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Dissertation

Derivation and Large-Time Asymptotics of Diffusion Models in Spintronics and Optical Lattices

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Univ.-Prof. Dr. Ansgar Jüngel

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von

Philipp Rudolf Holzinger

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Kurzfassung

Diese Arbeit widmet sich der Herleitung makroskopischer Modelle von Elektronenensembles und deren Eigenschaften, insbesondere Energie und Spin und der Untersuchung von Langzeitverhalten. Da das Thema breit gefächert ist, werden drei ausgewählte Themen behandelt, die jedoch in einer gewissen Art miteinander verbunden sind.

Ziel des ersten Teils ist es ein makroskopisches Modell der Teilchendichte und Energiedichte von ultrakalten Fermionenwolken rigoros herzuleiten, startend von einer Halbleitergleichung des Boltzmann-Typs. Außerdem wird gezeigt, dass das System exponentiell zu einem Fermi-Dirac-Gleichgewicht konvergiert und dass die Dichten gegen ihre Mittelwerte konvergieren.

Der zweite Teil konzentriert sich auf die Herleitung eines Modells für alle Richtungen des Spins, ausgehend von der Von-Neumann-Gleichung. Der Hamilton-Operator in dieser Gleichung enthält eine Beschreibung einer bestimmten Spin-Orbit-Wechselwirkung, der sogenannte Rashba-Effekt. Von dort aus entwickeln wir das System in den Wigner-Formalismus (ähnlich zum Phasenraum), ausgestattet mit einer Relaxation zum lokalen Equilibrium, mit Hilfe des Quantenentropieprinzips. Das volle Quantenmodell wird erreicht, indem wir den Linien des klassischen Chapman-Enskog-Verfahrens folgen. Um ein praktischeres Modell zu erhalten, entwickeln wir das Equilibrium semiklassisch, was zu einem approximierten makroskopischen Modell der Spindichten führt.

Ein bereits vorhandenes makroskopisches Modell eines Elektronenensembles und ihrer Spins, auf einen beschränkten Bereich, ist der Ausgangspunkt des letzten Teils. Wenn man annimmt, dass der mittlere Spin am Rand verschwindet und dass sich das System bereits nahe des Gleichgewichtszustands befindet, führt das zu einem exponentiellen Abfall der Spindichten in Richtung des stationären Zustands des Systems.

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Abstract

The thesis is dedicated to derive macroscopic descriptions of electron ensembles and their properties, in particular energy and spin, and to study their long-time behaviour. Since it is a topic with a wide range of fields, three selected topics are chosen, which are connected but still different.

The goal of the first part is the rigorous derivation of a macroscopic description for the particle density and energy density of an ultracold cloud of fermions, starting form a semiconductor Boltzmann-type equation. Additionally it is shown that the system converges exponentially to a Fermi-Dirac equilibrium, as well as the densities converge to their mean values respectively.

The second part focuses on the search of a model for all directions of the spin. To obtain this the chosen starting equation is the von Neumann equation. The Hamiltonian occurring in this equation includes a description of a particular spin-orbit interaction, the so called Rashba-effect. From there the system is transformed into the Wigner picture, endowed with a relaxation to the local equilibrium obtained by the quantum entropy principle. Following the lines of the classical Chapman-Enskog procedure, the full quantum drift diffusion model is derived. To obtain a more practical model, the semiclassical expansion of the equilibrium leads to an approximated macroscopic description of the spin densities.

Another already derived macroscopic description of an electron ensemble and their spins on a bounded domain is the starting point of the last part. Considering that the average spin vanishes on the boundary and that the system is close to the equilibrium state, leads to the exponential decay of the spin densities towards the steady state of the system.

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Danksagung

Diese Arbeit hätte ich nicht in diesem Ausmaß bewerkstelligen können, ohne die Hilfe ganz besonderer Menschen, und ich möchte mir hier die Zeit nehmen und jenen danken.

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Als nächstes möchte ich mich bei Professor Luigi Barletti bedanken, der mich während meiner Italienaufenthalte unter die Fittiche nahm. Dank ihm konnte ich mein Verständnis über die Materie weiter ausbauen und dank ihm kam der zündende Gedanke zur Lösung eines der größten Schwierigkeiten in meiner Arbeit. Er hat sich auch immer geduldig Zeit für mich genommen, auch wenn ich manches mal länger gebraucht habe und er hat mich in die italienische Kultur eingeführt. Seine ruhige und verständisvolle Art findet man kein zweites Mal.

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haben immer gut getan, und unsere gemeinsamen Spieleabende waren eine willkommende und notwendige Abwechslung zum Alltag.

Danke auch an meine langjährigen Mathematikkollegen und Freunde Dominik Forkert, Jakob Hruby, Philipp Kniefacz und Andreas Kreumel, die mit mir gemeinsam durch dick und dünn gegangen sind und mir dadurch das Studium erleichtert haben. Außerdem waren unsere Brettspielschlachten legendär.

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Euch allen vielen vielen Dank für eure Unterstützung,
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Wien, am ....
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1. Introduction

1.1. Motivation

Technology has become indispensable in our modern way of life, the advances seem unlimited and electronic devices get smaller and faster every year. Therefore it is nearly unimaginable that the basic language of such electronic devices is binary, meaning that still everything is encoded with zeros and ones (or ”on” and ”off”). One of the basic tools in modern electronics are transistors, which are used as switches for electrical power and implement that language in electric circuits. These transistors are usually built from semiconductors (such as silicon, germanium or graphene) and have the ability to become either a conductor or an insulator, depending on the purpose and as such the transistor controls if there is an electron flow $(= 1)$ or if there is no current at all $(= 0)$.
Moore’s law [Moo65] predicted in 1965 that the number of transistors packed into integrated circuits will increase, and in 1975 the rate was estimated to double every two years. This is evident in the fact that manufacturing technology has gone from 6μm in 1976 to 7nm in 2019, making the same chip roughly 850 times smaller. As an example, a smartphone like the Samsung Galaxy S8, has about 460 billion transistors (an idea how many that is, 1 million seconds are roughly 11 days, but 1 billion seconds are roughly 31 years). This progress has slowed down since the year 2000, due to the limits of engineering and because quantum mechanical effects occur. Electrons have a remarkable ability called *tunnelling*: If there is a thin ”wall” (e.g. created by a potential energy barrier), it is possible for the electrons to ”tunnel” to the other side. Hence, if a semiconductor is too small, the electrons can tunnel through the device, making it hard to distinguish if there is a current or not.

A solution to resolve this issue could be using the spin of electrons. Spin is an intrinsic form of angular momentum carried by elementary particles, discovered by the Stern-Gerlach experiment in 1922. The study of spin transport electronics (short: Spintronics) emerged from discoveries in the 1980s revolving around spin-dependent electron transport phenomena in solid-state devices, for details see [Ban08, WAB$^+$01, WCT06]. The simplified idea behind spintronics is to control the spin and use it as information transport. For example if we take a single electron and look in which direction its spin points, let it pass the device and check the spin again at the end. If it remains the same, no information is passed $(= 0)$, and if the spin changes it gives us information $(=1)$. This idea is easier said than done, since it is already quite a challenge to check in which direction the spin points in the beginning. Less troublesome is to check if the spin looks ”upwards” (has positive component in the z-axis) or ”downwards” (has negative component in the z-axis), which we will call spin-up and spin-down respectively for short. Going a step further, we could gain much more information from a single electron, if we know how the spin behaves in each direction. Controlling the spin at this level, could open plenty more opportunities for new devices. Using each direction of the spin as another information could tremendously increase calculation speed, and tunnelling would pose no problem, since we want the electrons to pass the device.

Before we go into details we would like to mention what kind of models exist. Roughly speaking there are three types of models, namely the microscopic, the mesoscopic and the macroscopic one. The microscopic models are based on the investigation of the individual

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elements of the system using equations such as the Schrödinger equation, and give a very detailed description of the model. This is the maximal possible ”zoom” level, and in most cases these models are too detailed. Comparing it with a river, it is as if we are trying to describe the evolution of every particle in the river separately, having the information of where they are and in which direction they go for all times. For academic purposes this is indeed interesting but for practical use it is way too complicated to compute. The usual ”zoom factor” we want to work with is the macroscopic one, where in most cases the starting model is averaged over the momentum. Comparing it again with a river, we notice that all particles in the river, move on average in the same direction, which coincides with our actual observation. Hence it is our main goal to derive such models. A scaling that is in between the micro- and macroscopic is the mesoscopic scaling, which is grounded in mathematics and introduces a more statistical point of view. This type is closer to a microscopic model, but it does not treat every particle on its own. An interpretation of the mesoscopic type is that all particles are identical and behave similarly, and its description gives us the distribution of these identical particles. One famous example for a mesoscopic equation is the Boltzmann equation.
Why did we use a river as comparison, when we are talking about electrons in a semiconductor? The answer is quite simple: We are interested in a macroscopic description of an electron ensemble, and in some sense we can interpret their movement as a motion of a fluid, see for example the picture below taken from [TDB+17].

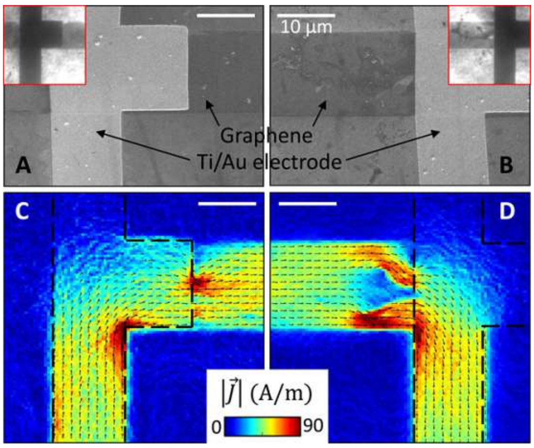

Figure 1.1.: The electron flow looks similar to water flowing through a canal.

As much as we mathematicians love details and theory, we are also interested in practical use of our achievements. One of the most interesting processes to study is diffusion, because this phenomenon is well observed for long times in many situations (short observation times for us). The usual procedure to derive a macroscopic diffusion model, simplified for now, is to start at either the microscopic or the mesoscopic level, use the right scaling, average over the momentum and pass formally to the diffusive limit (which will be explained in the next section). So what is the right level to start?
Using the microscopic level gives us a lot of information and details from which we can derive intricate models. These are in most cases highly non-local, complex and contain many quantum terms. Since such models are hard to understand and most of the find no applications in numerics, it makes sense to approximate these with some similar objects from classical physics, and ”add” some quantum terms. This procedure is known as the semiclassical approximation (and will be treated in Section 3.6). Deeper into the thesis we will see that

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starting from the microscopic level is complicated and requires much background knowledge, but is then rewarded with a more detailed model, which can be then approximated with as much accuracy as we wish.
Alternatively one can start with the mesoscopic one. The idea in this case would be to compare quantum particles with larger particles that behave classically, like gas molecules. Using such a classical approach to describe a quantum setting, already assumes a semiclassical approximation. The advantage of this choice is that the calculations that follow are simpler and will not need to be approximated any further.

Our goal in this thesis is to derive equations which model electrons and their quantum properties, and explore their long time behaviour. Before we go into details of the separate chapters let us mention, that this is a mathematical thesis, which is highly connected to physics. Since we are interested to also give motivation for our choices and provide the reader some background knowledge, it is possible that some physical statements will not be very accurate and could be very naive from a physicists point of view. We apologize in advance and ask for understanding.

1.2. Details on the chapters

Chapter 2 revolves around the behaviour of an ultracold cloud of fermions (particles with 1/2 spin, e.g. electrons), which appear in quantum information processing and quantum optics, where we focus on the latter. Due to low temperatures (close to 0), the fermions behave similar to particles in condensed matter and are therefore also used as quantum simulation for solid state physics. The advantage of optical lattices is that atoms can be imaged directly, which in comparison is difficult in solids, and all parameters of the quantum system can be controlled.
Our aim here is to derive rigorously moment equations for the particle density and the total energy of the system. This chapter relies on the work of Marcel Braukhoff [Bra17] and the paper of Golse and Poupaud [GP92]. Starting from the semiconductor Boltzmann equation (mesoscopic level), where we in particular assume that the spatial variable x and the momentum variable p lie both in the $d-$dimensional Torus $\mathbb{T}^d$. We assume zero potential energy, we study the entropy functional, the Fermi-Dirac distribution and state an appropriate H-Theorem. Let us point out that the Fermi-Dirac distribution is introduced here as the minimizer of the entropy under the condition of having the same particle density and total energy as that of the solution of the semiconductor Boltzmann equation.

Formal derivations of associated macroscopic diffusive models have already been done, see for instance [JKP11] and [Bra17], but we are interested in a rigorous derivation. The question for us is therefore, in which sense the diffusive limit and solutions exist. Similar theories exist, as in [GP92] and [BADG96]. Our work however has two main differences: Firstly, we consider a spatial variable that lies in the d-dimensional torus instead of $\mathbb{R}^d$, which is similar to assuming that the Bravais lattice is of primitive cubic type (CUB, see [AM76]). Secondly, we consider different type of collisions, namely a collision operator of Barthnagar-Gross-Krook (BGK) type ([BGK54]), instead of an electron-electron scattering operator. As far as we know, this is the first time that this setting was chosen for such a derivation.

The idea to achieve the rigorous diffusive limit relies on a boundedness result of [GP92] and Fermi-Dirac analysis from [Bra17]. We adapt the boundedness result for our purposes

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which leads together with the Aubin Lions Lemma, to a convergence result for our desired densities. The well known Chapman-Enskog expansion (e.g. [JÖ9]) is also introduced here, which will not only prepare the path for our derivation, but will also be used in the following chapter. Even tough the Fermi-Dirac distribution is well known [DF26, JÖ9, AM76], with the analysis of [Bra17], we are able to extend the theory a bit further, which will be an important ingredient of our convergence result. Besides the appealing mathematics, the advantages of the rigorous derivation is that it provides solutions for the limit equations, as long as the starting equation has already one. Due to the desire to keep the chapter as comprehensible as possible, this existence was stated as a hypothesis, so that we are able to focus on the derivation itself.

In the end of this chapter we will check the long time behaviour of the system and introduce the relative entropy of it as well as some apriori estimates to this entropy. The adapted version of the boundedness result of Golse and Poupaud will serve as useful tool here, along with the H-Theorem. Finally, we will use a Gronwall argument to show that our rigorously derived weak solution converges in norm towards equilibrium, with an exponential decay rate.

A second purpose of Chapter 2 is to introduce the reader to the concepts of deriving macroscopic models and studying long time behaviour of a system. We will see that in Chapter 3, which deals with the derivation of a full spin model, it is already at a formal level quite challenging and not easy to understand. In addition, the last chapter, where we study the long time behaviour of the spin, will need a different trick to bypass issues with the limit of t going to infinity.

Chapter 3 of this thesis is devoted to the derivation of quantum diffusive equations for a bidimensional gas of spinors with spin-orbit interaction. The physical situation that we have in mind is that of electrons that are confined in a two-dimensional potential well and are subject to the so-called Rashba effect. Such a system is often used for interesting applications to spintronics [icvacFDS04].

In the literature two kinds of spin drift-diffusion models are usually considered. In one approach, the dynamical variables of the model are the densities of spin-up and spin-down electrons (with respect to a given direction) or, equivalently, the total density and the polarization. In turn, such models can be either semiclassical [EH14], i.e. derived from a spinorial Boltzmann equation, or quantum. The quantum model is derived from the von Neumann equation (statistical Schrödinger) together with a quantum version of the Maximum Entropy Principle (Q-MEP) [DR03, DMR05, JÖ9]. The fully-quantum model obtained in this way can be semiclassically expanded (i.e. in powers of $\hbar$), up to a desired order. Typically the second order is enough to observe important quantum features, such as the Bohm potential. Examples of semiclassical bipolar drift-diffusion models are given in [EH14, PN11], while a quantum bipolar drift-diffusion model is treated in [BM10, BMNP15].

The second approach to such models considers the complete spin vectors, and not only their projection on a given direction. Such models, therefore, have four dynamical variables: the particle density and the densities of the three spin components. A semiclassical model of this kind has also been developed in [EH14] starting from the spinorial Boltzmann equation. However, to our knowledge, no quantum drift-diffusion model for the full spin structure has been considered in literature so far. The presented work aims exactly to fill this gap, with the derivation of quantum drift-diffusion equations for fully-structured spinors.

We consider a two-dimensional electron gas of electrons confined in an asymmetric two-dimensional potential well. In such conditions, electrons experience a spin-orbit interaction of Rashba type [BR84, icvacFDS04]. This is a small effect due to the relativistic conversion of the

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electrostatic field into a magnetic one. The resulting effective magnetic field is perpendicular to both the electron motion and the confinement direction, see Figure 1.2. At a kinetic level

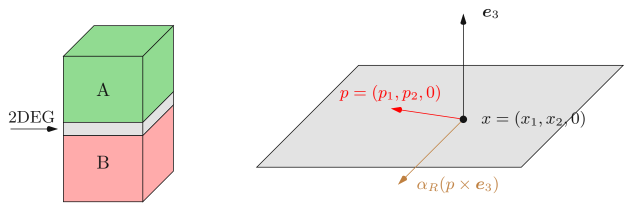

Figure 1.2.: **(left)**: The two different semiconductors, A and B, provide an asymmetric, planar potential well where a two-dimensional electron gas (2DEG) is confined; **(right)**: the electrons of the 2DEG experience the Rashba effect i.e. an effective magnetic field $\alpha_R(p \times \boldsymbol{e}_3)$ orthogonal to both the electron momentum p and the confinement direction $\boldsymbol{e}_3$.

we shall work in the framework of phase-space formulation of quantum mechanics (Wigner). The Wigner formalism is a "classical looking" version of the density operator formalism (von Neumann). Although the two versions are equivalent, the former has the advantage of making the derivation of the model and its semiclassical expansion more intuitive.

The purely Hamiltonian dynamics described by the spinor Wigner equation is endowed with a collisional term of Bhatnagar-Gross-Krook (BGK) type [BGK54, Arn96], describing the relaxation of the system to the equilibrium state. Such equilibrium state is provided by the Q-MEP, and is represented by a matrix-valued Wigner function that minimizes the quantum free-energy functional under the constraint of given position and spin densities. Then, the formal asymptotic analysis, with respect to the scaled relaxation time, is performed on basis of the usual techniques in kinetic theory, namely the already mentioned Chapman-Enskog expansion [Cer69, Jö09]. However, differently to the standard classical and quantum cases [BM10, Cer69, DMR05, Jö09], it turns out that the leading order of the expansion does carry a current, so that the usual diffusive scaling must be replaced by a hydrodynamic one (even though the collisions do not conserve the particle momentum but only the particle number and spin). This analysis leads to spinorial quantum drift-diffusion equations for the position and spin densities. Such equations are non-local, since they contain a functional dependence on the unknown densities.

In order to be able to compute an explicit semiclassical expansion, i.e. an expansion in powers of the scaled Planck constant ε, we make the assumption that the system is in a regime of small polarization. More precisely, we assume that the spin densities are of order ε, which amounts to assume that the macroscopic polarization of the electron gas is small. Then, the quantum non-local model is semiclassically expanded up to the order $\varepsilon^m \alpha^l$, where $m + l = 2$ and α is the scaled Rashba constant (measuring the intensity of the spin-orbit interaction). We obtain in this way a system of four local equations having the form of semiclassical drift-diffusion equations with "quantum corrections", including the Bohm potential and their spinorial counterparts.

The structure of Chapter 3 is the following: We start with some background from physics, by presenting the Rashba spin-orbit Hamiltonian, together with the corresponding von Neumann equation. Afterwards we introduce mathematical tools, such as the Wigner-Weyl transformation, the Moyal product and the Pauli algebra, which allow us to transform the von Neumann equation into a four-component Wigner equation. The Wigner equation is then scaled into non-dimensional form, where we will introduce the scaled Planck constant ε. Then

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we use the Q-MEP to define the local-equilibrium Wigner function ("quantum Maxwellian") and the corresponding BGK collisional operator in the Wigner equation, and present our assumption of small polarization with a short discussion there. We will see that issues related to the diffusive time-scaling arise, where we give a general characterization of all systems that show a non-vanishing current in the equilibrium state, thus requiring a hydrodynamic scaling instead of the usual diffusive one. With the previous preparation we use the hydrodynamic scaling on our Wigner equation, where a new non-dimensional parameter, the scaled collisional time τ, appears. The first main result of this chapter will be the full quantum drift-diffusion model which appears in Section 3.5, where an adapted version of Chapman-Enskog expansion will be introduced and applied. Afterwards we introduce in Section 3.6 the quadratic semiclassical approximation, and its connection to semiclassical expansions of the quantum Maxwellian and the Lagrange multiplier, and achieve our desired model. Finally, in the last part of the chapter we draw several conclusions and show that our model can be seen as a generalization of the other models mentioned in this Introduction.

Let us finally remark that some of the results about this non-local model have been anticipated, without proofs, in [BHJ].

In the very last chapter (Chapter 4), which is mostly cited from our paper [HJ20], we are interested in what happens to the spin in a bounded domain, if the spin on the boundary is on average zero.

Semiconductor lasers and transistor devices may be improved by taking into account spin-polarized electron injection. We choose a different model than our derived model in Chapter 3, but the corresponding semiconductor models should include the spin effects in an accurate way. A widely used model is the two-component spin drift-diffusion model which can be derived for strong spin-orbit coupling from the spinorial Boltzmann equation in the diffusion limit [EH14]. When the spin-orbit coupling is only moderate, the diffusion limit in the spinorial Boltzmann equation leads to a matrix spin drift-diffusion model for the electron density matrix [EH14, PN11]. This model contains much more information than the two-component model, but the strong coupling between the four spin components makes the mathematical analysis very challenging. The driving force to consider this model ([EH14, PN11]), rather than one of the models derived in Chapter 3, was that our models have more involved terms and are more complicated to investigate (even the approximated one). Another reason for this choice is the fact that the existence of global weak solutions for [EH14, PN11] was already shown in [JNS15]. After some investigation, we are able to show the large-time asymptotics of the density matrix towards a near-equilibrium steady state.

Our idea is to decompose the matrix equation into two equations modelling the spin up and spin down densities and a third equation regarding a perpendicular direction of the spin. Interestingly these three equations do still contain all the information needed for the spin. Simply put we will see that the spin up and spin down densities will cancel themselves out (in the sense they converge to a steady state) and the perpendicular direction will vanish for long times. Details are given in Section 4.2.

1.3. Scaling and Performing Limits

This section is designed to give intuition and ideas, why and how we want to scale equations. Since in this work different settings are considered, we will keep everything as general and easy as possible. This means that no details about existence and spaces are given, and the specific choices will be given in the appropriate chapters.

Let $f = f(t, x, p)$ be the distribution function of a cloud of indistinguishable particles in

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a force field $F(x,t)$, then these particles can be modelled by a *semiconductor Boltzmann equation* (SBE), (see [CIP94, JÖ9, JÖ1, MRS90]), namely

$$\partial_t f(t,x,p) + v(p)\cdot\nabla_x f(t,x,p) + F(t,x)\cdot\nabla_p f(t,x,p) = \mathcal{Q}(f(t,x,.))(p). \tag{1.1}$$

with $v(p)$ being the velocity. To keep it simple, we consider the case where the velocity is proportional to the momentum. For free particles for example, the dispersive relation is given by $\varepsilon(p) = |p|^2/2m$, where m is the mass of each particle. Therefore we have

$$v(p) = \nabla_p E_{kinetic} = \nabla_p \varepsilon(p) = \frac{p}{m}.$$

We also restrict ourselves to the case where the force field $F(t,x)$ comes from a potential $V(t,x)$, i.e. $F(t,x) = \nabla_x V(t,x)$. The right hand side $\mathcal{Q}$ in (1.1) is in general non-local in p and describes short ranged collisions of the particles.
Scaling is a tool of simplification and better understanding. It puts everything in relation. For example it is easier to say on a road trip that we are half way through, rather to tell the exact amount of meters travelled. Therefore it is useful to look at reference quantities and define them. In many cases we consider the reference length x_0 (the device diameter for example), and the reference time t_0 (the time how long we want to observe the system). Next let us denote the reference energy, reference temperature and reference momentum by E_0, T_0 and p_0 respectively, where only one of these needs to be given, since they are related:

$$k_B T_0 = E_0, \qquad E_0 = \frac{p_0^2}{m}, \tag{1.2}$$

where k_B is the Boltzmann constant. Now we are able to define the dimensionless variables

$$\tilde{t} := \frac{t}{t_0}, \qquad \tilde{x} := \frac{x}{x_0}, \qquad \tilde{p} := \frac{p}{p_0}.$$

Further we introduce the scaled functions

$$\tilde{f}(\tilde{t},\tilde{x},\tilde{p}) := f(t_0\tilde{t}, x_0\tilde{x}, p_0\tilde{p}), \qquad \tilde{V}(\tilde{t},\tilde{x}) := \frac{1}{E_0} V(t_0\tilde{t}, x_0\tilde{x}).$$

Looking for example at the time derivative of f, and using the fact that $t = t_0\tilde{t}(t)$, we have that

$$\partial_t f(t,x,p) = \partial_t f(t_0\tilde{t}(t), x_0\tilde{x}(x), p_0\tilde{p}(p)) = \frac{1}{t_0}\partial_{\tilde{t}} f(t_0\tilde{t}(t), x_0\tilde{x}(x), p_0\tilde{p}(p)) = \frac{1}{t_0}\partial_{\tilde{t}}\tilde{f}(\tilde{t},\tilde{x},\tilde{p}).$$

It is rare to use the scaled variables as functions, due to the tendency for confusion, and hence we will also drop this. In the literature the notation $t \to t_0\tilde{t}$, $x \to x_0\tilde{x}$, $p \to p_0\tilde{p}$, $V \to E_0\tilde{V}$ is much more common. Using this transformation in SBE (1.1), we obtain the following equation

$$\frac{1}{t_0}\partial_{\tilde{t}}\tilde{f}(\tilde{t},\tilde{x},\tilde{p}) + \frac{p_0\tilde{p}}{m x_0}\cdot\nabla_{\tilde{x}}\tilde{f}(\tilde{t},\tilde{x},\tilde{p}) + \frac{E_0}{x_0 p_0}\nabla_{\tilde{x}}\tilde{V}(\tilde{t},\tilde{x})\cdot\nabla_{\tilde{p}}\tilde{f}(\tilde{t},\tilde{x},\tilde{p}) = \mathcal{Q}(\tilde{f}(\tilde{t},\tilde{x},.))(\tilde{p}). \tag{1.3}$$

One may notice that the above equation is not totally dimensionless, since the left hand side depends on "*seconds*$^{-1}$". Before we describe the time scaling , we briefly discuss our collision operator $\mathcal{Q}$ on the right side. For the interested reader we suggest [JÖ9] for more information about collision operators. In this work the main collision operator that will be used is of Bhatnagar-Gross-Krook-type (BGK-type) ([BGK54]), which drives the relaxation of the system to a local equilibrium $\mathcal{F}$. Closely connected to it is the measure of disorder,

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known as the entropy functional, which minimized over given constraints provides exactly this local equilibrium. These constraints depend on the conserved quantities of the system. For example: Equation (1.3) conserves the zeroth moment, the macroscopic density $n := \int f dp$. The minimizer $\mathcal{F}$ is therefore the distribution with the lowest measure of disorder that has the same macroscopic density $\int \mathcal{F}\, dp = n$. That the particle density n should be conserved, is the least we expect (in Chapter 2 and Chapter 3 additionally the total energy or all directions of the spin are conserved). Since the constraints depend on the solution f, we will denote this dependence in the minimizer by writing $\mathcal{F}(f;p)$ in this introduction.
Let t_c be the typical collision time (describes the "average time" between two collisions), which in this work will be assumed to be constant for the sake of simplicity, and define the *collision operator* for a distribution f as

$$\mathcal{Q}(f(t,x,.))(p) = \frac{1}{t_c}\left(\mathcal{F}(f;p) - f(t,x,p)\right). \tag{1.4}$$

If we now drop the tilde notation and substitute the definition for $\mathcal{Q}$ in (1.3), we obtain

$$\frac{1}{t_0}\partial_t f + \frac{p_0 p}{m x_0}\cdot \nabla_x f + \frac{E_0}{x_0 p_0}\nabla_x V \cdot \nabla_p f = \frac{1}{t_c}\left(\mathcal{F}(f;p) - f(t,x,p)\right).$$

With the typical collision time we can now introduce the *mean free path* x_c, which is the distance an electron travels between two consecutive collisions. As a basic example, a possible way to calculate it would be to multiply the reference velocity $v_0 = p_0/m$ by the typical collision time t_c, giving us $x_c = p_0 t_c/m$. The ratio between the mean free path x_c and the reference length x_0 is then called the *Knudsen number* $\tau = x_c/x_0$. This ratio details if our system has many collisions ($i.e. \tau \ll 1$) or not.
The time an electron with reference energy E_0 needs to pass through the device is called in the literature the energy time scale (cf. [BFM14]) , which we will denote by t_E. The formula for the energy time scale t_E is given by dividing the reference length x_0 by the reference velocity, which is $t_E = x_0 m/p_0$. An immediate consequence is then that the ratio between the typical collision time and the energy time scale, needs to equal the ratio between the mean free path and the reference length. Indeed we see

$$\frac{t_c}{t_E} = \frac{t_c p_0}{m x_0} = \frac{x_c}{x_0}.$$

Therefore the Knudsen number is also given by $\tau = t_c/t_E$. With this we obtain the non dimensional semiconductor Boltzmann equation (NDSBE)

$$\frac{t_c}{t_0}\partial_t f + \tau\left(p\cdot\nabla_x f + \nabla_x V\cdot\nabla_p f\right) = \mathcal{F}(f;p) - f. \tag{1.5}$$

We are left with choosing the observing time t_0. For our purposes we will have two possibilities.

- The hydrodynamic regime: This regime has the shorter time scale of the two, and it appears when we are interested in the current of the electrons. In that case the right choice as observation time would be $t_0 = t_E$, leading to the hydrodynamic scaled semiconductor Boltzmann equation (HSBE)

$$\tau\partial_t f + \tau\left(p\cdot\nabla_x f + \nabla_x V\cdot\nabla_p f\right) = \mathcal{F}(f;p) - f. \tag{1.6}$$

- The diffusive regime: The longer timescale of this regime provides the possibility to observe diffusion of the particles in the device. In this regime we want to maintain

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the ratio given by the Knudsen number. The choice here would be $t_0 = t_E/\tau$, because then the ratio between the energy time scale and observation time coincides with the Knudsen number. Substituting this in (1.5) gives us the diffusive scaled Boltzmann equation (DSBE)

$$\tau^2 \partial_t f + \tau \left(p \cdot \nabla_x f + \nabla_x V \cdot \nabla_p f \right) = \mathcal{F}(f;p) - f. \tag{1.7}$$

As the DSBE will be our main focus in attaining the macroscopic models in the Chapters 2 and 3, hence we will use it to continue our motivation. As mentioned in the introduction, in the macroscopic scaling we want to see "the motion of the river" and not how every particle behaves. Applying this idea to the DSBE (1.7) we want to average the equation over the momentum, which is achieved by integrating with respect to p. If f_τ is the solution of (1.7), then the macroscopic particle density n_τ is given via $n_\tau(t,x) = \int f_\tau(t,x,p)dp$. Since $\mathcal{F}(f_\tau;p)$ has the same particle density as f_τ we obtain formally

$$\partial_t n_\tau + \frac{1}{\tau} \int \left(p \cdot \nabla_x + \nabla_x V \cdot \nabla_p \right) f_\tau dp = 0, \tag{1.8}$$

a potentially simpler equation.
When one considers many collisions, the Knudsen number τ is really small ($\sim \mathcal{O}(10^{-2})$). Since this is close to zero, we expect a good approximation of passing to the limit $\tau \to 0$. Moreover, we notice that if τ goes to zero, t_0 has to go to infinity, which means that we investigate the system for long times. Looking at (1.8), we notice that taking τ to zero seems like a trivial task, but we expect that the family $(n_\tau)_{\tau>0}$ has a limit function n and that the equation (1.8) converges to a parabolic equation like

$$\partial_t n - \operatorname{div}_x(J(n,V)) = 0, \tag{1.9}$$

where J describes the flux of the system, the term $\operatorname{div}_x(J)$ contains second order derivatives and as well as the diffusion. Notice that equation (1.9) is still time dependent. For long time behaviour we will study therefore the limit

$$\lim_{t\to\infty} n(t,x).$$

Here we expect that the particle density will converge to a steady state, but what this means depends on the system we are looking at. The derivation of equations in form of (1.9) and the study of long times regarding the macroscopic densities is exactly what we will focus on in this thesis.

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2. Effective Energy Transport Model and Longtime Behaviour

2.1. Setting and Scaling

As mentioned before we want to study the behaviour of an ultracold cloud of fermions (particles with 1/2 spin, e.g. electrons), in an optical lattice. Such a lattice is generated by lasers and their standing waves, which create a periodic structure, similar to the ones that can be found in crystals and semiconductors. For our purposes we assume that the spatial variable lies in a cube $[0, x_0]^d$, where opposite sides are identified, i.e. a d-dimensional Torus $x \in \mathbb{T}^d_{x_0}$ and x_0 is defined as the typical length, i.e. the lattice constant. Further we assume that the momentum variable p lies in a d-dimensional torus $p \in \mathbb{T}^d_{p_0}$ as well, where p_0 denotes the periodicity of the energy.
It was shown in [KZPH18] that a laser generated rectangular square lattice with a hole in the middle can be turned into the surface of a torus, which justifies our first assumption on the spatial variable. Since we are looking at optical lattices, electrons are assumed to be in potential wells with periodic potentials. In that case, a connected bounded subset $B \subset \mathbb{R}^d$, the so called first Brillouin zone, describes the momentum space well enough. In the theory of semiconductors this is a well-known fact, since it is a consequence of the Bloch Theorem [Blo29]. One of the simplest forms is to assume $B = \mathbb{T}^d_{p_0}$, similar as in [BADG96].
We choose a semiclassical approach to describe the behaviour of these particles, *given by the semiconductor Boltzmann equation*

$$\partial_t f(t,x,p) + v(p) \cdot \nabla_x f(t,x,p) + F(t,x) \cdot \nabla_p f(t,x,p) = \mathcal{Q}(f(t,x,.))(p), \tag{2.1}$$

where the spatial variable x and the momentum variable p lie in the d-dimensional torus $\mathbb{T}^d_{x_0}$ and $\mathbb{T}^d_{p_0}$ respectively, and the time variable t lies in $\mathbb{R}$.
For this work we specifically chose that there is no external force $F = 0$, to keep it simpler and the velocity $v(p)$ is given by the gradient of the dispersion relation $\varepsilon(p)$ which in turn is given by

$$\varepsilon : \mathbb{T}^d \to \mathbb{R}, \quad p = (p_1, \ldots, p_d) \mapsto -\varepsilon_0 \sum_{i=1}^{d} \cos\left(2\pi \frac{p_i}{p_0}\right), \qquad \text{for } \varepsilon_0 > 0. \tag{2.2}$$

The factor p_0 is the reference momentum, which describes the periodicity of the energy and ε_0 represents the amplitude. The function $\varepsilon(p)$ represents a particular kinetic energy, where tunnelling is considered and for example finds usage in the so called Hubbard Model, see [SHR+12]. As in the Introduction mentioned the collision operator $\mathcal{Q}$ on the right hand side of (2.1) is considered to be of BGK-type (see [BGK54]), which describes the relaxation towards equilibrium. Let therefore $\mathcal{F}(f;p)$ be a nonlinear function of f and p, representing the local equilibrium, and let t_c denote the typical collision time, assuming to be constant, then we can write

$$\mathcal{Q}(f(t,x,.))(p) = \frac{1}{t_c} \left(\mathcal{F}(f;p) - f \right).$$

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At this point we also mention that we want to describe a closed system with elastic collisions, which means that the total amount of particles and the mean Energy remain the same. Details about that and discussion of the local equilibrium $\mathcal{F}$ requires more work and is therefore postponed to Section 2.2. With all these adjustments our model equation reads as follows

$$\partial_t f(t,x,p) + \nabla_p \varepsilon(p) \cdot \nabla_x f(t,x,p) = \frac{1}{t_c}(\mathcal{F}(f;p) - f(t,x,p)). \tag{2.3}$$

For the derivation of a macroscopic model, the right choice to observe long time behaviour of the system, is the diffusive one. Starting with putting (2.3) in its non-dimensional form, we introduce the scaled quantities

$$t \to t_0 \tilde{t}, \qquad x \to x_0 \tilde{x}, \qquad p \to p_0 \tilde{p},$$

where t_0, x_0 are the reference time and space. The scaled variables $\tilde{x}$ and $\tilde{p}$ lie both now in $\mathbb{T}^d = [0,1]^d$ and $\tilde{t}$ still lies in $\mathbb{R}$. As reference velocity, denoted by v_0, we choose the maximal possible velocity, which is the same in every direction p_i,

$$v_0 \coloneqq \sup_{p \in \mathbb{T}^d} |\partial_{p_i} \varepsilon(p)| = 2\pi \frac{\varepsilon_0}{p_0}, \qquad \forall i \in \{1, \dots, d\}$$

Using the above we can introduce the scaled dispersion relation with

$$\tilde{\varepsilon}(\tilde{p}) \coloneqq \frac{1}{2\pi\varepsilon_0} \varepsilon(p_0 \tilde{p}) = -\frac{1}{2\pi} \sum_{i=1}^{d} \cos(2\pi \tilde{p}_i). \tag{2.4}$$

If we look at the partial derivative of $\varepsilon(p)$, with the above scaling we see

$$\partial_{p_i} \varepsilon(p) = -\partial_{p_i} \varepsilon_0 \sum_{i=1}^{d} \cos\left(2\pi \frac{p_i}{p_0}\right) = 2\pi \frac{\varepsilon_0}{p_0} \sin\left(2\pi \frac{p_i}{p_0}\right) = -\frac{\varepsilon_0}{p_0} \partial_{\tilde{p}_i} \cos(2\pi \tilde{p}_i) = 2\pi \frac{\varepsilon_0}{p_0} \partial_{\tilde{p}_i} \tilde{\varepsilon}(\tilde{p})$$

and hence

$$\nabla_p \varepsilon(p) = v_0 \nabla_{\tilde{p}} \tilde{\varepsilon}(\tilde{p}). \tag{2.5}$$

Let the energy time scale t_E of an electron be defined as the minimum time an electron needs through the device with diameter x_0, given by

$$t_E \coloneqq \frac{x_0}{v_0}.$$

We obtain the non dimensional semiconductor Boltzmann equation

$$\frac{1}{t_0} \partial_{\tilde{t}} \tilde{f}(\tilde{t}, \tilde{x}, \tilde{p}) + \frac{1}{t_E} \nabla_{\tilde{p}} \tilde{\varepsilon}(\tilde{p}) \cdot \nabla_{\tilde{x}} \tilde{f}(\tilde{t}, \tilde{x}, \tilde{p}) = \frac{1}{t_c}(\tilde{\mathcal{F}}(\tilde{f}; \tilde{p}) - \tilde{f}(\tilde{t}, \tilde{x}, \tilde{p})).$$

Applying the diffusive scaling means that the relation of the energy time scale and the reference time coincide with the Knudsen number τ, such that $t_E/t_0 = \tau$, where $\tau = t_c/t_E$. Dropping the tilde notation, this leads us to the diffusive scaled semiconductor Boltzmann equation (DSSBE)

$$\tau \partial_t f + \nabla_p \varepsilon(p) \cdot \nabla_x f = \frac{1}{\tau}(\mathcal{F}(f;p) - f). \tag{2.6}$$

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Remark 2.1.1. In this particular case we could have chosen another way of scaling to obtain the DSSBE. First assume that the given momentum is already scaled. Furthermore define the average collision distance $x_c = t_c v_0$. Then we can define the Knudsen number as usual, namely as $\tau = x_c/x_0$. Then the scaling could be quicken up by choosing the transformation

$$t \to \frac{\tilde{t}}{\tau^2}, \qquad x \to \frac{\tilde{x}}{\tau}$$

which would lead to the exact same equation as in (2.6), see [Bra17, JÖ9]. ■

Notation 2.1.2. *From now on $\varepsilon(p)$ will always denote the scaled dispersion relation given in* (2.4)*, which we recall*

$$\varepsilon(p) = -\frac{1}{2\pi}\sum_{i=1}^{d}\cos(2\pi p_i). \tag{2.7}$$

Also notice that the scaled spatial variable x and the scaled momentum variable p lie both in $\mathbb{T}^d$, which is from now on the cube $[0,1]^d$ with opposite sides identified.

In the end we define even and odd functions on the torus.

Definition 2.1.3. *We call a function $g \in \mathrm{L}^1(\mathbb{T}^d)$ even on $\mathbb{T}^d$ in p_i for $i \in \{1,\dots,d\}$ if*

$$g(p_1,\dots,(1/2)+p_i,\dots,p_d) = g(p_1,\dots,(1/2)-p_i,\dots,p_d) \qquad \forall p_i \in [0,(1/2)],$$

and we call the function g odd on $\mathbb{T}^d$ in p_i for $i \in \{1,\dots,d\}$, if

$$-g(p_1,\dots,(1/2)+p_i,\dots,p_d) = g(p_1,\dots,(1/2)-p_i,\dots,p_d) \qquad \forall p_i \in [0,(1/2)],$$

The function $g \in \mathrm{L}^1(\mathbb{T}^d)$ is called even or odd, if it is even in p_i for all $i \in \{1,\dots,d\}$ or odd in p_i for all $i \in \{1,\dots,d\}$.

Example 2.1.4. The function $\varepsilon(p)$ is thanks to the cosine an even function on $\mathbb{T}^d$. If we derive $\varepsilon(p)$ partially we obtain that $\partial_{p_j}\varepsilon(p)$ is odd on $\mathbb{T}^d$, due to the properties of the sine. Moreover for an even function $g \in \mathrm{L}^2(\mathbb{T}^d)$ we obtain the following

$$\int_0^1 \partial_{p_j}\varepsilon(p)g(p)dp_j = \int_0^{\frac{1}{2}} \partial_{p_j}\varepsilon(p)g(p)dp_j + \int_{\frac{1}{2}}^1 \partial_{p_j}\varepsilon(p)g(p)dp_j = 0,$$

and hence

$$\int_{\mathbb{T}^d} \partial_{p_j}\varepsilon(p)g(p)\ dp = \int_0^1 \cdots \int_0^1 \partial_{p_j}\varepsilon(p)g(p)\ dp_1\cdots dp_d = 0$$

■

2.2. Entropy and Equilibrium

2.2.1. The Mean Particle Density, the Mean Energy, and their Relation

The equation DSSBE (2.6) requires an initial value f_0 to be well stated. At the moment it is enough to choose f_0 in $\mathrm{L}^1(\mathbb{T}^d \times \mathbb{T}^d)$ with $0 \le f_0 \le 1$. The initial condition f_0 provides the *mean particle density* and *mean energy* by

$$\bar{n} := \int_{\mathbb{T}^d}\int_{\mathbb{T}^d} f_0(x,p)dpdx \qquad \bar{E} := \int_{\mathbb{T}^d}\int_{\mathbb{T}^d} \varepsilon(p)f_0(x,p)dpdx. \tag{2.8}$$

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Considering that our system is closed and having elastic collisions, the quantities $\bar{n}, \bar{E}$ are both conserved at all times. In particular if $f(t,x,p)$ describes the system, i.e. is the solution to the DSSBE (2.6) with initial condition f_0, then the macroscopic densities $n_f := \int f dp$ and $E_f := \int \varepsilon f dp$ should fulfill at any time $t \geq 0$

$$\int_{\mathbb{T}^d} n_f(t,x)dx = \bar{n}, \qquad \int_{\mathbb{T}^d} E_f(t,x)dx = \bar{E}. \tag{2.9}$$

The energy of a system relies totally on the particle density. If for example there are no particles in the system ($\bar{n} = 0$) there cannot be energy due to the lack of motion. If conversely, the system has full density, ($\bar{n} = 1$), there is no movement and therefore the mean energy is again zero, which is reflected in the dispersion relation by

$$\int_{\mathbb{T}^d} \varepsilon(p)dp = 0.$$

In the upcoming lemma, we will show that the possible range for the energy depends on the particle density of the system.

Lemma 2.2.1. *Let $f_0 \in \mathrm{L}^1(\mathbb{T}^d \times \mathbb{T}^d)$ be given with $0 \leq f_0(x,p) \leq 1$ for all x and p in $\mathbb{T}^d$ and define $\bar{n}$ and $\bar{E}$ as in (2.8). Let $C \in \mathbb{R}$ be such that*

$$\operatorname{meas}\left(\left\{p \in \mathbb{T}^d : \varepsilon(p) \geq C\right\}\right) = \bar{n},$$

where meas (.) *denotes the d-dimensional Lebesgue measure, then we have the following inequality*

$$\left|\bar{E}\right| \leq \int_{\left\{p \in \mathbb{T}^d : \varepsilon(p) \geq C\right\}} \varepsilon(p)dp.$$

Proof. From [Bra17] Remark 5.1.3 we deduce, due to $\mathbb{T}^d$ being a connected set and $\varepsilon(p)$ being continuous, that the image of $\varepsilon(\mathbb{T}^d)$ equals an interval I and that the function

$$h : \bar{I} \to \mathbb{R}; \quad C \mapsto \operatorname{meas}\left(\left\{p \in \mathbb{T}^d : \varepsilon(p) \geq C\right\}\right),$$

is continuous and decreases strict monotonically. The interval $\bar{I}$ is given by $[-d/(2\pi), d/(2\pi)]$. If $C = -d/(2\pi)$ we get that $h(C) = \operatorname{meas}\left(\mathbb{T}^d\right) = 1$ and for $C = d/(2\pi)$ we have that $h(C) = \operatorname{meas}\left(\{((1/2), \ldots, (1/2))\}\right) = 0$. Since h decreases strict monotonically and is continuous, we obtain that $h(\bar{I}) = [0,1]$ and therefore exists a unique C for every $\bar{n} \in [0,1]$.
Let C be now the unique solution for $\bar{n} = \left\{p \in \mathbb{T}^d : \varepsilon(p) \geq C\right\}$ and define the short notation

$$\mathfrak{C} := \left\{p \in \mathbb{T}^d : \varepsilon(p) \geq C\right\}.$$

Additionally we have for $\bar{f}(p) := \int_{\mathbb{T}^d} f_0(x,p)dx$ the following identity

$$\int_{\mathfrak{C}} 1 dp = \int_{\mathbb{T}^d} \mathbb{1}_{\mathfrak{C}}(p)dp = \int_{\mathbb{T}^d} \bar{f}(p)dp = \int_{\mathfrak{C}} \bar{f}(p)dp + \int_{\mathfrak{C}^c} \bar{f}(p).dp \tag{2.10}$$

For $\bar{f}$ the inequalities $0 \leq \bar{f}(p) \leq 1$ still hold for all p in $\mathbb{T}^d$, as well as $\bar{E} = \int_{\mathbb{T}^d} \varepsilon(p)\bar{f}(p)dp$. We have

$$\bar{E} = \int_{\mathbb{T}^d} \varepsilon(p)\bar{f}(p)dp = \int_{\mathfrak{C}} \varepsilon(p)\bar{f}(p)dp + \int_{\mathfrak{C}^c} \varepsilon(p)\bar{f}(p)dp \leq \int_{\mathfrak{C}} \varepsilon(p)\bar{f}(p)dp + C\int_{\mathfrak{C}^c} \bar{f}(p)dp.$$

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From (2.10) we deduce that

$$\int_{\mathfrak{C}} (1 - \bar{f}(p))dp = \int_{\mathfrak{C}^c} \bar{f}(p)dp.$$

Since $0 \le \bar{f} \le 1$ and $\varepsilon(p) \ge C$ on $\mathfrak{C}$ we have that for all $p \in \mathfrak{C}$ that

$$0 \le (\varepsilon(p) - C)\bar{f}(p) \le \varepsilon(p) - C,$$

which yields the estimate

$$\bar{E} \le \int_{\mathfrak{C}} (\varepsilon(p) - C)\bar{f}(p)dp + \int_{\mathfrak{C}} C dp \le \int_{\{p \in \mathbb{T}^d : \varepsilon(p) \ge C\}} \varepsilon(p)dp. \tag{2.11}$$

For the lower bound we first notice that the integral over the torus $\mathbb{T}^d$ is translation invariant, meaning that for any $a \in \mathbb{R}^d$ and all $f \in \mathrm{L}^1(\mathbb{T}^d)$ that

$$\int_{\mathbb{T}^d} f(p)dp = \int_{\mathbb{T}^d} f(p + a)dp,$$

see for example [Gra08]. Additionally for the cosine we know that $\cos(y + \pi) = -\cos(y)$ for any $y \in \mathbb{R}$. Defining the vector $a := (1/2)(1, 1, ...1) \in \mathbb{T}^d$ provides $\varepsilon(p + a) = -\varepsilon(p)$. The function $g(p) := \bar{f}(p + a)$ fulfills, due to the properties of $\mathbb{T}^d$, that

$$\bar{n} = \int_{\mathbb{T}^d} \bar{f}(p)dp = \int_{\mathbb{T}^d} \bar{f}(p + a)dp = \int_{\mathbb{T}^d} g(p)dp,$$
$$\bar{E} = \int_{\mathbb{T}^d} \varepsilon(p)\bar{f}(p)dp = \int_{\mathbb{T}^d} \varepsilon(p + a)f(p + a)dp = -\int_{\mathbb{T}^d} \varepsilon(p)g(p) =: -E_g.$$

Applying the first part of the proof to g and E_g, gives us $E_g \le \int_{\mathfrak{C}} \varepsilon(p)dp$, and therefore

$$-\bar{E} = -\int_{\mathbb{T}^d} \varepsilon(p)\bar{f}(p)dp = \int_{\mathbb{T}^d} \varepsilon(p)g(p)dp = E_g \le \int_{\{p \in \mathbb{T}^d : \varepsilon(p) \ge C\}} \varepsilon(p)dp,$$

which concludes the proof. □

Motivated from Lemma 2.2.1 we give the following

Definition 2.2.2. *Let us define therefore the energy bound for given $n \in [0, 1]$:*

$$e_{max}(n) := \int_{\{p \in \mathbb{T}^d : \varepsilon(p) \ge C\}} \varepsilon(p)dp, \qquad \textit{where } \operatorname{meas}\left(\left\{p \in \mathbb{T}^d : \varepsilon(p) \ge C\right\}\right) = n, \tag{2.12}$$

and define the set of all admissible particle and energy densities as

$$\mathfrak{D} := \left\{(n, E) \in \mathbb{R}^2 : 0 \le n \le 1; \ -e_{max}(n) \le E \le e_{max}(n)\right\}. \tag{2.13}$$

Example 2.2.3. Interesting is the depiction of $\mathfrak{D}$. For $d = 1$ we have that the dispersion relation is given by $\varepsilon(p) = -(1/2\pi)\cos(2\pi p)$ with the graph

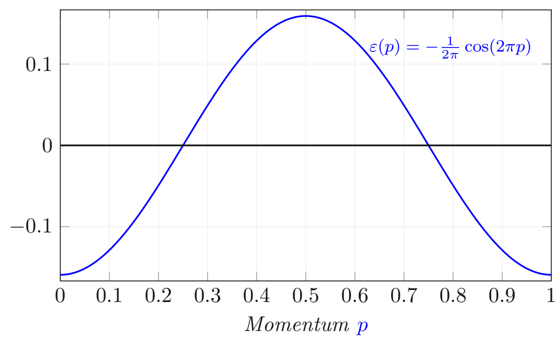

Figure 2.1.: The dispersion relation $\varepsilon(p)$ for $d = 1$.

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Using similar notation as in the proof of Lemma 2.2.1 we have

$$\mathfrak{C}_n = \left\{ p \in \mathbb{T}^d : \varepsilon(p) \geq C(n) \right\}, \qquad \text{where } C(n) \text{ is implicit given, such that meas}\,(\mathfrak{C}_n) = n.$$

From Figure 2.1 we read of that the set $\mathfrak{C}_n$ has to be an interval with centre $1/2$, which in the particular 1D case we expect to be given by $\mathfrak{C}_n = [(1-n)/2, (1+n)/2]$. To prove this we need an explicit formula for $C(n)$, hence we take a closer look onto the condition $\varepsilon(p) \geq C(n)$. The intersection $\varepsilon(p) = C(n)$ has two solutions, namely

$$p_1 = \frac{1}{2\pi} \arccos(-2\pi C(n)) \qquad \text{and} \qquad p_2 = \frac{1}{2} + \frac{1}{2\pi} \arccos(2\pi C(n)). \tag{2.14}$$

Using that $\arccos(-x) = 1/2 - \arccos(x)$ we obtain for

$$p_1 = \frac{1}{2} - \frac{1}{2\pi} \arccos(2\pi C(n))$$

Notice that for all $p \in [p_1, p_2]$ the condition $\varepsilon(p) \geq C(n)$ is always fulfilled and for $p \notin [p_1, p_2]$ we have that $\varepsilon(p) < C(n)$ and hence $\mathfrak{C}_n = [p_1, p_2]$. Since meas $(\mathfrak{C}_n) = n$ has to hold for all n in $[0, 1]$, we obtain the equation

$$\text{meas}\,(\mathfrak{C}_n) = n \qquad \Leftrightarrow \qquad \int_{\frac{1}{2} - \frac{1}{2\pi} \arccos(2\pi C(n))}^{\frac{1}{2} + \frac{1}{2\pi} \arccos(2\pi C(n))} dp = n.$$

Resolving the integral on the right side and using again $\arccos(-x) = 1/2 - \arccos(x)$, yields

$$\frac{1}{\pi} \arccos(2\pi C(n)) = n \qquad \Leftrightarrow \qquad C(n) = \frac{1}{2\pi} \cos(\pi n).$$

Substituting the formula for $C(n)$ into (2.14), we really obtain $\mathfrak{C}_n = [(1-n)/2, (1+n)/2]$. Since $C(n) = (1/2\pi)\cos(\pi n)$ we deduce that the range of $C(n)$ is the intervall $[-1/2\pi, 1/2\pi]$ and that it is monotonically decreasing for n from zero to one. Next we evaluate the maximal energy for a given density n:

$$e_{max}\,(n) = \int_{\mathfrak{C}_n} \varepsilon(p) dp = -\frac{1}{2\pi} \int_{\frac{1}{2} - \frac{n}{2}}^{\frac{1}{2} + \frac{n}{2}} \cos(2\pi p) dp = -\frac{1}{4\pi^2} (\sin(\pi(1+n)) - \sin(\pi(1-n))).$$

Using the identities $\sin(\pi + x) = -\sin(x)$ and $\sin(x) = \sin(\pi - x)$, leads us then to

$$e_{max}\,(n) = -\frac{1}{4\pi^2} (\sin(\pi(1+n)) - \sin(\pi(1-n))) = \frac{1}{4\pi^2} (\sin(\pi n) + \sin(\pi n)) = \frac{1}{2\pi^2} \sin(\pi n).$$

Plotting the above yields

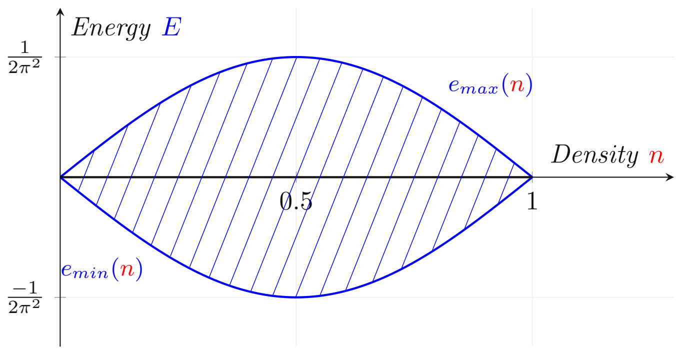

Figure 2.2.: The set $\mathfrak{D}$ for $d = 1$.

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For $d > 1$ the treatment is much more difficult, due to the fact that $C(n)$ and $\mathfrak{C}_n$ are harder to determine. We expect that $\mathfrak{D}$ should, up to some constants, always have the same shape as in Figure 2.2 ■

Remark 2.2.4. For any given particle density $n \in [0,1]$, the interval $[-e_{max}(n), e_{max}(n)]$ is the possible range for the energy of the system. The function $e_{max}(n)$ is only zero if $n \in \{0,1\}$, which coincides with the fact mentioned in the beginning of this section. Moreover the integral of $\varepsilon(p)$ is at maximum, if we integrate over the set where $\varepsilon(p) > 0$, which coincides with $C(n) = 0$ and $n = (1/2)$ for all dimensions $d \in \mathbb{N}$. Therefore we obtain for any $n \in [0,1]$

$$e_{max}(n) \leq e_{max}\left(\frac{1}{2}\right) = -\frac{d}{(2\pi)^2}\left(\sin\left(2\pi\frac{3}{4}\right) - \sin\left(2\pi\frac{1}{4}\right)\right) = \frac{d}{2\pi^2} =: e_{max}. \tag{2.15}$$

This can be interpreted as achieving the highest possible energy when the system is "*half full*" (is also reflected in our picture of $\mathfrak{D}$, see Figure 2.2). ■

The Fermi Dirac distribution

The set $\mathfrak{D}$ defined in (2.13) will be important for our diffusive limit, hence it is worth to have a closer look on it. With the help of the so called *Fermi Dirac distribution* we will be able to find for every pair (n, E) in $\mathfrak{D}$ a function f from $\mathrm{L}^1(\mathbb{T}^d)$, which integrated with respect to the zeroth and second momentum equals that pair. The next Lemma is cited from [Bra17] and justifies that assumption.

Lemma 2.2.5. *Let $\mathfrak{D}$ be the set given in* (2.13)*, then*

$$\begin{aligned}\mathfrak{D} &= \Big\{(n,E) \in \mathbb{R}^2 : 0 \leq n \leq 1; \ -e_{max}(n) \leq E \leq e_{max}(n)\Big\}\\ &= \Big\{\int_{\mathbb{T}^d}(1,\varepsilon(p))f(p)dp : f \in \mathrm{L}^1(\mathbb{T}^d);\ 0 \leq f \leq 1\Big\}\end{aligned}$$

Proof. We give here a short sketch and for details we refer to [Bra17], Lemma 5.1.14., where η has to be chosen as one.
The first equality is the definition of the set D and the second equality is a standard set comparison, where we give a rough idea. With Lemma (2.2.1), we obtain the inclusion "$\supseteq$". For the other direction "$\subseteq$, let (n, E) be given, then the key point is to construct a function of the form

$$\xi_s(p) := s\mathbb{1}_{\{p\in\mathbb{T}^d:\varepsilon(p)\geq C\}}(p)+(1-s)\mathbb{1}_{\{p\in\mathbb{T}^d:\varepsilon(p)\leq -C\}}(p), \text{ with } \operatorname{meas}\left(\Big\{p \in \mathbb{T}^d : \varepsilon(p) \geq C\Big\}\right) = n$$

for $s \in [0,1]$. Then it is possible to find a suitable s_0 such, that $\int_{\mathbb{T}^d}(1,\varepsilon(p))\xi_{s_0}(p)dp = (n, E)$. □

The next definition will give us a clue, what the local equilibrium of the system will be.

Definition 2.2.6. *For $(\lambda_0, \lambda_1, p) \in \mathbb{R}^2 \times \mathbb{T}^d$ define the generalized Fermi Dirac distribution*

$$\mathcal{F}(\lambda_0, \lambda_1; p) := \frac{1}{1 + \exp(-\lambda_0 - \lambda_1\varepsilon(p))}. \tag{2.16}$$

Not trivial is the upcoming proposition, which we also cite from [Bra17]. It shows the relation between the set $\mathfrak{D}$ and the Fermi Dirac distribution, given in the above Definition.

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Proposition 2.2.7. *Let $\mathfrak{D}$ be the set defined in* (2.13) *and denote by $\mathfrak{D}^\circ$ the interior of it, then the mapping*

$$\mathfrak{b} : \mathbb{R}^2 \to \mathfrak{D}^\circ, \qquad (\lambda_0, \lambda_1) \mapsto \int_{\mathbb{T}^d} (1, \varepsilon(p)) \mathcal{F}(\lambda_0, \lambda_1; p) dp,$$

is bijective and smooth. Moreover, its inverse is smooth as well.

Proof. This is proven in [Bra17], where we set $\eta = 1$. Notice that the author made in his Proposition a typing mistake and that he meant exactly what we have written in Proposition 2.2.7. We give a short sketch of the proof here and refer for details to [Bra17] Proposition 5.1.8 in Chapter 5. First define the functions

$$\tilde{n}(\lambda_0, \lambda_1) := \int_{\mathbb{T}^d} \mathcal{F}(\lambda_0, \lambda_1; p) dp, \quad \tilde{E}(\lambda_0, \lambda_1) := \int_{\mathbb{T}^d} \varepsilon(p) \mathcal{F}(\lambda_0, \lambda_1; p) dp.$$

Then it possible to show that the Jacobian determinant $\det \partial_{\lambda_0, \lambda_1}(\tilde{n}, \tilde{E})$ is positive. This just proves that $(\lambda_0, \lambda_1) \mapsto (\tilde{n}(\lambda_0, \lambda_1), \tilde{E}(\lambda_0, \lambda_1))$ is just a local isomorphism. To proof that this isomorphism is indeed global, it is possible to show the existence of a unique function $\phi : \mathbb{R} \to \mathbb{R}$, such that for every (n, E) given in $\mathfrak{D}^\circ$ there exists a unique $\lambda_1 \in \mathbb{R}$ such that

$$(n, E) = \int_{\mathbb{T}^d} (1, \varepsilon(p)) \mathcal{F}(\phi(\lambda_1), \lambda_1; p) dp.$$

The fact that $\det \partial_{\lambda_0, \lambda_1}(\tilde{n}, \tilde{E})$ is positive ensures that the Jacobian of $\mathfrak{b}$ is invertible and the implicit function theorem ensures therefore the smoothness of the inverse $\mathfrak{b}^{-1}$. □

The upcoming statement is deduced from the above and gives a detailed insight on the interior of $\mathfrak{D}$.

Corollary 2.2.8. *Let $\mathfrak{D}$ be the set defined in* (2.13), *then the interior of $\mathfrak{D}$ is given by*

$$\begin{aligned} \mathfrak{D}^\circ &= \Big\{ (n, E) \in \mathbb{R}^2 : 0 < n < 1; \;\; -e_{max}(n) < E < e_{max}(n) \Big\} \\ &= \Big\{ \int_{\mathbb{T}^d} (1, \varepsilon(p)) f(p) dp : f \in \mathrm{L}^1(\mathbb{T}^d); \;\; 0 < f < 1 \Big\} \end{aligned}$$

Proof. The first equality comes from basic topology, therefore we focus on the second equality. Starting with "$\supseteq$" we deduce from Lemma 2.2.5 that for every $f \in \mathrm{L}^1(\mathbb{T}^d)$ with $0 < f < 1$ there exist a representative (n_f, E_f) in $\mathfrak{D}$, which is given by

$$(n_f, E_f) = \int_{\mathbb{T}^d} (1, \varepsilon(p)) f(p) dp.$$

Hence it is enough to show that (n_f, E_f) lies in the interior of $\mathfrak{D}$. Since $0 < f(p) < 1$ we have clearly that $0 < n_f < 1$. For E_f we look into the estimate (2.11) in proof of Lemma 2.2.1. At that point we can estimate with a strict "$<$" since f is strict smaller than one. Therefore we obtain that $E_f < e_{max}(n_f)$. Following the same proof further we also obtain for the same reason the strict estimate $-e_{max}(n_f) < E_f$, which proves the first inclusion.
For the other direction let $(n, E) \in \mathfrak{D}^\circ$ be given. Recalling Definition 2.2.6 we obtain with Proposition 2.2.7, since $n \notin \{0, 1\}$, that for (n, E) there exist unique $(\lambda_{(0,n,E)}, \lambda_{(1,n,E)}) \in \mathbb{R}^2$ such that

$$\int_{\mathbb{T}^d} (1, \varepsilon(p)) \mathcal{F}(\lambda_{(0,n,E)}, \lambda_{(1,n,E)}, p) dp = (n, E).$$

Looking at the definition of $\mathcal{F}$ we see immediately that it has to be in $\mathrm{L}^1(\mathbb{T}^d)$ and that the function fulfills $0 < \mathcal{F}(\lambda_{(0,n,E)}, \lambda_{(1,n,E)}, p) < 1$ for all $p \in \mathbb{T}^d$, which concludes the proof. □

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Remark 2.2.9. Before we pass to the next section, we state facts about the Fermi Dirac distribution and give for our purposes important results about the bijection $\mathfrak{b}$ coming from [Bra17]. $\mathcal{F}$ can be rewritten as composition of two functions

$$\mathcal{F}(\lambda_0, \lambda_1; p) = G'(\lambda_0 + \lambda_1 \varepsilon(p)), \qquad \text{where} \quad G : \mathbb{R} \to \mathbb{R}, \quad s \mapsto \log(1 + \exp(s)).$$

An immediate consequence is that the Fermi-Dirac distribution is even on the $\mathbb{T}^d$ in the sense of Definition 2.1.3, for all $(\lambda_0, \lambda_1) \in \mathbb{R} \times \mathbb{R}$, since $\varepsilon(p)$ is even on $\mathbb{T}^d$. The derivatives of G are

$$G'(s) = \frac{\exp(s)}{1 + \exp(s)} = \frac{1}{1 + \exp(-s)}, \qquad G''(s) = \frac{\exp(s)}{(1 + \exp(s))^2}, \qquad \forall s \in \mathbb{R}.$$

They have the following properties for all $s \in \mathbb{R}$ and $r \in (0, 1)$

$$G'(s) \in (0, 1), \qquad G''(s) = G'(s)(1 - G'(s)), \qquad (G')^{-1}(r) = \log \frac{r}{1 - r}.$$

We introduce the notation

$$\lambda := (\lambda_0, \lambda_1), \qquad \mathfrak{b}(\lambda) \widehat{=} \begin{pmatrix} \tilde{n}(\lambda) \\ \tilde{E}(\lambda) \end{pmatrix} \qquad \mathfrak{b}^{-1}(n, E) \widehat{=} \begin{pmatrix} \lambda_0(n, E) \\ \lambda_1(n, E) \end{pmatrix}.$$

Using the properties of G we see that for $i, j \in \{0, 1\}$

$$\partial_{\lambda_i} \mathfrak{b}_j(\lambda) = \partial_{\lambda_i} \int_{\mathbb{T}^d} \varepsilon(p)^j \mathcal{F}(\lambda; p) dp = \int_{\mathbb{T}^d} \varepsilon(p)^{i+j} \mathcal{F}(\lambda; p)(1 - \mathcal{F}(\lambda; p)) dp.$$

From the above we deduce immediately that $\partial_{\lambda_0} \tilde{n}(\lambda)$ has to be positive and in [Bra17] was shown that the Jacobian matrix $D_{\lambda_0, \lambda_1} \mathfrak{b}(\lambda)$ has a positive determinant (see Lemma 5.1.10 in [Bra17]). Hence we can conclude with the main minors that $D_{\lambda_0, \lambda_1} \mathfrak{b}$ $(\widehat{=} D_{\lambda_0, \lambda_1}(\tilde{n}(\lambda), \tilde{E}(\lambda)))$ is a symmetric and positive definite matrix. Moreover with the inverse function theorem and the fact that $\partial_{\lambda_1} \tilde{E}(\lambda) > 0$, we also obtain for the inverse $\mathfrak{b}^{-1}$, that its Jacobian matrix $D_{n,E}(\lambda)$ is symmetric and positive definite. ■

2.2.2. The Local Equilibrium and the H-Theorem

As mentioned in the beginning, the DSSBE (2.6) is not fully described yet, since we have not given an explicit form of $\mathcal{F}(f; p)$. The local equilibrium of our system is defined as the minimizer of the measure of disorder, *the entropy functional*, under the constraints having the same particle density and total energy as that of the distribution describing the system at the moment (coming from the elastic collisions). We will show in this section that the Fermi Dirac distribution is exactly this minimizer we are looking for. The entropy functional for an ultracold cloud of fermions comes from degenerate Fermi statistics and is defined by

$$\mathcal{H}(f) := \int_{\mathbb{T}^d} \int_{\mathbb{T}^d} h(f) dp dx, \qquad \text{where } h(f) := f \log(f) + (1 - f) \log(1 - f), \tag{2.17}$$

see as examples [Jü09, Hug83, Dol94, Lu08a, Lu01]. We see that the above functional is well defined for all functions f in $\mathrm{L}^1(\mathbb{T}^d \times \mathbb{T}^d)$ with $0 \leq f \leq 1$.

Remark 2.2.10. Since the function $\mathcal{H}$ will be of great value for this chapter, we give here some facts about it.

- Looking at the function $h(y) = y \log(y) + (1 - y) \log(1 - y)$ for $y \in (0, 1)$, we have the derivatives

$$h(y) = y \log \left(\frac{y}{1 - y} \right) + \log(1 - y), \qquad h'(y) = \log \left(\frac{y}{1 - y} \right), \qquad h''(y) = \frac{1}{y(1 - y)}.$$

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- The function $h(y)$ has a minimum at $y = 2^{-1}$ and hence $h(y) > \log(1/2),\ \forall y \in (0,1)$.
- Looking at the first derivative we see that h' is the inverse function of

$$g : \mathbb{R} \to (0,1), \qquad s \mapsto \frac{1}{1 + exp(-s)}.$$

- Observe that $h'' > 0$ and therefore h is a convex function. Additionally $h''(y)$ has a minimum at $y = 1/2$, hence $h''(y) \geq 4$ for all $y \in (0,1)$.
- The Taylor expansion of $h(y)$ at the point $y_0 \in (0,1)$ is given by

$$h(y) = h(y_0) + h'(y_0)(y - y_0) + \frac{1}{2}h''(\xi)(y - y_0)^2$$

for some $\xi \in (0,1)$. Since $h''(y)$ has a minimum at $y = 1/2$ we have the estimate

$$h(y) \geq h(y_0) + h'(y_0)(y - y_0) + 2(y - y_0)^2 \tag{2.18}$$

■

Theorem 2.2.11. *Let (n, E) be given in $\mathfrak{D}^\circ$, then the solution to*

$$\min_{f \in L^1(\mathbb{T}^d)} \left\{ \mathcal{H}(f) \middle| \ 0 < f < 1, \quad \int_{\mathbb{T}^d} f(p)dp = n, \quad \int_{\mathbb{T}^d} \varepsilon(p) f(p) dp = E \right\} \tag{2.19}$$

is given by the Fermi Dirac distribution

$$\mathcal{F}(n, E; p) = \frac{1}{1 + \exp(-\lambda_0(n,E) - \lambda_1(n,E)\varepsilon(p))}, \tag{2.20}$$

where λ_0, λ_1 are given by the bijection in Proposition 2.2.7.

Proof. Notice that we have for now no dependence on the spatial variable x, hence the entropy functional $\mathcal{H}$ reduces to

$$\mathcal{H}(f) = \int_{\mathbb{T}^d} \int_{\mathbb{T}^d} h(f(p)) dx dp = \int_{\mathbb{T}^d} h(f(p)) dp.$$

Also observe that the set over we minimize is due to Corollary 2.2.8 not empty. Proposition 2.2.7 provides for $(n, E) \in \mathfrak{D}^\circ$ the existence of unique $\lambda_0(n, E), \lambda_1(n, E)$ such that

$$\int_{\mathbb{T}^d} (1, \varepsilon(p)) \mathcal{F}(\lambda_0(n,E), \lambda_1(n,E); p) dp = (n, E),$$

and with $\mathcal{F}$ being clearly a function in $L^1(\mathbb{T}^d)$, it is a valid candidate. The remaining part is to prove that $\mathcal{F}$ is really a minimizer, and let therefore $f \in L^1(\mathbb{T}^d)$ with $f \neq \mathcal{F}$ fulfill the constraints given in (2.19). Using the Taylor series of h around $\mathcal{F}$, we obtain with (2.18) that

$$h(f(p)) \geq h(\mathcal{F}(p)) + h'(\mathcal{F}(p))(f(p) - \mathcal{F}(p)) + 2(f(p) - \mathcal{F}(p))^2, \qquad \forall p \in \mathbb{T}^d. \tag{2.21}$$

From Remark 2.2.10 we deduce that $h'(\mathcal{F}(p)) = \lambda_0(n, E) + \lambda_1(n, E)\varepsilon(p)$, and since f and $\mathcal{F}$ fulfill the constraints in (2.19), we get

$$\int_{\mathbb{T}^d} h'(\mathcal{F}(p))(f(p) - \mathcal{F}(p)) dp = \lambda_0 \int_{\mathbb{T}^d} (f(p) - \mathcal{F}(p)) dp + \lambda_1 \int_{\mathbb{T}^d} \varepsilon(p)(f(p) - \mathcal{F}(p)) dp = 0.$$

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Integrating the previous estimate (2.21) with respect to the momentum p, we obtain with the above identity that

$$\mathcal{H}(f) \geq \mathcal{H}(\mathcal{F}) + 2\int_{\mathbb{T}^d} (f(p) - \mathcal{F}(p))^2 dp.$$

Since $(f - \mathcal{F})^2 \geq 0$ we obtain that for given $(n, E) \in \mathfrak{D}^\circ$ and for all $f \in \mathrm{L}^1(\mathbb{T}^d)$, fulfilling the constraints given in (2.19), that

$$\mathcal{H}(\mathcal{F}) \leq \mathcal{H}(f).$$

□

Remark 2.2.12. To avoid over-notation we will denote the Fermi Dirac distribution with $\mathcal{F}(n, E; p)$ (instead of $\mathcal{F}(\lambda_0(n, E), \lambda_1(n, E); p)$), to show the dependence on the constraints given in (2.19).
Looking at a distribution function $f \in \mathrm{L}^1(\mathbb{R} \times \mathbb{T}^d \times \mathbb{T}^d)$ with $0 < f(t, x, p) < 1$ for all (t, x, p) in $\mathbb{R} \times \mathbb{T}^d \times \mathbb{T}^d$ and defining

$$(n(t, x), E(t, x)) := \int_{\mathbb{T}^d} (1, \varepsilon(p)) f(t, x, p) dp \in \mathfrak{D}^\circ, \qquad \forall (t, x) \in \mathbb{R} \times \mathbb{T}^d,$$

we see that the Fermi Dirac distribution $\mathcal{F}(n(t, x), E(t, x); p)$ is well defined and depends through f on the variables t and x. ■

Finally with all the prework we have done so far, we are able to give the definition for the collision operator of BGK-type.

Definition 2.2.13. *Let f be a function in $\mathrm{L}^1(\mathbb{R} \times \mathbb{T}^d \times \mathbb{T}^d)$ with $0 < f(t, x, p) < 1$ for all $(t, x, p) \in \mathbb{R} \times \mathbb{T}^d \times \mathbb{T}^d$, then we define the collision operator as follows:*

$$\mathcal{Q}_\tau(f) := \frac{1}{\tau}\left(\mathcal{F}\left(\int_{\mathbb{T}^d} f(t, x, \tilde{p}) d\tilde{p}, \int_{\mathbb{T}^d} \varepsilon(\tilde{p}) f(t, x, \tilde{p}) d\tilde{p}; p\right) - f(t, x, p)\right) \tag{2.22}$$

Since we want to lay our focus on the rigorous derivation of a macroscopic model and the long time behaviour of it, we state for further progress a hypothesis about the existence of a solution to our model equation with a sufficiently smooth initial condition.

Hypothesis 2.2.14. *Let f_0 be a function in $C^1(\mathbb{T}^d \times \mathbb{T}^d)$ with $0 < f_0(x, p) < 1$ for all $(x, p) \in \mathbb{T}^d \times \mathbb{T}^d$, let $\mathcal{F}$ be the Fermi-Dirac distribution as defined in (2.20) and let $\mathcal{Q}_\tau$ be the collision operator defined in (2.22). Then the equation*

$$\tau \partial_t f_\tau + \nabla_p \varepsilon \cdot \nabla_x f_\tau = \mathcal{Q}_\tau(f_\tau), \qquad f_\tau(0, x, p) = f_0(x, p) \tag{2.23}$$

has a unique solution f_τ in $C^1(\mathbb{R}^+ \times \mathbb{T}^d \times \mathbb{T}^d)$ for all $\tau > 0$.

Remark 2.2.15. First we point out that some decisions about the above conditions could have been chosen less restrictive, but for the purpose of keeping an good overview we decided to choose them specifically as they are. To show that the equation (2.23) has under specific conditions a solution can be found in the literature. For example one of our main reference paper [GP92] has shown that the solution f_τ lies in $\mathrm{L}^\infty(\mathbb{R} \times \mathbb{R}^3 \times B)$ where B is the first Brillouin zone. There a more general setting was considerd.
Another approach was performed by Xuguang [Lu08b], where the right side of (2.23) was chosen differently and very soft collision kernels were an condition.
Mustieles [Mus90] and the follow up work with Francisco [Mus91], found global existance

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of classical (for $d = 1, 2$) and weak solutions ($d = 3$), and also uniqueness under certain assumptions, where again the right hand side differs from our choice. Also the velocity was considered of linear dependence regarding the momentum, which is in our setting not the case.
We think that it is possible to show the existence of a solution of (2.23), which is at least L^∞ (comparing with the above results), but due to time issues and the desire to keep it simple, we did not prove the hypothesis here. ■

Definition 2.2.16. *Let f_τ be the solution to the diffusive scaled semiconductor Boltzmann equation* (2.23)*, then we define the macroscopic particle density n_τ and energy density E_τ of the system by*

$$n_\tau(t,x) := \int_{\mathbb{T}^d} f_\tau(t,x,p)dp, \qquad E_\tau(t,x) := \int_{\mathbb{T}^d} \varepsilon(p) f_\tau(t,x,p)dp. \tag{2.24}$$

Remark 2.2.17. If the solution f_τ lies in $C^1(\mathbb{R}^+ \times \mathbb{T}^d \times \mathbb{T}^d)$, then we have clearly that also its moments n_τ and E_τ (see (2.24)) lie in $C^1(\mathbb{R}^+ \times \mathbb{T}^d)$ for every $\tau > 0$. With Proposition 2.2.7 we obtain then that also the functions $\lambda_0(n_\tau, E_\tau) : \mathbb{R}^+ \times \mathbb{T}^d \to \mathbb{R}^2$ and $\lambda_1(n_\tau, E_\tau) : \mathbb{R}^+ \times \mathbb{T}^d \to \mathbb{R}^2$ are at least in $C^1(\mathbb{R}^+ \times \mathbb{T}^d)$ and hence we conclude that then the Fermi-Dirac distribution $\mathcal{F}(n_\tau, E_\tau; p)$ is a composition of C^1-functions and therefore itself in $C^1(\mathbb{R}^+ \times \mathbb{T}^d \times \mathbb{T}^d)$ for all $\tau > 0$. ■

The starting distribution f_0 defines the mean particle density $\bar{n}$ and mean energy $\bar{E}$ (see (2.8)) of the system which should be the same at all times. Now the function with the lowest measure of disorder, with the same mean particle density and mean energy, is the equilibrium of our system. Explicit we have the following.

Definition 2.2.18. *For given $f_0 \in \mathrm{L}^1(\mathbb{T}^d \times \mathbb{T}^d)$, with $0 < f_0 < 1$, let $\bar{n}$ and $\bar{E}$ be the mean particle density and mean energy given by* (2.8)*. Then we define the equilibrium of the system*

$$\mathcal{F}_{eq}(p) := \mathcal{F}(\bar{n}, \bar{E}; p). \tag{2.25}$$

Remark 2.2.19. $\mathcal{F}_{eq}(p)$ in Definition 2.2.18 is well defined due to the fact, that if $0 < f_0 < 1$ we also have that $(\bar{n}, \bar{E}) \in \mathfrak{D}^\circ$, see Corollary 2.2.8.
Moreover if the system is already at equilibrium from the start, i.e. if we set in our model equation (2.23) for any $(\bar{n}, \bar{E}) \in \mathfrak{D}^\circ$

$$f_0(x,p) := \mathcal{F}(\bar{n}, \bar{E}, p),$$

the solution is given by the equilibrium state $\mathcal{F}_{eq}$. The left hand side of (2.23) vanishes, because $\mathcal{F}_{eq}$ is constant in time and space. For the right hand side we notice that

$$\mathcal{F}\left(\int_{\mathbb{T}^d} \mathcal{F}_{eq}(p)dp, \int_{\mathbb{T}^d} \varepsilon(p)\mathcal{F}_{eq}(p)dp; p\right) = \mathcal{F}(\bar{n}, \bar{E}; p) = \mathcal{F}_{eq}(p),$$

and therefore $\mathcal{Q}_\tau(\mathcal{F}(\bar{n}, \bar{E}, p)) = 0$. This reflects the natural behaviour we would expect, if the system is in equilibrium from the start, it remains in this state. ■

We state now an appropriate H-Theorem, which will play a major role in the diffusive limit and studying the long time behaviour.

Theorem 2.2.20 (H-Theorem)**.** *Let f_τ be the solution to the semiconductor Boltzmann equation* (2.23)*, and define the functions*

$$n_\tau := \int_{\mathbb{T}^d} f_\tau(t,x,p)dp, \quad E_\tau := \int_{\mathbb{T}^d} \varepsilon(p) f_\tau(t,x,p)dp, \quad P_\tau(t) := \|\mathcal{Q}_\tau(f_\tau(t))\|^2_{\mathrm{L}^2(\mathbb{T}^d \times \mathbb{T}^d)},$$

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where $\mathcal{Q}_\tau$ is defined in (2.22) *and $\mathcal{F}(n_\tau, E_\tau; p)$ denotes the Fermi Dirac distribution defined in* (2.20)*. Then the time derivative of the entropy functional decays*

$$\frac{d}{dt}\mathcal{H}(f_\tau(t)) \leq 0 \qquad \forall \tau > 0.$$

Moreover the following estimate holds for all $s, t \in \mathbb{R}_0^+$ with $s \leq t$:

$$\mathcal{H}(f_\tau(t)) + 2\int_s^t P_\tau(\sigma)d\sigma \leq \mathcal{H}(f_\tau(s)), \qquad \forall \tau > 0. \tag{2.26}$$

Proof. For the sake of simplicity we fix $\tau > 0$ and drop the lower index notation on f_τ, n_τ, E_τ, $\mathcal{F}(n_\tau, E_\tau; p)$, $\mathcal{Q}_\tau$ and will just write f, n, E, $\mathcal{F}$, $\mathcal{Q}$ respectively instead. Now since f is a solution of (2.23), we have that $f \in C^1(\mathbb{R}^+ \times \mathbb{T}^d \times \mathbb{T}^d)$ and $0 < f < 1$. The time derivative of $\mathcal{H}(f(t))$ is given by

$$\frac{d}{dt}\mathcal{H}(f) = \int_{\mathbb{T}^d}\int_{\mathbb{T}^d}\frac{d}{dt}h(f)dxdp = \int_{\mathbb{T}^d}\int_{\mathbb{T}^d}(\partial_t f)h'(f)\ dxdp.$$

Using that f is a solution to (2.23) provides

$$\begin{aligned}
\frac{d}{dt}\mathcal{H}(f) &= \int_{\mathbb{T}^d}\int_{\mathbb{T}^d}\left(\frac{1}{\tau^2}(\mathcal{F} - f) - \frac{1}{\tau}\nabla_p\varepsilon(p)\cdot\nabla_x f\right)h'(f)dxdp \\
&= \int_{\mathbb{T}^d}\int_{\mathbb{T}^d}\frac{1}{\tau^2}(\mathcal{F} - f)\,h'(f)dxdp - \int_{\mathbb{T}^d}\int_{\mathbb{T}^d}\frac{1}{\tau}(\nabla_p\varepsilon(p)\cdot\nabla_x f)h'(f)dxdp \\
&= \int_{\mathbb{T}^d}\int_{\mathbb{T}^d}\frac{1}{\tau^2}(\mathcal{F} - f)\,h'(f)dxdp - \int_{\mathbb{T}^d}\int_{\mathbb{T}^d}\frac{1}{\tau}\nabla_p\varepsilon(p)\cdot\nabla_x h(f)dxdp \\
&= \int_{\mathbb{T}^d}\int_{\mathbb{T}^d}\frac{1}{\tau^2}(\mathcal{F} - f)\,h'(f)dxdp.
\end{aligned}$$

Through the convexity of h (see Remark 2.2.10) we have that the tangent on every point $h(f)$ evaluated at $\mathcal{F}$ is smaller than $h(\mathcal{F})$

$$h'(f)(\mathcal{F} - f) + h(f) \leq h(\mathcal{F}), \tag{2.27}$$

which leads us to

$$\begin{aligned}
\frac{d}{dt}\mathcal{H}(f) &= \int_{\mathbb{T}^d}\int_{\mathbb{T}^d}\frac{1}{\tau^2}(\mathcal{F} - f)\,h'(f)dxdp \leq \frac{1}{\tau^2}\int_{\mathbb{T}^d}\int_{\mathbb{T}^d}(h(\mathcal{F}) - h(f))dxdp \\
&= \frac{1}{\tau^2}(\mathcal{H}(\mathcal{F}) - \mathcal{H}(f)).
\end{aligned} \tag{2.28}$$

Since (n, E) lies in $\mathfrak{D}^\circ$ for all $(t, x) \in \mathbb{R}^+ \times \mathbb{T}^d$ and $\mathcal{F}$ being a minimizer of $\mathcal{H}$ (Theorem 2.2.11), we deduce

$$\frac{d}{dt}\mathcal{H}(f_\tau(t)) \leq 0 \qquad \forall \tau > 0.$$

For estimate (2.26) we use the Taylor expansion of $h(f)$ at $\mathcal{F}$ (see Remark 2.2.10) and obtain

$$(f - \mathcal{F})^2 \leq \frac{1}{2}(h(f) - h(\mathcal{F}) - h'(\mathcal{F})(f - \mathcal{F})).$$

Integrating left and right hand side with respect to x and p leads to

$$\int_{\mathbb{T}^d}\int_{\mathbb{T}^d}(f - \mathcal{F})^2 dxdp \leq \frac{1}{2}(\mathcal{H}(f) - \mathcal{H}(\mathcal{F})) - \frac{1}{2}\int_{\mathbb{T}^d}\int_{\mathbb{T}^d}h'(\mathcal{F})(f - \mathcal{F})dxdp. \tag{2.29}$$

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From Remark 2.2.10 we deduce that $h'(\mathcal{F}) = \lambda_0(n,E) + \lambda_1(n,E)\varepsilon(p)$, and since f and $\mathcal{F}$ fulfill the constraints in (2.19), we get for all (t,x) in $\mathbb{R}^+ \times \mathbb{T}^d$ that

$$\int_{\mathbb{T}^d} h'(\mathcal{F})(f-\mathcal{F})dp = \lambda_0 \int_{\mathbb{T}^d} (f-\mathcal{F})dp + \lambda_1 \int_{\mathbb{T}^d} \varepsilon(p)(f-\mathcal{F})dp = 0.$$

Hence the integral over $\mathbb{T}^d$ with respect to the spatial variable x is also zero. Using the previous estimates (2.28) and (2.29), we obtain for the time derivative of $\mathcal{H}$

$$\frac{d}{dt}\mathcal{H}(f) \leq \frac{1}{\tau^2}(\mathcal{H}(\mathcal{F}) - \mathcal{H}(f)) \leq -\frac{2}{\tau^2}\int_{\mathbb{T}^d}\int_{\mathbb{T}^d}(f-\mathcal{F})^2 dx dp.$$

Integrating both sides from s to t for $0 \leq s \leq t$, we get the desired estimate for all $\tau > 0$

$$\mathcal{H}(f_\tau(t)) + 2\int_s^t P_\tau(\sigma)d\sigma \leq \mathcal{H}(f_\tau(s)).$$

□

As last result of this section we apply the H-Theorem, and show that the family $(\mathcal{Q}_\tau)_{\tau>0}$ is uniformly bounded.

Corollary 2.2.21. *Let for all $\tau > 0$, f_τ be the solution to* (2.23)*, let f_0 be the initial value for all $\tau > 0$ and let $\mathcal{Q}_\tau$ the belonging collision operator, see* (2.22)*. Then the family $(\mathcal{Q}(f_\tau))_{\tau>0}$ is uniformly bounded for all intervals $I \subseteq \mathbb{R}_0^+$, i.e.*

$$\|\mathcal{Q}_\tau(f_\tau)\|^2_{\mathrm{L}^2(I;\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))} \leq \mathcal{H}(f_0) - \log(1/2). \tag{2.30}$$

Proof. Let t_0, t_1 such that $\bar{I} = [t_0, t_1]$ and recall from the H-theorem the definition

$$P_\tau(t) := \|\mathcal{Q}_\tau(f_\tau(t))\|^2_{\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)}.$$

From Remark 2.2.10 we have that $h(f_\tau(t)) > \log(1/2)$ for all $t \in \mathbb{R}^+$ and all $\tau > 0$. With that and the fact that $P_\tau(t)$ is positive for all $\tau > 0$, we deduce

$$\forall t \in \mathbb{R}^+: \qquad \log(1/2) \leq \mathcal{H}(f_\tau(t)) \leq \mathcal{H}(f_\tau(0)) = \mathcal{H}(f_0).$$

Therefore we conclude from the H-theorem that

$$\|\mathcal{Q}_\tau(f_\tau)\|^2_{\mathrm{L}^2(I;\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))} = \int_{t_0}^{t_1} \|\mathcal{Q}_\tau(f_\tau(t))\|^2_{\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)} dt = \int_{t_0}^{t_1} P_\tau(t)dt \leq \mathcal{H}(f_0) - \log(1/2).$$

Since the above holds for all t_0, t_1 in $\mathbb{R}_0^+$ we have that it holds for all intervals $I_N := [0, N]$, $N \in \mathbb{N}$. Passing to the limit N to infinity, we obtain that the estimate holds also for $\mathbb{R}_0^+$. □

2.3. The Diffusive Limit

Recalling that our main goal is to derive rigorously a macroscopic description of the ultracold cold cloud of fermions. To prepare the path we want to follow, we look first at the formal limit. For the convenience of the reader we recall the starting equation (diffusive scaled semiconductor Boltzmann equation (DSSBE)):

$$(2.23): \quad \tau\partial_t f_\tau + \nabla_p\varepsilon \cdot \nabla_x f_\tau = \mathcal{Q}_\tau(f_\tau), \qquad f_\tau(0,x,p) = f_0(x,p), \qquad \forall \tau > 0.$$

and the definitions of the macroscopic densities

$$n_\tau(t,x) := \int_{\mathbb{T}^d} f_\tau(t,x,p)dp, \qquad E_\tau(t,x) := \int_{\mathbb{T}^d} \varepsilon(p) f_\tau(t,x,p)dp. \tag{2.31}$$

The formal diffusive limit is given by:

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Theorem 2.3.1 (Formal Limit)**.** *Let f_τ be the solution to the DSSBE* (2.23) *and let n_τ and E_τ be defined as in* (2.31)*, and let them be sufficiently smooth with*

$$(n_\tau(t,x), E_\tau(t,x)) \in \mathfrak{D}^\circ \quad \forall (t,x) \in \mathbb{R}^+ \times \mathbb{T}^d.$$

If the the family of collision operators $(\mathcal{Q}_\tau)_{\tau>0}$ is bounded and if the families $(n_\tau)_{\tau>0}$ and $(E_\tau)_{\tau>0}$ converge towards limit functions n and E such that

$$\forall (t,x) \in \mathbb{R}^+ \times \mathbb{T}^d : \qquad (n(t,x), E(t,x)) \in \mathfrak{D}^\circ,$$

then the limit functions n and E solve the following equations:

$$\partial_t n - \operatorname{div}_x \left(\int_{\mathbb{T}^d} (\nabla_p \varepsilon(p) \cdot \nabla_x \mathcal{F}(n,E;p)) \nabla_p \varepsilon(p) dp \right) = 0 \tag{2.32}$$

$$\partial_t E - \operatorname{div}_x \left(\int_{\mathbb{T}^d} \varepsilon(p) (\nabla_p \varepsilon(p) \cdot \nabla_x \mathcal{F}(n,E;p)) \nabla_p \varepsilon(p) dp \right) = 0. \tag{2.33}$$

The proof of Theorem 2.3.1 is given in Subsection 2.3.1, where we also introduce the *Chapman-Enskog expansion*, which is the main idea of the formal derivation. In the end of Subsection 2.3.1 we take a closer look the formal limit equations, see the belonging remark.

For the rigorous derivation we cannot expect that the limit functions n and E exist and that their range lies in $\mathfrak{D}^\circ$. Therefore the Fermi-Dirac distribution, as given in (2.20), would not be enough and would not be well defined. Starting with the definition of the *Fermi energy* ϵ_F we will be able to extend the Fermi-Dirac distribution onto $\mathfrak{D}$.

Definition 2.3.2. *For $n \in [0,1]$ define $\epsilon_F(n) \in \overline{\varepsilon(\mathbb{T}^d)} = [-d/(2\pi), d/(2\pi)]$ as the unique solution of*

$$\operatorname{meas}\left(\left\{ p \in \mathbb{T}^d : \varepsilon(p) < \epsilon_F(n) \right\} \right) = n, \tag{2.34}$$

The parameter $\epsilon_F(n)$ is called the Fermi Energy.

That the Fermi energy is well defined follows from the proof of Lemma 2.2.1, where we defined a similar function. Let us now introduce the extension of the Fermi-Dirac distribution:

Definition 2.3.3. *Let $\mathcal{F}$ be the Fermi-Dirac distribution, as given in* (2.20)*. The extension $\bar{\mathcal{F}}$ of $\mathcal{F}$ from $\mathfrak{D}^\circ$ to $\mathfrak{D}$ is then defined by*

$$\bar{\mathcal{F}}(n,E;p) := \begin{cases} n & \text{if } n \in \{0,1\}, \\ \mathcal{F}(n,E;p) & \text{if } (n,E) \in \mathfrak{D}^\circ, \\ \mathbb{1}_{\{\mp\varepsilon(p) < \epsilon_F(n)\}}(p) & \text{if } E = \pm e_{max}(n). \end{cases}$$

We see that $\bar{\mathcal{F}}$ is now defined for all pairs $(n,E) \in \mathfrak{D}$ and another immediate observation is, that $\bar{\mathcal{F}}$ also fulfills

$$\int_{\mathbb{T}^d} (1, \varepsilon(p)) \bar{\mathcal{F}}(n,E;p) dp = (n,E), \qquad \forall (n,E) \in \mathfrak{D}.$$

In Section 2.3.4 we treat the extension $\bar{\mathcal{F}}$ in more detail and show for sequences (n,E) in $\mathfrak{D}$, that there exists a subsequence $(n_{k_j}, E_{k_j})_{j\in\mathbb{N}}$ such that

$$\lim_{j\to\infty} \left\| \bar{\mathcal{F}}(n_{k_j}, E_{k_j}; .) - \bar{\mathcal{F}}(n,E;.) \right\|_{\mathrm{L}^q(I;\mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d))} = 0, \tag{2.35}$$

for any compact $I \subset \mathbb{R}_0^+$ and $q \in [1,\infty)$. This convergence result will be an important tool for the upcoming Main Theorem. Next we give the definition of the weak formulation regarding the diffusive equations (2.32)- (2.33).

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Definition 2.3.4. *We call functions $\tilde{n}$ and $\tilde{E}$ weak solutions of* (2.32)- (2.33) *if*

(i) $\tilde{n}, \tilde{E}$ *are in* $\mathrm{L}^2_{loc}(\mathbb{R}^+_0; \mathrm{L}^2(\mathbb{T}^d))$ *and* $\partial_t \tilde{n}, \partial_t \tilde{E}$ *are in* $\mathrm{L}^2(\mathbb{R}^+_0; \mathrm{H}^{-1}(\mathbb{T}^d))$

(ii) Define the space of functions that have a weak divergence with respect to the spatial variable as

$$\mathrm{H}_{\mathrm{div}_x}(\mathbb{T}^d \times \mathbb{T}^d) := \left\{ g \in (\mathrm{L}^2(\mathbb{T}^d \times \mathbb{T}^d))^d : \mathrm{div}_x \, g \in \mathrm{L}^2(\mathbb{T}^d \times \mathbb{T}^d) \right\}. \tag{2.36}$$

The functions $\tilde{n}$ and $\tilde{E}$ have to fulfill

$$(\nabla_p \varepsilon) \bar{\mathcal{F}}(\tilde{n}, \tilde{E}; .), \;\; \varepsilon(\nabla_p \varepsilon) \bar{\mathcal{F}}(\tilde{n}, \tilde{E}; .) \in \mathrm{L}^2_{loc}(\mathbb{R}^+_0; \mathrm{H}_{\mathrm{div}_x}(\mathbb{T}^d \times \mathbb{T}^d)).$$

(iii) For all φ in $\mathrm{H}^1_0(\mathbb{R}^+_0 \times \mathbb{T}^d)$ the following equations hold:

$$\int_{\mathbb{R}^+} \langle \partial_t n, \varphi \rangle_{\mathrm{H}^{-1}(\mathbb{T}^d)} - \int_{\mathbb{R}^+} \int_{\mathbb{T}^d \times \mathbb{T}^d} \mathrm{div}_x (\nabla_p \varepsilon(p) \bar{\mathcal{F}}(n, E; p))(\nabla_p \varepsilon(p) \cdot \nabla_x \varphi) = 0, \tag{2.37}$$

$$\int_{\mathbb{R}^+} \langle \partial_t E, \varphi \rangle_{\mathrm{H}^{-1}(\mathbb{T}^d)} - \int_{\mathbb{R}^+} \int_{\mathbb{T}^d \times \mathbb{T}^d} \varepsilon(p) \, \mathrm{div}_x (\nabla_p \varepsilon(p) \bar{\mathcal{F}}(n, E; p))(\nabla_p \varepsilon(p) \cdot \nabla_x \varphi) = 0. \tag{2.38}$$

With the above we are now able to state the first main result of this thesis, which gives us the macroscopic model equation for our system.

Main Theorem 2.3.5 (Rigorous Limit)**.** *Let $f_0 \in C^1(\mathbb{T}^d \times \mathbb{T}^d)$ with $0 < f_0(x,p) < 1$ for all (x,p) in $\mathbb{T}^d \times \mathbb{T}^d$ and for all $\tau > 0$ denote by f_τ the solution to the DSSBE* (2.23) *in the sense of Hypothesis 2.2.14 and define the macroscopic densities $(n_\tau)_{\tau>0}$ and $(E_\tau)_{\tau>0}$ as in* (2.31)*. Then there exist functions n and E in $\mathrm{L}^2_{loc}(\mathbb{R}^+, \mathbb{T}^d \times \mathbb{T}^d)$ and a subsequence of the families $(n_\tau)_{\tau>0}$ and $(E_\tau)_{\tau>0}$ such that*

$$\lim_{\tau_k \to 0} n_{\tau_k} = n, \qquad \lim_{\tau_k \to 0} E_{\tau_k} = E, \qquad \text{in } \mathrm{L}^2_{loc}(\mathbb{R}^+_0; \mathrm{L}^2(\mathbb{T}^d \times \mathbb{T}^d)). \tag{2.39}$$

and the functions n and E are weak solutions in the sense of Definition 2.3.4. As additional consequence we have that

$$\lim_{\tau_k \to 0} f_{\tau_k} = \bar{\mathcal{F}}(n, E; p), \qquad \text{in } \mathrm{L}^2_{loc}(\mathbb{R}^+_0; \mathrm{L}^2(\mathbb{T}^d \times \mathbb{T}^d)),$$

The proof of Main Theorem 2.3.5 is split into three parts. First we need to show that there exists a converging subsequence of the family $(n_\tau, E_\tau)_{\tau>0}$. Even tough we have quite strong conditions, it is not an easy undertaking. The functions f_τ, n_τ and E_τ are at all times bounded, but that does not ensure that the integrals over $\mathbb{R}^+$ with respect to time, are also bounded. One of the main tools to obtain these bounds comes from the work of Golse and Poupaud [GP92], which will be introduced in Subsection 2.3.2. This is still too less to apply the Aubin Lions Lemma, because we need estimates for compact intervals $I \subset \mathbb{R}^+$. Therefore we adapted the result from Golse and Poupand and obtained such estimates, which are stated and proven in Subsection 2.3.2. The Subsection 2.3.3 will then deal with the proof regarding the existence of a converging subsequence, where we check the requirements for the Aubin Lions Lemma and apply then a diagonal argument.

Then Subsection 2.3.4 is reserved for the treatment of the Fermi-Dirac extension. For the L^1-convergence (2.35) we follow first [Bra17], by doing some variable changes for the Lagrange multiplicands λ_0, λ_1 and study their behavior if $(E_\tau)_{\tau>0}$ converges towards a limit on the boundary $\partial\mathfrak{D}$. After that it is classic analysis.

The proof of Main Theorem 2.3.5 is presented in Section 2.3, where we follow the lines of the formal limit (Theorem 2.3.1) and look closely in which sense everything exists or converges.

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2.3.1. Formal Derivation

The major tool used for the proof of Theorem 2.3.1 is the already mentioned *Chapman-Enskog expansion*, which is frequently used for formal derivations of macroscopic models (see [JÖ9, BF10, EH14, CC70]). This method will be applied in an adapted version in Chapter 3, hence we introduce it here.

1. It exists a bounded family of functions $(g_\tau)_{\tau>0}$ such that we can express the solution f_τ of the DSSBE (2.23) with
$$f_\tau(t,x,p) = \mathcal{F}(n_\tau(t,x), E_\tau(t,x); p) + \tau g_\tau(t,x,p). \tag{2.40}$$
Passing to the limit $\tau \to 0$ should then lead to $\lim_{\tau\to 0} f_\tau = \mathcal{F}(n, E; p)$.
2. Next step is to evaluate the limit (if it exists) of the family $(g_\tau)_{\tau>0}$ for τ going to zero. This comes from substituting the Ansatz (2.40) into the model equation and passing there to the limit τ to zero. Denote the limit with g.
3. As last step we substitute the Ansatz (2.40), with the explicit forms from step 1 and step 2 into the model equation (in our case the DSSBE), integrate with respect to the moments (in this chapter we are interested into the zeroth moment and the second moment) and pass to the limit $\tau \to 0$. In the end we expect to obtain equations for n and E that are dependent on $\mathcal{F}$ and g.

We state here just a formal proof, since the equations (2.32)-(2.33) only exist, if the limit functions (n, E) lie in $\mathfrak{D}^\circ$. Also just for this proof let us assume that every appearing function is sufficiently smooth.

Proof of Theorem 2.3.1. We will divide the proof into the steps of the Chapman-Enskog expansion. Also to keep it simple we will introduce the short notations $\mathcal{F}_\tau \hat{=} \mathcal{F}(n_\tau, E_\tau; p)$ and $\mathcal{Q}_\tau \hat{=} \mathcal{Q}_\tau(f_\tau)$

Step 1: Our candidate for the family $(g_\tau)_{\tau>0}$ is the family of collision operators $(\mathcal{Q}_\tau)_{\tau>0}$, since
$$\mathcal{F}_\tau - \tau\mathcal{Q}_\tau = \mathcal{F}_\tau + f_\tau - \mathcal{F}_\tau = f_\tau.$$
Due to the smoothness of n_τ, E_τ and $\mathcal{F}_\tau$ and the boundedness of $(\mathcal{Q}_\tau)_{\tau>0}$, we can pass to the limit for τ to zero and obtain that
$$\lim_{\tau\to 0} f_\tau = \mathcal{F}(n, E; p)$$

Step 2: We take the Ansatz $f_\tau = \mathcal{F}_\tau - \tau\mathcal{Q}_\tau$ and substitute it into the DSSBE (2.23) and obtain
$$\tau\partial_t\mathcal{F}_\tau - \tau^2\partial_t\mathcal{Q}_\tau + \nabla_p\varepsilon\cdot\nabla_x\mathcal{F}_\tau - \tau\nabla_p\varepsilon\cdot\nabla_x\mathcal{Q}_\tau = \mathcal{Q}_\tau \tag{2.41}$$
Passing to the limit τ to zero, yields
$$\mathcal{Q}_0 = \nabla_p\varepsilon\cdot\nabla_x\mathcal{F}(n, E; .).$$

Step 3: Last step is the derivation of the equations for the densities n and E. To obtain the first equation, integrate (2.41) with respect to p. For the second equation multiply (2.41) first with $\varepsilon(p)$ and then integrate it with respect to p. This gives us
$$\partial_t n_\tau - \tau\int_{\mathbb{T}^d}\partial_t\mathcal{Q}_\tau dp + \frac{1}{\tau}\int_{\mathbb{T}^d}\nabla_p\varepsilon\cdot\nabla_x\mathcal{F}_\tau dp - \int_{\mathbb{T}^d}\nabla_p\varepsilon\cdot\nabla_x\mathcal{Q}_\tau dp = \int_{\mathbb{T}^d}\mathcal{Q}_\tau dp$$
$$\partial_t E_\tau - \tau\int_{\mathbb{T}^d}\varepsilon\partial_t\mathcal{Q}_\tau dp + \frac{1}{\tau}\int_{\mathbb{T}^d}\varepsilon\nabla_p\varepsilon\cdot\nabla_x\mathcal{F}_\tau dp - \int_{\mathbb{T}^d}\varepsilon\nabla_p\varepsilon\cdot\nabla_x\mathcal{Q}_\tau dp = \int_{\mathbb{T}^d}\varepsilon\mathcal{Q}_\tau dp$$

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After exchanging derivation and integral in the first integral on the left side, we obtain through the definition of the collision operator, that it vanishes. This holds also for the integral on the right hand side. The second integrator on the left hand side is odd with respect to p,see Remark 2.3.18, hence it vanishes too. Passing to the limit τ to zero gives us then the formal equations for the limits n and E

$$\partial_t n - \operatorname{div}_x \left(\int_{\mathbb{T}^d} (\nabla_p \varepsilon(p) \cdot \nabla_x \mathcal{F}(n, E; p)) \nabla_p \varepsilon(p) dp \right) = 0$$
$$\partial_t E - \operatorname{div}_x \left(\int_{\mathbb{T}^d} \varepsilon(p)(\nabla_p \varepsilon(p) \cdot \nabla_x \mathcal{F}(n, E; p)) \nabla_p \varepsilon(p) dp \right) = 0.$$

□

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Another way to obtain existence theory for the model (2.32)-(2.33) is to study directly these formal derived equations (e.g [Mar86, MRS90]). This would exceed our purposes, but we give a short analysis of the obtained formal limit.

Remark 2.3.6. The formal derived limit equations (2.32)-(2.33) have an alternative form which we will derive here with some comments. Let us first recall that

$$\mathcal{F}(n, E; p) \widehat{=} \mathcal{F}(\lambda_0(n, E), \lambda_1(n, E); p),$$

where λ_0 and λ_1 are the two components of the inverse $\mathfrak{b}^{-1}$ given in Proposition 2.2.7 (for each $(t, x) \in \mathbb{R}_0^+ \times \mathbb{T}^d$). By using Remark 2.2.9, denoting $D_{n,E}(\lambda)$ as Jacobi matrix, we are able to evaluate the gradient of $\mathcal{F}$:

$$\begin{aligned}\nabla_x \mathcal{F}(n, E; p) =& \mathcal{F}(n, E; p)(1 - \mathcal{F}(n, E; p))(1, \varepsilon(p)) \nabla_x (\lambda_0(n, E), \lambda_1(n, E)) \\ =& \mathcal{F}(n, E; p)(1 - \mathcal{F}(n, E; p))(1, \varepsilon(p))(D_{n,E}(\lambda)(n, E)) \nabla_x (n, E) \\ =& \mathcal{F}(n, E; p)(1 - \mathcal{F}(n, E; p))((\partial_n \lambda_0 + \varepsilon(p) \partial_n \lambda_1) \nabla_x n + (\partial_E \lambda_0 + \varepsilon(p) \partial_E \lambda_1) \nabla_x E),\end{aligned}$$

where $\partial_{n,E} \lambda_k$ are evaluated at (n, E) for $k \in \{0, 1\}$. Next we can rewrite the integrator as

$$(\nabla_p \varepsilon(p) \cdot \nabla_x \mathcal{F}(n, E; p)) \nabla_p \varepsilon(p) = (\nabla_p \varepsilon(p) \otimes \nabla_p \varepsilon(p)) \cdot \nabla_x \mathcal{F}(n, E; p),$$

where "$\otimes$" describes the Tensor product such that $(\nabla_p \varepsilon(p) \otimes \nabla_p \varepsilon(p))_{ij} = \partial_{p_i} \varepsilon(p) \partial_{p_j} \varepsilon(p)$ for $i, j \in \{1, \dots, d\}$. Hence we have for the $j-$th component

$$((\nabla_p \varepsilon \otimes \nabla_p \varepsilon) \cdot \nabla_x \mathcal{F})_j = \sum_{i=1}^{d} \mathcal{F}(1 - \mathcal{F}) \partial_{p_j} \varepsilon \partial_{p_i} \varepsilon ((\partial_n \lambda_0 + \varepsilon \partial_n \lambda_1) \partial_{x_i} n + (\partial_E \lambda_0 + \varepsilon \partial_E \lambda_1) \partial_{x_i} E)$$

Define now the following block matrix $A(n, E) \in \mathbb{R}^{2d \times 2d}$

$$\begin{aligned} A(n, E) &:= \begin{pmatrix} A^{00}(n, E) & A^{01}(n, E) \\ A^{10}(n, E) & A^{11}(n, E) \end{pmatrix}, \qquad A^{kl}(n, E) \in \mathbb{R}^{d \times d}, && \text{for } k, l \in \{0, 1\}, \\ A^{00}_{ij}(n, E) &:= \int_{\mathbb{T}^d} \mathcal{F}(1 - \mathcal{F}) \partial_{p_j} \varepsilon \partial_{p_i} \varepsilon ((\partial_n \lambda_0(n, E) + \varepsilon \partial_n \lambda_1(n, E)) dp, && \text{for } i, j \in \{1, \dots, d\}, \\ A^{01}_{ij}(n, E) &:= \int_{\mathbb{T}^d} \mathcal{F}(1 - \mathcal{F}) \partial_{p_j} \varepsilon \partial_{p_i} \varepsilon (\partial_E \lambda_0(n, E) + \varepsilon \partial_E \lambda_1)(n, E)) dp, && \text{for } i, j \in \{1, \dots, d\}, \\ A^{10}_{ij}(n, E) &:= \int_{\mathbb{T}^d} \varepsilon \mathcal{F}(1 - \mathcal{F}) \partial_{p_j} \varepsilon \partial_{p_i} \varepsilon (\partial_n \lambda_0(n, E) + \varepsilon \partial_n \lambda_1(n, E)) dp, && \text{for } i, j \in \{1, \dots, d\}, \\ A^{11}_{ij}(n, E) &:= \int_{\mathbb{T}^d} \varepsilon \mathcal{F}(1 - \mathcal{F}) \partial_{p_j} \varepsilon \partial_{p_i} \varepsilon (\partial_E \lambda_0(n, E) + \varepsilon \partial_E \lambda_1(n, E)) dp && \text{for } i, j \in \{1, \dots, d\}, \end{aligned}$$

which gives us a matrix written form of (2.32)-(2.33):

$$\partial_t \begin{pmatrix} n \\ E \end{pmatrix} - \operatorname{div}_x \left(A(n,E) \cdot \nabla_x \begin{pmatrix} n \\ E \end{pmatrix} \right) = 0 \tag{2.42}$$

The above divergence is to understand as the sum over the $i-$th derivative of the $i-$th column with respect to x. Interesting for further investigations is the question, if matrix A has a particular structure.
We notice that all blocks A^{kl} for $k,l \in \{0,1\}$ are diagonal matrices. This comes from the fact that $\mathcal{F}$ and $\varepsilon(p)$ are even functions in p over $\mathbb{T}^d$, in the sense of Definition 2.1.3, and that $\partial_{p_j}\varepsilon\partial_{p_i}\varepsilon$ is odd for $i \neq j$. If we interpret the functions n and E as functions of $\lambda = (\lambda_0, \lambda_1)$ (recall notation from Remark 2.2.9) we can rewrite the equations (2.32)-(2.33) in the way that

$$\partial_t \begin{pmatrix} \tilde{n}(\lambda(t,x)) \\ \tilde{E}(\lambda(t,x)) \end{pmatrix} - \operatorname{div}_x \left(\mathcal{D}(\lambda(t,x))\nabla_x\lambda(t,x)\right) = 0$$

where $\mathcal{D}(\lambda) \in \mathbb{R}^{2d\times 2d}$ is defined as

$$\begin{aligned}
\mathcal{D}(\lambda) &:= \begin{pmatrix} \mathcal{D}^{00}(\lambda) & \mathcal{D}^{01}(\lambda) \\ \mathcal{D}^{10}(\lambda) & \mathcal{D}^{11}(\lambda) \end{pmatrix}, \qquad \mathcal{D}^{kl}(\lambda) \in \mathbb{R}^{d\times d}, && \text{for } k,l \in \{0,1\}, \\
\mathcal{D}^{00}_{ij}(\lambda) &:= \int_{\mathbb{T}^d} \mathcal{F}(\lambda;p)(1-\mathcal{F}(\lambda;p))\partial_{p_j}\varepsilon(p)\partial_{p_i}\varepsilon(p)dp, && \text{for } i,j \in \{1,\dots,d\}, \\
\mathcal{D}^{01}_{ij}(\lambda) &:= \int_{\mathbb{T}^d} \varepsilon(p)\mathcal{F}(\lambda;p)(1-\mathcal{F}(\lambda;p))\partial_{p_j}\varepsilon(p)\partial_{p_i}\varepsilon(p)dp, && \text{for } i,j \in \{1,\dots,d\}, \\
\mathcal{D}^{10}_{ij}(\lambda) &:= \int_{\mathbb{T}^d} \varepsilon(p)\mathcal{F}(\lambda;p)(1-\mathcal{F}(\lambda;p))\partial_{p_j}\varepsilon(p)\partial_{p_i}\varepsilon(p)dp, && \text{for } i,j \in \{1,\dots,d\}, \\
\mathcal{D}^{11}_{ij}(\lambda) &:= \int_{\mathbb{T}^d} \varepsilon(p)^2\mathcal{F}(\lambda;p)(1-\mathcal{F}(\lambda;p))\partial_{p_j}\varepsilon(p)\partial_{p_i}\varepsilon(p)dp && \text{for } i,j \in \{1,\dots,d\},
\end{aligned}$$

First we observe that $\mathcal{D}(\lambda(n,E)) \cdot D_{n,E}\lambda(n,E) = A(n,E)$ and that $\mathcal{D}^{01} = \mathcal{D}^{10}$. Since $(\mathcal{D}^{kl})_{k,l\in\{0,1\}}$ are obviously all symmetric, we get that $\mathcal{D}(\lambda)$ is also symmetric. Moreover we also see, as before, that due to the oddness of $\partial_{p_j}\varepsilon(p)\partial_{p_i}\varepsilon(p)$ for $i \neq j$ we also have that $(\mathcal{D}^{kl})_{k,l\in\{0,1\}}$ are all diagonal matrices. Hence we obtain for $z = (\xi, \zeta) \neq 0$ and $\xi, \zeta \in \mathbb{R}^d$ that

$$z^T\mathcal{D}(\lambda)z = \sum_{i=1}^d \int_{\mathbb{T}^d} (\xi_i + \varepsilon(p)\zeta_i)^2(\partial_{p_i}\varepsilon(p))^2\mathcal{F}(\lambda;p)(1-\mathcal{F}(\lambda;p))dp > 0$$

and therefore we have that $\mathcal{D}(\lambda)$ is also a positive definite matrix. ■

2.3.2. Boundedness with Fourier

Since we need Fourier transformation on the Torus, we post for the convenience of the reader the most important statements that will be used As reference and for further content we refer to basic literature like [Gra08]. Starting simple by defining the Fourier transformation.

Definition 2.3.7. *Let g be a complex valued function in $\mathrm{L}^1(\mathbb{T}^d)$ and $l \in \mathbb{Z}^d$, then we define the l-th Fourier coefficient of g as*

$$\mathfrak{F}_x(g)(l) := \int_{\mathbb{T}^d} g(x)e^{-2\pi i l\cdot x}dx.$$

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The properties of the Fourier transformation on $\mathbb{R}^d$ can be directly applied to the Fourier coefficients. Using $\mathfrak{F}_x(.)$ is unconventional, but for our purposes more convenient. One of the most important properties for this work, is the Plancherel's identity, which is given on the torus as the following.

Proposition 2.3.8. *Let g be a function in $\mathrm{L}^2(\mathbb{T}^d)$, then the Plancherel's identity holds*

$$\|g\|^2_{\mathrm{L}^2(\mathbb{T}^d)} = \sum_{l\in\mathbb{Z}^d} |\mathfrak{F}_x(g)(l)|^2. \tag{2.43}$$

Proof. See Proposition 3.1.16. in [Gra08]. □

Next we define the $\mathrm{H}^s(\mathbb{T}^d)$-space which can be identified with the fractional Sobolev spaces, see [DPV12], but we do not need this identification.

Definition 2.3.9. *Let $s \in (0,1)$ and g be a function in $\mathrm{L}^2(\mathbb{T}^d)$. We define the semi-norm*

$$[g]^2_{\mathrm{H}^s(\mathbb{T}^d)} := \sum_{l\in\mathbb{Z}^d} |l|^{2s}|\mathfrak{F}_x(g)(l)|^2. \tag{2.44}$$

The space $\mathrm{H}^s(\mathbb{T}^d)$ is then defined as all functions g in $\mathrm{L}^2(\mathbb{T}^d)$ such that the semi-norm is bounded

$$\mathrm{H}^s(\mathbb{T}^d) := \left\{ g \in \mathrm{L}^2(\mathbb{T}^d) : [g]_{\mathrm{H}^s(\mathbb{T}^d)} < \infty \right\} \tag{2.45}$$

Remark 2.3.10. For $g \in \mathrm{H}^s(\mathbb{T}^d)$ the norm is defined as

$$\|g\|_{\mathrm{H}^s(\mathbb{T}^d)} := \|g\|_{\mathrm{L}^2(\mathbb{T}^d)} + [g]_{\mathrm{H}^s(\mathbb{T}^d)} \tag{2.46}$$

Since $|l|^{2s} \geq 1$ for all $l \in \mathbb{Z}^d \setminus \{0\}$ and $s \in (0,1)$ and thanks to Plancherel's identity (2.43) we can estimate the above norm with

$$\|g\|^2_{\mathrm{H}^s(\mathbb{T}^d)} \leq 2\left(\|g\|^2_{\mathrm{L}^2(\mathbb{T}^d)} + [g]^2_{\mathrm{H}^s(\mathbb{T}^d)}\right) \leq 2\left(2[g]^2_{\mathrm{H}^s(\mathbb{T}^d)} + \left|\int_{\mathbb{T}^d} g(x)dx\right|^2\right), \tag{2.47}$$

which will be used to study the long time behaviour. ■

As given in [GP92] we state a geometric result, which seems first out of context, but will be needed for the proof of the upcoming Proposition. It is already in the one dimensional case quite troublesome to prove, hence we will not show the proof here.

Hypothesis 2.3.11. *There exist constants $C \in \mathbb{R}$ and $\beta > 0$ such that for all $(a_1, a_2) \in \mathbb{R}^d \times \mathbb{R}$ with $|(a_1, a_2)| = 1$ we have that*

$$\operatorname{meas}\left(\left\{p \in \mathbb{T}^d : |a_1 \cdot \nabla_p \varepsilon(p) + a_2|\right\} < \tilde{\delta}\right) \leq C\tilde{\delta}^\beta,$$

where $\varepsilon(p)$ is the scaled dispersion relation defined in (2.4) *and* meas(.) *denotes the d-dimensional Lebesgue measure.*

We come to one of our key elements of this chapter, which is an adapted version of Proposition 3.2 in [GP92]. In [GP92] the statement is given with the spatial variable x lying in $\mathbb{R}^d$, whereas in our version we have that $x \in \mathbb{T}^d$. Since the theory of Fourier analysis on $\mathbb{R}^d$ is similar to the the Fourier analysis on the torus $\mathbb{T}^d$, we can adapt the proof of [GP92].

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Proposition 2.3.12. *Let the families* $(f_\tau)_{\tau>0}$ *and* $(\mathcal{Q}_\tau)_{\tau>0}$ *be bounded in* $\mathrm{L}^2(\mathbb{R};\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))$ *such that the following holds a.e. for all* $\tau>0$

$$\tau\partial_t f_\tau + \nabla_p\varepsilon\cdot\nabla_x f_\tau = \mathcal{Q}_\tau, \tag{2.48}$$

with $\varepsilon(p)$ *being the scaled dispersion relation* (2.4)*. Then the families* $(n_\tau)_{\tau>0}$ *and* $(E_\tau)_{\tau>0}$*, given by*

$$n_\tau(t,x)=\int_{\mathbb{T}^d} f_\tau(t,x,p)dp, \qquad E_\tau(t,x)=\int_{\mathbb{T}^d}\varepsilon(p)f_\tau(t,x,p)dp, \qquad \forall\tau>0,$$

are bounded in $\mathrm{L}^2(\mathbb{R};\mathrm{H}^s(\mathbb{T}^d))$ *for* $s=\beta/(4+\beta)$*, and* β *being the constant from Hypothesis 2.3.11. Moreover the following estimates hold for arbitrary* $\delta>0$ *and a constant* $D_\delta>0$*,*

$$\left\|[n_\tau]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(\mathbb{R})} \le D_\delta\left\|\mathcal{Q}_\tau\right\|^2_{\mathrm{L}^2(\mathbb{R};\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))}+\delta\left\|f_\tau\right\|^2_{\mathrm{L}^2(\mathbb{R};\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))} \tag{2.49}$$

$$\left\|[E_\tau]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(\mathbb{R})} \le D_\delta\varepsilon_\infty\left\|\mathcal{Q}_\tau\right\|^2_{\mathrm{L}^2(\mathbb{R};\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))}+\delta\varepsilon_\infty\left\|f_\tau\right\|^2_{\mathrm{L}^2(\mathbb{R};\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))} \tag{2.50}$$

where $\varepsilon_\infty := \|\varepsilon\|^2_{\mathrm{L}^\infty(\mathbb{T}^d)}$.

Proof. It is enough to prove all the statements for the family $(n_\tau)_{\tau>0}$, because the statements for the family $(E_\tau)_{\tau>0}$ are then direct consequences and will be therefore postponed to the end of the proof. Let us follow the proof of Proposition 3.2 from [GP92]. Denote by $\mathfrak{F}_t(n_\tau)(\mu,x)$ the Fourier transform of n_τ with respect to the time variable t. Then we have with Plancherel's identity (on $\mathbb{R}$) that

$$\left\|[n_\tau]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(\mathbb{R})} = \left\|[\mathfrak{F}_t(n_\tau)]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(\mathbb{R})}. \tag{2.51}$$

Applying the Fourier transformation with respect to time and space (not. $\mathfrak{F}_{t,x}(.)$) to identity (2.48), gives us, due to the properties of the Fourier transformation, for all $\mu\in\mathbb{R}$ and $l\in\mathbb{Z}^d$:

$$\begin{aligned}\mathfrak{F}_{t,x}\left(\tau\partial_t f_\tau+\nabla_p\varepsilon(p)\cdot\nabla_x f_\tau\right)(\mu,l,p)&=\mathfrak{F}_{t,x}(\mathcal{Q}_\tau)(\mu,l,p),\\ i(\tau\mu+\nabla_p\varepsilon(p)\cdot l)\mathfrak{F}_{t,x}(f_\tau)(\mu,l,p)&=\mathfrak{F}_{t,x}(\mathcal{Q}_\tau)(\mu,l,p).\end{aligned} \tag{2.52}$$

We define $z(\mu,l,p):=(\tau\mu+\nabla_p\varepsilon(p)\cdot l)$ and will denote it shortly with z. The reader should notice that $z\in\mathbb{R}$ for all $(\mu,l,p)\in\mathbb{R}\times\mathbb{Z}^d\times\mathbb{T}^d$. Thanks to Plancherel's identity (2.51) we obtain further

$$\begin{aligned}\left\|[\mathfrak{F}_t(n_\tau)]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(\mathbb{R})} &= \int_{\mathbb{R}}\sum_{l\in\mathbb{Z}^d}|l|^{2s}|\mathfrak{F}_x(\mathfrak{F}_t(n_\tau))(\mu,l)|^2 d\mu\\ &= \int_{\mathbb{R}}\sum_{l\in\mathbb{Z}^d}|l|^{2s}\left|\int_{\mathbb{T}^d}\mathfrak{F}_{t,x}(f_\tau)(\mu,l,p)dp\right|^2 d\mu.\end{aligned}$$

Next we introduce the bump function $\chi_{\tilde\delta}(r):\mathbb{R}\to[0,1]$, with

$$\chi_{\tilde\delta}(r)=\begin{cases}0 \text{ for } & |r|<\tilde\delta,\\ 1 \text{ for } & |r|>2\tilde\delta.\end{cases}$$

where $\chi_{\tilde\delta}$ in $C^\infty(\mathbb{R})$ and there exist a constant C independent from $\tilde\delta$, such that $\left|r\chi'_{\tilde\delta}(r)\right|\le C\chi_{\tilde\delta}(r)$ for all $r\in\mathbb{R}$. For more details we refer to standard literature like [Lee13]. We will

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use the bump functions and (2.52) to estimate the absolute value of the integral of $\mathfrak{F}_{t,x}(f_\tau)$ with respect to p.

$$\begin{aligned}\left|\int_{\mathbb{T}^d}\mathfrak{F}_{t,x}(f_\tau)\,dp\right|^2 &= \left|\int_{\mathbb{T}^d}\left(1-\chi_{\tilde\delta}(z)+\frac{\chi_{\tilde\delta}(z)}{z}z\right)\mathfrak{F}_{t,x}(f_\tau)(\mu,l,p)dp\right|^2\\ &= \left|\int_{\mathbb{T}^d}(1-\chi_{\tilde\delta}(z))\,\mathfrak{F}_{t,x}(f_\tau)(\mu,l,p)+\frac{\chi_{\tilde\delta}(z)}{z}\frac{1}{\mathrm{i}}\mathfrak{F}_{t,x}(\mathcal{Q}_\tau)(\mu,l,p)dp\right|^2\\ &\le 2\underbrace{\left|\int_{\mathbb{T}^d}(1-\chi_{\tilde\delta}(z))\,\mathfrak{F}_{t,x}(f_\tau)(\mu,l,p)dp\right|^2}_{=:I_1}+2\underbrace{\left|\int_{\mathbb{T}^d}\frac{\chi_{\tilde\delta}(z)}{z}\mathfrak{F}_{t,x}(\mathcal{Q}_\tau)(\mu,l,p)dp\right|^2}_{=:I_2}.\end{aligned}$$

The two above integrals will be treated separately. For the first integral I_1, we use Hölder inequality, the fact that $(1-\chi_{\tilde\delta}(z))^2\le 1$ and Hypothesis 2.3.11 to get

$$\begin{aligned}I_1 &\le \int_{\mathbb{T}^d}(1-\chi_{\tilde\delta}(z))^2dp\,\|\mathfrak{F}_{t,x}(f_\tau)(\mu,l,.)\|^2_{\mathrm{L}^2(\mathbb{T}^d)}\\ &= \int_{\{|z|<2\tilde\delta\}\cap\mathbb{T}^d}(1-\chi_{\tilde\delta}(z))^2dp\,\|\mathfrak{F}_{t,x}(f_\tau)(\mu,l,.)\|^2_{\mathrm{L}^2(\mathbb{T}^d)}\\ &= \operatorname{meas}\left(\left\{p\in\mathbb{T}^d:|\tau\mu+\nabla_p\varepsilon(p)\cdot l|<2\tilde\delta\right\}\right)\|\mathfrak{F}_{t,x}(f_\tau)(\mu,l,.)\|^2_{\mathrm{L}^2(\mathbb{T}^d)}\\ &= \operatorname{meas}\left(\left\{p\in\mathbb{T}^d:\frac{1}{|(\tau\mu,l)|}|\tau\mu+\nabla_p\varepsilon(p)\cdot l|<\frac{2}{|(\tau\mu,l)|}\tilde\delta\right\}\right)\|\mathfrak{F}_{t,x}(f_\tau)(\mu,l,.)\|^2_{\mathrm{L}^2(\mathbb{T}^d)}\\ &\le C\left|\tau^2\mu^2+|l|^2\right|^{-\frac{\beta}{2}}\tilde\delta^\beta\,\|\mathfrak{F}_{t,x}(f_\tau)(\mu,l,.)\|^2_{\mathrm{L}^2(\mathbb{T}^d)}\\ &\le C|l|^{-\beta}\tilde\delta^\beta\,\|\mathfrak{F}_{t,x}(f_\tau)(\mu,l,.)\|^2_{\mathrm{L}^2(\mathbb{T}^d)}.\end{aligned}$$

The integral I_2 needs less effort to estimate. We obtain again with Hölder and $\operatorname{meas}\left(\mathbb{T}^d\right)=1$

$$\begin{aligned}I_2 &\le \int_{\mathbb{T}^d}\left(\frac{\chi_{\tilde\delta}(z)}{z}\right)^2dp\,\|\mathfrak{F}_{t,x}(\mathcal{Q}_\tau)(\mu,l,.)\|^2_{\mathrm{L}^2(\mathbb{T}^d)}\\ &\le \int_{\{|z|>\tilde\delta\}\cap\mathbb{T}^d}\left(\frac{\chi_{\tilde\delta}(z)}{z}\right)^2dp\,\|\mathfrak{F}_{t,x}(\mathcal{Q}_\tau)(\mu,l,.)\|^2_{\mathrm{L}^2(\mathbb{T}^d)}\\ &\le \int_{\{|z|>\tilde\delta\}\cap\mathbb{T}^d}\left(\frac{1}{z^2}\right)dp\,\|\mathfrak{F}_{t,x}(\mathcal{Q}_\tau)(\mu,l,.)\|^2_{\mathrm{L}^2(\mathbb{T}^d)}\\ &\le \frac{1}{\tilde\delta^2}\|\mathfrak{F}_{t,x}(\mathcal{Q}_\tau)(\mu,l,.)\|^2_{\mathrm{L}^2(\mathbb{T}^d)}.\end{aligned}$$

Using the estimates for I_1 and I_2, leads us to

$$\begin{aligned}&\left\|[\mathfrak{F}_t(n_\tau)]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(\mathbb{R})}\le\\ &\quad\le 2\int_{\mathbb{R}}\sum_{l\in\mathbb{Z}^d}C|l|^{(2s-\beta)}\tilde\delta^\beta\,\|\mathfrak{F}_{t,x}(f_\tau)(\mu,l,.)\|^2_{\mathrm{L}^2(\mathbb{T}^d)}+|l|^{2s}\frac{1}{\tilde\delta^2}\|\mathfrak{F}_{t,x}(\mathcal{Q}_\tau)(\mu,l,.)\|^2_{\mathrm{L}^2(\mathbb{T}^d)}\,d\mu.\end{aligned}$$

Setting $s=\beta/(4+\beta)$ and $\tilde\delta=2^{-\frac{1}{\beta}}C^{-\frac{1}{\beta}}\delta^{\frac{1}{\beta}}|l|^{(s+1)/2}$, for some $\delta>0$, gives us

$$\begin{aligned}&\left\|[\mathfrak{F}_t(n_\tau)]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(\mathbb{R})}\le\\ &\quad\le \int_{\mathbb{R}}\sum_{l\in\mathbb{Z}^d}\delta\,\|\mathfrak{F}_{t,x}(f_\tau)(\mu,l,.)\|^2_{\mathrm{L}^2(\mathbb{T}^d)}+2^{\frac{2+\beta}{\beta}}|l|^{(s-1)}C^{\frac{2}{\beta}}\delta^{-\frac{2}{\beta}}\|\mathfrak{F}_{t,x}(\mathcal{Q}_\tau)(\mu,l,.)\|^2_{\mathrm{L}^2(\mathbb{T}^d)}\,d\mu.\end{aligned}$$

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Since $|l|^{s-1} \leq 1$ holds for all $l \in \mathbb{Z}^d$, $l \neq 0$ and $s-1<0$, we can estimate it with one. The case where $l=0$ needs no estimate, since everything is zero then. Using Plancherel's identity in space and time and defining $D_\delta := 2^{\frac{2+\beta}{\beta}} C^{\frac{2}{\beta}} \delta^{-\frac{2}{\beta}}$ we obtain

$$\begin{aligned}\left\| [n_\tau]_{\mathrm{H}^s(\mathbb{T}^d)} \right\|^2_{\mathrm{L}^2(\mathbb{R})} &\leq \int_{\mathbb{R}} \sum_{l \in \mathbb{Z}^d} \delta \left\| \mathfrak{F}_{t,x}(f_\tau)(\mu, l, .) \right\|^2_{\mathrm{L}^2(\mathbb{T}^d)} + D_\delta \left\| \mathfrak{F}_{t,x}(\mathcal{Q}_\tau)(\mu, l, .) \right\|^2_{\mathrm{L}^2(\mathbb{T}^d)} d\mu \\ &= \delta \left\| f_\tau \right\|^2_{\mathrm{L}^2(\mathbb{R}\times\mathbb{T}^d\times\mathbb{T}^d)} + D_\delta \left\| \mathcal{Q}_\tau \right\|^2_{\mathrm{L}^2(\mathbb{R}\times\mathbb{T}^d\times\mathbb{T}^d)}.\end{aligned}$$

The family $(n_\tau)_{\tau>0}$ is bounded in $\mathrm{L}^2(\mathbb{R}; \mathrm{H}^s(\mathbb{T}^d))$ since the families $(f_\tau)_{\tau>0}$ and $(\mathcal{Q}_\tau)_{\tau>0}$ are bounded in $\mathrm{L}^2(\mathbb{R}; \mathrm{L}^2(\mathbb{T}^d \times \mathbb{T}^d))$. More detailed, we see this by using the definition of the $\mathrm{H}^s(\mathbb{T}^d)$-norm (2.46) combined with the previously derived estimate for the semi-norm (2.49):

$$\begin{aligned}\|n_\tau\|_{\mathrm{L}^2(\mathbb{R};\mathrm{H}^s(\mathbb{T}^d))} &\leq \|n_\tau\|_{\mathrm{L}^2(\mathbb{R};\mathrm{L}^2(\mathbb{T}^d))} + \left\| [n_\tau]_{\mathrm{H}^s(\mathbb{T}^d)} \right\|_{\mathrm{L}^2(\mathbb{R})} \\ &= \|f_\tau\|_{\mathrm{L}^2(\mathbb{R};\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))} + \left\| [n_\tau]_{\mathrm{H}^s(\mathbb{T}^d)} \right\|_{\mathrm{L}^2(\mathbb{R})}.\end{aligned}$$

Last we look onto the family $(E_\tau)_{\tau>0}$. We have the estimate

$$|E_\tau| = \left| \int_{\mathbb{T}^d} \varepsilon(p) f_\tau(t,x,p) dp \right| \leq \sqrt{\varepsilon_\infty} |n_\tau|,$$

and therefore

$$\left\| [E_\tau]_{\mathrm{H}^s(\mathbb{T}^d)} \right\|^2_{\mathrm{L}^2(\mathbb{R})} = \left\| [\mathfrak{F}_t(E_\tau)]_{\mathrm{H}^s(\mathbb{T}^d)} \right\|^2_{\mathrm{L}^2(\mathbb{R})} \leq \varepsilon_\infty \int_{\mathbb{R}} \sum_{l \in \mathbb{Z}^d} |l|^{2s} \left| \int_{\mathbb{T}^d} \mathfrak{F}_{t,x}(f_\tau)(\mu, l, p) dp \right|^2 d\mu.$$

The integral on the right is the same we estimated with I_1 and I_2, hence we can conclude the statements for $(E_\tau)_{\tau>0}$ directly from the results regarding the family $(n_\tau)_{\tau>0}$ and obtain the estimate (2.50). The boundedness of $(E_\tau)_{\tau>0}$ in $\mathrm{L}^2(\mathbb{R}; \mathrm{H}^s(\mathbb{T}^d))$ follows in the same way as for the family $(n_\tau)_{\tau>0}$.

□

We will need the results from Proposition 2.3.12 restricted to compact intervals in $\mathbb{R}_0^+$ instead of the whole space $\mathbb{R}$. The problem is that we cannot conclude this directly from the above results, or adapt the proof, since the Fourier transformation is not defined on compact intervals. We remind the reader, that we are interested for the limit τ going to zero, hence all indices τ are considered small or at least smaller than some constant in $\mathbb{R}_0^+$.

Proposition 2.3.13. *If $(f_\tau)_{\tau>0}$ is bounded in $\mathrm{L}^\infty(\mathbb{R}_0^+ \times \mathbb{T}^d \times \mathbb{T}^d)$, if $(\mathcal{Q}_\tau)_{\tau>0}$ is bounded in $\mathrm{L}^2(\mathbb{R}_0^+; \mathrm{L}^2(\mathbb{T}^d \times \mathbb{T}^d))$ and if*

$$a.e.\ \tau > 0: \qquad \tau \partial_t f_\tau + \nabla_p \varepsilon \cdot \nabla_x f_\tau = \mathcal{Q}_\tau, \qquad a.e.\ on\ \mathbb{R}_0^+ \times \mathbb{T}^d \times \mathbb{T}^d,$$

then we have for every compact interval $I \subseteq \mathbb{R}_0^+$ that the families $(n_\tau)_{\tau>0}$ and $(E_\tau)_{\tau>0}$ (defined as in Proposition 2.3.12) fulfill the estimates

$$\begin{aligned}\left\| [n_\tau]_{\mathrm{H}^s(\mathbb{T}^d)} \right\|^2_{\mathrm{L}^2(I)} &\leq D_\delta \left\| \mathcal{Q}_\tau \right\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \delta \left\| f_\tau \right\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \tau C^2(\delta + D_\delta), \\ \left\| [E_\tau]_{\mathrm{H}^s(\mathbb{T}^d)} \right\|^2_{\mathrm{L}^2(I)} &\leq \varepsilon_\infty D_\delta \left\| \mathcal{Q}_\tau \right\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \varepsilon_\infty \delta \left\| f_\tau \right\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \tau \varepsilon_\infty C^2(\delta + D_\delta),\end{aligned}$$

where $\varepsilon_\infty, s, \delta, D_\delta$ are the same as in Proposition 2.3.12.

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Proof. The main idea is to construct two families of functions, which are extensions of f_τ and $\mathcal{Q}_\tau$ onto the whole space, such that the requirements of Proposition 2.3.12 are met, and then apply the latter. We need to choose the extensions cleverly, such that we obtain the desired estimates on the compact interval $I \subset \mathbb{R}_0^+$. Let $C > 0$ be the constant that bounds the family $(f_\tau)_{\tau>0}$ in $\mathrm{L}^\infty(\mathbb{R}_0^+ \times \mathbb{T}^d \times \mathbb{T}^d)$ and let $I = [t_0, t_1]$ for some $t_0, t_1 \in \mathbb{R}_0^+$. Define for $\tau > 0$ the function $g_\tau : \mathbb{R} \times \mathbb{T}^d \times \mathbb{T}^d \to \mathbb{R}$:

$$g_\tau(t,x,p) = \begin{cases} f_\tau(t_0, x - \frac{t-t_0}{\tau}\nabla_p\varepsilon(p), p) & \text{for } t < t_0, \\ f_\tau(t,x,p) & \text{for } t \in [t_0,t_1], \\ f_\tau(t_1, x - \frac{t-t_1}{\tau}\nabla_p\varepsilon(p), p) & \text{for } t > t_0. \end{cases}$$

Since we are on the torus $\mathbb{T}^d$, the x coordinate in our above definition is well defined, due to the equivalence classes. We also have that the family $(g_\tau)_{\tau>0}$ is bounded in $\mathrm{L}^\infty(\mathbb{R} \times \mathbb{T}^d \times \mathbb{T}^d)$ with the same constant C as the family $(f_\tau)_{\tau>0}$. Furthermore we have for $t \notin [t_0, t_1]$ that

$$\tau\partial_t g_\tau + \nabla_p\varepsilon \cdot \nabla_x g_\tau = \tau\left(-\frac{1}{\tau}\nabla_x g_\tau \cdot \nabla_p\varepsilon\right) + \nabla_p\varepsilon \cdot \nabla_x g_\tau = 0.$$

Therefore the following equation holds a.e. on $\mathbb{R} \times \mathbb{T}^d \times \mathbb{T}^d$

$$\tau\partial_t g_\tau + \nabla_p\varepsilon(p) \cdot \nabla_x g_\tau = \mathcal{R}_\tau, \qquad \text{where } \mathcal{R}_\tau = \begin{cases} 0 & \text{for } t < t_0, \\ \mathcal{Q}_\tau & \text{for } t \in [t_0,t_1], \\ 0 & \text{for } t > t_1. \end{cases}$$

At this point we cannot assure that g is in any L^q-space for $q \in [1, \infty)$, hence we have to adjust g. We introduce for $\alpha > 0$ the functions

$$f_{\tau,\alpha}(t,x,p) \coloneqq \varphi_\alpha g_\tau(t,x,p), \qquad \text{where } \varphi_\alpha(t) = \begin{cases} e^{\alpha(t-t_0)} & \text{for } t < t_0 \\ 1 & t \in [t_0,t_1], \\ e^{-\alpha(t-t_1)} & \text{for } t > 0. \end{cases}$$

We show that the family $(f_{\tau,\alpha})_{\tau>0}$ is bounded in $\mathrm{L}^q(\mathbb{R}; \mathrm{L}^q(\mathbb{T}^d \times \mathbb{T}^d))$ for $1 \leq q < \infty$ and $\alpha > 0$. Since there exists a constant $C > 0$, such that $\|g_\tau\|_{\mathrm{L}^\infty} \leq C$ a.e. for all $\tau > 0$, we get

$$\begin{aligned} \|f_{\tau,\alpha}\|^q_{\mathrm{L}^q(\mathbb{R};\mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d))} &= \int_{\mathbb{R}} \|\varphi_\alpha(t) g_\tau(t)\|^q_{\mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d)}\, dt \\ &\leq C^q \int_{-\infty}^{t_0} |\varphi_\alpha|^q dt + \int_{t_0}^{t_1} \|\varphi_\alpha(t) g_\tau(t)\|^q_{\mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d)}\, dt + C^q \int_{t_1}^{\infty} |\varphi_\alpha|^q dt \\ &\leq C^q \int_{-\infty}^{t_0} e^{q\alpha(t-t_0)} dt + C^q \int_{t_1}^{\infty} e^{-q\alpha(t-t_1)} dt + \|f_\tau\|^q_{\mathrm{L}^q(I;\mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d))} \\ &= C^q \frac{2}{q\alpha} + \|f_\tau\|^q_{\mathrm{L}^q(I;\mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d))}\,. \end{aligned} \tag{2.53}$$

Recall that the constant C is also a bound of the family $(f_\tau)_{\tau>0}$, hence $\|f\|^q_{\mathrm{L}^q(I;\mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d))}$ is bounded by $C^q \operatorname{meas}(I)$ for all $q \in [0, \infty)$. So we deduce from (2.53), that the family $(f_{\tau,\alpha})_{\tau>0}$ is in particular bounded in $\mathrm{L}^2(\mathbb{R}; \mathrm{L}^2(\mathbb{T}^d \times \mathbb{T}^d))$ for all $\alpha > 0$. Next we define another family of functions, namely

$$\Phi_{\tau,\alpha}(t,x,p) \coloneqq \begin{cases} \tau\alpha\varphi_\alpha(t) g_\tau(t,x,p) & \text{for } t < t_0, \\ \mathcal{Q}_\tau(t,x,p) & \text{for } t \in [t_0,t_1], \\ \tau\alpha\varphi_\alpha(t) g_\tau(t,x,p) & \text{for } t > t_1. \end{cases}$$

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To prove that the family $(\Phi_{\tau,\alpha})_{\tau>0}$ is bounded in $\mathrm{L}^2(\mathbb{R};\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))$ for all $\alpha>0$ we estimate firstly

$$\begin{aligned}\|\Phi_{\tau,\alpha}\|_{\mathrm{L}^2(\mathbb{R};\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))} \leq & \int_{-\infty}^{t_0}(\tau\alpha C)^2|\varphi_\alpha|^2dt+\int_{t_0}^{t_1}\|\mathcal{Q}_\tau\|^2_{\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)}\,dt+\int_{t_1}^{\infty}(\tau\alpha C)^2|\varphi_\alpha|^2dt\\ =&C^2\tau^2\alpha+\|\mathcal{Q}_\tau\|^2_{\mathrm{L}^2(I;\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))}.\end{aligned} \tag{2.54}$$

Since τ can be considered to be bounded by some constant in $\mathbb{R}^+$ and since the family $(\mathcal{Q}_\tau)_{\tau>0}$ is bounded in $\mathrm{L}^2(\mathbb{R}^+_0;\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))$, we see that the family $(\Phi_{\tau,\alpha})_{\tau>0}$ is indeed bounded in $\mathrm{L}^2(\mathbb{R};\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))$ for all $\alpha>0$. Moreover we have that $f_{\tau,\alpha}$ and $\Phi_{\tau,\alpha}$ fulfill for all $\tau,\alpha>0$ and a.e. in $\mathbb{R}\times\mathbb{T}^d\times\mathbb{T}^d$ the equation

$$\tau\partial_t f_{\tau,\alpha}+\nabla_p\varepsilon\cdot\nabla_x f_{\tau,\alpha}=\Phi_{\tau,\alpha}, \tag{2.55}$$

due to the fact that

$$\tau\partial_t f_\alpha+\nabla_p\varepsilon(p)\cdot\nabla_x f_\alpha=\tau(\partial_t\varphi_\alpha)g+\varphi_\alpha(\tau\partial_t g+\nabla_p\varepsilon\cdot\nabla_x g).$$

Therefore the families $(f_{\tau,\alpha})_{\tau,\alpha>0}$ and $(\Phi_{\tau,\alpha})_{\tau,\alpha>0}$ satisfy the requirements of Proposition 2.3.12. Hence we obtain for the families $(n_{\tau,\alpha})_{\tau,\alpha>0}$ and $(E_{\tau,\alpha})_{\tau,\alpha>0}$, given by

$$n_{\tau,\alpha}:=\int_{\mathbb{T}^d}f_{\tau,\alpha}dp,\qquad E_{\tau,\alpha}:=\int_{\mathbb{T}^d}\varepsilon f_{\tau,\alpha}dp,$$

by using Proposition 2.3.12 the estimates

$$\begin{aligned}\left\|[n_{\tau,\alpha}]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(\mathbb{R})}&\leq D_\delta\|\Phi_{\tau,\alpha}\|^2_{\mathrm{L}^2(\mathbb{R};\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))}+\delta\|f_{\tau,\alpha}\|^2_{\mathrm{L}^2(\mathbb{R};\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))},\\ \left\|[E_{\tau,\alpha}]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(\mathbb{R})}&\leq D_\delta\varepsilon_\infty\|\Phi_{\tau,\alpha}\|^2_{\mathrm{L}^2(\mathbb{R};\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))}+\delta\varepsilon_\infty\|f_{\tau,\alpha}\|^2_{\mathrm{L}^2(\mathbb{R};\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))}.\end{aligned}$$

That $f_\tau(t)$ coincides with $f_{\tau,\alpha}(t)$ for all t in $[t_0,t_1]$ and all $\tau,\alpha>0$, implies the same for n_τ and $n_{\tau,\alpha}$, and E_τ and $E_{\tau,\alpha}$. Hence

$$\left\|[n_\tau]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(I)}=\left\|[n_{\tau,\alpha}]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(I)}\leq\left\|[n_{\tau,\alpha}]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(\mathbb{R})}. \tag{2.56}$$

$$\left\|[E_\tau]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(I)}=\left\|[E_{\tau,\alpha}]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(I)}\leq\left\|[E_{\tau,\alpha}]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(\mathbb{R})}. \tag{2.57}$$

Using the estimates we obtained from Proposition 2.3.12, the estimates we obtained for $(f_{\tau,\alpha})_{\tau,\alpha>0}$ and $(\Phi_{\tau,\alpha})_{\tau,\alpha>0}$ in (2.53) and (2.54) respectively, and the inequalities above (2.56)-(2.57), yields for all $\alpha>0$

$$\begin{aligned}\left\|[n_\tau]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(I)}&\leq D_\delta\left(C^2\tau^2\alpha+\|\mathcal{Q}_\tau\|^2_{\mathrm{L}^2(I;\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))}\right)+\delta\left(\frac{C^2}{\alpha}+\|f_\tau\|^2_{\mathrm{L}^2(I;\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))}\right),\\ \left\|[E_\tau]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(I)}&\leq D_\delta\varepsilon_\infty\left(C^2\tau^2\alpha+\|\mathcal{Q}_\tau\|^2_{\mathrm{L}^2(I;\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))}\right)+\delta\varepsilon_\infty\left(\frac{C^2}{\alpha}+\|f_\tau\|^2_{\mathrm{L}^2(I;\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))}\right).\end{aligned}$$

Choosing now $\alpha^{-1}=\tau$, provides the desired estimates. □

Remark 2.3.14. What is not immediately apparent, is that in Proposition 2.3.12 and in the bounded version (Proposition 2.3.13) the families $(f_\tau)_{\tau>0}$ and $(\mathcal{Q}_\tau)_{\tau>0}$ are arbitrary and only connected over the equation (2.48). We also notice that an initial value is not necessary to fulfill the requirements of those propositions. This will be important later, when we want to show the long time behaviour. ■

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2.3.3. Existence of a Converging Subsequence

Recalling from our Hypothesis 2.2.14, let f_τ be the solution to our model equation (2.23) for $\tau > 0$ and recall also the definitions for the macroscopic particle density n_τ and macroscopic energy density E_τ

$$(2.31): \qquad n_\tau(t,x) = \int_{\mathbb{T}^d} f_\tau(t,x,p)dp, \qquad E_\tau(t,x) = \int_{\mathbb{T}^d} \varepsilon(p) f_\tau(t,x,p)dp.$$

In this section we will prove that these families have converging subsequences. One of the tools for the proof will be the *Aubin Lions Lemma*, where the original version can be found in [Aub63], and the version we use is from Showalter [Sho97]:

Lemma 2.3.15 (Aubin-Lions-Lemma). *Let the spaces X, Y, B be Banach-spaces and let X be compactly embedded in B (not.: $X \subset\subset B$), and let B continuously be embedded in Y (not.: $B \hookrightarrow Y$). If for $p \in (1,\infty)$ and $r > 1$ the subsets $U \subseteq \mathrm{L}^p(I;X)$ and $\{\partial_t u : u \in U\} \subseteq \mathrm{L}^r(I,Y)$ are bounded on a compact interval I, then the set U is relatively compact in $\mathrm{L}^p(I;B)$.*

Proof. See [Sho97] p.106. □

Remark 2.3.16. We recall here some standard facts, which can be found in basic literature for PDEs or Sobolev spaces. The embedding $\mathrm{H}^1_0(\mathbb{T}^d) \hookrightarrow \mathrm{L}^2(\mathbb{T}^d)$ is dense and continuous. Since $\mathrm{L}^2(\mathbb{T}^d)$ is a Hilbert space, it can be identified with its dual space and therefore the embedding $\mathrm{L}^2(\mathbb{T}^d) \hookrightarrow \mathrm{H}^{-1}(\mathbb{T}^d) := (\mathrm{H}^1_0(\mathbb{T}^d))'$ is also dense and continuous. Moreover it holds

$$\langle u, \varphi \rangle_{\mathrm{H}^{-1}(\mathbb{T}^d)} = (u,\varphi)_{\mathrm{L}^2(\mathbb{T}^d)} \qquad \text{for } u \in \mathrm{L}^2(\mathbb{T}^d),\ \varphi \in \mathrm{H}^1_0(\mathbb{T}^d). \tag{2.58}$$

This will be important for the operator norm in $\mathrm{H}^{-1}(\mathbb{T}^d)$ and the weak formulation. In particular

$$\|u\|_{\mathrm{H}^{-1}(\mathbb{T}^d)} = \sup_{\|\varphi\|_{\mathrm{H}^1_0(\mathbb{T}^d)}=1} \langle u,\varphi\rangle_{\mathrm{H}^{-1}(\mathbb{T}^d)} = \sup_{\|\varphi\|_{\mathrm{H}^1_0(\mathbb{T}^d)}=1} (u,\varphi)_{\mathrm{L}^2(\mathbb{T}^d)}.$$

■

The next proposition will be crucial for the use of Aubin's Lemma, and the proof is postponed to the appendix

Proposition 2.3.17. *For all $s \in (0,1)$ the embedding $\mathrm{H}^s(\mathbb{T}^d) \hookrightarrow \mathrm{L}^2(\mathbb{T}^d)$ is compact for all dimensions $d \in \mathbb{N}$ (not.: $\mathrm{H}^s(\mathbb{T}^d) \subset\subset \mathrm{L}^2(\mathbb{T}^d)$).*

Proof. See Appendix A.1. □

Remark 2.3.18. Recall the Definition 2.1.3 when a function is even or odd on the torus. We have seen in the Example 2.1.4 that the function $\varepsilon(p)$ is even in p and that $\partial_{p_i}\varepsilon(p)$ is odd on the torus. Also recall from Remark 2.2.9 that the Fermi Dirac distribution also is even in p for all $(n,E) \in \mathfrak{D}^\circ$. Hence we see that the following integrals vanish:

$$\int_{\mathbb{T}^d} \nabla_p \varepsilon(p) \nabla_x \mathcal{F}(n_\tau, E_\tau, p)dp = 0 = \int_{\mathbb{T}^d} \varepsilon(p)\nabla_p\varepsilon(p)\nabla_x\mathcal{F}(n_\tau,E_\tau,p)dp, \qquad \tau > 0.$$

■

Theorem 2.3.19. *Let $(n_\tau)_{\tau>0}$ and $(E_\tau)_{\tau>0}$ be the families defined in (2.31). Then there exists subsequences $(n_{\tau_k})_{k\in\mathbb{N}}$ and $(E_{\tau_k})_{k\in\mathbb{N}}$ that converge in $\mathrm{L}^2_{loc}([0,\infty);\mathrm{L}^2(\mathbb{T}^d))$ towards limit functions n and E respectively.*

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Proof. The proof is split into two parts. First we show that for arbitrary compact intervals in $\mathbb{R}_0^+$, we find converging subsequences. The second part concludes through a diagonal argument that we can find limit functions $n(t,x)$ and $E(t,x)$, that are defined for all $t \in \mathbb{R}_0^+$.

Let $I \subset \mathbb{R}^+$ be a compact interval and since we want to apply the Aubin-Lions-Lemma (Lemma 2.3.15), we need that the families $(n_\tau)_{\tau>0}$, $(E_\tau)_{\tau>0}$, and $(\partial_t n_\tau)_{\tau>0}$, $(\partial_t E_\tau)_{\tau>0}$ are bounded in $\mathrm{L}^2(I;\mathrm{H}^s(\mathbb{T}^d))$ and $\mathrm{L}^2(I,\mathrm{H}^{-1}(\mathbb{T}^d))$ respectively. Then we are able to conclude that these families $(n_\tau)_{\tau>0}$, $(E_\tau)_{\tau>0}$ are relatively compact in $\mathrm{L}^2(I,\mathrm{L}^2(\mathbb{T}^d))$, since we have the embeddings $\mathrm{H}^s(\mathbb{T}^d) \subset\subset \mathrm{L}^2(\mathbb{T}^d) \hookrightarrow \mathrm{H}^{-1}(\mathbb{T}^d)$, thanks to Proposition 2.3.17.
Introducing the short notations for the Fermi Dirac distribution $\mathcal{F}_\tau \coloneqq \mathcal{F}(n_\tau, E_\tau, p)$ and for the collision operator $\mathcal{Q}_\tau \coloneqq \mathcal{Q}(f_\tau) = (\tau^{-1})(\mathcal{F}_\tau - f_\tau)$. Due to our assumption on the solutions f_τ (see Hypothesis 2.2.14) we have that the family $(f_\tau)_{\tau>0}$ is bounded in $\mathrm{L}^\infty(\mathbb{R}_0^+ \times \mathbb{T}^d \times \mathbb{T}^d)$ by the constant 1 (this holds also for $f_\tau(0) = f_0$ and f_0, since the initial condition has range in $(0,1)$). Then we recall that the family $(\mathcal{Q}_\tau)_{\tau>0}$ is due to Corollary 2.2.21 uniformly bounded for all $\tau > 0$ by

$$\|\mathcal{Q}_\tau\|_{\mathrm{L}^2(\mathbb{R}_0^+;\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))} \le \mathcal{H}(f_0) - \log(1/2).$$

Therefore the requirements of Proposition 2.3.13 are satisfied, which implies that the families $(n_\tau)_{\tau>0}$ and $(E_\tau)_{\tau>0}$ fulfill the estimates:

$$\left\|[n_\tau]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(I)} \le D_\delta \|\mathcal{Q}_\tau\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \delta \|f_\tau\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \tau(\delta + D_\delta)$$
$$\left\|[E_\tau]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(I)} \le \varepsilon_\infty D_\delta \|\mathcal{Q}_\tau\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \varepsilon_\infty\delta \|f_\tau\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \tau\varepsilon_\infty(\delta + D_\delta)$$

Recalling the definition of $\bar{n}$ and $\bar{E}$ we have for all $\tau > 0$

$$(\bar{n}, \bar{E}) = \int_{\mathbb{T}^d} (n_\tau(t,x), E_\tau(t,x))dx.$$

With the estimate (2.47) in Remark 2.3.10 we obtain then for the family $(n_\tau)_{\tau>0}$

$$\begin{aligned}
\|n_\tau\|^2_{\mathrm{L}^2(I;\mathrm{H}^s(\mathbb{T}^d))} &= \int_I \|n_\tau(t)\|^2_{\mathrm{H}^s(\mathbb{T}^d)}\, dt \\
&\le \int_I 2\left(2[n_\tau]^2_{\mathrm{H}^s(\mathbb{T}^d)} + \bar{n}^2\right) \\
&= 4\left\|[n_\tau]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(I)} + 2\,\mathrm{meas}\,(I)\,\bar{n}^2 \\
&\le 4\left(D_\delta \|\mathcal{Q}_\tau\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \delta\|f_\tau\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \tau(\delta + D_\delta)\right) + 2\,\mathrm{meas}\,(I)\,\bar{n}^2.
\end{aligned}$$

Since the family $(\mathcal{Q}_\tau)_{\tau>0}$ is uniformly bounded (Corollary 2.2.21) and $|f_\tau| < 1$ for all $\tau > 0$ we get

$$\|n_\tau\|^2_{\mathrm{L}^2(I;\mathrm{H}^s(\mathbb{T}^d))} \le 4\left(D_\delta\left(\mathcal{H}(f_0) - \log\frac{1}{2}\right) + \delta\,\mathrm{meas}\,(I) + \tau(\delta + D_\delta)\right) + 2\,\mathrm{meas}\,(I)\,\bar{n}^2. \tag{2.59}$$

The same argumentation provides for the family $(E_\tau)_{\tau>0}$

$$\|E_\tau\|^2_{\mathrm{L}^2(I;\mathrm{H}^s(\mathbb{T}^d))} \le 4\varepsilon_\infty\left(D_\delta\left(\mathcal{H}(f_0) - \log\frac{1}{2}\right) + \delta\,\mathrm{meas}\,(I) + \tau(\delta + D_\delta)\right) + 2\,\mathrm{meas}\,(I)\,\bar{E}^2. \tag{2.60}$$

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If we choose the subfamilies, where $\tau \in (0, C)$ for any constant $C \in \mathbb{R}$, we see that the estimates (2.59)-(2.60), give a uniform bound for those subfamilies and therefore we have that these families are bounded in $\mathrm{L}^2(I; \mathrm{H}^s(\mathbb{T}^d))$.
Next to check for the Aubin Lions Lemma, is that the families $(\partial_t n_\tau)_{\tau>0}$ and $(\partial_t E_\tau)_{\tau>0}$ are bounded in $\mathrm{L}^2(I; \mathrm{H}^{-1}(\mathbb{T}^d))$. For this express our function f_τ also as

$$f_\tau = \mathcal{F}_\tau - \tau \mathcal{Q}_\tau. \tag{2.61}$$

Substituting the above (2.61) into our semiconductor Boltzmann equation and in the same equation multiplicated by $\varepsilon(p)$ we get

$$\tau\partial_t(\mathcal{F}_\tau - \tau\mathcal{Q}_\tau) + \nabla_p\varepsilon \cdot \nabla_x\mathcal{F}_\tau - \tau\nabla_p\varepsilon \cdot \nabla_x\mathcal{Q}_\tau = \mathcal{Q}_\tau, \tag{2.62}$$

$$\tau\partial_t(\varepsilon\mathcal{F}_\tau - \tau\varepsilon\mathcal{Q}_\tau) + \varepsilon\nabla_p\varepsilon \cdot \nabla_x\mathcal{F}_\tau - \varepsilon\tau\nabla_p\varepsilon \cdot \nabla_x\mathcal{Q}_\tau = \varepsilon\mathcal{Q}_\tau. \tag{2.63}$$

Dividing equations (2.62)-(2.63) through τ and integrating them over the momentum p leads to

$$\partial_t n_\tau + \frac{1}{\tau}\int_{\mathbb{T}^d} \nabla_p\varepsilon \cdot \nabla_x\mathcal{F}_\tau dp - \int_{\mathbb{T}^d} \nabla_p\varepsilon \cdot \nabla_x\mathcal{Q}_\tau dp = 0, \tag{2.64}$$

$$\partial_t E_\tau + \frac{1}{\tau}\int_{\mathbb{T}^d} \varepsilon\nabla_p\varepsilon \cdot \nabla_x\mathcal{F}_\tau dp - \int_{\mathbb{T}^d} \varepsilon\nabla_p\varepsilon \cdot \nabla_x\mathcal{Q}_\tau dp = 0, \tag{2.65}$$

where the integrals of $\mathcal{Q}_\tau$, and $\varepsilon\mathcal{Q}_\tau$ vanish. The terms with the factor τ^{-1} also vanish, thanks to Remark 2.3.18, hence

$$\partial_t n_\tau = \int_{\mathbb{T}^d} \nabla_p\varepsilon \cdot \nabla_x\mathcal{Q}_\tau dp \tag{2.66}$$

$$\partial_t E_\tau = \int_{\mathbb{T}^d} \varepsilon\nabla_p\varepsilon \cdot \nabla_x\mathcal{Q}_\tau dp \tag{2.67}$$

We notice that all the above equations are well stated due to Remark 2.2.17 and therefore n_τ and E_τ solve (2.66) and (2.67). Integrating (φ(2.66)) with respect to p, where $\varphi \in \mathrm{H}_0^1(\mathbb{T}^d)$, yields for all $t > 0$

$$\begin{aligned}
\left|\int_{\mathbb{T}^d} \partial_t n_\tau(t,x)\varphi(x)dx\right| &= \left|\int_{\mathbb{T}^d}\int_{\mathbb{T}^d} (\nabla_p\varepsilon(p) \cdot \nabla_x\mathcal{Q}_\tau(t,x,p))dp\ \varphi(x)dx\right| \\
&= \left|\int_{\mathbb{T}^d}\int_{\mathbb{T}^d} \mathrm{div}_x(\mathcal{Q}_\tau(t,x,p)\nabla_p\varepsilon(p))\varphi(x)\ dpdx\right| \\
&= \left|-\int_{\mathbb{T}^d}\int_{\mathbb{T}^d} \mathcal{Q}_\tau(t,x,p)\nabla_p\varepsilon(p) \cdot \nabla_x\varphi(x)\ dpdx\right| \\
&\leq \|\mathcal{Q}_\tau(t)\|_{\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)} \|\nabla_p\varepsilon\|_{\mathrm{L}^\infty(\mathbb{T}^d)} \|\varphi\|_{\mathrm{H}_0^1(\mathbb{T}^d)}.
\end{aligned}$$

As already mentioned, the family $(\mathcal{Q}_\tau)_{\tau>0}$ is uniformly bounded in $\mathbb{R}_0^+$, which provides the estimate

$$\begin{aligned}
\|\partial_t n_\tau\|^2_{\mathrm{L}^2(I;\mathrm{H}^{-1}(\mathbb{T}^d))} = &\int_I \sup_{\|\varphi\|=1} \left|(\partial_t n_\tau(t),\varphi)_{\mathrm{L}^2(\mathbb{T}^d)}\right|^2 dt \leq \int_I \|\mathcal{Q}_\tau(t)\|^2_{\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)} \|\nabla_p\varepsilon\|^2_{\mathrm{L}^\infty(\mathbb{T}^d)} dt \\
\leq &(\mathcal{H}(f_0) - \log(1/2)) \|\nabla_p\varepsilon\|^2_{\mathrm{L}^\infty(\mathbb{T}^d)},
\end{aligned}$$

and hence the family $(\partial_t n_\tau)_{\tau>0}$ is uniformly bounded in $\mathrm{L}^2(I; \mathrm{H}^{-1}(\mathbb{T}^d))$. For $(\partial_t E_\tau)_{\tau>0}$ we obtain similarly from (2.67) that

$$\begin{aligned}
\left|\int_{\mathbb{T}^d} \partial_t E_\tau(t,x)\varphi(x)dx\right| &= \left|\int_{\mathbb{T}^d}\int_{\mathbb{T}^d} (\varepsilon(p)\nabla_p\varepsilon(p) \cdot \nabla_x\mathcal{Q}_\tau(t,x,p))dp\ \varphi(x)dx\right| \\
&\leq \frac{d}{2\pi}\|\mathcal{Q}_\tau(t)\|^2_{\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)} \|\nabla_p\varepsilon\|^2_{\mathrm{L}^\infty(\mathbb{T}^d)} \|\varphi\|^2_{\mathrm{H}_0^1(\mathbb{T}^d)},
\end{aligned}$$

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and then we see that the family $(\partial_t E_\tau)_{\tau>0}$ is also uniformly bounded in $\mathrm{L}^2(I;\mathrm{H}^{-1}(\mathbb{T}^d))$, since

$$\|\partial_t E_\tau\|^2_{\mathrm{L}^2(I;\mathrm{H}^{-1}(\mathbb{T}^d))} = \int_I \sup_{\|\varphi\|=1} \left|(\partial_t E_\tau(t),\varphi)_{\mathrm{L}^2(\mathbb{T}^d)}\right|^2 dt \le \frac{d}{2\pi}\int_I \|\mathcal{Q}_\tau(t)\|^2_{\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)} \|\nabla_p\varepsilon\|^2_{\mathrm{L}^\infty(\mathbb{T}^d)}\, dt$$
$$\le \frac{d}{2\pi}(\mathcal{H}(f_0)-\log(1/2))\,\|\nabla_p\varepsilon\|^2_{\mathrm{L}^\infty(\mathbb{T}^d)}\,.$$

Therefore we can apply Aubin-Lions Lemma to the families $(n_\tau)_{\tau\in(0,C)}$ and $(E_\tau)_{\tau\in(0,C)}$, and find $n^{(I)}, E^{(I)} \in \mathrm{L}^2(I;\mathrm{L}^2(\mathbb{T}^d))$ such that there are subsequences which converge in the sense that

$$n_{\tau_k} \xrightarrow[k\to\infty]{} n^{(I)}, \qquad E_{\tau_k} \xrightarrow[k\to\infty]{} E^{(I)}, \qquad \text{in } \mathrm{L}^2(I;\mathrm{L}^2(\mathbb{T}^d)).$$

For the general limit we first define the intervals $I_N \coloneqq [0,N]$ for $N\in\mathbb{N}$, and define for the first interval I_1 the subsequences $(n_{(\tau_k,1)})_{k\in\mathbb{N}}$, and $(E_{(\tau_k,1)})_{k\in\mathbb{N}}$, which converge towards the limits $n^{(1)}$, and $E^{(1)}$, i.e.

$$n_{(\tau_k,1)} \xrightarrow[k\to\infty]{} n^{(1)}, \qquad E_{(\tau_k,1)} \xrightarrow[k\to\infty]{} E^{(1)}, \qquad \text{in } \mathrm{L}^2(I_1;\mathrm{L}^2(\mathbb{T}^d))$$

Now these sequences $(n_{(\tau_k,1)})_{k\in\mathbb{N}}$, and $(E_{(\tau_k,1)})_{k\in\mathbb{N}}$ also fulfill, as subsequences of the families $(n_\tau)_{\tau\in(0,C)}$ and $(E_\tau)_{\tau\in(0,C)}$, the criteria of the Aubin Lions Lemma for any compact interval $I\subset\mathbb{R}_0^+$. Hence there exist for the interval I_2 converging subsequences $(n_{(\tau_k,2)})_{k\in\mathbb{N}}$ and $(E_{(\tau_k,2)})_{k\in\mathbb{N}}$ from the sequences $(n_{(\tau_k,1)})_{k\in\mathbb{N}}$, and $(E_{(\tau_k,1)})_{k\in\mathbb{N}}$, with limits $n^{(2)}$ and $E^{(2)}$, in the sense that

$$n_{(\tau_k,2)} \xrightarrow[k\to\infty]{} n^{(2)}, \qquad E_{(\tau_k,2)} \xrightarrow[k\to\infty]{} E^{(2)} \qquad \text{in } \mathrm{L}^2(I_2;\mathrm{L}^2(\mathbb{T}^d)).$$

We notice that the functions $n^{(2)}$ and $E^{(2)}$, restricted to I_1, coincide with $n^{(1)}$ and $E^{(1)}$ respectively, since $(n_{(\tau_k,2)})_{k\in\mathbb{N}}$ and $(E_{(\tau_k,2)})_{k\in\mathbb{N}}$ are subsequences of $(n_{(\tau_k,1)})_{k\in\mathbb{N}}$ and $(E_{(\tau_k,1)})_{k\in\mathbb{N}}$. Proceeding iteratively now for $N\in\mathbb{N}$, $N\ge 1$, playing the same game, we obtain a family of sequences $((n_{(\tau_k,N)})_{k\in\mathbb{N}};(E_{(\tau_k,N)})_{k\in\mathbb{N}})_{N\in\mathbb{N}}$ that fulfill the following:

1. $(n_{(\tau_k,N)})_{k\in\mathbb{N}} \supseteq (n_{(\tau_k,N+1)})_{k\in\mathbb{N}}$, and $(E_{(\tau_k,N)})_{k\in\mathbb{N}} \supseteq (E_{(\tau_k,N+1)})_{k\in\mathbb{N}}$, $\forall N\in\mathbb{N}$
2. $(n_{(\tau_k,N)})_{k\in\mathbb{N}}$; $(E_{(\tau_k,N)})_{k\in\mathbb{N}}$ converge towards $n^{(N)}$; $E^{(N)}$ in $\mathrm{L}^2(I_N;\mathrm{L}^2(\mathbb{T}^d))$, $\forall N\in\mathbb{N}$
3. $n^{(N)}|_{I_J} \widehat{=} n^{(J)}$, $E^{(N)}|_{I_J} \widehat{=} E^{(J)}$ for all $N\in\mathbb{N}$ and for $J\le N, J\in\mathbb{N}$.

Define the functions n and E on $\mathbb{R}_0^+\times\mathbb{T}^d\to\mathfrak{D}$, with the mapping rule

$$n(t,x) \coloneqq n^{(N)}(t,x),\ E(t,x) \coloneqq E^{(N)}(t,x) \qquad \text{for } t\in[N-1,N],\ N\in\mathbb{N},\ x\in\mathbb{T}^d. \tag{2.68}$$

Due to the fact that $n^{(N)}|_{I_{N-1}} \widehat{=}\ n^{(N-1)}$ and $E^{(N)}|_{I_{N-1}} \widehat{=}\ E^{(N-1)}$, the above functions n and E are well defined on $\mathbb{R}_0^+\times\mathbb{T}^d$. Looking at the diagonal sequences $(n_{(\tau_N,N)})_{N\in\mathbb{N}}$ and $(E_{(\tau_N,N)})_{N\in\mathbb{N}}$, we observe that for every compact interval $I\subseteq\mathbb{R}_0^+$, there exists a $J\in\mathbb{N}$ such that $I\subseteq I_J$ and therefore

$$\lim_{N\to\infty} n_{(\tau_N,N)} = n^{(J)} = n|_{I_J}, \qquad \lim_{N\to\infty} E_{(\tau_N,N)} = E^{(J)} = E|_{I_J}, \qquad \text{in } \mathrm{L}^2(I_J;\mathrm{L}^2(\mathbb{T}^d)).$$

Finally we obtain, that

$$\lim_{N\to\infty} n_{(\tau_N,N)} = n, \qquad \lim_{N\to\infty} E_{(\tau_N,N)} = E, \qquad \text{in } \mathrm{L}^2_{loc}(\mathbb{R}_0^+;\mathrm{L}^2(\mathbb{T}^d)).$$

□

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Corollary 2.3.20. *For the families $(n_\tau)_{\tau>0}$ and $(E_\tau)_{\tau>0}$, defined in* (2.31)*, exist subsequences $(n_{\tau_k})_{k\in\mathbb{N}}$ and $(E_{\tau_k})_{k\in\mathbb{N}}$ that converge in $\mathrm{L}^2_{loc}(\mathbb{R}_0^+;\mathrm{L}^2(\mathbb{T}^d))$ towards the limits n and E, such that these limits have a weak derivative $\partial_t n$ and $\partial_t E$ that lie in $\mathrm{L}^2(\mathbb{R}_0^+;\mathrm{H}^{-1}(\mathbb{T}^d))$.*

Proof. From the previous Theorem 2.3.19 we obtain converging subsequences $(n_{\tau_k})_{k\in\mathbb{N}}$ and $(E_{\tau_k})_{k\in\mathbb{N}}$ that converge in $\mathrm{L}^2_{loc}(\mathbb{R}_0^+;\mathrm{L}^2(\mathbb{T}^d))$ towards the limits n and E. In the proof of Theorem 2.3.19 we also derived the estimates for all intervals $I\subseteq\mathbb{R}_0^+$ and $\tau>0$

$$\begin{aligned}\|\partial_t n_\tau\|^2_{\mathrm{L}^2(I;\mathrm{H}^{-1}(\mathbb{T}^d))} &\leq (\mathcal{H}(f_0)-\log(1/2))\,\|\nabla_p\varepsilon\|^2_{\mathrm{L}^\infty(\mathbb{T}^d)}\,,\\ \|\partial_t E_\tau\|^2_{\mathrm{L}^2(I;\mathrm{H}^{-1}(\mathbb{T}^d))} &\leq \frac{d}{2\pi}(\mathcal{H}(f_0)-\log(1/2))\,\|\nabla_p\varepsilon\|^2_{\mathrm{L}^\infty(\mathbb{T}^d)}\,.\end{aligned}$$

These estimates hold also for the subsequences $(\partial_t n_{\tau_k})_{k\in\mathbb{N}}$ and $(\partial_t E_{\tau_k})_{k\in\mathbb{N}}$ and $I=\mathbb{R}_0^+$. Since $\mathrm{L}^2(\mathbb{R}_0^+;\mathrm{H}^{-1}(\mathbb{T}^d))$ is reflexive, Theorem of Eberlein-Šmuljan (see [Zei90a] Theorem 21.D) provides weak converging subsequences (denoting with the same indices) $(\partial_t n_{\tau_k})_{k\in\mathbb{N}}$ and $(\partial_t E_{\tau_k})_{k\in\mathbb{N}}$. Let us denote these weak limits with g_n, and g_E, then we have for all φ in $C_c^\infty(\mathbb{R}_0^+\times\mathbb{T}^d)$

$$\begin{aligned}\int_{\mathbb{R}_0^+}\int_{\mathbb{T}^d} n\partial_t\varphi dxdt &= \lim_{k\to\infty}\int_{\mathbb{R}_0^+}\int_{\mathbb{T}^d} n_{\tau_k}\partial_t\varphi dxdt = \lim_{k\to\infty} -\int_{\mathbb{R}_0^+}\int_{\mathbb{T}^d}\partial_t n_{\tau_k}\varphi dxdt\\ &= -\int_{\mathbb{R}_0^+}\int_{\mathbb{T}^d} g_n\varphi dxdt\end{aligned}$$

Therefore g_n is the weak derivative of n, and with the same argumentation we have that g_E is the weak derivative of E. Since g_n, g_E are elements of $\mathrm{L}^2(\mathbb{R}_0^+;\mathrm{H}^{-1}(\mathbb{T}^d))$ we have that the weak derivatives $\partial_t n$ and $\partial_t E$ are in $\mathrm{L}^2(\mathbb{R}_0^+;\mathrm{H}^{-1}(\mathbb{T}^d))$ as well. □

2.3.4. A Convergence Result for the Fermi Dirac Distribution

As already mentioned in the beginning of Section 2.3, we want to prove the convergence result

$$(2.35):\qquad \lim_{j\to\infty}\left\|\bar{\mathcal{F}}(n_{k_j},E_{k_j};.)-\bar{\mathcal{F}}(n,E;.)\right\|_{\mathrm{L}^q(I;\mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d))}=0,$$

which should hold for all compact intervals $I\subset\mathbb{R}_0^+$, for all $q\in[1,\infty)$, and all sequences in $\mathfrak{D}^\circ$ with limit in $\mathfrak{D}$. Recall that $\bar{\mathcal{F}}$ is the extension of $\mathcal{F}$ from $\mathfrak{D}^\circ$ to $\mathfrak{D}$, given by (2.3.3), where we do not need the definition for now. The start of this subsection will be some results taken from the thesis of Braukoff [Bra17], since in his work a lot has already been done regarding the treatment of $\mathcal{F}$ and its extension. Then we state in Theorem 2.3.27 the first convergence result, and in the end we will prove the convergence result we are looking for. We recall for $n\in[0,1]$ the definition of the Fermi energy $\epsilon_F(n)\in\overline{\varepsilon(\mathbb{T}^d)}$, which is defined being the unique solution of

$$\mathrm{meas}\left(\left\{p\in\mathbb{T}^d:\varepsilon(p)<\epsilon_F(n)\right\}\right)=n.$$

Remark 2.3.21. (Taken from [Bra17]) The Fermi Energy ϵ_F describes the energy level below which every state is occupied at zero temperature and is well defined, since it is similar to the function h defined in Lemma 2.2.1 and we have, thanks to the symmetry of $\varepsilon(p)$, that

$$\mathrm{meas}\left(\left\{p\in\mathbb{T}^d:\varepsilon(p)>-\epsilon_F(n)\right\}\right)=n.$$

With its relation to h in Lemma 2.2.1, we notice that $\epsilon_F(n)$ is a continuous and strict increasing function. At this point we mention also that for every $C\in\mathbb{R}$ we have that

$$\mathrm{meas}\left(\left\{p\in\mathbb{T}^d:\varepsilon(p)=C\right\}\right)=0,$$

■

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Let us further recall that actually the Fermi Dirac distribution depends on the two parameters (λ_0, λ_1), which in turn depend on the densities $(n, E) \in \mathfrak{D}^\circ$. In Proposition 2.2.7, we stated that the mapping $(\lambda_0, \lambda_1) \to (n, E)$ is bijective and smooth, as well as the inverse (see also Remark 2.2.9).

Notation 2.3.22. *To avoid confusion we will for this section be more precise on the dependences. When we are talking about the bijection from $\mathbb{R}^2 \to \mathfrak{D}^\circ$ we will denote it via the tilde notation*

$$(\lambda_0, \lambda_1) \mapsto (\tilde{n}(\lambda_0, \lambda_1), \tilde{E}(\lambda_0, \lambda_1)) \quad \textit{or vice versa} \quad (n, E) \mapsto (\tilde{\lambda}_0(n, E), \tilde{\lambda}_1(n, E)).$$

The mentioned bijection is one way to describe the dependence. Next we introduce analogous representations of elements in $\mathfrak{D}^\circ$ and cite the next two Lemmas and the following Remark from [Bra17].

Lemma 2.3.23. *Let $n \in (0, 1)$, then there exists a unique smooth function $\phi : \mathbb{R} \to \mathbb{R}$ such that*

$$n = \int_{\mathbb{T}^d} \mathcal{F}(\phi(\lambda_1), \lambda_1; p) dp. \tag{2.69}$$

In particular, it holds $\phi(0) = \log \frac{n}{1-n}$ and we have

$$\phi(\lambda_1) \mp \epsilon_F(n)\lambda_1 = o(\lambda_1) \ \textit{as} \ \lambda_1 \to \pm\infty.$$

Proof. We give here only the idea of the proof and for details we suggest the reader to see Lemma 5.1.11 in [Bra17]. It can be shown that for fixed $\lambda_1 \in \mathbb{R}$ the function

$$\lambda_0 \mapsto \int_{\mathbb{T}^d} \mathcal{F}(\lambda_0, \lambda_1; p) dp$$

is strictly monotone and continuous in λ_0. Therefore with the mean-value theorem it is possible to show that there exists a unique function ϕ as in (2.69).
For the convergence rate we look at the function $r_\pm(\lambda_1) := \phi(\lambda_1) \mp \epsilon_F(n)\lambda_1$. First assume that $r_\pm(\lambda_1)/\lambda_1$ is bounded as $\lambda_1 \to \pm\infty$, then it is possible to show that this holds only if $r_\pm(\lambda_1)/\lambda_1$ goes to zero. Assuming that $r_\pm(\lambda_1)/\lambda_1$ diverges for $\lambda_1 \to \pm\infty$, then we find that this is only the case if $n = 0$, which this is a contradiction to our requirement $n \in (0, 1)$. □

Lemma 2.3.24. *Let $n \in (0, 1)$ and ϕ be given by Lemma 2.3.23. Then for every $-e_{max}(n) < E < e_{max}(n)$, there exists a unique $\lambda_1 \in \mathbb{R}$ such that*

$$E = \int_{\mathbb{T}^d} \varepsilon(p) \mathcal{F}(\phi(\lambda_1), \lambda_1; p) dp. \tag{2.70}$$

Proof. Again we only provide the idea, and refer for details to Lemma 5.1.15 in [Bra17]. The key elements are to prove that the function $\tilde{E}(\phi(\lambda_1), \lambda_1)$ fulfills two requirements:

$$\frac{d}{d\lambda_1} \tilde{E}(\phi(\lambda_1), \lambda_1) > 0, \qquad \text{and} \qquad \lim_{\lambda_1 \to \pm\infty} \tilde{E}(\phi(\lambda_1), \lambda_1) = \pm e_{max}(n).$$

If these two properties are met, by the mean-value theorem it holds that there exists a unique $\lambda_1 \in \mathbb{R}$, such that (2.70) is fulfilled. □

Remark 2.3.25. The parameters λ_0, λ_1 are sometimes called the *entropy parameters*. Note that λ_1 has the same sign as $\tilde{E}(\phi(\lambda_1), \lambda_1)$, since the energy increases in λ_1 and we may observe that $E(\phi(0), 0)$ vanishes. ■

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To show our convergence result, we need these analogous representations. The last important result we need is what happens to $\tilde{\lambda}_1$ if the sequence of energies $(E_k)_{k\in\mathbb{N}}$ converges towards the boundary $\partial\mathfrak{D}$. This will be an important case in the upcoming Theorem 2.3.27.

Lemma 2.3.26. *Let $(n_k, E_k)_{k\in\mathbb{N}}$ be a sequence in $\mathfrak{D}^\circ$. If the sequence converges such that*

$$(n_k, E_k) \to (n, \pm e_{max}(n)), \qquad n \in (0,1)$$

then we have that $\tilde{\lambda}_1(n_k, E_k) \to \pm\infty$.

Proof. Without loss of generality we take first $E_k \to e_{max}(n)$ and then we assume that

$$\lim_{k\to\infty} \left|\tilde{\lambda}_1(n_k, E_k)\right| = \lambda_1 < \infty \qquad \text{and} \qquad \lim_{k\to\infty} \left|\tilde{\lambda}_0(n_k, E_k)\right| = \lambda_0 < \infty.$$

The pair (λ_0, λ_1) would be the representative in $\mathbb{R}^2$ such that

$$(n, e_{max}(n)) = \int_{\mathbb{T}^d} (1, \varepsilon(p))\mathcal{F}(\lambda_0, \lambda_1; p)dp.$$

If $(\lambda_0, \lambda_1) \in \mathbb{R}^2$, Proposition 2.2.7 states that then $(n, e_{max}(n)) \in \mathfrak{D}^\circ$, which is a contradiction. Next assume that

$$\lim_{k\to\infty} \left|\tilde{\lambda}_1(n_k, E_k)\right| = \lambda_1 < \infty \qquad \text{and} \qquad \lim_{k\to\infty} \left|\tilde{\lambda}_0(n_k, E_k)\right| = \infty.$$

So if $\tilde{\lambda}_0$ diverges either to $+\infty$ or $-\infty$ we have

$$\lim_{k\to\infty} \mathcal{F}(\tilde{\lambda}_0(n_k, E_k), \tilde{\lambda}_1(n_k, E_k); p) = \begin{cases} 1 & \text{if } \tilde{\lambda}_0 \to +\infty \\ 0 & \text{if } \tilde{\lambda}_0 \to -\infty. \end{cases}$$

Now that is again a contradiction to $n \in (0,1)$, and therefore it must hold that

$$\lim_{k\to\infty} (n_k, E_k) = (n, \pm e_{max}(n)), \quad \text{with } n \in (0,1), \quad \Longrightarrow \quad \lim_{k\to\infty} \left|\tilde{\lambda}_1(n_k, E_k)\right| = \infty.$$

What remains to show is that the signs of the limits coincide. We refer here to Lemma 2.3.24 and Remark 2.3.25. Since $(n_k, E_k)_{k\in\mathbb{N}}$ is in $\mathfrak{D}^\circ$, there exists for every E_k a $\lambda_{1,k}$ such that

$$E_k = \int_{\mathbb{T}^d} \varepsilon(p)\mathcal{F}(\phi(\lambda_{1,k}), \lambda_{1,k}; p)dp.$$

Because of uniqueness we have that $\tilde{\lambda}_1(n_k, E_k) = \lambda_{1,k}$ and that $E_k = \tilde{E}(\phi(\lambda_{1,k}), \lambda_{1,k})$. Now if $E_k \to e_{max}(n)$ there exists an index $k_0 \in \mathbb{N}$ such that for all $k > k_0$ we have that $E_k > 0$ and therefore we have also that $\tilde{E}(\phi(\lambda_{1,k}), \lambda_{1,k}) > 0$ for all $k > k_0$. Since the sign of $\tilde{E}(\phi(\lambda_{1,k}), \lambda_{1,k})$ coincides with $\lambda_{1,k}$ (see Remark 2.3.25), we get that $\lambda_{1,k} > 0$ for all $k > k_0$. With this we conclude that $\lambda_1(n_k, E_k) > 0$ for all $k > k_0$ which gives us the implication

$$\lim_{k\to\infty} (n_k, E_k) = (n, e_{max}(n)) \qquad \Longrightarrow \qquad \lim_{k\to\infty} \lambda_1(n_k, E_k) = \infty.$$

With the same argumentation we obtain that if $(E_k)_{k\in\mathbb{N}}$ converges to $-e_{max}(n)$ we have that $(\tilde{\lambda}_1(n_k, E_k))_{k\in\mathbb{N}}$ diverges to $-\infty$. □

Now we come to our first convergence result, where we need all the previous preparation.

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Theorem 2.3.27. *If the sequence* $(n_k, E_k)_{k\in\mathbb{N}} \subset \mathfrak{D}^\circ$ *converges to a limit* $(n, E) \in \mathfrak{D}$, *then*

$$\lim_{k\to\infty} \mathcal{F}(n_k, E_k; p) = \begin{cases} n & \text{if } n \in \{0,1\}, \\ \mathcal{F}(n, E; p) & \text{if } (n, E) \in \mathfrak{D}^\circ, \\ \mathbb{1}_{\{\mp\varepsilon(p)<\epsilon_F(n)\}}(p) & \text{if } E = \pm e_{max}(n), \end{cases}$$

where the above convergence is to understand in the $\mathrm{L}^1(\mathbb{T}^d)$ *norm.*

Proof. First let $(n_k)_{k\in\mathbb{N}}$ converge to $n \in \{0,1\}$. Then clearly we have that $e_{max}(n) = -e_{max}(n) = 0$ and therefore $(E_k)_{k\in\mathbb{N}}$ has to converge to zero. We have for all $k \in \mathbb{N}$ and for all $p \in \mathbb{T}^d$, that $0 < \mathcal{F}(\tilde\lambda_0(n_k, E_k), \tilde\lambda_1(n_k, E_k); p) < 1$. In the case where the limit is $n = 1$ we see

$$\begin{aligned}\left\|1 - \mathcal{F}(\tilde\lambda_0(n_k, E_k), \tilde\lambda_1(n_k, E_k); p)\right\|_{\mathrm{L}^1(\mathbb{T}^d)} &= \int_{\mathbb{T}^d} \left|1 - \mathcal{F}(\tilde\lambda_0(n_k, E_k), \tilde\lambda_1(n_k, E_k); p)\right| dp \\ &= 1 - \int_{\mathbb{T}^d} \mathcal{F}(\tilde\lambda_0(n_k, E_k), \tilde\lambda_1(n_k, E_k); p) dp \\ &= 1 - n_k,\end{aligned}$$

which converges to 0 for k to infinity. In the other case, where the limit is $n = 0$ we have

$$\left\|\mathcal{F}(\tilde\lambda_0(n_k, E_k), \tilde\lambda_1(n_k, E_k); p)\right\|_{\mathrm{L}^1(\mathbb{T}^d)} = \int_{\mathbb{T}^d} \left|\mathcal{F}(\tilde\lambda_0(n_k, E_k), \tilde\lambda_1(n_k, E_k); p)\right| dp = n_k,$$

which also converges for k to infinity to zero. Therefore the first convergence is proven. Now if the sequence $(n_k, E_k)_{k\in\mathbb{N}}$ converges to an element (n, E) in $\mathfrak{D}^\circ$, we have that thanks to Proposition 2.2.7 the mappings $\tilde\lambda_0$ and $\tilde\lambda_1$ are continuous on $\mathfrak{D}^\circ$. Therefore we obtain as composition of continuous mappings

$$\lim_{k\to\infty} \mathcal{F}(\tilde\lambda_0(n_k, E_k), \tilde\lambda_1(n_k, E_k); p) = \mathcal{F}(\tilde\lambda_0(n, E), \tilde\lambda_1(n, E); p).$$

which is the Fermi Dirac distribution of the densities (n, E). Now since it converges point wise for all $p \in \mathbb{T}^d$ we can use the dominated convergence theorem and obtain the convergence in $\mathrm{L}^1(\mathbb{T}^d)$ such that

$$\lim_{k\to\infty} \left\|\mathcal{F}(n, E; p) - \mathcal{F}(\tilde\lambda_0(n_k, E_k), \tilde\lambda_1(n_k, E_k); p)\right\|_{\mathrm{L}^1(\mathbb{T}^d)} = 0.$$

The last case where $n \in (0,1)$ and $(E_k)_{k\in\mathbb{N}}$ converges to either $e_{max}(n)$ or $-e_{max}(n)$, needs slightly more treatment. For this we define the functions

$$\omega_j(\lambda_0, \lambda_1) := \int_{\mathbb{T}^d} \varepsilon(p)^j \mathcal{F}(\lambda_0, \lambda_1; p)(1 - \mathcal{F}(\lambda_0, \lambda_1; p)) dp \qquad j \in \mathbb{N}.$$

Now from Lemma 2.3.23 we recall that for every n in $(0,1)$ there exists a unique smooth function $\phi : \mathbb{R} \to \mathbb{R}$ that depends on λ_1, such that

$$n = \int_{\mathbb{T}^d} \mathcal{F}(\phi(\lambda_1), \lambda_1; p) dp.$$

Now it makes sense to choose ϕ also dependent on n, such that the above holds for all (n, λ_1) in $(0,1) \times \mathbb{R}$, (not.: $\phi(n, \lambda_1)$). Next we define the function $g : (0,1) \times \mathbb{R} \to (0,1)$ with

$$g(n, \lambda_1) := \int_{\mathbb{T}^d} \mathcal{F}(\phi(n, \lambda_1), \lambda_1; p) dp.$$

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This is may a bit be an exaggeration since $g(n,\lambda_1) = n$ for all $\lambda_1 \in \mathbb{R}$, but it will help us to make the next step more vivid. We have for the partial derivative with respect to λ_1 on one hand $\partial_{\lambda_1} g = 0$ (since $g(n,\lambda_1) = n$) and on the other hand (compare with Remark 2.2.9)

$$\begin{aligned}\partial_{\lambda_1} g =& \int_{\mathbb{T}^d} \partial_{\lambda_1} \mathcal{F}(\phi(n,\lambda_1),\lambda_1;p)dp\\ =& \int_{\mathbb{T}^d} \mathcal{F}(\phi(n,\lambda_1),\lambda_1;p)(1-\mathcal{F}(\phi(n,\lambda_1),\lambda_1;p))(\partial_{\lambda_1}\phi(n,\lambda_1)+\varepsilon(p))dp\\ =&\omega_1(\phi(n,\lambda_1),\lambda_1)+\omega_0(\phi(n,\lambda_1),\lambda_1)\partial_{\lambda_1}\phi(n,\lambda_1).\end{aligned}$$

This together leads us to the ODE

$$0 = \omega_1 + \omega_0 \partial_{\lambda_1}\phi, \qquad \text{with } \phi(n,0) = \log\frac{n}{1-n},$$

which has the implicit form

$$\phi(n,\lambda_1) = \log\frac{n}{1-n} - \int_0^{\lambda_1} \frac{\omega_1(\phi(n,\mu),\mu)}{\omega_0(\phi(n,\mu),\mu)} d\mu.$$

Now Braukhoff has proven in [Bra17] (see Remark 5.2.8) that

$$\frac{1}{\lambda_1}\int_0^{\lambda_1} \frac{\omega_1(\phi(n,\mu),\mu)}{\omega_0(\phi(n,\mu),\mu)} d\mu \xrightarrow{\lambda_1\to\pm\infty} \mp\epsilon_F(n) \quad \text{uniformly in } n, \tag{2.71}$$

where $\epsilon_F(n)$ is the Fermi energy defined in Definition 2.3.2. From Lemma 2.3.26 we have that for $(n_k, E_k) \to (n, \pm e_{max}(n))$ that $\tilde{\lambda}_1(n_k,E_k)$ diverges to $\pm\infty$. With the uniform convergence (2.71) we obtain then

$$\lim_{k\to\infty} \frac{1}{\tilde{\lambda}_1(n_k,E_k)}\phi(n_k,\tilde{\lambda}_1(n_k,E_k)) = \begin{cases}\epsilon_F(n) & \text{for } E_k \to e_{max}(n),\\ -\epsilon_F(n) & \text{for } E_k \to -e_{max}(n).\end{cases} \tag{2.72}$$

We introduce the short notation $\tilde{\lambda}_{1,k} \hat{=} \tilde{\lambda}_1(n_k,E_k)$ and $\phi_k \hat{=} \phi(n_k,\tilde{\lambda}_{1,k})$ and without loss of generality we choose that $(E_k)_{k\in\mathbb{N}}$ converges to $e_{max}(n)$. Since $n \in (0,1)$ we have that $\epsilon_F(n) \in (-d/2\pi, d/2\pi)$ (the cases where $\epsilon_F(n) \in \{-d/2\pi, d/2\pi\}$ is given when $n \in \{0,1\}$ respectively). Therefore there exists a $\gamma_0 > 0$ such that

$$B_{\gamma_0}(-\epsilon_F(n)) \subset (-d/2\pi, d/2\pi) \qquad \text{and} \qquad B_{\gamma_0}(\epsilon_F(n)) \subset (-d/2\pi, d/2\pi).$$

From Remark 2.3.21 we deduce that

$$\text{meas}\left(\left\{p\in\mathbb{T}^d : \varepsilon(p) \in B_{\gamma_0}(-\epsilon_F(n))\right\}\right) \xrightarrow{\gamma\to 0} 0.$$

Hence for $\delta > 0$ exists a $\gamma_1 \in (0,\gamma_0]$ (that depends on δ) such that

$$B_{\gamma_1}(-\epsilon_F(n)) \subset (-d/2\pi, d/2\pi) \qquad \text{and} \qquad \text{meas}\left(\left\{p\in\mathbb{T}^d : \varepsilon(p) \in B_{\gamma_1}(-\epsilon_F(n))\right\}\right) < \frac{\delta}{4}.$$

Since $|-\epsilon_F(n) \pm \gamma_1| < d/2\pi$, we also obtain for our choice of γ_1 that

$$\begin{aligned}\text{meas}\left(\left\{p\in\mathbb{T}^d : \varepsilon(p) > (-\epsilon_F(n)+\gamma_1)\right\}\right) > 0,\\ \text{meas}\left(\left\{p\in\mathbb{T}^d : \varepsilon(p) < (-\epsilon_F(n)-\gamma_1)\right\}\right) > 0.\end{aligned}$$

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We define the sets

$$D_+ \coloneqq \left\{p \in \mathbb{T}^d : \varepsilon(p) > (-\epsilon_F(n) + \gamma_1)\right\},$$
$$D_- \coloneqq \left\{p \in \mathbb{T}^d : \varepsilon(p) < (-\epsilon_F(n) - \gamma_1)\right\},$$
$$D_0 \coloneqq \left\{p \in \mathbb{T}^d : \varepsilon(p) \in B_{\gamma_1}(-\epsilon_F(n))\right\}.$$

Obviously we have $\overline{D_+ \cup D_- \cup D_0} = \mathbb{T}^d$. Since we are in the case $E_k \to e_{max}(n)$, there exists an index $\tilde{k} \in \mathbb{N}$, such that $E_k > 0$ for all $k > \tilde{k}$. This implies that $\tilde{\lambda}_{1,k} > 0$ for all $k > \tilde{k}$ (see Remark 2.3.25). Furthermore, thanks to (2.72), there exists a $k_0 \in \mathbb{N}$, with $k_0 > \tilde{k}$ such that

$$\forall k > k_0 : \qquad \tilde{\lambda}_{1,k}^{-1}\phi_k \in B_\gamma(\epsilon_F(n)) \text{ and } \tilde{\lambda}_{1,k} > 0.$$

We observe that

$$\forall k > k_0, \forall p \in D_+ : \qquad \tilde{\lambda}_{1,k}^{-1}\phi_k + \varepsilon(p) > \epsilon_F(n) - \gamma + \varepsilon(p) > 0,$$
$$\forall k > k_0, \forall p \in D_- : \qquad \tilde{\lambda}_{1,k}^{-1}\phi_k + \varepsilon(p) < \epsilon_F(n) + \gamma + \varepsilon(p) < 0.$$

This and $\tilde{\lambda}_{1,k} > 0$ for all $k > k_0$ imply

$$\forall k > k_0, \forall p \in D_+ : \qquad -\tilde{\lambda}_{1,k}\left(\tilde{\lambda}_{1,k}^{-1}\phi_k + \varepsilon(p)\right) < 0,$$
$$\forall k > k_0, \forall p \in D_- : \qquad -\tilde{\lambda}_{1,k}\left(\tilde{\lambda}_{1,k}^{-1}\phi_k + \varepsilon(p)\right) > 0,$$

and hence with Lemma 2.3.26 ($\tilde{\lambda}_{1,k} \to \infty$)

$$\forall p \in D_+ : \lim_{k\to\infty} \mathcal{F}(\phi_k, \tilde{\lambda}_{1,k}; p) = \lim_{k\to\infty} \frac{1}{1 + \exp\left(-\tilde{\lambda}_{1,k}\left(\tilde{\lambda}_{1,k}^{-1}\phi_k + \varepsilon(p)\right)\right)} = 1,$$
$$\forall p \in D_- : \lim_{k\to\infty} \mathcal{F}(\phi_k, \tilde{\lambda}_{1,k}; p) = \lim_{k\to\infty} \frac{1}{1 + \exp\left(-\tilde{\lambda}_{1,k}\left(\tilde{\lambda}_{1,k}^{-1}\phi_k + \varepsilon(p)\right)\right)} = 0.$$

With the above we find $k_1 \geq k_0$ such that

$$\forall k > k_1,\ \forall p \in D_+ : \quad \left|1 - \mathcal{F}(\phi_k, \tilde{\lambda}_{1,k}; p)\right| \leq \frac{\delta}{4},$$
$$\forall k > k_1,\ \forall p \in D_- : \quad \left|\mathcal{F}(\phi_k, \tilde{\lambda}_{1,k}; p)\right| \leq \frac{\delta}{4}.$$

Since $\mathbb{1}_{\{-\varepsilon(p)<\epsilon_F(n)\}}(p) = \mathbb{1}_{\{\varepsilon(p)>-\epsilon_F(n)\}}(p)$ (see Remark 2.3.21), we have for all $k \geq k_1$ that

$$\begin{aligned}
\left\|\mathbb{1}_{\{\varepsilon(p)>-\epsilon_F(n)\}} - \mathcal{F}(\phi_k, \tilde{\lambda}_{1,k}; .)\right\|_{L^1(\mathbb{T}^d)} &= \int_{\mathbb{T}^d}\left|\mathbb{1}_{\{\varepsilon(p)>-\epsilon_F(n)\}}(p) - \mathcal{F}(\phi_k, \tilde{\lambda}_{1,k}; p)\right|dp \\
&= \int_{D_+}\left|1 - \mathcal{F}(\phi_k, \tilde{\lambda}_{1,k}; p)\right|dp \\
&\quad + \int_{D_0}\left|\mathbb{1}_{\{\varepsilon(p)>-\epsilon_F(n)\}}(p) - \mathcal{F}(\phi_k, \tilde{\lambda}_{1,k}; p)\right|dp \\
&\quad + \int_{D_-}\left|\mathcal{F}(\phi_k, \tilde{\lambda}_{1,k}; p)\right|dp
\end{aligned}$$

For the integral over D_0, we chose γ_1 such that meas $(D_0) < \delta/4$, and estimate the integrator with just one, and obtain for all $k \geq k_1$

$$\left\|\mathbb{1}_{\{\varepsilon(p)>-\epsilon_F(n)\}} - \mathcal{F}(\phi_k, \tilde{\lambda}_{1,k}; .)\right\|_{L^1(\mathbb{T}^d)} \leq \frac{\delta}{4} + \frac{\delta}{4} + \frac{\delta}{4} < \delta.$$

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Since $\delta > 0$ was chosen arbitrary we conclude that for $(E_k)_{k\in\mathbb{N}}$ converging to $e_{max}(n)$ we have that

$$\lim_{k\to\infty} \mathcal{F}(n_k, E_k; .) = \lim_{k\to\infty} \mathcal{F}(\tilde{\lambda}_0(n_k, E_k), \tilde{\lambda}_1(n_k, E_k); .) = \lim_{k\to\infty} \mathcal{F}(\phi_k, \tilde{\lambda}_{1,k}; .) = \mathbb{1}_{\{-\varepsilon(p)<\epsilon_F(n)\}}$$

in $\mathrm{L}^1(\mathbb{T}^d)$. For $\lim_{k\to\infty} E_k = -e_{max}(n)$ we obtain with the same calculations, except we have to change the signs of $\epsilon_F(n)$, that

$$\lim_{k\to\infty} \left\| \mathbb{1}_{\{\varepsilon(p)<\epsilon_F(n)\}} - \mathcal{F}(n_k, E_k; .) \right\|_{\mathrm{L}^1(\mathbb{T}^d)} = 0.$$

□

With Theorem 2.3.27 we can finally prove the convergence result we will use in the end. Recall therefore the definition of the extension $\bar{\mathcal{F}}$ of the Fermi Dirac distribution

$$\bar{\mathcal{F}}(n, E; p) = \begin{cases} n & \text{if } n \in \{0, 1\}, \\ \mathcal{F}(n, E; p) & \text{if } (n, E) \in \mathfrak{D}^\circ, \\ \mathbb{1}_{\{\mp\varepsilon(p)<\epsilon_F(n)\}}(p) & \text{if } E = \pm e_{max}(n). \end{cases}$$

Corollary 2.3.28. *Let $(n_k)_{k\in\mathbb{N}}$ and $(E_k)_{k\in\mathbb{N}}$ be converging sequences in $\mathrm{L}^2_{loc}(\mathbb{R}_0^+; \mathrm{L}^2(\mathbb{T}^d))$ with limit functions $n, E \in \mathrm{L}^2_{loc}(\mathbb{R}_0^+; \mathrm{L}^2(\mathbb{T}^d))$, such that*

$$\forall (t, x) \in \mathbb{R}_0^+ \times \mathbb{T}^d, \forall k \in \mathbb{N} : \qquad (n_k(t, x), E_k(t, x)) \in \mathfrak{D}^\circ.$$

Then there exist subsequences $(n_{k_j})_{j\in\mathbb{N}}$ and $(E_{k_j})_{j\in\mathbb{N}}$ such that for all compact intervals $I \subset \mathbb{R}_0^+$ and all $q \in [1, \infty)$

$$\lim_{j\to\infty} \left\| \mathcal{F}(n_{k_j}, E_{k_j}; .) - \bar{\mathcal{F}}(n, E; .) \right\|_{\mathrm{L}^q(I; \mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d))} = 0.$$

Proof. Let I be a compact interval in $\mathbb{R}_0^+$, then the sequences $(n_k)_{k\in\mathbb{N}}$ and $(E_k)_{k\in\mathbb{N}}$ converge to n and E in $\mathrm{L}^2(I; \mathrm{L}^2(\mathbb{T}^d))$ and there exists subsequences $(n_{k_j})_{j\in\mathbb{N}}$ and $(E_{k_j})_{j\in\mathbb{N}}$ that converge point wise a.e. on $I \times \mathbb{T}^d$ (see for example Brezis [Bre11], Theorem 4.9.). With Theorem 2.3.27 we obtain for almost all $(t, x) \in I \times \mathbb{T}^d$:

$$\lim_{j\to\infty} \left\| \mathcal{F}(n_{k_j}(t, x), E_{k_j}(t, x); .) - \bar{\mathcal{F}}(n(t, x), E(t, x); .) \right\|_{\mathrm{L}^1(\mathbb{T}^d)} = 0.$$

Since we have $\mathrm{L}^1(\mathbb{T}^d)$ convergence, there exists subsequences (using again the same indexing) $(n_{k_j})_{j\in\mathbb{N}}$ and $(E_{k_j})_{j\in\mathbb{N}}$ such that

$$\lim_{j\to\infty} \mathcal{F}(n_{k_j}(t, x), E_{k_j}(t, x); p) = \bar{\mathcal{F}}(n(t, x), E(t, x); p), \qquad \text{a.e. } on\ I \times \mathbb{T}^d \times \mathbb{T}^d.$$

Now since $\mathcal{F}(n_{k_j}, E_{k_j}; p) \leq 1$ for all $j \in \mathbb{N}$ and obviously $1 \in \mathrm{L}^q(I; \mathrm{L}^q(\mathbb{T}^d \times \mathbb{T}^d))$ for all $q \in [1, \infty)$, we can apply the dominated convergence theorem and get

$$\lim_{j\to\infty} \left\| \mathcal{F}(n_{k_j}, E_{k_j}; .) - \bar{\mathcal{F}}(n, E; .) \right\|_{\mathrm{L}^q(I; \mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d))} = 0.$$

With the similar diagonal argument as in the proof of Theorem 2.3.27 we find subsequences of $(n_{k_j})_{j\in\mathbb{N}}$ and $(E_{k_j})_{j\in\mathbb{N}}$ (using again the same indexing) such that these subsequences fulfill for all compact intervals I in $\mathbb{R}_0^+$ the desired convergence. □

Since $\mathcal{F}$ coincides with $\bar{\mathcal{F}}$ on $\mathfrak{D}^\circ$, (2.35) is clearly fulfilled.

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2.3.5. The Rigorous Limit

In this section we give the proof of Main Theorem 2.3.5 and show, under the assumptions of Hypothesis 2.2.14, the existence of a weak solution in the sense of Definition 2.3.4. The idea is to follow the Chapman-Enskog expansion, presented in Section 2.3.1, and check in what sense the limits exist.

Proof of Main Theorem 2.3.5. The existence of converging subsequences of the families $(n_\tau)_{\tau>0}$ and $(E_\tau)_{\tau>0}$ is deduced directly from Theorem 2.3.19. Let us denote this converging subsequences and their limits with

$$n_{\tau_k} \xrightarrow{k\to\infty} n, \quad E_{\tau_k} \xrightarrow{k\to\infty} E, \qquad \text{in } \mathrm{L}^2_{loc}(\mathbb{R}_0^+;\mathrm{L}^2(\mathbb{T}^d)),$$

where τ_k converges to 0. We now go through the steps of the Chapman-Enskog expansion

Step 1: We make the ansatz

$$f_\tau = \mathcal{F}(n_\tau, E_\tau; p) - \tau \mathcal{Q}_\tau(f_\tau). \tag{2.73}$$

It is clear from the definition of the collision operators (see Definition 2.22) that this expression is well defined for all $\tau > 0$. Recall that the family $(\mathcal{Q}_\tau(f_\tau))_{\tau>0}$ is, thanks to Corollary 2.2.21, bounded in $\mathrm{L}^2(\mathbb{R}_0^+;\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))$, with the estimate (2.30)

$$\|\mathcal{Q}_\tau(f_\tau)\|^2_{\mathrm{L}^2(\mathbb{R}_0^+;\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))} \le \mathcal{H}(f_0) - \log(1/2).$$

This boundedness provides

$$\lim_{\tau\to 0} \tau \mathcal{Q}_\tau(f_\tau) = 0, \qquad \text{in } \mathrm{L}^2(\mathbb{R}_0^+;\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)).$$

From Corollary 2.3.28 we know that there exists subsequences of $(n_{\tau_k})_{k\in\mathbb{N}}$ and $(E_{\tau_k})_{k\in\mathbb{N}}$ (using again the same indices) such that for all compact intervals $I\subset\mathbb{R}_0^+$ and $q\in[1,\infty)$

$$\lim_{k\to\infty} \left\|\mathcal{F}(n_{\tau_k}, E_{\tau_k}; .) - \bar{\mathcal{F}}(n,E;.)\right\|_{\mathrm{L}^q(I;\mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d))} = 0.$$

For the subsequence $(f_{\tau_k})_{k\in\mathbb{N}}$ of the family of solutions $(f_\tau)_{\tau>0}$ we have for every compact interval $I\subset\mathbb{R}_0^+$ and $q\in[1,\infty)$ that

$$\begin{aligned}\left\|f_{\tau_k} - \bar{\mathcal{F}}(n,E;.)\right\|_{\mathrm{L}^q(I;\mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d))} &\le \\ \le \left\|\mathcal{F}(n_{\tau_k}, E_{\tau_k}; .) - \bar{\mathcal{F}}(n,E;.)\right\|_{\mathrm{L}^q(I;\mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d))} &+ \tau_k \left\|\mathcal{Q}_{\tau_k}(f_{\tau_k})\right\|_{\mathrm{L}^q(I;\mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d))},\end{aligned}$$

and therefore we obtain especially for $q=2$, that

$$\lim_{k\to\infty} f_{\tau_k} = \bar{\mathcal{F}}(n,E;.) \qquad \text{in } \mathrm{L}^2_{loc}(\mathbb{R}_0^+;\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)).$$

Step 2: Following the second step of the Chapman-Enskog Expansion we want to find out if and in which way the family of collision operators $(\mathcal{Q}_\tau(f_\tau))_{\tau>0}$ converges for τ going to zero. Recall the model equation

$$(2.23): \qquad \tau\partial_t f_\tau + \nabla_p\varepsilon\cdot\nabla_x f_\tau = \mathcal{Q}_\tau(f_\tau), \qquad f_\tau(0,x,p) = f_0(x,p).$$

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Thanks to Remark 2.2.17, we know that $\mathcal{F}(n_\tau, E_\tau; .)$ and $\mathcal{Q}_\tau(f_\tau)$ are both in $C^1(\mathbb{R}^+ \times \mathbb{T}^d \times \mathbb{T}^d)$ for all $\tau > 0$, and hence we are able to substitute our ansatz (2.73) into the DSSBE (2.23) and obtain (using the short notation $\mathcal{F}_\tau \hat{=} \mathcal{F}(n_\tau, E_\tau; p)$ and $\mathcal{Q}_\tau \hat{=} \mathcal{Q}_\tau(f_\tau)$)

$$\tau \partial_t \mathcal{F}_\tau - \tau^2 \partial_t \mathcal{Q}_\tau + \nabla_p \varepsilon \cdot \nabla_x \mathcal{F}_\tau - \tau \nabla_p \varepsilon \cdot \nabla_x \mathcal{Q}_\tau = \mathcal{Q}_\tau. \tag{2.74}$$

As mentioned above, the subsequence $(\mathcal{F}_{\tau_k})_{k\in\mathbb{N}}$ converges in $\mathrm{L}^2_{loc}(\mathbb{R}^+_0; \mathrm{L}^2(\mathbb{T}^d \times \mathbb{T}^d))$ towards $\bar{\mathcal{F}}(n, E; p)$. Since the family $(\mathcal{Q}_\tau(f_\tau))_{\tau>0}$ is bounded in $\mathrm{L}^2(\mathbb{R}^+_0; \mathrm{L}^2(\mathbb{T}^d \times \mathbb{T}^d))$ we have with the Theorem of Eberlein-Šmuljan (see [Zei90a] Theorem 21.D) at least that there exists a weak converging subsequence (using the same indices) $(\mathcal{Q}_{\tau_k}(f_{\tau_k}))_{k\in\mathbb{N}}$ and a function $\mathcal{Q}^{(0)}$ in $\mathrm{L}^2(\mathbb{R}^+_0; \mathrm{L}^2(\mathbb{T}^d \times \mathbb{T}^d))$, such that

$$\mathcal{Q}_{\tau_k}(f_{\tau_k}) \xrightharpoonup{k\to\infty} \mathcal{Q}^{(0)} \qquad \text{in } \mathrm{L}^2(\mathbb{R}^+_0; \mathrm{L}^2(\mathbb{T}^d \times \mathbb{T}^d)). \tag{2.75}$$

Multiply equation (2.74) with a a test function $\varphi \in C_c^\infty(\mathbb{R}^+_0 \times \mathbb{T}^d \times \mathbb{T}^d)$ and integrate it with respect to all variables we get

$$\int_0^\infty \int_{\mathbb{T}^d\times\mathbb{T}^d} \tau \partial_t \mathcal{F}_\tau \varphi - \tau^2 \partial_t \mathcal{Q}_\tau \varphi + \nabla_p \varepsilon \cdot \nabla_x \mathcal{F}_\tau \varphi - \tau \nabla_p \varepsilon \cdot \nabla_x \mathcal{Q}_\tau \varphi = \int_0^\infty \int_{\mathbb{T}^d\times\mathbb{T}^d} \mathcal{Q}_\tau \varphi. \tag{2.76}$$

For the left hand side, denoting with $\operatorname{supp}\varphi$ the support of φ, it follows from the Cauchy-Schwarz inequality and partial integration that

$$\begin{aligned} \tau |(\partial_t \mathcal{F}_\tau, \varphi)_{\mathrm{L}^2}| &\le \tau \operatorname{meas}(\operatorname{supp}\varphi) \|\partial_t \varphi\|_{\mathrm{L}^2(\mathbb{R}^+\times\mathbb{T}^d\times\mathbb{T}^d)}, \\ \tau^2 |(\partial_t \mathcal{Q}_\tau, \varphi)_{\mathrm{L}^2}| &\le \tau^2 (\mathcal{H}(f_0) - \log(1/2)) \|\partial_t \varphi\|_{\mathrm{L}^2(\mathbb{R}^+\times\mathbb{T}^d\times\mathbb{T}^d)}, \\ \tau |(\nabla_p \varepsilon \cdot \nabla_x \mathcal{Q}_\tau, \varphi)_{\mathrm{L}^2}| &\le \tau \|\nabla_p \varepsilon\|_{\mathrm{L}^\infty(\mathbb{T}^d)} (\mathcal{H}(f_0) - \log(1/2)) \|\nabla_x \varphi\|_{\mathrm{L}^2(\mathbb{R}^+\times\mathbb{T}^d\times\mathbb{T}^d)}. \end{aligned}$$

Therefore all the above terms vanish if we pass to the limit τ to zero. For the last term, that is not multiplied by τ, we have with partial integration.

$$\begin{aligned} \int_0^\infty \int_{\mathbb{T}^d\times\mathbb{T}^d} (\nabla_p \varepsilon \cdot \nabla_x \mathcal{F}_\tau)\varphi &= \int_0^\infty \int_{\mathbb{T}^d\times\mathbb{T}^d} \operatorname{div}_x ((\nabla_p \varepsilon)\mathcal{F}_\tau)\varphi \\ &= -\int_0^\infty \int_{\mathbb{T}^d\times\mathbb{T}^d} ((\nabla_p \varepsilon)\mathcal{F}_\tau) \cdot \nabla_x \varphi. \end{aligned}$$

All results above, starting from (2.76), hold for all $\tau > 0$ and therefore in particular for the subsequence $(\tau_k)_{k\in\mathbb{N}}$. Since the sequence $(\mathcal{F}_{\tau_k})_{k\in\mathbb{N}}$ converges in $\mathrm{L}^2_{loc}(\mathbb{R}^+_0)$ towards $\bar{\mathcal{F}}(n, E; p)$ and since (2.75) holds, passing to the limit $\tau_k \to 0$ in (2.76) then provides for all $\varphi \in C_c^\infty(\mathbb{R}^+_0 \times \mathbb{T}^d \times \mathbb{T}^d)$

$$\begin{aligned} &\int_0^\infty \int_{\mathbb{T}^d\times\mathbb{T}^d} \mathcal{Q}^{(0)}(t,x,p)\varphi(t,x,p) = \\ &\qquad = -\int_0^\infty \int_{\mathbb{T}^d\times\mathbb{T}^d} ((\nabla_p \varepsilon(p))\bar{\mathcal{F}}(n(t,x), E(t,x); p)) \cdot \nabla_x \varphi(t,x,p) \end{aligned}$$

Hence we get two outputs from the above

a) Since the above equality holds for all $\varphi \in C_c^\infty(\mathbb{R}^+_0 \times \mathbb{T}^d \times \mathbb{T}^d)$ we have that

$$(\nabla_p \varepsilon)\bar{\mathcal{F}} \in \mathrm{L}^2_{loc}(\mathbb{R}^+_0; \mathrm{H}_{\operatorname{div}_x}(\mathbb{T}^d \times \mathbb{T}^d)),$$

where we defined $\mathrm{H}_{\operatorname{div}_x}(\mathbb{T}^d \times \mathbb{T}^d)$ as the space of weak divergences with respect to the spatial variable x (see (2.36)).

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b) Additionally we have for the sequence $(\mathcal{Q}_{\tau_k})_{k\in\mathbb{N}}$ the weak convergence

$$\mathcal{Q}_{\tau_k}(f_{\tau_k}) \xrightarrow{k\to\infty} \operatorname{div}_x\left(\bar{\mathcal{F}}(n,E;.)\nabla_p\varepsilon\right) \qquad \text{in } \mathrm{L}^2(\mathbb{R}_0^+;\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)).$$

Step 3: Last step is now to derive the drift diffusion equations for the functions n and E in the sense of Definition 2.3.4. and to achieve this, we follow the third step of the Chapman Enskog expansion. For the first equation we divide (2.74) through τ and integrate it with respect to the momentum p, which gives us

$$\partial_t n_\tau - \tau\int_{\mathbb{T}^d}\partial_t\mathcal{Q}_\tau dp + \frac{1}{\tau}\int_{\mathbb{T}^d}\nabla_p\varepsilon\cdot\nabla_x\mathcal{F}_\tau dp - \int_{\mathbb{T}^d}\nabla_p\varepsilon\cdot\nabla_x\mathcal{Q}_\tau dp = \int_{\mathbb{T}^d}\mathcal{Q}_\tau dp. \quad (2.77)$$

The integral on the right hand side vanishes, due to the definition of the collision operator

$$\int_{\mathbb{T}^d}\mathcal{Q}_\tau dp = \frac{1}{\tau}\int_{\mathbb{T}^d} f_\tau - \mathcal{F}(n_\tau,E_\tau;p)dp = n - n = 0$$

In the first integral of (2.77) we can exchange integration and the derivative, and see that the integral vanishes for all $\tau > 0$ due to the same reason as above. Also the second integral in (2.77) vanishes, since $\nabla_p\varepsilon\cdot\nabla_x\mathcal{F}_\tau$ is an odd function in p in the sense of Definition 2.1.3 (see Remark 2.3.18). Therefore from (2.77) remains

$$\partial_t n_\tau(t,x) - \int_{\mathbb{T}^d}\nabla_p\varepsilon(p)\cdot\nabla_x\mathcal{Q}_\tau(t,x,p)dp = 0. \quad (2.78)$$

We multiply equation (2.78) with a test function $\varphi\in C_c^\infty(\mathbb{R}_0^+\times\mathbb{T}^d)$, integrate it respect to the time- and space variables, and obtain with partial integration

$$\int_0^\infty\int_{\mathbb{T}^d} n_\tau\partial_t\varphi dxdt - \int_0^\infty\int_{\mathbb{T}^d\times\mathbb{T}^d}\mathcal{Q}_\tau(\nabla_p\varepsilon\cdot\nabla_x\varphi)dxdpdt = 0.$$

Now we know that there exists subsequences $(n_{\tau_k})_{k\in\mathbb{N}}$ and $(\mathcal{Q}_{\tau_k})_{k\in\mathbb{N}}$ such that $(n_{\tau_k})_{k\in\mathbb{N}}$ converges in $\mathrm{L}^2_{loc}(\mathbb{R}_0^+;\mathrm{L}^2(\mathbb{T}^d))$ and $(\mathcal{Q}_{\tau_k})_{k\in\mathbb{N}}$ converges weakly in $\mathrm{L}^2(\mathbb{R}_0^+;\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))$. The function $\nabla_p\varepsilon\cdot\nabla_x\varphi$ lies obviously in $C_c^\infty(\mathbb{R}_0^+\times\mathbb{T}^d\times\mathbb{T}^d)$ for all $\varphi\in C_c^\infty(\mathbb{R}_0^+\times\mathbb{T}^d)$, hence we obtain that for all $\varphi\in C_c^\infty(\mathbb{R}_0^+\times\mathbb{T}^d)$

$$\begin{aligned}\lim_{k\to\infty}\int_0^\infty\int_{\mathbb{T}^d} n_{\tau_k}\partial_t\varphi dxdt - &\int_0^\infty\int_{\mathbb{T}^d\times\mathbb{T}^d}\mathcal{Q}_{\tau_k}(\nabla_p\varepsilon\cdot\nabla_x\varphi)dtdxdp \\ &= \int_0^\infty\int_{\mathbb{T}^d} n\partial_t\varphi dtdx - \int_0^\infty\int_{\mathbb{T}^d\times\mathbb{T}^d}\mathcal{Q}^{(0)}(\nabla_p\varepsilon\cdot\nabla_x\varphi)dxdpdt.\end{aligned}$$

It was shown that $\mathcal{Q}^{(0)}$ is the weak divergence with respect to the spatial variable of $(\nabla_p\varepsilon)\bar{\mathcal{F}}$ and in Corollary 2.3.20 we have proven that n has also a weak derivative $\partial_t n$ in $\mathrm{L}^2(\mathbb{R}_0^+;\mathrm{H}^{-1}(\mathbb{T}^d))$, hence we obtain for all $\varphi\in C_c^\infty(\mathbb{R}_0^+\times\mathbb{T}^d)$ that

$$\int_0^\infty\langle\partial_t n,\varphi\rangle_{\mathrm{H}^{-1}(\mathbb{T}^d)}dt - \int_0^\infty\int_{\mathbb{T}^d\times\mathbb{T}^d}\operatorname{div}_x(\nabla_p\varepsilon(p)\bar{\mathcal{F}}(n,E;p))(\nabla_p\varepsilon(p)\cdot\nabla_x\varphi)dxdpdt = 0 \quad (2.79)$$

The second equation of our macroscopic model, is achieved in a similar way. Going back to equation (2.74), we multiply it with $\varepsilon(p)$, divide it through τ and integrate it with respect to the momentum p. With Remark 2.3.18, the fact that the integral of $\varepsilon\mathcal{Q}_\tau$ with respect to the momentum vanishes for all $\tau > 0$, we get for all $\tau > 0$ that

$$\partial_t E_\tau(t,x) - \int_{\mathbb{T}^d}\varepsilon(p)\nabla_p\varepsilon(p)\cdot\nabla_x\mathcal{Q}_\tau(t,x,p)dp = 0.$$

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We have that the subsequence $(E_{\tau_k})_{k\in\mathbb{N}}$ converges in $\mathrm{L}^2_{loc}(\mathbb{R}_0^+;\mathrm{L}^2(\mathbb{T}^d))$ towards E and the subsequence $(\mathcal{Q}_{\tau_k})_{k\in\mathbb{N}}$ converges as mentioned weakly towards $\mathrm{div}_x(\nabla_p\varepsilon\bar{\mathcal{F}}(n,E;.))$. The function E has, thanks to Corollary 2.3.20 a weak derivative $\partial_t E$ that lies in $\mathrm{L}^2(\mathbb{R}_0^+;\mathrm{H}^{-1}(\mathbb{T}^d))$. The function $\varepsilon(\nabla_p\varepsilon\cdot\nabla_x\varphi)$ is an element of $C_c^\infty(\mathbb{R}_0^+\times\mathbb{T}^d\times\mathbb{T}^d)$ for all $\varphi\in C_c^\infty(\mathbb{R}_0^+\times\mathbb{T}^d)$ and passing to the limit for k to infinity we obtain for all φ in $C_c^\infty(\mathbb{R}_0^+\times\mathbb{T}^d)$

$$\int_0^\infty \langle\partial_t E,\varphi\rangle_{\mathrm{H}^{-1}(\mathbb{T}^d)}\,dt = \int_0^\infty\int_{\mathbb{T}^d\times\mathbb{T}^d}\varepsilon(p)\,\mathrm{div}_x(\nabla_p\varepsilon(p)\bar{\mathcal{F}}(n,E;p))(\nabla_p\varepsilon(p)\cdot\nabla_x\varphi)dxdpdt \tag{2.80}$$

With the standard density argument (see for example [Eva10]), we obtain that functions n and E solve equations (2.79) - (2.80) for all φ in $\mathrm{H}_0^1(\mathbb{R}_0^+\times\mathbb{T}^d)$ and are therefore weak solutions in the sense of Definition 2.3.4.

□

2.4. Long Time Behaviour

The second main result revolves around the weak solutions n,E and the limit function $\bar{\mathcal{F}}(n,E;p)$ and their behaviour for time going to infinity. Now from physics we expect that the limit function converges towards the equilibrium $\mathcal{F}_{eq}$ (see Definition 2.2.18) and that the macroscopic limit densities will distribute equally, i.e. converge towards the mean values $\bar{n}$ and $\bar{E}$ respectively. We are able to show this converges with even exponential decay. The most important quantities to recall are the definitions of the mean densities and the equilibrium (see Subsection 2.2), which are given by

$$\bar{n}=\int_{\mathbb{T}^d}\int_{\mathbb{T}^d}f_0(x,p)dpdx,\quad \bar{E}=\int_{\mathbb{T}^d}\int_{\mathbb{T}^d}\varepsilon(p)f_0(x,p)dpdx,\quad \mathcal{F}_{eq}(p)=\mathcal{F}(\bar{n},\bar{E};p),$$

where f_0 is the initial value of the system (in our case given via Hypothesis 2.2.14).

Main Theorem 2.4.1 (Long Time Behavior)**.** *As in Main Theorem 2.3.5 let $(f_\tau)_{\tau>0}$ be the family of solutions to the model equation* (2.23)*, and let n and E be the weak solutions in the sense of Definition 2.3.4, then there exists constants $C,K>0$ such that*

$$\left\|\bar{\mathcal{F}}(n(t,.),E(t,.);.)-\mathcal{F}_{eq}\right\|^2_{\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)}\le Ke^{-Ct}.$$

With the same constants as above we also have exponential decay for the solutions n and E towards their means,

$$\|n(t,.)-\bar{n}\|^2_{\mathrm{L}^2(\mathbb{T}^d)}\le Ke^{-Ct},\quad \left\|E(t,.)-\bar{E}\right\|^2_{\mathrm{L}^2(\mathbb{T}^d)}\le\varepsilon_\infty Ke^{-Ct},\qquad \text{for a.e. } t\in\mathbb{R}_0^+, \tag{2.81}$$

where $\varepsilon_\infty=\|\varepsilon\|_{\mathrm{L}^\infty(\mathbb{T}^d)}$.

We postpone the proof of Main Theorem 2.4.1 to Subsection 2.4.2, since we need some preparation. The main tools for the proof are the so called "*relative Entropy*" and the H-Theorem (Theorem 2.2.20). We split this section into two subsections, where the first one introduces the relative entropy and its properties. There we obtain lower and upper estimates and we will see that the relative entropy differs only by a constant to the entropy functional $\mathcal{H}$ (see (2.17)). To finally get the exponential decay, we use estimates obtained from the previous Section 2.3, show some kind of Lipschitz continuity of $\bar{\mathcal{F}}$ and use then a Gronwall argument. For details we refer to Subsection 2.4.2.

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2.4.1. The Relative Entropy

The relative entropy describes the measure of the distance from a given state to the equilibrium. Using the relative entropy to estimate the decay of a solution towards the equilibrium is a quite common idea, like in [CJM+01, JÏ6]. New is the combination of the relative entropy and the estimates obtained for $(n_\tau)_{\tau>0}$ and $(E_\tau)_\tau$ in $\mathrm{L}^2(I;\mathrm{H}^s(\mathbb{T}^d))$ from Subsection 2.3.2 to achieve the desired decay.

Definition 2.4.2. *Define the function*

$$S^\infty : [0,1]\times(0,1)\to\mathbb{R}, \qquad S^\infty(r|s) = \begin{cases} -\log(1-s) & r=0,\\ r\log\left(\frac{r}{s}\right)+(1-r)\log\left(\frac{1-r}{1-s}\right) & r\in(0,1),\\ -\log(s) & r=1, \end{cases}$$

then we call for $f\in\mathrm{L}^2(\mathbb{R}_0^+;\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d))$, with $0\le f\le 1$, the function

$$\mathcal{H}^f_{\mathcal{F}_{eq}}(t) := \int_{\mathbb{T}^d}\int_{\mathbb{T}^d} S^\infty(f(t)|\mathcal{F}_{eq})dpdx$$

the relative entropy of the system.

Remark 2.4.3. We point out that since $(\bar{n},\bar{E})\in\mathfrak{D}^\circ$ we have that $\mathcal{F}_{eq}$ only takes values in $(0,1)$ for all $p\in\mathbb{T}^d$ and hence the relative entropy is well defined. Moreover we can show that there exists a constant $a\in(0,(1/2)]$ such that $\mathcal{F}_{eq}(\bar{n},\bar{E};p)\in[a,1-a]$ for all $p\in\mathbb{T}^d$. First notice that $(\bar{n},\bar{E})$ is fixed and hence are the values $\lambda_0(\bar{n},\bar{E})$ $(\widehat{=}\lambda_0)$ and $\lambda_1(\bar{n},\bar{E})$ $(\widehat{=}\lambda_1)$ which are both in $\mathbb{R}$. If $\lambda_0=0=\lambda_1$ then we have that $\mathcal{F}_{eq}=1/2$ and therefore $a=1/2$. Without loss of generality assume $\lambda_1>0$ and $\lambda_0\in\mathbb{R}$ (the case where $\lambda_1<0$ goes similarly). Then we have for all $p\in\mathbb{T}^d$:

$$\begin{aligned} -\frac{d}{2\pi} \le \varepsilon(p) &\le \frac{d}{2\pi},\\ \lambda_1\frac{d}{2\pi} \ge -\lambda_1\varepsilon(p) &\ge -\lambda_1\frac{d}{2\pi},\\ -\left(\lambda_0-\lambda_1\frac{d}{2\pi}\right) \ge -(\lambda_0+\lambda_1\varepsilon(p)) &\ge -\left(\lambda_0+\lambda_1\frac{d}{2\pi}\right),\\ 1+\exp\left(-\left(\lambda_0-\lambda_1\frac{d}{2\pi}\right)\right) \ge 1+\exp(-(\lambda_0+\lambda_1\varepsilon(p))) &\ge 1+\exp\left(-\left(\lambda_0+\lambda_1\frac{d}{2\pi}\right)\right),\\ a_1 := \frac{1}{1+\exp\left(-\left(\lambda_0-\lambda_1\frac{d}{2\pi}\right)\right)} \le \mathcal{F}(\bar{n},\bar{E};p) &\le \frac{1}{1+\exp\left(-\left(\lambda_0+\lambda_1\frac{d}{2\pi}\right)\right)} =: 1-a_2. \end{aligned}$$

Define now $a:=\min\{a_1,a_2\}$. We see immediately that $a\in(0,(1/2)]$ and therefore we have that $a\le\mathcal{F}_{eq}\le 1-a$. ∎

The next Lemma is crucial for the L^2- estimates of the limit functions n, E and $\bar{\mathcal{F}}(n,E;p)$ and it also provides the beginning for the estimate regarding the exponential decay.

Lemma 2.4.4. *For any $a\in(0,(1/2)]$, there exists a constant C_a, such that the function S^∞, defined in Definition 2.4.2, fulfills the estimate*

$$|r-s|^2 \le S^\infty(r|s) \le C_a|r-s|^2 \qquad \forall(r,s)\in[0,1]\times[a,1-a]. \tag{2.82}$$

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Proof. Let us recall the function h from the definition of the entropy functional $\mathcal{H}$ in (2.17),

$$h : (0,1) \to \mathbb{R}, \qquad h(r) = r \log\left(\frac{r}{1-r}\right) + \log(1-r).$$

with the derivatives

$$h'(r) = \log\left(\frac{r}{1-r}\right), \qquad h''(r) = \frac{1}{r(1-r)}.$$

As in Remark 2.2.10 we develop h around $s \in [a, 1-a]$ and obtain

$$h(r) = h(s) + h'(s)(r-s) + \frac{1}{2}h''(\xi_s)(r-s)^2 \qquad \text{for some } \xi_s \in [a, 1-a].$$

With rewriting S^∞ we see that for all $(r,s) \in (0,1) \times [a, 1-a]$

$$\begin{aligned}
S^\infty(r|s) =& r \log\left(\frac{r}{s}\right) + (1-r)\log\left(\frac{1-r}{1-s}\right) \\
=& r\left(\log\left(\frac{r}{1-r}\right) - \log\left(\frac{s}{1-s}\right)\right) + \log(1-r) - \log(1-s) \\
=& h(r) - r\log\left(\frac{s}{1-s}\right) - \left(s\log\left(\frac{s}{1-s}\right) + \log(1-s)\right) + s\log\left(\frac{s}{1-s}\right) \\
=& h(r) - h(s) - h'(s)(r-s) \\
=& \frac{1}{2}h''(\xi_s)(r-s)^2.
\end{aligned}$$

In Remark 2.2.10 we showed that h'' has a minimum at $1/2$ and that $h''(r) \geq 4$ for all $r \in (0,1)$. Hence we obtain the lower estimate for all $(r,s) \in (0,1) \times [a, 1-a]$

$$(r-s)^2 \leq 4(r-s)^2 \leq \frac{1}{2}h''(\xi_s)(r-s)^2 = S^\infty(r|s).$$

Next we go to the upper estimate. Since $a \in (0, (1/2)]$, the interval $[a, 1-a]$ has as middle point $(1/2)$. Additionally we have that $h''(a) = h(1-a)''$ and moreover $h''(a) > h(s)$ for all s in $[a, 1-a]$. Defining $C_a \coloneqq (1/2)h''(a)$, we obtain for all $(r,s) \in (0,1) \times [a, 1-a]$

$$S^\infty(r|s) = \frac{1}{2}h''(\xi_s)(r-s)^2 \leq C_a(r-s)^2.$$

Passing to the limits r to zero or one, we obtain (2.82). □

As already mentioned, we show that the relative entropy and the entropy functional are related, in particular they just differ by a constant independent of time.

Lemma 2.4.5. *Let f_τ be the solution of the model equation* (2.23)*, in the sense of Hypothesis 2.2.14. Then the time derivative of the entropy functional (see* (2.17)*) coincides with the time derivative of the relative entropy, i.e.*

$$\frac{d}{dt}\mathcal{H}^{f_\tau}_{\mathcal{F}_{eq}} = \frac{d}{dt}\mathcal{H}(f_\tau) \qquad \forall \tau > 0. \tag{2.83}$$

Proof. Recall that for all $\tau > 0$ the range of f_τ lies in $(0,1)$ and that f_τ solves (2.23)

$$\tau \partial_t f_\tau + \nabla_p \varepsilon(p) \cdot \nabla_x f_\tau = \mathcal{Q}_\tau(f_\tau), \qquad \forall \tau > 0.$$

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We calculate first the derivative of $\mathcal{H}^{f_\tau}_{\mathcal{F}_{eq}}$. For this we will use the alternative Form of S^∞ on $(0,1)\times(0,1)$, which is given by

$$S^\infty(f_\tau|\mathcal{F}_{eq}) = f_\tau \left(\log\left(\frac{f_\tau}{1-f_\tau}\right) - \log\left(\frac{\mathcal{F}_{eq}}{1-\mathcal{F}_{eq}}\right)\right) + \log(1-f_\tau) - \log(1-\mathcal{F}_{eq}).$$

We remember that the equilibrium is independent of space and time, that $\lambda_0(\bar{n},\bar{E})$ $(\widehat{=}\lambda_0)$ and $\lambda_1(\bar{n},\bar{E})$ $(\widehat{=}\lambda_1)$ are constants in $\mathbb{R}$, and observe that

$$\begin{aligned}-\log\left(\frac{\mathcal{F}_{eq}}{1-\mathcal{F}_{eq}}\right) =& \log\left(\frac{\exp(-(\lambda_0+\lambda_1\varepsilon(p)))}{1+\exp(-(\lambda_0+\lambda_1\varepsilon(p)))}(1+\exp(-(\lambda_0+\lambda_1\varepsilon(p))))\right)\\ =& -(\lambda_0+\lambda_1\varepsilon(p)).\end{aligned}$$

Since we can exchange integration and differentiation we calculate first the time derivative of $S^\infty(f_\tau|\mathcal{F}_{eq})$ and get

$$\begin{aligned}&\frac{d}{dt}\left(f_\tau\left(\log\left(\frac{f_\tau}{1-f_\tau}\right)-(\lambda_0+\lambda_1\varepsilon(p))\right)\right) = (\partial_t f_\tau)\left(\log\left(\frac{f_\tau}{1-f_\tau}\right)-(\lambda_0+\lambda_1\varepsilon(p))\right)+\frac{\partial_t f_\tau}{1-f_\tau},\\ &\frac{d}{dt}\log(1-f_\tau) = -\frac{\partial_t f_\tau}{1-f_\tau}.\end{aligned}$$

This and the fact that f_τ solves equation (2.23), gives us for the derivative of $\mathcal{H}^{f_\tau}_{\mathcal{F}_{eq}}$

$$\begin{aligned}\frac{d}{dt}\mathcal{H}^{f_\tau}_{\mathcal{F}_{eq}} =& \int_{\mathbb{T}^d}\int_{\mathbb{T}^d}\frac{d}{dt}S^\infty(f_\tau|\mathcal{F}_{eq})dxdp\\ =& \int_{\mathbb{T}^d}\int_{\mathbb{T}^d}(\partial_t f_\tau)\left(\log\left(\frac{f_\tau}{1-f_\tau}\right)-(\lambda_0+\lambda_1\varepsilon(p))\right)dxdp\\ =& \int_{\mathbb{T}^d}\int_{\mathbb{T}^d}(\partial_t f_\tau)\log\left(\frac{f_\tau}{1-f_\tau}\right)-(\mathcal{Q}_\tau(f_\tau)-\nabla_p\varepsilon(p)\cdot\nabla_x f_\tau)(\lambda_0+\lambda_1\varepsilon(p))dxdp\end{aligned}$$

Due to the definition of $\mathcal{Q}_\tau(f_\tau)$ we obtain that

$$\int_{\mathbb{T}^d}\int_{\mathbb{T}^d}\mathcal{Q}_\tau(f_\tau)(\lambda_0+\lambda_1\varepsilon(p))dxdp = 0,$$

and since $(\lambda_0+\lambda_1\varepsilon(p))$ is independent of the spatial variable x we get

$$\begin{aligned}\int_{\mathbb{T}^d}\int_{\mathbb{T}^d}(-\nabla_p\varepsilon(p)\cdot\nabla_x f_\tau)(\lambda_0+\lambda_1\varepsilon(p))dxdp =& -\int_{\mathbb{T}^d}\int_{\mathbb{T}^d}\mathrm{div}_x(f_\tau\nabla_p\varepsilon(p))(\lambda_0+\lambda_1\varepsilon(p))dxdp\\ =& \int_{\mathbb{T}^d}\int_{\mathbb{T}^d}f_\tau\nabla_p\varepsilon(p)\cdot\nabla_x(\lambda_0+\lambda_1\varepsilon(p))dxdp\\ =& 0.\end{aligned}$$

Therefore we obtain

$$\frac{d}{dt}\mathcal{H}^{f_\tau}_{\mathcal{F}_{eq}} = \int_{\mathbb{T}^d}\int_{\mathbb{T}^d}(\partial_t f_\tau)\log\left(\frac{f_\tau}{1-f_\tau}\right)dxdp. \tag{2.84}$$

The time derivative of the entropy functional $\mathcal{H}$ is quicker derived. Let us recall the function h from the definition of the entropy functional in (2.17),

$$h:(0,1)\to\mathbb{R}, \qquad h(r) = r\log\left(\frac{r}{1-r}\right)+\log(1-r).$$

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The time derivative of h is given by

$$\frac{d}{dt}h(f_\tau) = (\partial_t f_\tau)h'(f_\tau) = (\partial_t f_\tau)\log\left(\frac{f_\tau}{1-f_\tau}\right),$$

and hence we obtain for the entropy functional

$$\frac{d}{dt}\mathcal{H}(f_\tau) = \frac{d}{dt}\int_{\mathbb{T}^d}\int_{\mathbb{T}^d} h(f_\tau)dxdp = \int_{\mathbb{T}^d}\int_{\mathbb{T}^d}(\partial_t f_\tau)\log\left(\frac{f_\tau}{1-f_\tau}\right)dxdp.$$

Comparing the above with (2.84) shows that the time derivatives of the relative entropy and the entropy functional coincide for the family $(f_\tau)_{\tau>0}$. □

2.4.2. Exponential Decay

For the proof of Main Theorem 2.4.1, we use an interesting form of Gronwall's Theorem as stated in [Bee75], which we cite from [FL16]. To save the reader time looking up the proof, we will also cite it from [FL16].

Lemma 2.4.6. *Let $\psi(t)$ be an integrate-able function over $[0,T]$ for $T \in \mathbb{R}^+$. If there exists a constant $K > 0$ such that*

$$\psi(t_1) + K\int_{t_0}^{t_1}\psi(s)ds \le \psi(t_0), \qquad \textit{for a.e. } 0 \le t_0 \le t_1 \le T, \tag{2.85}$$

then

$$\psi(t_1) \le \psi(t_0)e^{-K(t_1-t_0)}, \qquad \textit{for a.e. } 0 \le t_0 \le t_1 \le T. \tag{2.86}$$

Proof. As mentioned we cite here the proof of [FL16]: First, we perform in (2.85) the change of variables $t = -r$ and $\psi(-r) = \tilde{\psi}(r)$ and obtain

$$\psi(t_1) + K\int_{-t_1}^{r_0}\tilde{\psi}(r)dr \le \tilde{\psi}(r_0), \qquad \text{for a.e. } -T \le -t_1 \le r_0 \le 0. \tag{2.87}$$

Then, we define $\Psi(r) = \int_{-t_1}^{r}\tilde{\psi}(\omega)d\omega$ and calculate with $\dot{\Psi}(r) = \tilde{\psi}(r) \ge \psi(t_1) + K\Psi(r)$ the well defined derivative

$$\begin{aligned}\frac{d}{dr}\left(\Psi(r)e^{-K(r+t_1)}\right) \ge&(\psi(t_1) + K\Psi(r))e^{-K(r+t_1)} - K\Psi(r)e^{-K(r+t_1)}\\ \ge&\psi(t_1)e^{-K(r+t_1)}.\end{aligned}$$

Then integration over $[-t_1, r_0]$ and division by $e^{-K(r_0+t_1)}$ yields

$$\Psi(r_0) \ge \frac{\psi(t_1)}{K}\left(e^{K(r_0+t_1)} - 1\right),$$

and further with (2.87) and $\int_{-t_1}^{r_0}\tilde{\psi}(r) = \Psi(r_0)$

$$\tilde{\psi}(r_0) \ge \psi(t_1)e^{K(r_0+t_1)}.$$

Then returning to the original variables $t_0 = -r_0$ and $\psi(-r_0) = \tilde{\psi}(r_0)$, yields (2.86). □

Before we go to the proof of exponential decay, we need one last property. The distance between the function $\mathcal{F}(n, E; p)$ and the equilibrium is always smaller than the distance between $(n, E) \in \mathfrak{D}$ and the mean values $(\bar{n}, \bar{E})$, times a constant that only depends on the latter.

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Lemma 2.4.7. *Let $(\bar{n}, \bar{E})$ be in $\mathfrak{D}^\circ$ fixed, then there exists a constant $L > 0$ such that*

$$\sup_{p\in\mathbb{T}^d} \left|\bar{\mathcal{F}}(n, E; p) - \mathcal{F}(\bar{n}, \bar{E}; p)\right| \leq \tilde{L}\left(\left|(n, E) - (\bar{n}, \bar{E})\right|\right)$$

for all (n, E) in $\mathfrak{D}$, where $|.|$ denotes the euclidean norm.

Proof. Since $(\bar{n}, \bar{E})$ lies in the open set $\mathfrak{D}^\circ \subset \mathbb{R}^2$, we can find a $\gamma > 0$ such that the closed ball $K_\gamma((\bar{n}, \bar{E}))$ with radius γ lies completely in $\mathfrak{D}^\circ$. Since $\bar{\mathcal{F}}$ coincides with $\mathcal{F}$ on $K_\gamma((\bar{n}, \bar{E}))$, both functions are smooth, as compositions of smooth functions. The derivatives of those functions are bounded on the compact set $K_\gamma((\bar{n}, \bar{E}))$ and hence there exists a Lipschitz constant L_γ on $K_\gamma((\bar{n}, \bar{E}))$ such that

$$\sup_{p\in\mathbb{T}^d} \left|\bar{\mathcal{F}}(n, E; p) - \mathcal{F}(\bar{n}, \bar{E}; p)\right| \leq L_\gamma\left(\left|(n, E) - (\bar{n}, \bar{E})\right|\right), \qquad \forall (n, E) \in K_\gamma((\bar{n}, \bar{E})).$$

If now (n, E) lies not in $K_\gamma((\bar{n}, \bar{E}))$ then we have, since $\bar{\mathcal{F}}$ and $\mathcal{F}$ are smaller or equal one, that

$$\sup_{p\in\mathbb{T}^d} \left|\bar{\mathcal{F}}(n, E; p) - \mathcal{F}(\bar{n}, \bar{E}; p)\right| \leq \frac{1}{\gamma}\gamma \leq \frac{1}{\gamma}\left(\left|(n, E) - (\bar{n}, \bar{E})\right|\right), \qquad \forall (n, E) \notin K_\gamma((\bar{n}, \bar{E})).$$

Choosing now $\tilde{L} \coloneqq \max\{L_\gamma, (1/\gamma)\}$ provides the desired estimate. ∎

Corollary 2.4.8. *Let $(\bar{n}, \bar{E})$ be in $\mathfrak{D}^\circ$ fixed, then there exists a constant $L > 0$ such that*

$$\left\|\bar{\mathcal{F}}(n(t, .), E(t, .); .) - \mathcal{F}(\bar{n}, \bar{E}; .)\right\|_{L^2(\mathbb{T}^d\times\mathbb{T}^d)} \leq L\left(\|n_k(t, .) - \bar{n}\|^2_{L^2(\mathbb{T}^d)} + \left\|E_k(t, .) - \bar{E}\right\|^2_{L^2(\mathbb{T}^d)}\right),$$

for all n and E in $L^2_{loc}(\mathbb{R}^+_0, L^2(\mathbb{T}^d))$ with $n(t, x), E(t, x) \in \mathfrak{D}$ for all $(t, x) \in \mathbb{R}^+_0 \times \mathbb{T}^d$.

Proof. With Lemma 2.4.7 we have for all $(t, x) \in \mathbb{R}^+_0 \times \mathbb{T}^d$:

$$\left|\bar{\mathcal{F}}(n(t, x), E(t, x); p) - \mathcal{F}(\bar{n}, \bar{E}; p)\right|^2 \leq \tilde{L}^2\left(|n(t, x) - \bar{n}|^2 + \left|E(t, x) - \bar{E}\right|^2\right).$$

Since $\operatorname{meas}\left(\mathbb{T}^d\right) = 1$, we can integrate both sides with respect to p and then over x and set $L \coloneqq \tilde{L}^2$, which finishes the proof. ∎

Proof of Theorem 2.4.1:

Proof. We introduce for this proof the short notation for the index $\tau_k \hat{=} k$. Let $(f_k)_{k\in\mathbb{N}}$, $(n_k)_{k\in\mathbb{N}}$ and $(E_k)_{k\in\mathbb{N}}$ (where) be the subsequences of the families $(f_\tau)_{\tau>0}$, $(n_\tau)_{\tau>0}$ and $(E_\tau)_{\tau>0}$ such that

$$\lim_{k\to\infty} \|n_k - n\|_{L^2_{loc}(\mathbb{R}^+_0;L^2(\mathbb{T}^d))} + \|E_k - E\|_{L^2_{loc}(\mathbb{R}^+_0;L^2(\mathbb{T}^d))} + \left\|f_k - \bar{\mathcal{F}}(n, E; .)\right\|_{L^2_{loc}(\mathbb{R}^+_0;L^2(\mathbb{T}^d))} = 0.$$

where n and E are weak solutions in the sense of Definition 2.3.4. From Remark 2.4.3 we obtain a constant $a \in (0, (1/2)]$ such that $\mathcal{F}_{eq}(p) \in [a, 1 - a]$ for all $p \in \mathbb{T}^d$. Since f_k only takes values in $(0, 1)$ we can apply Lemma 2.4.4 and obtain for all $k \in \mathbb{N}$ and all $(t, x, p) \in \mathbb{R}^+_0 \times \mathbb{T}^d \times \mathbb{T}^d$

$$(f_k(t, x, p) - \mathcal{F}_{eq}(p))^2 \leq S^\infty(f_k(t, x, p)|\mathcal{F}_{eq}(p)) \leq C_a(f_k(t, x, p) - \mathcal{F}_{eq}(p))^2. \tag{2.88}$$

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The lower estimate will be important for the final conclusion. For now we make use of the upper estimate and obtain by integrating (2.88) with respect to p and x

$$\begin{aligned}\mathcal{H}^{f_k}_{\mathcal{F}_{eq}}(t) \leq & C_a \|f_k(t) - \mathcal{F}_{eq}\|^2_{\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)} \\ \leq & 2C_a \left(\|f_k(t) - \mathcal{F}(n_k(t), E_k(t))\|^2_{\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)} + \|\mathcal{F}(n_k(t), E_k(t)) - \mathcal{F}_{eq}\|^2_{\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)}\right),\end{aligned}$$

where $\mathcal{F}(n_k, E_k)$ is the Fermi Dirac distribution (2.20). For the last term we have with Corollary 2.4.8 the following estimate for all $t \in \mathbb{R}^+_0$

$$\|\mathcal{F}(n_k(t,.), E_k(t,.)) - \mathcal{F}_{eq}\|^2_{\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)} \leq L\left(\|n_k(t) - \bar{n}\|^2_{\mathrm{L}^2(\mathbb{T}^d)} + \left\|E_k(t) - \bar{E}\right\|^2_{\mathrm{L}^2(\mathbb{T}^d)}\right).$$

Next we want to apply Proposition 2.3.13 onto the families $(f_k - \mathcal{F}_{eq})_{k\in\mathbb{N}}$ and $(\mathcal{Q}_k(f_k))_{k\in\mathbb{N}}$. Notice that $|f_k - \mathcal{F}_{eq}| \leq 1$ for all $k \in \mathbb{N}$, which gives us that the family $(f_k - \mathcal{F}_{eq})_{k\in\mathbb{N}}$ is bounded in $\mathrm{L}^\infty(\mathbb{R}^+_0 \times \mathbb{T}^d \times \mathbb{T}^d)$, and the boundedness of $(\mathcal{Q}_k(f_k))_{k\in\mathbb{N}}$ in $\mathrm{L}^2(\mathbb{R}^+_0, \mathrm{L}^2(\mathbb{T}^d \times \mathbb{T}^d))$ is given by Corollary 2.2.21. Then we see that the families fulfill the equation

$$\tau_k\partial_t(f_k - \mathcal{F}_{eq}) + \nabla_p\varepsilon \cdot \nabla_x(f_k - \mathcal{F}_{eq}) = \mathcal{Q}_k(f_k),$$

because the equilibrium $\mathcal{F}_{eq}$ is independent of time and space and $\mathcal{Q}_\tau(\mathcal{F}_{eq}) = 0$. Hence the families meet the requirements of Proposition 2.3.13, and therefore we obtain for the families $(n_k - \bar{n})_{k\in\mathbb{N}}$ and $(E_k - \bar{E})_{k\in\mathbb{N}}$ the estimates for any compact interval $I \subset \mathbb{R}^+_0$

$$\begin{aligned}\left\|[n_k - \bar{n}]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(I)} &\leq D_\delta \|\mathcal{Q}_k\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \delta \|f_k - \mathcal{F}_{eq}\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \tau_k(\delta + D_\delta), \\ \left\|[E_k - \bar{E}]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(I)} &\leq \varepsilon_\infty \left(D_\delta \|\mathcal{Q}_k\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \delta \|f_k - \mathcal{F}_{eq}\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \tau_k(\delta + D_\delta)\right).\end{aligned}$$

The $\mathrm{H}^s(\mathbb{T}^d)$ - norm can be estimated by its semi norm and the average (for details see inequality (2.47) in Remark 2.3.10), which gives us for all times $t \in \mathbb{R}^+_0$:

$$\begin{aligned}\|n_k(t) - \bar{n}\|^2_{\mathrm{H}^s(\mathbb{T}^d)} &\leq 2\left(2[n_k(t) - \bar{n}]^2_{\mathrm{H}^s(\mathbb{T}^d)} + \left|\int_{\mathbb{T}^d} n_k(t,x) - \bar{n}dx\right|^2\right) = 4[n_k(t) - \bar{n}]^2_{\mathrm{H}^s(\mathbb{T}^d)}, \\ \left\|E_k(t) - \bar{E}\right\|^2_{\mathrm{H}^s(\mathbb{T}^d)} &\leq 2\left(2[E_k(t) - \bar{E}]^2_{\mathrm{H}^s(\mathbb{T}^d)} + \left|\int_{\mathbb{T}^d} E_k(t,x) - \bar{E}dx\right|^2\right) = 4[E_k(t) - \bar{E}]^2_{\mathrm{H}^s(\mathbb{T}^d)},\end{aligned}$$

where we used the fact that n_k and E_k integrated with respect to x at any time t has to coincide with $\bar{n}$ and $\bar{E}$, due to our conservation assumption (see (2.9)). This gives us for any compact interval $I \subset \mathbb{R}^+_0$

$$\begin{aligned}\|n_k - \bar{n}\|^2_{\mathrm{L}^2(I;\mathrm{L}^2(\mathbb{T}^d))} &\leq \|n_k - \bar{n}\|^2_{\mathrm{L}^2(I;\mathrm{H}^s(\mathbb{T}^d))} \leq 4\left\|[n_k - \bar{n}]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(I)}, \\ \left\|E_k - \bar{E}\right\|^2_{\mathrm{L}^2(I;\mathrm{L}^2(\mathbb{T}^d))} &\leq \left\|E_k - \bar{E}\right\|^2_{\mathrm{L}^2(I;\mathrm{H}^s(\mathbb{T}^d))} \leq 4\left\|[E_k - \bar{E}]_{\mathrm{H}^s(\mathbb{T}^d)}\right\|^2_{\mathrm{L}^2(I)}.\end{aligned}$$

And together with the estimates obtained from Proposition 2.3.13 we get

$$\begin{aligned}\|n_k - \bar{n}\|^2_{\mathrm{L}^2(I;\mathrm{L}^2(\mathbb{T}^d))} \leq & 4\left(D_\delta \|\mathcal{Q}_k\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \delta \|f_k - \mathcal{F}_{eq}\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \tau_k(\delta + D_\delta)\right), \\ \left\|E_k - \bar{E}\right\|^2_{\mathrm{L}^2(I;\mathrm{L}^2(\mathbb{T}^d))} \leq & 4\varepsilon_\infty\left(D_\delta \|\mathcal{Q}_k\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \delta \|f_k - \mathcal{F}_{eq}\|^2_{\mathrm{L}^2(I\times\mathbb{T}^d\times\mathbb{T}^d)} + \tau_k(\delta + D_\delta)\right).\end{aligned}$$

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Let us take a closer look on the term $\delta \left\| f_k - \mathcal{F}_{eq} \right\|^2_{L^2(I\times\mathbb{T}^d\times\mathbb{T}^d)}$ in the above estimates. We can rewrite f_k as in the Chapman- Enskog expansion, i.e. $f_k = \mathcal{F}(n_k, E_k; .) - \tau_k \mathcal{Q}_k$, and apply again Corollary 2.4.8, (short notation L^2 for the space $L^2(I, L^2(\mathbb{T}^d \times \mathbb{T}^d))$):

$$\begin{aligned}\left\| f_k - \mathcal{F}_{eq} \right\|^2_{L^2} \leq& 2\left(\left\| \tau_k \mathcal{Q}_k \right\|^2_{L^2} + \left\| \mathcal{F}(n_k, E_k; .) - \mathcal{F}_{eq} \right\|^2_{L^2} \right) \\ \leq& 2\left(\tau_k^2 \left\| \mathcal{Q}_k \right\|^2_{L^2} + L\left(\left\| n_k - \bar{n} \right\|^2_{L^2} + \left\| E_k - \bar{E} \right\|^2_{L^2} \right) \right).\end{aligned}$$

The estimates we obtained from Proposition 2.3.13, include a constant $\delta > 0$, which can be chosen arbitrarily. Indeed we can choose it separately for the families $(n_k - \bar{n})_{k\in\mathbb{N}}$ and $(E_k - \bar{E})_{k\in\mathbb{N}}$. For the first family we choose $\delta_1 = (1/32L)$ and for the second family $\delta_2 = (1/32L\varepsilon_\infty)$, then we obtain (not.: $L^2 \mathrel{\widehat{=}} L^2(I, L^2(\mathbb{T}^d \times \mathbb{T}^d))$ or $L^2 \mathrel{\widehat{=}} L^2(I, L^2(\mathbb{T}^d))$, which should be clear from the contex):

$$\begin{aligned}&\left\| n_k - \bar{n} \right\|^2_{L^2} \leq \\ &\quad \leq 4\left((D_{\delta_1} + 2\tau_k^2) \left\| \mathcal{Q}_k \right\|^2_{L^2} + \frac{1}{16}\left(\left\| n_k - \bar{n} \right\|^2_{L^2} + \left\| E_k - \bar{E} \right\|^2_{L^2} \right) + \tau_k(\delta_1 + D_{\delta_1}) \right), \\ &\left\| E_k - \bar{E} \right\|^2_{L^2} \leq \\ &\quad \leq 4\varepsilon_\infty \left((D_{\delta_2} + 2\tau_k^2) \left\| \mathcal{Q}_k \right\|^2_{L^2} + \frac{1}{16\varepsilon_\infty}\left(\left\| n_k - \bar{n} \right\|^2_{L^2} + \left\| E_k - \bar{E} \right\|^2_{L^2} \right) + \tau_k(\delta_2 + D_{\delta_2}) \right).\end{aligned}$$

Adding together both estimates provides

$$\begin{aligned}\left\| n_k - \bar{n} \right\|^2_{L^2} + \left\| E_k - \bar{E} \right\|^2_{L^2} \leq& 4\left((D_{\delta_1} + 2\tau_k^2 + \varepsilon_\infty(D_{\delta_2} + 2\tau_k^2)) \right) \left\| \mathcal{Q}_k \right\|^2_{L^2} + \\ &+ \frac{1}{2}\left(\left\| n_k - \bar{n} \right\|^2_{L^2} + \left\| E_k - \bar{E} \right\|^2_{L^2} \right) + \\ &+ 4\tau_k \left(\delta_1 + D_{\delta_1} + \varepsilon_\infty(\delta_2 + D_{\delta_2}) \right).\end{aligned}$$

Define $C_{\tau_k} := 8(D_{\delta_1} + \varepsilon_\infty D_{\delta_2} + 2\tau_k^2(1 + \varepsilon_\infty))$ and $\tilde{C} := 8(\delta_1 + D_{\delta_1} + \varepsilon_\infty(\delta_2 + D_{\delta_2}))$, then the above becomes

$$\left\| n_k - \bar{n} \right\|^2_{L^2} + \left\| E_k - \bar{E} \right\|^2_{L^2} \leq C_{\tau_k} \left\| \mathcal{Q}_k \right\|^2_{L^2} + \tau_k^2 \tilde{C}.$$

Putting everything together that came after (2.88), using again the Chapman-Enskog ansatz (2.61), and integrating over t_0, t in $\mathbb{R}_0^+$ yields

$$\begin{aligned}\int_{t_0}^t \mathcal{H}^{f_k}_{\mathcal{F}_{eq}}(r)dr \leq& 2C_a \left(\left\| f_k - \mathcal{F}(n_k, E_k) \right\|^2_{L^2([t_0,t];L^2)} + \left\| \mathcal{F}(n_k, E_k) - \mathcal{F}_{eq} \right\|^2_{L^2([t_0,t];L^2)} \right) \\ \leq& 2C_a \left(\tau_k^2 \left\| \mathcal{Q}_k \right\|^2_{L^2([t_0,t];L^2)} + L\left(\left\| n_k - \bar{n} \right\|^2_{L^2([t_0,t];L^2)} + \left\| E_k - \bar{E} \right\|^2_{L^2([t_0,t];L^2)} \right) \right) \\ \leq& 2C_a \left(\tau_k^2 \left\| \mathcal{Q}_k \right\|^2_{L^2([t_0,t];L^2)} + L\left(C_{\tau_k} \left\| \mathcal{Q}_k \right\|^2_{L^2([t_0,t];L^2)} + \tau_k^2 \tilde{C} \right) \right) \\ =& 2C_a(\tau_k^2 + LC_{\tau_k}) \left\| \mathcal{Q}_k \right\|^2_{L^2([t_0,t];L^2)} + \tau_k^2 2C_a L\tilde{C}.\end{aligned}$$

Recall the result of the H-Theorem (see Theorem 2.2.20)

$$\left\| \mathcal{Q}_k \right\|^2_{L^2([t_0,t];L^2)} \leq \frac{1}{2}(\mathcal{H}(f_k(t_0)) - \mathcal{H}(f_k(t))), \qquad \forall t, t_0 \in \mathbb{R}_0^+.$$

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In Lemma 2.4.5 we have shown that the time derivatives of the entropy functional and the relative entropy coincide and hence we have

$$\|\mathcal{Q}_k\|^2_{\mathrm{L}^2([t_0,t];\mathrm{L}^2)} \leq \frac{1}{2}(\mathcal{H}^{f_k}_{\mathcal{F}_{eq}}(t_0) - \mathcal{H}^{f_k}_{\mathcal{F}_{eq}}(t)), \qquad \forall t, t_0 \in \mathbb{R}^+_0.$$

which gives us in turn the estimate ($C_{(\tau_k,a)} := C_a(\tau_k^2 + LC_{\tau_k})$ and $\tilde{C}_a := 2C_aL\tilde{C}$)

$$\int_{t_0}^t \mathcal{H}^{f_k}_{\mathcal{F}_{eq}}(r)dr \leq C_{(\tau_k,a)}(\mathcal{H}^{f_k}_{\mathcal{F}_{eq}}(t_0) - \mathcal{H}^{f_k}_{\mathcal{F}_{eq}}(t)) + \tau_k^2\tilde{C}_a, \qquad \forall t, t_0 \in \mathbb{R}^+_0. \tag{2.89}$$

There exists now a subsequence of $(f_k)_{k\in\mathbb{N}}$ (using the same indices) such that it converges towards $\bar{\mathcal{F}}(n, E; .)$ point wise a.e. on $\mathbb{R}^+_0 \times \mathbb{T}^d \times \mathbb{T}^d$. With the continuity of S^∞ we obtain

$$\lim_{k\to\infty} \mathcal{H}^{f_k}_{\mathcal{F}_{eq}}(t) = \mathcal{H}^{\bar{\mathcal{F}}(n,E)}_{\mathcal{F}_{eq}}(t), \qquad \text{for a.e. } t \in \mathbb{R}^+_0.$$

Since $\lim_{k\to\infty} \tau_k = 0$, we have $\lim_{k\to\infty} C_{(\tau_k,a)} = 8LC_a(D_{\delta_1} + \varepsilon_\infty D_{\delta_2}) =: C^{-1}$. By taking the limit k to infinity on both sides in (2.89) and using the dominated convergence theorem, we obtain

$$\int_{t_0}^t \mathcal{H}^{\bar{\mathcal{F}}(n,E)}_{\mathcal{F}_{eq}}(r)dr \leq C^{-1}(\mathcal{H}^{\bar{\mathcal{F}}(n,E)}_{\mathcal{F}_{eq}}(t_0) - \mathcal{H}^{\bar{\mathcal{F}}(n,E)}_{\mathcal{F}_{eq}}(t)), \qquad \text{for a.e. } t, t_0 \in \mathbb{R}^+_0.$$

The constant C is greater than zero and therefore the above becomes

$$\mathcal{H}^{\bar{\mathcal{F}}(n,E)}_{\mathcal{F}_{eq}}(t) + C\int_{t_0}^t \mathcal{H}^{\bar{\mathcal{F}}(n,E)}_{\mathcal{F}_{eq}}(r)dr \leq \mathcal{H}^{\bar{\mathcal{F}}(n,E)}_{\mathcal{F}_{eq}}(t_0), \qquad \text{for a.e. } t, t_0 \in \mathbb{R}^+_0.$$

With the Gronwall argument we stated before (see Lemma 2.4.6) and setting $t_0 = 0$ we get

$$\mathcal{H}^{\bar{\mathcal{F}}(n,E)}_{\mathcal{F}_{eq}}(t) \leq \mathcal{H}^{\bar{\mathcal{F}}(n,E)}_{\mathcal{F}_{eq}}(0)e^{-Ct}, \qquad \text{for a.e. } t \in \mathbb{R}^+_0. \tag{2.90}$$

The estimate given in Lemma 2.4.4 can now be applied, since $0 \leq \bar{\mathcal{F}}(n, E) \leq 1$ and $0 < a \leq \mathcal{F}_{eq} \leq 1 - a$, and defining $K := \mathcal{H}^{\bar{\mathcal{F}}(n,E)}_{\mathcal{F}_{eq}}(0)$ provides

$$\left\|\bar{\mathcal{F}}(n(t,.), E(t,.); .) - \mathcal{F}_{eq}\right\|^2_{\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)} \leq Ke^{-Ct}, \qquad \text{for a.e. } t \in \mathbb{R}^+_0.$$

The exponential decay of the macroscopic densities n and E towards the steady states $\bar{n}$ and $\bar{E}$, is now a direct consequence from the above. For the convenience of the reader we carry this out, starting with the density n. We have that

$$n(t,x) - \bar{n} = \int_{\mathbb{T}^d} \bar{\mathcal{F}}(n(t,x), E(t,x); p) - \mathcal{F}_{eq}(p)dp, \qquad \forall (t,x) \in \mathbb{R}^+_0 \times \mathbb{T}^d.$$

Taking the absolute value from the above and use Jensen's inequality we get (notice that $\operatorname{meas}\left(\mathbb{T}^d\right) = 1$)

$$|n(t,x) - \bar{n}|^2 \leq \int_{\mathbb{T}^d} \left|\bar{\mathcal{F}}(n(t,x), E(t,x); p) - \mathcal{F}_{eq}(p)\right|^2 dp, \qquad \forall (t,x) \in \mathbb{R}^+_0 \times \mathbb{T}^d,$$

and hence we obtain

$$\|n(t,.) - \bar{n}\|^2_{\mathrm{L}^2(\mathbb{T}^d)} \leq Ke^{-Ct}, \qquad \text{for a.e. } t \in \mathbb{R}^+_0.$$

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For the energy density E we have that

$$E(t,x)-\bar{E}=\int_{\mathbb{T}^d}\varepsilon(p)\bar{\mathcal{F}}(n(t,x),E(t,x);p)-\varepsilon(p)\mathcal{F}_{eq}(p)dp,\qquad \forall(t,x)\in\mathbb{R}_0^+\times\mathbb{T}^d.$$

Recalling the definition $\varepsilon_\infty=\|\varepsilon\|^2_{\mathrm{L}^\infty(\mathbb{T}^d)}$, estimate the above with $\sqrt{\varepsilon_\infty}$ times the integral, then we get with the same steps as before

$$\left\|E(t,.)-\bar{E}\right\|^2_{\mathrm{L}^2(\mathbb{T}^d)}\leq\varepsilon_\infty Ke^{-Ct},\qquad \text{for a.e. } t\in\mathbb{R}_0^+.$$

□

Last we state the exponential decay that holds for every L^q- norm, where $q\in[1,\infty)$.

Corollary 2.4.9. *Let the functions n, E, $\bar{\mathcal{F}}(n,E;p)$ and the constants C,K be the same as in Main Theorem 2.4.1, then for almost every t in $\mathbb{R}_0^+$ we have for all $q\in[1,\infty)$:*

$$\left\|\bar{\mathcal{F}}(n(t,.),E(t,.);.)-\mathcal{F}_{eq}\right\|_{\mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d)}\leq K^{\frac{1}{2}}e^{-\frac{C}{2}t},$$

and

$$\|n(t,.)-\bar{n}\|_{\mathrm{L}^q(\mathbb{T}^d)}\leq K^{\frac{1}{2}}e^{-\frac{C}{2}t},\qquad \left\|E(t,.)-\bar{E}\right\|_{\mathrm{L}^q(\mathbb{T}^d)}\leq(\varepsilon_\infty K)^{\frac{1}{2}}e^{-\frac{C}{2}t}.$$

Proof. It is enough to prove the above for $\bar{\mathcal{F}}$ since the estimates for n and E are then direct consequences, as in the proof before. The case $q=2$ comes from Theorem 2.4.1.
For $q\in[1,2)$ we obtain with Hölder inequality, by defining $r:=2q(2-q)^{-1}$, since $1\in\mathrm{L}^r(\mathbb{T}^d\times\mathbb{T}^d)$ and $q^{-1}=2^{-1}+r^{-1}$, that (using the short notation $\bar{\mathcal{F}}(t)\widehat{=}\bar{\mathcal{F}}(n(t,.),E(t,.);.)$)

$$\left\|\bar{\mathcal{F}}(t)-\mathcal{F}_{eq}\right\|_{\mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d)}\leq\left\|\bar{\mathcal{F}}(t)-\mathcal{F}_{eq}\right\|_{\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)}$$

For $q\in(2,\infty)$ we see immediately that, since $\left|f_\tau(t)-\mathcal{F}(\bar{n}_0,\bar{E}_0)\right|\leq 1$,

$$\begin{aligned}\left\|\bar{\mathcal{F}}(t)-\mathcal{F}_{eq}\right\|^q_{\mathrm{L}^q(\mathbb{T}^d\times\mathbb{T}^d)}&\leq\left\|\bar{\mathcal{F}}(t)-\mathcal{F}_{eq}\right\|^q_{\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)}\left\|\bar{\mathcal{F}}(t)-\mathcal{F}_{eq}\right\|^q_{\mathrm{L}^\infty(\mathbb{T}^d\times\mathbb{T}^d)}\\&\leq\left\|\bar{\mathcal{F}}(t)-\mathcal{F}_{eq}\right\|^q_{\mathrm{L}^2(\mathbb{T}^d\times\mathbb{T}^d)}.\end{aligned}$$

□

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3. Spin Drift Diffusion Model

The goal of this chapter is to derive a quantum description of electrons and their spin in spintronic devices. If we pack all the information into one density matrix N (details follow later), we expect a model of the form

$$\partial_t N = \operatorname{div}(J(N)) + S(N),$$

where $\operatorname{div}(J(N))$ describes the current and $S(N)$ represents quantum effects regarding spin. As mentioned in the introduction we rely mainly on two works, namely [EH14] and [BM10]. Since the first starts from a semiclassical approach, it cannot be considered as "full quantum" model, but it derives equations for all components and that rigorously. The second derives "full quantum" models for the "spin up" and "spin down" densities. We look here, for a combination of both. Since we are in a different setting than in the previous chapter and we want to focus completely on the spin of the electrons, we dismiss the total energy.

3.1. General Description and the Microscopic Picture

Spintronics aims at controlling the electron spins by means of electrostatic fields and, therefore, tame it with the same technology of electronics. A prototypical spintronic device consists of four main components: the source, the channel region, the gate and the collector. The electrons start in the source, pass through the channel region and are the collected in the collector. The spin of the electrons is only affected in the channel, if the gate is switched on, which we then see as passing information (=1).

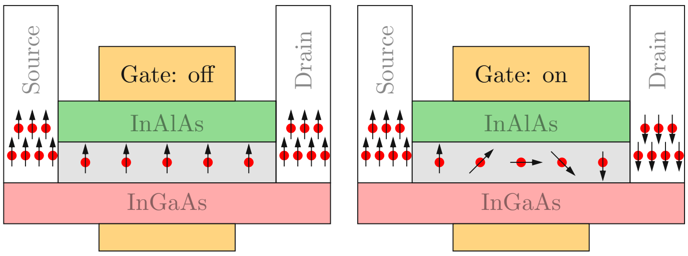

Figure 3.1.: A spintronic device with electrons passing through the channel region (here grey part). After activating the gate the average spin is changing the direction, which does not have to be the opposite.

Since the interesting effects happen in the channel region, it will be our target of modelling. Therefore we consider a two dimensional electron gas (2DEG) in the (x_1, x_2) plane as our ground setting for the channel region. The fact that the 2DEG is nearly a plane (see Figure 3.2), we mention at that point that the space variable x is 2 dimensional in $\mathbb{R}^3$ and will always be of the form $x = (x_1, x_2, 0)$. The same holds for the momentum p, since the electrons cannot move into the x_3 direction,therefore the momentum p, will always be of the form $p = (p_1, p_2, 0)$. Even tough the spin is still a vector in $\mathbb{R}^3$. The 2DEG is in between two layers of materials A,B (for example Indium aluminium arsenide (InAlAs) and Indium

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gallium arsenide (InGaAs) respectively) with different potentials. If the channel region is surrounded by suitable layers of semiconductors (e.g. InAlAs and InGaAs), so that to obtain an electron confinement into an asymmetric potential well, then the electrons experience the Rashba (or Bychkov-Rashba) spin-orbit effect. This effect manifests itself as an effective magnetic field orthogonal to the confinement direction and to the electron motion. Then, the spin orientation can be indirectly controlled by a gate voltage, which deviates the electrons, thus changing the direction of the effective magnetic field into the channel region. It is then possible to observe that the spin vector staggers around the direction of the effective field (see Figure 3.2). For a more detailed explanation of the Rashba effect at its application to spintronics we refer the reader to the work of Žutić and Fabian [icvacFDS04].

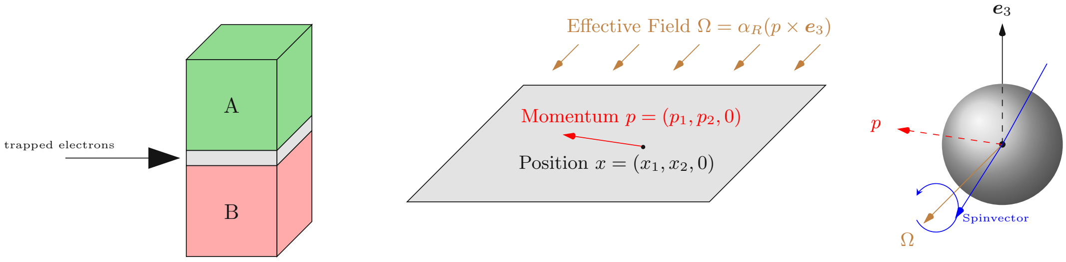

Figure 3.2.: **(left)**: Passage between two layers; **(middle)**: The passage (2DEG) presented as a plane, with an effective field; **(right)**: Staggering of the spin vector, due to the Rashba effect.

A two-dimensional electron gas in the (x_1, x_2)-plane with a Rashba spin-orbit interaction is described by the following Hamiltonian:

$$\mathcal{H} = \left(-\frac{\hbar^2}{2m}\Delta_{x_1,x_2} + V(x)\right) Id - \hbar\alpha_R \begin{pmatrix} 0 & i\partial_{x_2} - \partial_{x_1} \\ i\partial_{x_2} + \partial_{x_1} & 0 \end{pmatrix}, \tag{3.1}$$

where $x = (x_1, x_2, 0)$, Id is the 2×2 identity matrix, $\hbar$ is the reduced Planck constant, m is the electron effective mass, V is a given electric potential, and α_R is the Rashba constant [icvacFDS04].

The evolution equation for the density operator $\varrho = \varrho(t)$, representing the quantum statistical ("mixed") state of the system, is the *von Neumann equation*

$$i\hbar\partial_t\varrho = [\mathcal{H}, \varrho], \tag{3.2}$$

where $[.,.]$ denotes the commutator. We will consider also collisions in our system, but for the sake of simplicity they will be added later. The solution ϱ for the von Neumann equation is a (time-dependent) *density operator* on the space of the two-component wave functions $\mathrm{L}^2(\mathbb{R}, \mathbb{C}^2)$. Therefore we have for every instant of time, that ϱ is a self-adjoint and positive definite ($\langle\varrho\psi, \psi\rangle \geq 0, \forall\psi \in \mathrm{L}^2(\mathbb{R}, \mathbb{C}^2)$) operator, with unitary trace. This implies that ϱ is a *Hilbert-Schmidt operator.*

Definition 3.1.1. *An operator ϱ on $\mathrm{L}^2(\mathbb{R}^2, \mathbb{C}^2)$ is called a Hilbert-Schmidt operator, if it is an self-adjoint and positive definite (in the sense that $\langle\varrho\psi, \psi\rangle \geq 0$ for all ψ in $\mathrm{L}^2(\mathbb{R}, \mathbb{C}^2)$) operator with unitary trace. Additionally it has an unique integral kernel ρ in $\mathrm{L}^2(\mathbb{R}^2 \times \mathbb{R}^2, \mathbb{C}^{2\times 2})$ such that*

$$(\varrho\psi)(x) = \int_{\mathbb{R}^2} \rho(x, y)\psi(y)dy, \qquad \forall\psi \in \mathrm{L}^2(\mathbb{R}^2, \mathbb{C}^2),$$

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where the integral is to understand component wise. We define the space of all Hilbert-Schmidt operators on $L^2(\mathbb{R}^2, \mathbb{C}^2)$ *as* $\mathcal{HS}(L^2(\mathbb{R}^2, \mathbb{C}^2))$*.*

For detailed theory on Hilbert-Schmidt operators we refer to [RS80].

Remark 3.1.2. Let us roughly discuss the idea what a density operator describes. First we know that a wave function $\psi \in L^2(\mathbb{R}^2, \mathbb{C}^2)$ has every information about a particle encoded. Let us notice that wave functions encode information differently, than a distribution function f, like the one from the Boltzmann picture. For example if we look at the following for $\Omega \subset \mathbb{R}^3$

$$\int_\Omega f(t, x, p) dx, \qquad \int_\Omega |\psi(x)|^2 dx,$$

we obtain from the left the density of the particles in Ω at the current time t and given momentum p, whereas the right hand side will only give the probability to find a particle in Ω at the current state. There is a way to transform f into a probability density, but we are not going to delve into that.
To obtain information from a wave function ψ, we need an *observable*, which is an operator on the space of the wave functions. For example the position operator $\hat{x}$ applied to ψ reflects the expected density value of the particle in the state ψ, i.e.

$$\hat{x}(\psi) = \int_{\mathbb{R}^2} x |\psi(x)|^2 dx.$$

Having another wave function $\phi \in L^2(\mathbb{R}^2, \mathbb{C}^2)$, the L^2- scalar product of ϕ and ψ, gives us the probability of a particle to change from one state ψ to the other state ϕ. The density operator ϱ in (3.2) is an operator on the space of wave functions and can therefore be seen as an observable itself. Let $(\phi_k)_{k\in\mathbb{N}}$ be an orthonormal basis of $L^2(\mathbb{R}^2, \mathbb{C}^2)$, then we can describe ϱ through

$$\varrho(\psi) = \sum_{k=1}^{\infty} p_k \phi_k (\phi_k, \psi)_{L^2}, \qquad \text{where } p_k \in [0, 1], \text{ and } \sum_{k=0}^{\infty} p_k = 1.$$

Such a density operator is also called a *mixed state*. If we have $p_j = 1$ and $p_k = 0$ for all $k \in \mathbb{N}, k \neq j$, then we call ϱ a *pure state*. Now $\varrho(t)$, can be interpreted as the observable of being in the mixed state at the time t. In other words the quantity $(\psi, \varrho(t)\psi)_{L^2}$ gives us the probability to get from the state ψ into the mixed state ϱ at the time t. This looks at first hand quite complicated, but describing the system with operators has one big advantage: The Wigner formalism. ■

3.2. Transformation into Phase-Space

3.2.1. The Wigner Transformation

In view of the diffusive and semiclassical asymptotic analysis, that will be treated in the next sections, it is more handy to work with phase-space functions than with operators. For this reason we introduce at this point the common used *Wigner transformation*, which transforms a density operator, such as the ϱ occurring in the von Neumann equation (3.2), into a phase-space like distribution, named Wigner function. Of course, due to the Heisenberg's uncertainty relation, it is impossible to have the existence of a phase-space distribution in quantum mechanics and this means that the Wigner function is only formally similar to a phase-space distribution. The Wigner transformation is to be considered as a tool to simplify

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the calculations and to have a classical-like intuition of the physics behind the mathematical manipulations. Indeed, we shall use it for transforming the von Neumann equation into a kinetic Boltzmann equation. The Wigner formalism is treated detailed in the literature, as for example in the books [Fol89, JÖ9, ZFC05] or in the review paper [BFM14], but we will give here a short overview.
We start with the scalar valued Wigner transformation, which means that we look at wave functions that do not consider spin and lie therefore in $\mathrm{L}^2(\mathbb{R}^2,\mathbb{C})$. The definition for Hilbert-Schmidt operators on $\mathrm{L}^2(\mathbb{R}^2,\mathbb{C})$ is the same as in Definition 3.1.1, with the difference that we replace every appearing vector space over $\mathbb{C}$, with its field $\mathbb{C}$.

Definition 3.2.1. *Let ϱ be a Hilbert-Schmidt Operator on $\mathrm{L}^2(\mathbb{R}^2,\mathbb{C}^2)$ and ρ be its unique integral kernel. Then the Wigner transformation $\mathcal{W}$ is an operator from $\mathcal{HS}(\mathrm{L}^2(\mathbb{R}^2,\mathbb{C}))$ to $\mathrm{L}^2(\mathbb{R}^2\times\mathbb{R}^2,\mathbb{C})$ with*

$$\mathcal{W}(\varrho)(x,p)=\int_{\mathbb{R}^2}\rho(x+\tfrac{1}{2}\eta,x-\tfrac{1}{2}\eta)e^{-i\eta\cdot p/\hbar}d\eta,\qquad\forall\varrho\in\mathcal{HS}(\mathrm{L}^2(\mathbb{R}^2,\mathbb{C})).\tag{3.3}$$

The inverse of the Wigner transformation is given by the Weyl-quantization (will be proven later, see Remark 3.2.16).

Definition 3.2.2. *Let $w=\mathcal{W}(\varrho)$ be a Wigner function (alias Wigner transform of a Hilbert-Schmidt operator $\varrho\in\mathcal{HS}(\mathrm{L}^2(\mathbb{R}^2,\mathbb{C}))$) with values in $\mathbb{C}$, then the Weyl-quantization or inverse Wigner transformation is given by*

$$\mathcal{W}^{-1}(w)(x,y)=\frac{1}{(2\pi\hbar)^2}\int_{\mathbb{R}^2}w\left(\frac{x+y}{2},p\right)e^{i(x-y)\cdot p/\hbar}dp,\tag{3.4}$$

where $\mathcal{W}^{-1}(w)$ can be interpreted as the integral kernel of the Hilbert-Schmidt operator ϱ.

Remark 3.2.3. Let us stress again the fact that we are modelling in the 2DEG, which means that we are in a two dimensional setting regarding space and momentum. This is reflected by the fact that in the definition of Wigner/Weyl transformation we integrate over $\mathbb{R}^2$ and the factor in front of the integral in (3.4) is of power two. In literature, the standard case is that a three dimensional setting is considered, hence the other definitions slightly differ from our. ■

In Definition 3.2.1 we looked on operators that are defined on $\mathrm{L}^2(\mathbb{R}^2,\mathbb{C})$, whereas the latter space is the space for wave functions without the spin information. Wave functions that have also the spin encoded, "live" in $\mathrm{L}^2(\mathbb{R}^2,\mathbb{C}^2)$. Therefore the integral kernels of the Hilbert-Schmidt operators are 2×2 matrices, see Definition 3.1.1. Hence we have to extend the definition of the Wigner transformation for our purposes and we will use the same notation for it.

Definition 3.2.4. *Let ϱ be a Hilbert-Schmidt Operator on $\mathrm{L}^2(\mathbb{R}^2,\mathbb{C}^2)$ and ρ be its unique integral kernel. Then the Wigner transformation $\mathcal{W}$ is an operator from $\mathcal{HS}(\mathrm{L}^2(\mathbb{R}^2,\mathbb{C}^2))$ to $\mathrm{L}^2(\mathbb{R}^2\times\mathbb{R}^2,\mathbb{C}^{2\times 2})$ with*

$$\mathcal{W}(\varrho)(x,p)=\int_{\mathbb{R}^2}\rho(x+\tfrac{1}{2}\eta,x-\tfrac{1}{2}\eta)e^{-i\eta\cdot p/\hbar}d\eta,\qquad\forall\varrho\in\mathcal{HS}(\mathrm{L}^2(\mathbb{R}^2,\mathbb{C}^2)),\tag{3.5}$$

where the integral is to be understand component wise, in the sense that

$$(\mathcal{W}(\varrho)(x,p))_{kl}=\int_{\mathbb{R}^2}\rho(x+\tfrac{1}{2}\eta,x-\tfrac{1}{2}\eta)_{kl}\ e^{-i\eta\cdot p/\hbar}d\eta,\qquad \textit{for } k,l\in\{1,2\}.$$

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Remark 3.2.5. We see that the Wigner transformation in Definition 3.2.1 and 3.2.4 are barely distinguishable, hence we will use the same notation $\mathcal{W}$ for both, but use lowercase letters to denote scalar valued symbols (e.g. w) and capital letters for matrix valued symbols (e.g. W). The Weyl quantization of the matrix Wigner transformation is then to understand component wise. ■

Since we want to apply the Wigner transformation to the von Neumann equation (3.2), we need to extent the Wigner transformation to a greater variety of operators, due to the fact that the Hamiltonian (3.1) is definitely not a Hilbert-Schmidt operator. In fact the Wigner theory can be extended to such a wider class of distributional phase space functions [Fol89]. In such an extended setting, the Wigner transformation is still the inverse transformation of the *Weyl quantization*, which assigns to a phase-space function (or distribution) a quantum operator. The expression *symbols* for phase-space functions (or distributions) associated to operators via Wigner-Weyl transforms is often used in the literature, while the expression *Wigner function* will be reserved to the symbols that are the Wigner transforms of density operators. Also worth to mention is that in literature sometimes the notation $\mathrm{Op}_\hbar$ is used for the Weyl quantization and $\mathrm{Op}_\hbar^{-1}$ for the Wigner transformation. The Wigner-Weyl correspondence is summarized in Figure 3.3 cited from our work [BHJ].

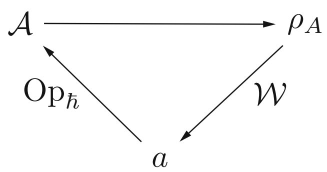

Figure 3.3.: The Wigner-Weyl correspondence: $\mathcal{A} = \mathrm{Op}_\hbar(a)$ is the operator associated to the phase-space function a, $\rho_\mathcal{A}$ is the integral kernel of $\mathcal{A}$, and $a = \mathcal{W}(\rho_\mathcal{A})$ is the Wigner transform of $\mathcal{A}$.

For a more detailed introduction to Weyl quantization and Wigner transform we refer the reader to Refs. [Fol89, ZFC05].

Remark 3.2.6. Furthermore for the sake of simplicity we drop from now any references on specific spaces and will just give formal definitions. ■

Example 3.2.7. The corresponding symbol to the Hamiltonian (3.1) is given by

$$\mathcal{W}(\mathcal{H})(x,p) = \begin{pmatrix} \frac{|p|^2}{2m} + V(x) & \alpha_R(p_2 + \mathrm{i}p_1) \\ \alpha_R(p_2 - \mathrm{i}p_1) & \frac{|p|^2}{2m} + V(x) \end{pmatrix}. \tag{3.6}$$

■

Applying the Wigner transformation to the von Neumann equation (3.2), the question arises what happens to the term $\mathcal{W}([\mathcal{H}, \varrho])$ and the next two subsections are dedicated to answer this question.

3.2.2. The Pauli Algebra

An very important fact is, that all the matrices we obtain from the Wigner-transform are hermitian $\left(A \in \mathbb{C}^{2\times 2} : A_{ij} = \bar{A}_{ji}\right)$. The Pauli algebra will simplify upcoming matrix-matrix

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multiplications and matrix-representation. The basis of hermitian matrices in $\mathbb{C}^{2\times 2}$ is given by the *Pauli matrices*:

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \ \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

with the multiplication table

Table 3.1.: Multiplication table for Pauli-matrices

$\cdot$	σ_0	σ_1	σ_2	σ_3
σ_0	σ_0	σ_1	σ_2	σ_3
σ_1	σ_1	σ_0	$\mathrm{i}\sigma_3$	$-\mathrm{i}\sigma_2$
σ_2	σ_2	$-\mathrm{i}\sigma_3$	σ_0	$\mathrm{i}\sigma_1$
σ_3	σ_3	$\mathrm{i}\sigma_2$	$-\mathrm{i}\sigma_1$	σ_0

With respect to such basis, each hermitian matrix in $\mathbb{C}^{2x2}$ has a representation with real scalar coefficients. Therefore for a general hermitian matrix $A \in \mathbb{C}^{2\times 2}$ exists unique *Pauli-components* $a_0, a_1, a_2, a_3 \in \mathbb{R}$ such that

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \sum_{j=0}^{3} a_j \sigma_j$$

with the relations

$$\begin{aligned} A_{11} &= a_0 + a_3, & a_0 &= \frac{1}{2}\left(A_{11} + A_{22}\right), \\ A_{12} &= a_1 - \mathrm{i}a_2, & a_1 &= \frac{1}{2}\left(A_{12} + A_{21}\right), \\ A_{21} &= a_1 + \mathrm{i}a_2, & a_2 &= \frac{1}{2}\left(A_{12} - A_{21}\right), \\ A_{22} &= a_0 - a_3, & a_3 &= \frac{1}{2}\left(A_{11} - A_{22}\right). \end{aligned}$$

This is also true, in particular, for the symbols associated to self-adjoint operators. Let $W := \mathcal{W}(\varrho)$ be a symbol associated to a density operator, i.e. a matrix-valued Wigner function. Then, we have that

$$W(x,p) = \sum_{j=0}^{3} w_j(x,p)\sigma_j = w_0(x,p)\sigma_0 + \boldsymbol{w}(x,p)\cdot\boldsymbol{\sigma},$$

with

$$\boldsymbol{w}(x,p) := \begin{pmatrix} w_1(x,p) \\ w_2(x,p) \\ w_3(x,p) \end{pmatrix}, \qquad \boldsymbol{\sigma} := \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{pmatrix},$$

and

$$w_j(x,p) = \frac{1}{2}\,\mathrm{tr}(W(x,p)\sigma_j), \qquad w_j \in \mathrm{L}^2(\mathbb{R}^2 \times \mathbb{R}^2, \mathbb{R}), \qquad j \in \{0,1,2,3\},$$

where ”tr” denotes the matrix trace.

Notation 3.2.8. *From now on we will drop the dependence on t if it is clear from the context. Matrix valued functions will be written in capital letters, vector valued functions will be denoted with bold small letters, and scalar functions will be denoted lowercase letters. For example we have for all $x, p \in \mathbb{R}^3$:*

$$W(x,p) \in \mathbb{C}^{2\times 2}, \qquad \boldsymbol{w}(x,p) \in \mathbb{R}^3, \qquad w_0(x,p) \in \mathbb{R}.$$

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Example 3.2.9. A good example for the usage of the Pauli-components is the transformed Hamiltonian (3.6). Defining $H := \mathcal{W}(\mathcal{H})$, the representation of H is given by:

$$H(x,p) = \left(\frac{|p|^2}{2m} + V(x)\right)\sigma_0 + \alpha_R p^\perp \cdot \boldsymbol{\sigma}, \tag{3.7}$$

where we define $p^\perp := p \times \boldsymbol{e}_3 = (p_2, -p_1, 0)$, with $\boldsymbol{e}_3 = (0,0,1)$. We also call H the *Hamiltonian symbol.* ■

Example 3.2.10. For this example let $A, B \in \mathbb{C}^{2\times 2}$ be hermitian matrices and a_j, b_j their Pauli-components for $j \in \{0,1,2,3\}$. With the given relations between the matrix entries and the Pauli-components we see immediately that the trace of a hermitian matrix stands in direct relation to the zeroth Pauli component, i.e.

$$\operatorname{tr}(A) = 2a_0.$$

With tabular 3.1 we can easily calculate the Pauli-components of the product AB:

$$\begin{aligned} AB =& (a_0\sigma_0 + \boldsymbol{a}\cdot\boldsymbol{\sigma})(b_0\sigma_0 + \boldsymbol{b}\cdot\boldsymbol{\sigma}) \\ =& (a_0 b_0 + \boldsymbol{a}\cdot\boldsymbol{b})\sigma_0 + (a_0\boldsymbol{b} + \boldsymbol{a}b_0 + \boldsymbol{a}\times\boldsymbol{b})\cdot\boldsymbol{\sigma}, \end{aligned} \tag{3.8}$$

where "$\cdot$" is the euclidean scalar product and "$\times$" is the cross product in $\mathbb{R}^3$. The representation (3.8) comes in quite handy calculating the trace of the product AB, because we obtain

$$\operatorname{tr}(AB) = 2(a_0 b_0 + \boldsymbol{a}\cdot\boldsymbol{b}).$$

■

3.2.3. The Moyal Product

The Moyal product (also called Weyl-Moyal or twisted product), introduced by Groenewold in 1946, will be one of our main tools for deriving the desired equations. The books [ZFC05, icvacFDS04, Fol89] cover the theory in detail, but their notation is different to ours. Therefore we introduce the most important theorems and statements which we will use, and prove them formally. Will also prove it for operators that have a unique integral kernel and are self adjoint. The extension to a greater class can then be done as same as mentioned in section 3.2.1.

Definition 3.2.11. *For two symbols f, g in $\mathrm{L}^2(\mathbb{R}^2\times\mathbb{R}^2, \mathbb{C})$ we define the Moyal product*

$$f\#g(x,p) := \frac{1}{(\hbar\pi)^4}\int_{\mathbb{R}^{2(\times 4)}} f(u_1,v_1)g(u_2,v_2)e^{\frac{2i}{\hbar}((x-u_2)v_1+(u_1-x)v_2-(u_1-u_2)p)}du_1du_2dv_1dv_2,$$

where $\mathbb{R}^{2(\times 4)} := \mathbb{R}^2\times\mathbb{R}^2\times\mathbb{R}^2\times\mathbb{R}^2$.

With the definition of the Moyal product and the Wigner/Weyl formalism, we are able to start answering the question, what happens to the term $\mathcal{W}[\mathcal{H}, \varrho]$. We start with the scalar case.

Lemma 3.2.12. *Let ϱ_1, ϱ_2 be two density operators on $\mathrm{L}^2(\mathbb{R}^2, \mathbb{C})$, with unique integral kernels ρ_1, ρ_2. Furthermore define $w_1 := \mathcal{W}(\varrho_1)$ and $w_2 := \mathcal{W}(\varrho_2)$, then*

$$\mathcal{W}(\varrho_1\varrho_2) = w_1\# w_2, \tag{3.9}$$

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Proof. For ψ in $L^2(\mathbb{R}^2, \mathbb{C})$, the operator product $\varrho_1\varrho_2$ applied on ψ can be rewritten with the help of the integral kernels:

$$\varrho_1(\varrho_2(\psi))(x) = \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \rho_1(x,y)\rho_2(y,z)\psi(z)dydz.$$

Using the Weyl quantization $\mathcal{W}^{-1}$ we obtain

$$\begin{aligned}\mathcal{W}(\varrho_1\varrho_2) =& \mathcal{W}(\mathcal{W}^{-1}(w_1)(\mathcal{W}^{-1}(w_2))) \\ =& \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \mathcal{W}^{-1}(w_1)\left(x+\frac{\eta}{2}, y\right)\mathcal{W}^{-1}(w_2)\left(y, x-\frac{\eta}{2}\right)e^{-\mathrm{i}\eta\cdot p/\hbar}dyd\eta \\ =& \frac{1}{(2\pi\hbar)^4}\int_{\mathbb{R}^{2(\times 4)}} w_1\left(\frac{x+y}{2}+\frac{\eta}{4}, v_1\right)e^{\frac{\mathrm{i}}{\hbar}\left((x-y+\frac{1}{2}\eta)\cdot v_1\right)} \\ & \qquad w_2\left(\frac{x+y}{2}-\frac{\eta}{4}, v_2\right)e^{\frac{\mathrm{i}}{\hbar}\left((y-x+\frac{1}{2}\eta)\cdot v_2\right)}e^{-\mathrm{i}\eta\cdot p/\hbar}dv_1dv_2dyd\eta.\end{aligned}$$

The transformation

$$\Phi(y,\eta) = (\tfrac{1}{2}(x+y)+\tfrac{1}{4}\eta, \tfrac{1}{2}(x+y)-\tfrac{1}{4}\eta), \quad |\det d\Phi| = 2^{-4},$$

with the inverse

$$\Phi^{-1}(u_1,u_2) = (u_1+u_2-x, 2(u_1-u_2)),$$

provides

$$\begin{aligned}\mathcal{W}(\varrho_1\varrho_2) =& \frac{1}{(\pi\hbar)^4}\int_{\mathbb{R}^{2(\times 4)}} w_1(u_1,v_1)w_2(u_2,v_2)e^{\frac{2\mathrm{i}}{\hbar}((x-u_2)\cdot v_1+(u_1-x)\cdot v_2-(u_1-u_2)\cdot p)}du_1du_2dv_1dv_2 \\ =& w_1\#w_2.\end{aligned}$$

□

Definition 3.2.13. *Let A and B be two symbols on $\mathbb{R}^2\times\mathbb{R}^2$ with values in $\mathbb{C}^{2\times 2}$. Then the matrix-Moyal product (not.: $A\#B$) between those symbols is defined as*

$$(A\#B(x,p))_{kl} := A_{k1}\#B_{1l}(x,p) + A_{k2}\#B_{2l}(x,p) \qquad \text{for } k,l\in\{1,2\}. \tag{3.10}$$

Since it is clear from the context, we will use the same notation for the Moyal product of either scalar-valued- or matrix-valued- symbols. Using Pauli components, the Moyal product of two hermitian matrix-valued symbols A and B can be also written as

$$A\#B = (a_0\#b_0 + \boldsymbol{a}\cdot_{\#}\boldsymbol{b})\,\sigma_0 + (a_0\#\boldsymbol{b} + \boldsymbol{a}\#b_0 + \mathrm{i}\boldsymbol{a}\times_{\#}\boldsymbol{b})\cdot\boldsymbol{\sigma}, \tag{3.11}$$

where $\cdot_{\#}$ and $\times_{\#}$ are to be understood as the scalar product and cross product, respectively, between two vectors in $\mathbb{R}^3$ where the multiplication is replaced by the Moyal product. The latter formula (3.11) will be used more frequently than (3.10), because we will work mostly with Pauli components.

Corollary 3.2.14. *Let ϱ_1, ϱ_2 be two density operators on $L^2(\mathbb{R}^2, \mathbb{C}^2)$, then we have the following:*

$$\mathcal{W}(\varrho_1\varrho_2) = \mathcal{W}(\varrho_1)\#\mathcal{W}(\varrho_2). \tag{3.12}$$

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Proof. We will show the proof just for Hilbert-Schmidt operators. The extension follows then as mentioned in Section 3.2.4 from [Fol89]. Therefore let ρ_1 and ρ_2 be the unique integral kernels in $\mathrm{L}^2(\mathbb{R}^2 \times \mathbb{R}^2, \mathbb{C}^{2\times 2})$ for ϱ_1 and ϱ_2 respectively. Furthermore define the operators on $\mathrm{L}^2(\mathbb{R}^2, \mathbb{C})$

$$(\varrho_m)_{kl}(\psi)(x) := \int_{\mathbb{R}^2} (\rho_m)_{kl}(x,y)\psi(y)dy, \qquad \text{for } m,k,l \in \{1,2\}, \text{ and } \forall \psi \in \mathrm{L}^2(\mathbb{R}^2,\mathbb{C}).$$

We have

$$\mathcal{W}(\varrho_1\varrho_2) = \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \rho_1\left(x+\frac{\eta}{2},y\right)\rho_2\left(y,x-\frac{\eta}{2}\right)e^{-i\eta\cdot p/\hbar}dyd\eta,$$

and therefore for $k,l \in \{1,2\}$ we obtain

$$\begin{aligned}(\mathcal{W}(\varrho_1\varrho_2))_{kl} &= \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \left(\rho_1\left(x+\frac{\eta}{2},y\right)\rho_2\left(y,x-\frac{\eta}{2}\right)\right)_{kl} e^{-\mathrm{i}\eta\cdot p/\hbar}dyd\eta,\\ &= \int_{\mathbb{R}^2}\int_{\mathbb{R}^2}\sum_{m=1}^{2}\left(\rho_1\left(x+\frac{\eta}{2},y\right)\right)_{km}\left(\rho_2\left(y,x-\frac{\eta}{2}\right)\right)_{ml} e^{-\mathrm{i}\eta\cdot p/\hbar}dyd\eta,\\ &= \sum_{m=1}^{2}\mathcal{W}\left((\varrho_1)_{km}(\varrho_2)_{ml}\right)\\ &= \sum_{m=1}^{2}\mathcal{W}(\varrho_1)_{km}\#\mathcal{W}(\varrho_2)_{ml}.\end{aligned}$$

□

For further progression we need a small ex-curse into the theory of distributions. Let therefore f be a symbol from $\mathbb{R}^2$ with values in $\mathbb{C}$. Recalling the definition of the Fourier-transform $\hat{\cdot}$ on $\mathbb{R}^2$

$$\hat{f}(\xi) := \frac{1}{2\pi}\int_{\mathbb{R}^2} f(x)\exp(-\mathrm{i}x\cdot\xi)dx. \tag{3.13}$$

Further recall also the definitions of the delta-distribution and the distribution generated from the constant one function

$$\delta(f) := f(0), \qquad \mathcal{T}_1(f) := \int_{\mathbb{R}^2} f(x)dx. \tag{3.14}$$

From the theory of distributions we know that we can define for every distribution ϕ the Fourier transform via $\hat{\phi}(f) := \phi(\hat{f})$. The distributions defined in (3.14) have a special relation, namely that

$$\hat{\delta}(f) = \delta(\hat{f}) = \hat{f}(0) = \frac{1}{2\pi}\int_{\mathbb{R}^2} f(x)dx = \frac{1}{2\pi}\mathcal{T}_1(f) \tag{3.15}$$

With the above we can show the following identity.

Lemma 3.2.15. *If f is a symbol, then we have for arbitrary z in $\mathbb{R}^2$:*

$$\frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} f(x)\exp(iy\cdot(x-z))dxdy = f(z). \tag{3.16}$$

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Proof. Define for simplicity the function $g(x) := f(z-x)$, then we have

$$\frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} f(x)\exp(-iy\cdot(z-x))dxdy = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} g(u)\exp(-iy\cdot(u))dudy = \frac{1}{2\pi}\int_{\mathbb{R}^2}\hat{g}(y)dy.$$

Using the definitions of $\delta, \mathcal{T}_1$, see (3.14), their relation $2\pi\hat{\delta}(f) = \mathcal{T}_1(f)$, see (3.15), and that $\hat{\hat{g}}(u) = g(-u)$, we conclude

$$\frac{1}{2\pi}\int_{\mathbb{R}^2}\hat{g}(y)dy = \frac{1}{2\pi}\mathcal{T}_1(\hat{g}) = \hat{\delta}(\hat{g}) = \delta\left(\hat{\hat{g}}\right) = g(0) = f(z).$$

□

Remark 3.2.16. An immediate consequence of Lemma 3.2.15 is that we can formally proof now that the Weyl quantization is the inverse of the Wigner transformation and vice versa. Let therefore $\varrho \in \mathcal{HS}$, $W = \mathcal{W}(\varrho)$ and let ρ be the integral kernel of ϱ. then using the transformation rule and (3.16), we obtain for a wave function $\psi \in \mathrm{L}^2(\mathbb{R}^2, \mathbb{C}^2)$

$$\begin{aligned}\int_{\mathbb{R}^2}\mathcal{W}^{-1}(\mathcal{W}(\varrho))(x,y)\psi(y)dy &= \int_{\mathbb{R}^2}\mathcal{W}^{-1}\left(\int_{\mathbb{R}^2}\rho(x+\tfrac{1}{2}\eta, x-\tfrac{1}{2}\eta)e^{-\mathrm{i}\eta\cdot p/\hbar}d\eta\right)(x,y)\psi(y)dy\\ &= \frac{1}{(2\pi\hbar)^2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2}\rho\left(\frac{x+y}{2}-\frac{1}{2}\eta, \frac{x+y}{2}+\frac{1}{2}\eta\right)e^{\mathrm{i}(\eta-(y-x))\cdot p/\hbar}d\eta dp\psi(y)dy\\ &= \int_{\mathbb{R}^2}\rho(x,y)\psi(y)dy,\end{aligned}$$

which coincides with $\varrho(\psi)(x)$ since ρ is the integral kernel of ϱ. For the other direction we obtain with similar argumentation:

$$\begin{aligned}\mathcal{W}(\mathcal{W}^{-1}(W))(x,p) &= \mathcal{W}\left(\frac{1}{(2\pi\hbar)^2}\int_{\mathbb{R}^2}W\left(\frac{x+y}{2}, p'\right)e^{\mathrm{i}(x-y)\cdot p'/\hbar}dp'\right)(x,p)\\ &= \frac{1}{(2\pi\hbar)^2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2}W(x,p')e^{\mathrm{i}\eta\cdot p'/\hbar}e^{-\mathrm{i}\eta\cdot p/\hbar}dp'd\eta\\ &= W(x,p).\end{aligned}$$

■

Coming back to the Moyal product, the next Proposition state two for us important properties.

Proposition 3.2.17. *Let f, g be two symbols with values in $\mathbb{C}$, then the following identity holds*

$$\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} f\#g(x,p)dxdp = \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} f(x,p)g(x,p)dxdp. \tag{3.17}$$

In particular if one of the functions is independent of one variable, e.g. $g(x,p) = g(x)$, then

$$\int_{\mathbb{R}^2} f\#g(x,p)dp = \int_{\mathbb{R}^2} f(x,p)dp\; g(x). \tag{3.18}$$

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Proof. To show our first equality (3.17) we will use identity (3.16) and use the shortcuts $du = du_1 du_2$ and $dv = dv_1 dv_2$:

$$
\begin{aligned}
&\int_{\mathbb{R}^{2(\times 2)}} f\#g(x,p)dxdp = \\
&= \frac{1}{(\hbar\pi)^4}\int_{\mathbb{R}^{2(\times 6)}} f(u_1,v_1)g(u_2,v_2)e^{\frac{2i}{\hbar}((x-u_2)\cdot v_1+(u_1-x)\cdot v_2-(u_1-u_2)\cdot p)}dudvdxdp \\
&= \frac{1}{(\hbar\pi)^4}\int_{\mathbb{R}^{2(\times 6)}} f(u_1,v_1)g(u_2,v_2)e^{\frac{2i}{\hbar}(u_1\cdot v_2-u_2\cdot v_1)}e^{\frac{2i}{\hbar}(v_1-v_2)\cdot x}dv_1dx\ e^{\frac{2i}{\hbar}(u_2-u_1)\cdot p}dudv_2dp \\
&= \frac{1}{(\hbar\pi)^2}\int_{\mathbb{R}^{2(\times 4)}} f(u_1,v_2)g(u_2,v_2)e^{\frac{2i}{\hbar}(u_1\cdot v_2-u_2\cdot v_2)}e^{\frac{2i}{\hbar}(u_2-u_1)\cdot p}du_2dpdu_1dv_2 \\
&= \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} f(u_1,v_2)g(u_1,v_2)du_1dv_2.
\end{aligned}
$$

To show the second equality (3.18), we proceed the same as for the first equality:

$$
\begin{aligned}
&\int_{\mathbb{R}^2} f(x,p)\#g(x)dp = \\
&= \frac{1}{(\hbar\pi)^4}\int_{\mathbb{R}^{2(\times 5)}} f(u_1,v_1)g(u_2)e^{\frac{2i}{\hbar}((x-u_2)\cdot v_1+(u_1-x)\cdot v_2-(u_1-u_2)\cdot p)}dudvdp \\
&= \frac{1}{(\hbar\pi)^4}\int_{\mathbb{R}^{2(\times 5)}} f(u_1,v_1)g(u_2)e^{\frac{2i}{\hbar}((x-u_2)\cdot v_1+(u_1-x)\cdot v_2)}e^{\frac{2i}{\hbar}(u_2-u_1)\cdot p}du_2dpdu_1dv \\
&= \frac{1}{(\hbar\pi)^2}\int_{\mathbb{R}^{2(\times 3)}} f(u_1,v_1)g(u_1)e^{\frac{2i}{\hbar}((x-u_1)v_1)}e^{\frac{2i}{\hbar}((u_1-x)\cdot v_2)}du_1dv_2dv_1 \\
&= \int_{\mathbb{R}^2} f(x,v_1)dv_1\ g(x).
\end{aligned}
$$

□

From the scalar case we obtain as a direct consequence

Corollary 3.2.18. *For two matrix-valued symbols A, B we have*

$$\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} A\#B(x,p)dxdp = \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} A(x,p)B(x,p)dxdp, \tag{3.19}$$

and if one function only depends on x, i.e. $A(x,p) = A(x)$, or i.e. $B(x,p) = B(x)$ then

$$\int_{\mathbb{R}^2} A\#B(x,p)dp = A(x)\int_{\mathbb{R}^2} B(x,p)dp, \quad or \quad \int_{\mathbb{R}^2} A\#B(x,p)dp = \int_{\mathbb{R}^2} A(x,p)dpB(x), \tag{3.20}$$

respectively.

Proof. Follows immediately from the definition of the matrix Moyal product (Definition 3.10) and Proposition 3.2.17. □

It is possible to develop the Moyal product into a special series, also called the semiclassical expansion (the concept will be introduced in more detail in Section 3.6).

Notation 3.2.19. *Recalling the definition of the multi-index. For a sufficiently smooth function f on $\mathbb{R}^n$ and $n \in \mathbb{N}$, we define the multi-index as $r = (r_1, \dots, r_n)$, with $r_j \in \mathbb{N}_0$ and the absolute value $|r| = \sum_{j=1}^n r_j$. Additionally we define*

$$\partial_x^r f := \frac{\partial^{|r|}}{\partial_{x_1}^{r_1}\partial_{x_2}^{r_2}\cdots\partial_{x_n}^{r_n}} f.$$

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Lemma 3.2.20. *For two scalar valued symbols f, g the semiclassical expansion with respect to $\hbar$ of their Moyal-product is given by:*

$$f\#g(x,p) = \sum_{j=0}^{\infty} \hbar^j f\#_{(j)} g \tag{3.21}$$

where the j-th order of the Moyal product equals

$$f\#_{(j)} g = \frac{1}{(2i)^j} \sum_{|r|+|s|=j} \frac{(-1)^{|r|}}{r!s!} \partial_x^r \partial_p^s f(x,p) \partial_p^r \partial_x^s g(x,p). \tag{3.22}$$

Proof. See [Zwo12] on Page 68, Theorem 4.12.. □

Remark 3.2.21. The first two orders in the Moyal product are quite interesting. Looking at the zeroth order we see that it becomes the usual product between two symbols, i.e. for scalar valued f and g we have

$$f\#_{(0)} g(x,p) = f(x,p) g(x,p).$$

For matrix valued symbols A, B we then clearly have $A\#_{(0)} B = A(x,p)B(x,p)$. The first order of the Moyal product gives for two scalar valued symbols f, g:

$$2\mathrm{i} f\#_{(1)} g = \nabla_p f \cdot \nabla_x g - \nabla_x f \cdot \nabla_p g, \tag{3.23}$$

which is also known as the *Poisson bracket* . ■

Remark 3.2.22. At this point we want to take the time and explain what it means to take the sum over a multi index. For example we have the sum

$$\sum_{|r|=j} \frac{1}{r!} \partial_x^r f(x,p),$$

where we assume that $x \in \mathbb{R}^n$, $r \in \mathbb{N}_0^n$. So we are looking at all n-tuples $(r_1, r_2, \ldots, r_n)$ such that the sum $\sum_{i=1}^n r_i$ equals j, which would be counted as combination with repetition, since the order does not play a role. In comparison if we would sort all the possible configurations of partial derivatives and if we differ $\partial_{x_{i_1}} \partial_{x_{i_2}}$ and $\partial_{x_{i_2}} \partial_{x_{i_1}}$, then all possible configurations would be a variation with repetition. The factor $\frac{1}{r!} = \frac{1}{r_1! r_2! \cdots r_n!}$ represents the ratio between a multi index r and all possible configurations of such belonging partial derivatives.
For example the multi index with $r_{i_1} = j-1$ and $r_{i_2} = 1$ for $i_1, i_2 \in \{1, 2, \ldots, n\}$ appears only once, but the mixed derivatives appear j times

$$\underbrace{\partial_{x_{i_1}}^{(j-1)} \partial_{x_{i_2}} f = \partial_{x_{i_1}}^{(j-2)} \partial_{x_{i_2}} \partial_{x_{i_1}} f = \partial_{x_{i_1}}^{(j-3)} \partial_{x_{i_2}} \partial_{x_{i_1}}^2 f = \cdots = \partial_{x_{i_2}} \partial_{x_{i_1}}^{(j-1)} f}_{j \text{ configurations}}.$$

In that case we have $\frac{1}{r!} = \frac{1}{(j-1)!1!} = \frac{j}{j!}$. Therefore we could rewrite the sum over the multi index into

$$\sum_{|r|=j} \frac{1}{r!} \partial_x^r f(x,p) = \frac{1}{j!} \sum_{i_1, i_2, \ldots, i_j = 1}^{n} \partial_{x_{i_1}} \partial_{x_{i_2}} \cdots \partial_{x_{i_j}} f(x,p). \tag{3.24}$$

■

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Example 3.2.23. We set in the formula (3.24) j=3 and $n = 3$. Therefore we obtain the formula

$$\sum_{|r|=3} \frac{1}{r!}\partial_x^r f(x,p) = \frac{1}{6}\sum_{i_1=1}^{3}\sum_{i_2=1}^{3}\sum_{i_3=1}^{3} \partial_{x_{i_1}}\partial_{x_{i_2}}\partial_{x_{i_3}} f(x,p).$$

■

Definition 3.2.24. *Let f and g be two scalar valued symbols, then the odd and even Moyal product are defined by*

$$f\#_{(odd)}g := \frac{1}{2}(f\#g - g\#f), \qquad f\#_{(even)}g := \frac{1}{2}(f\#g + g\#f). \tag{3.25}$$

Remark 3.2.25. The definition of the odd and even Moyal product make sense if we calculate these. We see with the expansion given in (3.21) and their orders (3.22) that by definition only either the odd or even orders remain. ■

3.2.4. The Pseudo Differential Operator

Applying the Wigner transformation to the von Neumann equation should make the problem more vivid. As already mentioned we cannot expect a classical equation, due to the Heißenberg uncertainty. This will be reflected in the transformed problem, by the pseudo differential.

Definition 3.2.26. *For two scalar valued symbols f and g on $\mathbb{R}^2 \times \mathbb{R}^2$, where f only depends on the space variable, i.e. $f(x,p) = f(x)$, we define the pseudo differential as*

$$(\Theta_\hbar[f]g)(x,p) := \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2\times\mathbb{R}^2} (\delta_\hbar[f])(x,\eta)g(x,p')e^{-i(p-p')\cdot\eta}d\eta dp',$$

where

$$(\delta_\hbar[f])(x,\eta) := \frac{1}{i\hbar}\left(f(x+\tfrac{\hbar}{2}\eta) - f(x-\tfrac{\hbar}{2}\eta)\right)$$

The above definition is the one that appears most frequently in the literature, but we will introduce another description of the pseudo-differential.

Lemma 3.2.27. *Let f,g and $\Theta_\hbar[f]g$ be the same as in Definition 3.2.26 then*

$$i\hbar(\Theta_\hbar[f]g) = 2f\#_{(odd)}g \tag{3.26}$$

Proof. We go from the right side to the left side using the definition of the Moyal product (see Definition 3.2.11) and the identity (3.16). The trick here is just to use a clever transformation to obtain the pseudo differential. Since the odd Moyal product is given by $2f\#_{(odd)}g = (f\#g - g\#f)$, see (3.25), we start with

$$\begin{aligned} f\#g(x,p) &= \frac{1}{(\hbar\pi)^4}\int_{\mathbb{R}^{2(\times 4)}} f(u_1)g(u_2,v_2)e^{\frac{2i}{\hbar}((x-u_2)v_1+(u_1-x)v_2-(u_1-u_2)p)}du_1du_2dv_1dv_2 \\ &= \frac{1}{(\hbar\pi)^4}\int_{\mathbb{R}^{2(\times 4)}} f(u_1)g(u_2,v_2)e^{\frac{2i}{\hbar}((u_1-x)v_2-(u_1-u_2)p)}e^{\frac{2i}{\hbar}(x-u_2)v_1}du_2dv_1du_1dv_2 \\ &= \frac{1}{(\hbar\pi)^2}\int_{\mathbb{R}^{2(\times 2)}} f(u_1)g(x,v_2)e^{\frac{2i}{\hbar}(u_1-x)(v_2-p)}du_1dv_2. \end{aligned}$$

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The transformation $\Phi(\eta) = x + \hbar 2^{-1}\eta$ with determinant $|\det d\Phi| = \hbar^2 2^{-2}$ and inverse $\Phi^{-1}(u_1) = 2\hbar^{-1}(u_1 - x)$, provides

$$f\#g(x,p) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2\times\mathbb{R}^2} f\left(x + \frac{\hbar}{2}\eta\right) g(x,v_2) e^{\mathrm{i}\eta\cdot(v_2-p)} d\eta dv_2.$$

Looking at the second term $g\#f$, we obtain with similar arguments the following

$$\begin{aligned}
g\#f(x,p) &= \frac{1}{(\hbar\pi)^4}\int_{\mathbb{R}^{2(\times 4)}} g(u_1,v_1)f(u_2)e^{\frac{2\mathrm{i}}{\hbar}((x-u_2)v_1+(u_1-x)v_2-(u_1-u_2)p)}du_1du_2dv_1dv_2\\
&= \frac{1}{(\hbar\pi)^4}\int_{\mathbb{R}^{2(\times 4)}} g(u_1,v_1)f(u_2)e^{\frac{2\mathrm{i}}{\hbar}((x-u_2)v_1-(u_1-u_2)p)}e^{\frac{2\mathrm{i}}{\hbar}(u_1-x)v_2}dv_2du_1du_2dv_1\\
&= \frac{1}{(\hbar\pi)^2}\int_{\mathbb{R}^{2(\times 2)}} g(x,v_1)f(u_2)e^{\frac{2\mathrm{i}}{\hbar}(x-u_2)(v_1-p)}du_2dv_1.
\end{aligned}$$

Choosing now the transformation $\Phi(\eta) = x - \frac{\hbar}{2}\eta$, with the determinant $|\det d\Phi| = \hbar^2 2^{-2}$ and inverse $\Phi^{-1}(u_1) = 2\hbar^{-1}(x - u_2)$, we obtain

$$g\#f(x,p) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2\times\mathbb{R}^2} g(x,v_1) f\left(x - \frac{\hbar}{2}\eta\right) e^{\mathrm{i}\eta\cdot(v_1-p)} d\eta dv_1.$$

Putting both calculations together we find

$$\begin{aligned}
(f\#g - g\#f)(x,p) &= \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2\times\mathbb{R}^2}\left(f\left(x+\frac{\hbar}{2}\eta\right) - f\left(x - \frac{\hbar}{2}\eta\right)\right) g(x,p')e^{\mathrm{i}\eta\cdot(p'-p)}d\eta dp'\\
&= \mathrm{i}\hbar\frac{1}{(2\pi)^2}\int_{\mathbb{R}^2\times\mathbb{R}^2}(\delta_\hbar[f])(x,\eta)g(x,p')e^{\mathrm{i}\eta\cdot(p'-p)}d\eta dp'\\
&= \mathrm{i}\hbar(\Theta_\hbar[f]g)(x,p)
\end{aligned}$$

□

Remark 3.2.28. Setting $f(x) = V(x)$, where V is the potential energy from the Hamiltonian H, and let g be any symbol. Applying now Lemma 3.2.27 provides

$$(\Theta_\hbar[V]g) = \frac{2}{\mathrm{i}\hbar}V\#_{(odd)}g = \nabla_x V\cdot\nabla_p g + \mathcal{O}(\hbar^2).$$

Comparing the above expression with the dimensionless semiconductor Boltzmann equation (1.5), we see the analogue. At zero order ($\hbar^0$) the pseudo differential coincides with the potential part of the "classical" picture. The operator is one of the reasons why we only speak formally of phase-space as mentioned in the beginning of this section. ■

3.2.5. The Wigner Picture

Finally we have everything at hand to apply the Wigner transform to the von Neumann equation (3.2). In the literature often we just see the result of this transformation, but in this thesis we think it is the right place to show the calculations to obtain the *Wigner-Boltzmann equation*.

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Theorem 3.2.29. *Let ϱ be the solution for the von Neumann equation (3.2) and $W \coloneqq \mathcal{W}(\varrho)$ its Wigner transform. Then the Pauli components of $W(x,p) = w_0(x,p)\sigma_0 + \boldsymbol{w}(x,p)\cdot\boldsymbol{\sigma}$ solve the Wigner-Boltzmann equation :*

$$\partial_t w_0 + \frac{p}{m}\cdot\nabla_x w_0 + \alpha_R \nabla_x^\perp \cdot \boldsymbol{w} - (\Theta_\hbar[V]w_0) = 0 \tag{3.27}$$

$$\partial_t \boldsymbol{w} + (\nabla_x \boldsymbol{w})\frac{p}{m} + \alpha_R \nabla_x^\perp w_0 - (\Theta_\hbar[V]\boldsymbol{w}) - \frac{2}{\hbar}\alpha_R p^\perp \times \boldsymbol{w} = 0, \tag{3.28}$$

where we define the planar gradient as $\nabla_x \coloneqq (\partial_{x_1}, \partial_{x_2}, 0)$, its orthogonal as

$$\nabla_x^\perp \coloneqq \nabla_x \times \boldsymbol{e}_3 = (\partial_{x_2}, -\partial_{x_1}, 0)$$

(so that $\nabla_x^\perp \cdot \boldsymbol{w} = \partial_{x_2} w_1 - \partial_{x_1} w_2$), $p^\perp = p \times \boldsymbol{e}_3$ and $\Theta_\hbar[V]$ is the pseudo differential.

Proof. By applying the Wigner transform to the von Neumann equation we obtain, due to the fact that $\mathcal{W}$ is linear,

$$\begin{aligned} \mathcal{W}(\mathrm{i}\hbar\partial_t\varrho) &= \mathcal{W}\left([\mathcal{H},\varrho]\right) \\ \mathrm{i}\hbar\partial_t W &= \mathcal{W}(\mathcal{H}\varrho) - \mathcal{W}(\varrho\mathcal{H}) \\ \mathrm{i}\hbar\partial_t W &= H\#W - W\#H, \end{aligned} \tag{3.29}$$

where $H = \mathcal{W}(\mathcal{H})$ is the Wigner transformed Hamiltonian, given by (3.6). The main part of this proof is to calculate the right hand side of the last equation. To achieve this we will make use of the Pauli algebra and the semiclassical expansion of the Moyal product, see Lemma 3.2.20. Referring to Example 3.2.9 we define

$$h_0(x,p) \coloneqq \frac{|p|^2}{2m} + V(x), \qquad \boldsymbol{h}(x,p) \coloneqq \alpha_R p^\perp.$$

Using the Pauli algebra combined with the Moyal product (see (3.11)) and the definition of the odd and even Moyal product (Def. 3.2.24) we obtain

$$H\#W - W\#H =$$
$$2\left(h_0\#_{(odd)}w_0 + \boldsymbol{h}\cdot_{\#_{(odd)}}\boldsymbol{w}\right)\sigma_0 + 2\left(h_0\#_{(odd)}\boldsymbol{w} + \boldsymbol{h}\#_{(odd)}w_0 + \mathrm{i}\boldsymbol{h}\times_{\#_{(even)}}\boldsymbol{w}\right)\cdot\boldsymbol{\sigma}.$$

The last factor comes from $\boldsymbol{h}\times_\# \boldsymbol{w} - \boldsymbol{w}\times_\# \boldsymbol{h} = 2(\boldsymbol{h}\times_{\#_{(even)}}\boldsymbol{w})$, which is shown by just evaluating the cross products and putting it back together. Comparing now the Pauli components of the left hand side with them on the right hand side in equation (3.29) we look at four equations which can be written as

$$\mathrm{i}\hbar\partial_t w_0 = 2\left(h_0\#_{(odd)}w_0 + \boldsymbol{h}\cdot_{\#_{(odd)}}\boldsymbol{w}\right), \tag{3.30}$$

$$\mathrm{i}\hbar\partial_t \boldsymbol{w} = 2\left(h_0\#_{(odd)}\boldsymbol{w} + \boldsymbol{h}\#_{(odd)}w_0 + \mathrm{i}\boldsymbol{h}\times_{\#_{(even)}}\boldsymbol{w}\right). \tag{3.31}$$

The special structure of h_0 and $\boldsymbol{h}$ simplifies calculations by far. Splitting h_0 into $|p|^2(2m)^{-1}$ and $V(x)$, we see immediately, due to Lemma 3.2.27, that

$$2V\#_{(odd)}w_0 = \mathrm{i}\hbar(\Theta_\hbar[V]w_0).$$

Since $\partial_p^\alpha |p|^2$ vanishes for every multi-index α with $|\alpha| \geq 3$ and $\partial_x^\alpha |p|^2 = 0$ for all $|\alpha| > 0$, we obtain with the Poisson bracket (formula (3.23))

$$2\left((2m)^{-1}\left(|p|^2\#_{(odd)}w_0\right)\right) = \frac{1}{m}\left(\frac{\hbar}{2\mathrm{i}}\left(|p|^2\#_{(1)}w_0\right)\right) = -\mathrm{i}\hbar\frac{p}{m}\cdot\nabla_x w_0.$$

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This leads to $h_0\#w_0 = \mathrm{i}\hbar((\Theta_\hbar[V]w_0) - \frac{p}{m} \cdot \nabla_x w_0)$. For the next term, we take a closer look onto $\boldsymbol{h} = \alpha_R p^\perp$. The derivative with respect to the momentum is clearly $\partial_p^\beta \boldsymbol{h} = 0$ for every multi-index β with $|\beta| \geq 2$ and the derivative with respect to x vanishes. Hence the only contributing term here is $\nabla_p h_j = \alpha_R(-\delta_{2j}, \delta_{1j}, 0)$ for $j \in \{1, 2, 3\}$ where δ_{kj} being the Kronecker delta symbol. We have

$$\begin{aligned} 2\boldsymbol{h} \cdot_{\#(odd)} \boldsymbol{w} =& 2\sum_{j=1}^{3} h_j \#_{(odd)} w_j = -i\hbar\alpha_R \sum_{j=1}^{3} \nabla_p h_j \cdot \nabla_x w_j = -i\hbar\alpha_R(\partial_{x_2} w_1 - \partial_1 w_2) \\ =& - i\hbar\alpha_R \nabla_x^\perp \cdot \boldsymbol{w}. \end{aligned}$$

With all terms for (3.30) at hand, dividing by $\mathrm{i}\hbar$ yields

$$\partial_t w_0 = -\frac{p}{m} \cdot \nabla_x w_0 - \alpha_R \nabla_x^\perp \cdot \boldsymbol{w} + \Theta_\hbar[V]w_0,$$

which proves the first equation (3.27). To obtain the second equation (3.28), we need to calculate the terms in (3.31). Looking at the first term in (3.31) we clarify that $(h_0\#\boldsymbol{w})_j = h_0\#w_j$ for $j \in \{1, 2, 3\}$, and the calculations for those terms are the same as for $h_0\#w_0$. Therefore we can write directly

$$2h_0\#\boldsymbol{w} = \mathrm{i}\hbar\left((\Theta_\hbar[V]\boldsymbol{w}) - (\nabla_x \boldsymbol{w})\, \frac{p}{m}\right),$$

where $(\Theta_\hbar[V]\boldsymbol{w})_j = (\Theta_\hbar[V]w_j)$ and $(\nabla_x \boldsymbol{w})\, p$ is simply a matrix-vector product. Same arguments as for $\boldsymbol{h} \cdot_{\#(odd)} \boldsymbol{w}$, yields for the second term in (3.31)

$$2\boldsymbol{h}\#_{(odd)} w_0 = -\mathrm{i}\hbar\alpha_R(\partial_{x_2} w_0, -\partial_{x_1} w_0, 0) = -\mathrm{i}\hbar\alpha_R \nabla_x^\perp w_0.$$

The last term in (3.31) needs a bit more treatment. Recall that $\times_\#$ denotes the $\mathbb{R}^3$ cross product, where we replace the product with the Moyal product. For $\boldsymbol{h} = \alpha_R p^\perp$ higher derivatives vanish ($\partial_x^\beta \boldsymbol{h} = 0 = \partial_p^\beta \boldsymbol{h}, |\beta| \geq 2$) and therefore only the zeroth order of the Moyal cross product remains. Hence

$$2\mathrm{i}\boldsymbol{h} \times_{\#(even)} \boldsymbol{w} = 2\mathrm{i}\boldsymbol{h} \times_{\#(0)} \boldsymbol{w} = 2\mathrm{i}\boldsymbol{h} \times \boldsymbol{w} = 2\mathrm{i}\alpha_R p^\perp \times \boldsymbol{w}.$$

Substituting our results into (3.31) and divide through $\mathrm{i}\hbar$ we obtain

$$\partial_t \boldsymbol{w} = -(\nabla_x \boldsymbol{w})\, \frac{p}{m} + (\Theta_\hbar[V]\boldsymbol{w}) - \alpha_R \nabla_x^\perp w_0 + \frac{2}{\hbar}\alpha_R p^\perp \times \boldsymbol{w},$$

which proves (3.28). □

3.2.6. The Non-Dimensional Form

In order to identify small parameters and to perform the asymptotic limits leading to the macroscopic models, we want to scale the Wigner-Boltzmann equation (3.27)-(3.28). This procedure can be found in similar works like in [BM10] and [BFM14] but we will show it here for the sake of completeness. Different is that we postpone the discussion of time scaling to Section 3.4, due to a problem that has not occurred in other works yet.

Let x_0 be the reference length, t_0 the reference time and T_0 the reference temperature (e.g., the temperature of a phonon bath). The reference momentum and energy are then defined as the thermal ones:

$$p_0 = \sqrt{mk_B T_0}, \qquad E_0 = \frac{p_0^2}{m},$$

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where k_B is the Boltzmann constant. Introducing the dimensionless variables

$$t \to t_0 \tilde{t}, \qquad x \to x_0 \tilde{x}, \qquad p \to p_0 \tilde{p}.$$

Just for this brisk moment we will write the Wigner Boltzmann equation in the new variables after the first scaling. For this define $\tilde{w}_0(\tilde{t},\tilde{x},\tilde{p}) := w_0(t_0\tilde{t}, x_0\tilde{x}, p_0\tilde{p})$, $\tilde{\boldsymbol{w}}(\tilde{t},\tilde{x},\tilde{p}) := \boldsymbol{w}(t_0\tilde{t}, x_0\tilde{x}, p_0\tilde{p})$ and $E_0\tilde{V}(\tilde{t},\tilde{x}) := V(t_0\tilde{t}, x_0\tilde{x})$, then we obtain (compare with Section 1.3)

$$\begin{aligned} \frac{1}{t_0}\partial_{\tilde{t}}\tilde{w}_0 &= -\frac{p_0\tilde{p}}{mx_0}\cdot\nabla_{\tilde{x}}\tilde{w}_0 - \frac{\alpha_R}{x_0}\nabla_{\tilde{x}}^{\perp}\cdot\tilde{\boldsymbol{w}} + \frac{p_0}{mx_0}\left(\Theta_{\frac{\hbar}{p_0x_0}}[\tilde{V}]\tilde{w}_0\right)\\ \frac{1}{t_0}\partial_{\tilde{t}}\tilde{\boldsymbol{w}} &= -\left(\nabla_{\tilde{x}}\tilde{\boldsymbol{w}}\right)\frac{p_0\tilde{p}}{mx_0} - \frac{\alpha_R}{x_0}\nabla_{\tilde{x}}^{\perp}\tilde{w}_0 + \frac{p_0}{mx_0}\left(\Theta_{\frac{\hbar}{p_0x_0}}[\tilde{V}]\tilde{\boldsymbol{w}}\right) + \frac{2}{\hbar}\alpha_R p_0\tilde{p}^{\perp}\times\tilde{\boldsymbol{w}}. \end{aligned}$$

Before we go on, we explain what happened to the pseudo differential and how the scaling affected it. We recall the representation from Lemma 3.2.27, where $\Theta_\hbar[V]w_j = (2/\mathrm{i}\hbar)(V\#_{(odd)}w_j)$ for $j\in\{0,1,2,3\}$. Therefore the index in $\Theta_\hbar$ comes from the factor $(1/\hbar)$ in front of the Moyal product. Using the above scaling, we have for $j\in\{0,1,2,3\}$

$$\Theta_\hbar[V]w_j = \frac{2}{\mathrm{i}\hbar}(V\#_{(odd)}w_j) = \frac{2E_0}{\mathrm{i}\hbar}(\tilde{V}\#_{(odd)}\tilde{w}_j) = \frac{2p_0^2x_0}{\mathrm{i}\hbar m x_0}(\tilde{V}\#_{(odd)}\tilde{w}_j) = \frac{p_0}{mx_0}\Theta_{\frac{\hbar}{p_0x_0}}[\tilde{V}]\tilde{w}_j.$$

From now we will drop the tilde notation again and identify the tilde variables with their original variables. Furthermore we introduce the Energy time scale t_E, which states how long an electron with Energy E needs to pass a device with length x_0. Further we introduce the scaled Planck constant ε , and the scaled Rashba constant α

$$t_E = \frac{mx_0}{p_0}, \qquad \varepsilon = \frac{\hbar}{x_0p_0}, \qquad \alpha = \frac{mx_0\alpha_R}{\hbar}. \tag{3.32}$$

Substituting the above into the Wigner Boltzmann equation (3.27)-(3.28), leads us to the *non dimensional Wigner Boltzmann equation*

$$\frac{t_E}{t_0}\partial_t w_0 = -\,p\cdot\nabla_x w_0 - \alpha\varepsilon\nabla_x^{\perp}\cdot\boldsymbol{w} + \Theta_\varepsilon[V]w_0, \tag{3.33}$$

$$\frac{t_E}{t_0}\partial_t \boldsymbol{w} = -\,(\nabla_x\boldsymbol{w})p - \alpha\varepsilon\nabla_x^{\perp}w_0 + \Theta_\varepsilon[V]\boldsymbol{w} + 2\alpha p^{\perp}\times\boldsymbol{w}. \tag{3.34}$$

For later use, we rewrite the above in a more concise form

$$\frac{t_E}{t_0}\partial_t W + \mathcal{T}W = 0, \tag{3.35}$$

where the transport operator $\mathcal{T}$ is defined as

$$\begin{aligned} \mathcal{T}W := &\Big((\nabla_x w_0)p + \alpha\varepsilon\nabla_x^{\perp}\cdot\boldsymbol{w} - \Theta_\varepsilon[V]w_0\Big)\,\sigma_0\\ &+\Big((\nabla_x\boldsymbol{w})p + \alpha\varepsilon\nabla_x^{\perp}w_0 - \Theta_\varepsilon[V]\boldsymbol{w} - 2\alpha p^{\perp}\times\boldsymbol{w}\Big)\cdot\boldsymbol{\sigma}. \end{aligned} \tag{3.36}$$

Notice that we changed the notation of $p\cdot\nabla_x w_0 \widehat{=} (\nabla_x w_0)p$. Since the representation of the Pauli components are unique for each hermitian matrix, the operator $\mathcal{T}$ is well defined. In particular, the chosen scaling of the Rashba constant proves necessary to obtain the correct behaviour in the semiclassical limit [BM10, BHJ]. For more detailed values of the physical quantities we refer to [KNAT02] and for the calculated non-dimensional variables in different spintronic devices table 1 in [BM10].

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The scaling we have done so far, has also an effect on the operators, where the Planck constant $\hbar$ appears. This will be important for our further work, since we need to remain dimensionless. The next examples deal with this scaling regarding the scaled Moyal product, the scaled transformed Hamiltonian, and the scaled Wigner-Weyl transformation. These calculations are standard and usually not present in literature, since its "simply" substituting $\hbar$ with ε, but we do it for the sake of completeness. For the scaling itself we use the same reference quantities as already introduced.

Example 3.2.30. (Scaled Moyal product) Let f and g be two scalar valued symbols, and define $\tilde{f}(\tilde{t},\tilde{x},\tilde{p}) := f(t_0\tilde{t}, x_0\tilde{x}, p_0\tilde{p})$ and $\tilde{g}(\tilde{t},\tilde{x},\tilde{p}) := g(t_0\tilde{t}, x_0\tilde{x}, p_0\tilde{p})$. Starting with the j-th order of the Moyal product, see (3.22), we obtain

$$\begin{aligned}(\tilde{f}\#_{(j)}\tilde{g})(\tilde{x},\tilde{p}) &= \frac{1}{(2\mathrm{i})^j(x_0p_0)^j}\sum_{|r|+|s|=j}\frac{(-1)^{|r|}}{r!s!}\partial_{\tilde{x}}^r\partial_{\tilde{p}}^s f(x_0\tilde{x},p_0\tilde{p})\partial_{\tilde{p}}^r\partial_{\tilde{x}}^s g(x_0\tilde{x},p_0\tilde{p})\\ &= \frac{1}{(2\mathrm{i})^j(x_0p_0)^j}\sum_{|r|+|s|=j}\frac{(-1)^{|r|}}{r!s!}\partial_{\tilde{x}}^r\partial_{\tilde{p}}^s \tilde{f}(\tilde{x},\tilde{p})\partial_{\tilde{p}}^r\partial_{\tilde{x}}^s \tilde{g}(\tilde{x},\tilde{p}).\end{aligned}$$

Dropping the tilde notation, using the definition of $\varepsilon = \hbar/(x_0p_0)$ we have the semiclassical expansion of the Moyal product with respect to the scaled Planck constant ε

$$f\#g = \sum_{j=0}^{\infty}\varepsilon^j f\#_{(j)}g \tag{3.37}$$

where the j-th order of the Moyal product equals

$$f\#_{(j)}g = \frac{1}{(2\mathrm{i})^j}\sum_{|r|+|s|=j}\frac{(-1)^{|r|}}{r!s!}\partial_x^r\partial_p^s f(x,p)\partial_p^r\partial_x^s g(x,p). \tag{3.38}$$

■

Example 3.2.31. (*Scaled Hamiltonian, H_ε*) Applying the scaling to the Wigner transformed Hamiltonian H given in Example 3.2.7 or Example 3.2.9 (using again the tilde notation to see the difference), we obtain

$$H(x,p) = H(x_0\tilde{x},p_0\tilde{p}) = \left(\frac{p_0^2}{m}\frac{|\tilde{p}|^2}{2} + V(x_0\tilde{x})\right)\sigma_0 + \alpha_R p_0\tilde{p}^\perp\cdot\boldsymbol{\sigma}$$

Thanks to the definitions of $E_0, \tilde{V}, \varepsilon, \alpha$ we define the scaled transformed Hamiltonian H_ε

$$H(x_0\tilde{x},p_0\tilde{p}) = \left(E_0\frac{|\tilde{p}|^2}{2} + E_0\tilde{V}(\tilde{x})\right)\sigma_0 + E_0\alpha\varepsilon\tilde{p}^\perp\cdot\boldsymbol{\sigma} =: E_0H_\varepsilon(\tilde{x},\tilde{p})$$

The scaled transformed Hamiltonian is explicit given by (without tilde notation)

$$H_\varepsilon(x,p) = \left(\frac{|p|^2}{2} + V(x)\right)\sigma_0 + \alpha\varepsilon p^\perp\cdot\boldsymbol{\sigma} \tag{3.39}$$

■

Example 3.2.32. (*Scaled Wigner Transformation*) Before we can go to scaling the transformation, we need to put the cart before the horse, because a scaled argument is needed.

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Let therefore ϱ be a density operator on $\mathrm{L}^2(\mathbb{R}^2, \mathbb{C}^2)$ with unique integral kernel $\rho \in \mathrm{L}^2(\mathbb{R}^2 \times \mathbb{R}^2, \mathbb{C}^{2\times 2})$. Define the scaled wave function $\tilde{\psi}(\tilde{x}) := \psi(x_0\tilde{x})$ for $\psi \in \mathrm{L}^2(\mathbb{R}^2, \mathbb{C}^2)$, then we get

$$\varrho(\psi)(x_0\tilde{x}) = \int_{\mathbb{R}^2} \rho\left(x_0\tilde{x}, x_0\frac{y}{x_0}\right)\psi\left(x_0\frac{y}{x_0}\right)dy = \int_{\mathbb{R}^2} x_0^2\rho\left(x_0\tilde{x}, x_0\tilde{y}\right)\psi\left(x_0\tilde{y}\right)d\tilde{y}.$$

Hence it makes sense to define the scaled integral kernel as $\tilde{\rho}(\tilde{x},\tilde{y}) := x_0^2\rho(x_0\tilde{x}, x_0\tilde{y})$ and with that we define the scaled density operator

$$\varrho(\psi)(x_0\tilde{x}) = \int_{\mathbb{R}^2} x_0^2\rho\left(x_0\tilde{x}, x_0\tilde{y}\right)\psi\left(x_0\tilde{y}\right)d\tilde{y} = \int_{\mathbb{R}^2} \tilde{\rho}(\tilde{x},\tilde{y})\tilde{\psi}(\tilde{y})d\tilde{y} =: \tilde{\varrho}(\tilde{\psi})(\tilde{x}).$$

Let $W(x,p) = \mathcal{W}(\varrho)(x,p)$ and recall the scaled Wigner function $\tilde{W}(\tilde{x},\tilde{p}) := W(x_0\tilde{x}, p_0\tilde{p})$. Looking at the latter, we obtain with the definition of $\mathcal{W}$, see (3.5),

$$\tilde{W}(\tilde{x},\tilde{p}) = W(x_0\tilde{x}, p_0\tilde{p}) = \int_{\mathbb{R}^2} \rho\left(x_0\left(\tilde{x} + \frac{\eta}{2x_0}\right), x_0\left(\tilde{x} - \frac{\eta}{2x_0}\right)\right) e^{-\mathrm{i}((\eta/x_0)\cdot\tilde{p})x_0p_0/\hbar}d\eta$$

Using the transformation rule and the definition of $\tilde{\rho}$ and ε, see (3.32), we obtain

$$\begin{aligned}\tilde{W}(\tilde{x},\tilde{p}) &= \int_{\mathbb{R}^2} x_0^2\rho\left(x_0\left(\tilde{x} + \frac{\tilde{\eta}}{2}\right), x_0\left(\tilde{x} - \frac{\tilde{\eta}}{2}\right)\right) e^{-\mathrm{i}(\tilde{\eta}\cdot\tilde{p})/\varepsilon}d\tilde{\eta} \\ &= \int_{\mathbb{R}^2} \tilde{\rho}\left(\tilde{x} + \frac{\tilde{\eta}}{2}, \tilde{x} - \frac{\tilde{\eta}}{2}\right) e^{-\mathrm{i}(\tilde{\eta}\cdot\tilde{p})/\varepsilon}d\tilde{\eta}.\end{aligned}$$

Therefore we see that the *scaled Wigner transformation* of a scaled density operator $\tilde{\varrho}$ is given by

$$\tilde{\mathcal{W}}(\tilde{\varrho})(\tilde{x},\tilde{p}) = \int_{\mathbb{R}^2} \tilde{\rho}\left(\tilde{x} + \frac{\tilde{\eta}}{2}, \tilde{x} - \frac{\tilde{\eta}}{2}\right) e^{-\mathrm{i}(\tilde{\eta}\cdot\tilde{p})/\varepsilon}d\tilde{\eta}. \tag{3.40}$$

With similar calculations we obtain that the *scaled Weyl quantization* is given by

$$\tilde{\mathcal{W}}^{-1}(\tilde{W})(\tilde{x},\tilde{y}) = \frac{1}{(2\pi\varepsilon)^2}\int_{\mathbb{R}^2} \tilde{W}\left(\frac{\tilde{x}+\tilde{y}}{2}, \tilde{p}\right) e^{\mathrm{i}(\tilde{x}-\tilde{y})\cdot\tilde{p}/\varepsilon}d\tilde{p}. \tag{3.41}$$

■

Remark 3.2.33. With the above examples we make clear that we could have scaled at any point. For example we see in [BM10] that scaling first the von Neumann equation (with our notation, without the time scaling and collision operator) and dropping the tilde notation, yields *non dimensional von Neumann equation*

$$\mathrm{i}\varepsilon\frac{t_E}{t_0}\partial_t\varrho = [\mathcal{H}_\varepsilon, \varrho]. \tag{3.42}$$

$\mathcal{H}_\varepsilon$ is the scaled Hamiltonian such that $\mathcal{H} = E_0\mathcal{H}_\varepsilon$, and is given by

$$\mathcal{H}_\varepsilon = \left(-\frac{\varepsilon^2}{2}\Delta_{x_1,x_2} + V(x)\right)Id - \varepsilon^2\alpha\begin{pmatrix} 0 & i\partial_{x_2} - \partial_{x_1} \\ i\partial_{x_2} + \partial_{x_1} & 0\end{pmatrix}. \tag{3.43}$$

Applying the scaled Wigner transformation (3.40) to the non dimensional von Neumann equation (3.42), results into

$$\mathrm{i}\varepsilon\frac{t_E}{t_0}\partial_t W = [H_\varepsilon, W]_\#,$$

where in the above we have the scaled Wigner function W, the scaled transformed Hamiltonian H_ε and the commutator with respect to the scaled Moyal product. Revolving the above equation as in Section 3.2.5 using the scaled versions, will lead us to the same non dimensional Wigner equation as obtained in (3.33)-(3.34). ■

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3.3. The Quantum Maximum Entropy Principle and Quantum Maxwellian

Before specifying the equilibrium we discuss roughly which *quantities* collisions should conserve. First of all we want that the number of particles in the system remains the same and since we want to observe spin, we assume that collisions do not affect the spin of the electrons. Since the collisions we are considering are in a thermal bath at a given temperature (e.g. with a phonon bath), we cannot expect that they conserve momentum nor energy. Hence we expect that collisions only conserve the particle density and the spin densities. To get there we take a small digression for better understanding.

3.3.1. Operator Trace and Definition of the Macroscopic Densities

The interpreted expected value of a physical observable, represented by the operator $\mathcal{A}$, when the system is in the state ϱ, is given by $\mathrm{Tr}(\mathcal{A}\varrho)$ (for details see [DR03], [WZ14], [Cas08]). We explain briefly the idea of the operator trace applied to a density operator ϱ and we consider for the beginning the scalar case. Let therefore $(\phi_k)_{k\in\mathbb{N}}$ be an orthonormal basis (ONB) of $\mathrm{L}^2(\mathbb{R}^2,\mathbb{C})$, recall that the operator trace of an operator $\mathcal{A}$ on $\mathrm{L}^2(\mathbb{R}^2,\mathbb{C})$ is given by

$$\mathrm{Tr}(\varrho) = \sum_{k=1}^{\infty} (\phi_k, \mathcal{A}(\phi_k))_{\mathrm{L}^2(\mathbb{R}^2,\mathbb{C})},$$

where $(.,.)_{\mathrm{L}^2(\mathbb{R}^2,\mathbb{C})}$ denotes the scalar product in $\mathrm{L}^2(\mathbb{R}^2,\mathbb{C})$. Let ϱ be a density operator on $\mathrm{L}^2(\mathbb{R}^2,\mathbb{C})$, describing a mixed state, it can be written as

$$\varrho(\psi)(x) = \sum_{k=1}^{\infty} p_k \phi_k(x) \, (\phi_k, \psi)_{\mathrm{L}^2(\mathbb{R}^2,\mathbb{C})}, \qquad \forall \psi \in \mathrm{L}^2(\mathbb{R}^2,\mathbb{C}),$$

where $p_k \in [0,1]$ for all $k \in \mathbb{N}$, and $\sum_{k=1}^{\infty} p_k = 1$. The values p_k can be interpreted as the possibility for a state ψ to change into the state ϕ_k and if ϱ depends on time, all p_k depend on time as well. If ϱ would be a *pure state*, the above would reduce to $\varrho(\psi)(x) \widehat{=} \phi_k(x)(\phi_k,\psi)$. With the previous work, we see why ϱ has trace one

$$\mathrm{Tr}(\varrho) = \sum_{k=1}^{\infty} (\phi_k, \varrho(\phi_k))_{\mathrm{L}^2(\mathbb{R}^2,\mathbb{C})} = \sum_{k=1}^{\infty} p_k \, (\phi_k, \phi_k)_{\mathrm{L}^2(\mathbb{R}^2,\mathbb{C})} = \sum_{k=1}^{\infty} p_k = 1.$$

Now if ϱ has an integral kernel $\rho(x,y)$ as representative, it should have the form

$$\rho(x,y) = \sum_{k=1}^{\infty} p_k \phi(x)\overline{\phi(y)}, \qquad \text{such that } \varrho(\psi)(x) = \int_{\mathbb{R}^2} \rho(x,y)\psi(y)dy, \qquad \forall \psi \in \mathrm{L}^2(\mathbb{R}^2,\mathbb{C}).$$

Looking back at the operator trace of ϱ, since $(\phi_k)_{k\in\mathbb{N}}$ is an ONB, we obtain formally

$$\mathrm{Tr}(\varrho) = \sum_{k=1}^{\infty} p_k \int_{\mathbb{R}^2} |\phi_k(x)|^2 dx = \int_{\mathbb{R}^2} \sum_{k=1}^{\infty} p_k \phi(x)\overline{\phi(x)}dx = \int_{\mathbb{R}^2} \rho(x,x)dx.$$

Now let $w(x,p) = \mathcal{W}(\varrho)(x,p)$ be the corresponding Wigner function (3.5) in the scalar case, then we obtain with the Weyl-quantization, $\mathcal{W}^{-1}$ given in (3.4), that the operator trace is also given by

$$\mathrm{Tr}(\varrho) = \int_{\mathbb{R}^2} \rho(x,x)dx = \frac{1}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} w(x,p)dpdx.$$

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Looking at two density operators ϱ_1, ϱ_2 with two integral kernels ρ_1, ρ_2 and corresponding Wigner functions w_1, w_2, we recall that the Wigner transform of the operator product $\varrho_1\varrho_2$ is given by $\mathcal{W}(\varrho_1\varrho_2) = w_1\#w_2$ (see Lemma 3.2.12). Since the Moyal product integrated with respect to space and momentum equals the integral of the product (see identity (3.17)), we have that

$$\begin{aligned}\mathrm{Tr}(\varrho_1\varrho_2) &= \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \rho_1(x,y)\rho_2(y,x)dydx = \frac{1}{(2\pi\hbar)^2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2}(w_1\#w_2)(x,p)dpdx = \\ &= \frac{1}{(2\pi\hbar)^2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} w_1(x,p)w_2(x,p)dpdx\end{aligned}$$

Next step is to understand what happens, if we apply the trace to density operators on $\mathrm{L}^2(\mathbb{R}^2,\mathbb{C}^2)$. Define therefore the set

$$\mathfrak{B} := \{e_l\phi_k : l \in \{1,2\},\ k \in \mathbb{N}\},$$

which is an ONB of $\mathrm{L}^2(\mathbb{R}^2,\mathbb{C}^2)$. Let $\mathcal{A} = (\mathcal{A}_{ij})_{i,j\in\{1,2\}}$ be an operator on $\mathrm{L}^2(\mathbb{R}^2,\mathbb{C}^2)$ with $\mathcal{A}_{ij}$ being an operator on $\mathrm{L}^2(\mathbb{R}^2,\mathbb{C})$. Then formally we have

$$\begin{aligned}\mathrm{Tr}_{(\mathrm{L}^2(\mathbb{R}^2,\mathbb{C}^2))}(\mathcal{A}) &= \sum_{l=1}^{2}\sum_{k=1}^{\infty}(e_l\phi_k, \mathcal{A}(e_l\phi_k))_{\mathrm{L}^2(\mathbb{R}^2,\mathbb{C}^2)} = \sum_{k=1}^{\infty}\left(\phi_k, \sum_{l=1}^{2} e_l^T\mathcal{A}e_l(\phi_k)\right)_{\mathrm{L}^2(\mathbb{R}^2,\mathbb{C}^2)} \\ &= \sum_{k=1}^{\infty}(\phi_k, \mathrm{tr}(\mathcal{A})(\phi_k))_{\mathrm{L}^2(\mathbb{R}^2,\mathbb{C})} = \mathrm{Tr}_{(\mathrm{L}^2(\mathbb{R}^2,\mathbb{C}))}(\mathrm{tr}(\mathcal{A})),\end{aligned}$$

where the lower indices indicates in which space we are taking the operator trace (will be dropped from now on) and "tr" denotes the usual matrix trace. For a density operator ϱ on $\mathrm{L}^2(\mathbb{R}^2,\mathbb{C}^2)$ with integral kernel $\rho(x,y)$ and Wigner function $W(x,p) = \mathcal{W}(\varrho)(x,p)$, we obtain with using the definition of the Weyl quantization (see (3.4))

$$\mathrm{Tr}(\varrho) = \int_{\mathbb{R}^2}\mathrm{tr}(\rho)(x,x)dx = \frac{1}{(2\pi\hbar)^2}\,\mathrm{tr}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} W(x,p)dpdx. \tag{3.44}$$

Looking especially at two density operators ϱ_1, ϱ_2 on $\mathrm{L}^2(\mathbb{R}^2,\mathbb{C}^2)$ and their corresponding Wigner functions W_1, W_2, we obtain thanks again to the integral identity of the Moyal product (see (3.17))

$$\mathrm{Tr}(\varrho_1\varrho_2) = \frac{1}{(2\pi\hbar)^2}\,\mathrm{tr}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} W_1(x,p)W_2(x,p)dpdx. \tag{3.45}$$

Next we introduce the *macroscopic particle density* of our electron ensemble and let therefore ϱ be again the solution to the von Neumann equation (3.2). As mentioned in Remark 3.1.2 we cannot obtain a function which gives us direct information about the distribution of the particles. Looking at

$$\mathrm{Tr}(\mathbb{1}_\Omega\varrho) = \mathrm{tr}\int_\Omega \rho(x,x)dx$$

gives us the expected value of the electron density in Ω. Hence (not rigorous) we can interpret this as the "*macroscopic particle density*" or "*charge density*" and define therefore

$$n_0(t,x) := \mathrm{tr}(\rho)(t,x,x). \tag{3.46}$$

This is one point where we see why the Wigner formalism gives the impression of phase-space behaviour. Using the Pauli algebra and the trace identity (3.44) we obtain

$$\mathfrak{n}_0(t,x) = \operatorname{tr}(\varrho)(t,x,x) = \frac{1}{(2\pi\hbar)^2}\operatorname{tr}\int_{\mathbb{R}^2} W(t,x,p)dp = \frac{1}{(2\pi\hbar)^2}\int_{\mathbb{R}^2}\operatorname{tr}(\sigma_0 W(t,x,p))dp = \\ = \frac{2}{(2\pi\hbar)^2}\int_{\mathbb{R}^2} w_0(t,x,p)dp.$$

The above looks familiar, up to the constant, to the common definition of the particle density from the Boltzmann picture (see for comparison Section 1.3 or Chapter 2).

Next we need the macroscopic description of the spin. Measuring spin, when we are in the state ϱ, is represented by the spin operators $\mathcal{S}_{x_1}, \mathcal{S}_{x_2}, \mathcal{S}_{x_3}$ which are given (up to a constant) by the Pauli matrices $\sigma_1, \sigma_2, \sigma_3$ respectively. Similarly as for the charge density $\mathfrak{n}_0$ we can define the *macroscopic spin densities*

$$\mathfrak{n}_j(t,x) := \operatorname{Tr}(\mathcal{S}_{x_j}\varrho) = \operatorname{tr}(\sigma_j\rho)(t,x,x) = \frac{2}{(2\pi\hbar)^2}\int_{\mathbb{R}^2} w_j(x,p)dp, \qquad \text{for } j \in \{1,2,3\}.$$

To have a better overview we pack the achieved into the following definition.

Definition 3.3.1. *Let ϱ be the solution to the von Neumann equation* (3.2) *and $\sigma_0, \sigma_1, \sigma_2, \sigma_3$ denote the Pauli matrices. Then we define as the macroscopic charge density $\mathfrak{n}_0$ and the macroscopic spin densities $\mathfrak{n}_j$ in direction of x_j*

$$\mathfrak{n}_j(t,x) = \operatorname{tr}(\sigma_j\rho)(t,x,x), \qquad \textit{for } j \in \{0,1,2,3\}.$$

Let $W = \mathcal{W}(\varrho)$ be the Wigner transform of the solutio ϱ, then we define the belonging Wigner macroscopic charge density n_0 and the Wigner macroscopic spin densities n_j in direction x_j as

$$n_j(t,x) := \int_{\mathbb{R}^2} w_j(t,x,p)dp, \qquad \textit{for } j \in \{0,1,2,3\},$$

where w_k is given by the matrix trace $(1/2)\operatorname{tr}(\sigma_j W)$. The scaled macroscopic densities are given via the scaled integral kernels/Wigner functions respectively.

Remark 3.3.2. At this point we mention that we will focus on the Wigner macroscopic densities, since we also work mostly with the Wigner formalism. Therefore we drop the term "Wigner" and will just refer to them as macroscopic densities. Also for the sake of simplicity we drop the notation on the time dependence and only mention it, when we think its necessary. ■

Remark 3.3.3. We can interpret that the quantities n_1, n_2, n_3 represent the local averages of the spin components with respect to p in the x_1, x_2, x_3-directions, respectively (see Figure 3.4).

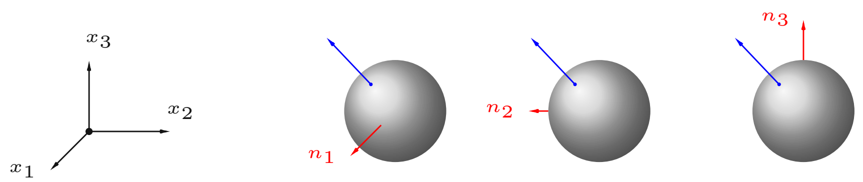

Figure 3.4.: **(Blue):** Spin of the electron, **(Red):** Projections on the x_j directions.

■

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3.3.2. Entropy, Equilibrium and a Smallness Assumption

The local equilibrium state of our system is assumed to be the solution to the minimization of an entropy functional, with the constraint of given macroscopic densities (i.e. n_k, $k = 0, 1, 2, 3$). This is called *(quantum) maximum entropy principle (not.:QMEP)* and can be interpreted as follows: the collisions drive the system towards the most probable microscopic state compatible with the observed macroscopic densities. The convenient entropy functional to be used in the diffusion regime (no momentum nor energy conservation) is the *quantum free energy*, see [BM10, DMR05]. It is given by

$$\mathcal{G}(\varrho) = \mathrm{Tr}\{k_B T_0 \varrho \ln(\varrho) - \varrho + \mathcal{H}\varrho\},$$

where "Tr" denotes the operator trace, k_B the Boltzmann constant, T_0 the reference temperature, ln is the operator logarithm and $\mathcal{H}$ is the Hamiltonian (see (3.1)). The quantum free energy in its non-dimensional form (again using tilde notation to differ), such that $E_0\tilde{G}(\tilde{\varrho}) = \mathcal{G}(\varrho)$, is then

$$\tilde{\mathcal{G}}(\tilde{\varrho}) = \mathrm{Tr}\{\tilde{\varrho}\ln(\tilde{\varrho}) - \tilde{\varrho} + \mathcal{H}_\varepsilon\tilde{\varrho}\},$$

where ε is the scaled Planck constant and $\mathcal{H}_\varepsilon$ is the non-dimensional form of the Hamiltonian $\mathcal{H}$, see (3.43). Note that the operator logarithm is well-defined for a positive-definite density operator.
Fur further progress we need now the definitions of the Wigner counterparts of the operator-exponential and logarithm.

Definition 3.3.4. *Let ϱ be a positive-definite density operator, define $W := \mathcal{W}(\varrho)$ the Wigner transform of ϱ and denote the Weyl-quantization with $\mathcal{W}^{-1}$, then we can define the quantum exponential and quantum logarithm by*

$$\mathcal{E}xp(W) := \mathcal{W}(\exp(\mathcal{W}^{-1}(W))), \qquad \mathcal{L}og(W) := \mathcal{W}(\log(\mathcal{W}^{-1}(W))) \tag{3.47}$$

where "exp" and "log" are the operator exponential and operator logarithm respectively. The scaled versions are defined in the same way by using the scaled versions of $\mathcal{W}, \mathcal{W}^{-1}$, see (3.40)*, on the scaled Wigner function.*

To obtain the quantum free energy in the Wigner picture, we apply the Trace-Product identity (3.45) and Definition 3.3.4 to $\mathcal{G}(\varrho)$

$$\begin{aligned}\mathcal{G}(\varrho) =& \frac{1}{(2\pi\hbar)^2}\,\mathrm{tr}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} E_0(W(x,p)\mathcal{L}og(W)(x,p) - W(x,p)) + H(x,p)W(x,p)dpdx \\ =:& \mathcal{E}(W).\end{aligned}$$

Scaling $\mathcal{E}(W)$ or using the scaled Weyl-quantization, see (3.41) on $\tilde{\mathcal{G}}(\tilde{\varrho})$ would lead to the same result, ergo the scaled entropy for the scaled Wigner function is given by

$$\begin{aligned}\frac{\mathcal{E}(W)}{E_0} =& \frac{1}{E_0(2\pi\hbar)^2}\,\mathrm{tr}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} E_0(W(x,p)\mathcal{L}og(W)(x,p) - W(x,p)) + H(x,p)W(x,p)dpdx \\ =& \frac{1}{(2\pi\varepsilon)^2}\,\mathrm{tr}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \tilde{W}(\tilde{x},\tilde{p})\tilde{\mathcal{L}og}(\tilde{W})(\tilde{x},\tilde{p}) - \tilde{W}(\tilde{x},\tilde{p}) + H_\varepsilon(\tilde{x},\tilde{p})\tilde{W}(\tilde{x},\tilde{p})d\tilde{p}d\tilde{x} \\ =:& \tilde{\mathcal{E}}(\tilde{W})\end{aligned}$$

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From now on we will only use the scaled entropy and scaled quantities, and drop therefore the tilde notation. Recalling the definition of the macroscopic densities (see Definition 3.3.1), we see the following relation between them (in the scaled version now)

$$\mathscr{n}_k = \frac{2}{(2\pi\varepsilon)^2} n_k, \qquad \text{for } k \in \{0,1,2,3\}.$$

As mentioned in the beginning, we want to minimize the entropy $\mathcal{E}$ under the condition that the macroscopic densities are conserved. Hence for given densities $\mathscr{n}_0, \mathscr{n}_1, \mathscr{n}_2, \mathscr{n}_3$ a symbol M is a minimizer, if it fulfills for all symbols W and for $k \in \{0,1,2,3\}$

$$\mathcal{E}(M) \le \mathcal{E}(W), \qquad \frac{2}{(2\pi\varepsilon)^2} \int_{\mathbb{R}^2} \operatorname{tr}(\sigma_k M(x,p))dp = \mathscr{n}_k(x) = \frac{2}{(2\pi\varepsilon)^2} n_k,$$

Since minimizing is independent of constants, we can drop the constant in $\mathcal{E}$ and redefine the entropy

$$\mathcal{E}(W) \coloneqq \operatorname{tr} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} W(x,p)\mathcal{L}og(W(x,p)) - W(x,p) + H_\varepsilon(x,p)W(x,p)dxdp. \tag{3.48}$$

Since minimizing the above with the constraints turns out to be extremely difficult to solve (even formally), but we found a way to reduce the amount of work by adjusting them a bit (which will be discussed in the remark below). For the sake of simplicity we will use only the Wigner macroscopic densities and state now precisely the constrained minimization problem corresponding to the quantum maximum entropy principle.

Problem 3.3.5 (Quantum Maximum Entropy Principle)**.** *Let n_0, n_1, n_2, n_3 be assigned, with*

$$n_0 > 0, \qquad n_1, n_2, n_3 \in \mathbb{R}, \qquad \varepsilon^2(n_1^2 + n_2^2 + n_3^2) < n_0^2, \qquad \boldsymbol{n} \coloneqq (n_1, n_2, n_3)^T. \tag{3.49}$$

Find a Wigner function W such that $\mathcal{E}(W)$ is minimal among all symbols $W = w_0\sigma_0 + \boldsymbol{w}\cdot\boldsymbol{\sigma}$ satisfying $\mathcal{W}^{-1}(W) > 0$ and

$$\langle w_0 \rangle = n_0, \qquad \langle \boldsymbol{w} \rangle = \varepsilon \boldsymbol{n}, \tag{3.50}$$

where $\langle . \rangle$ denotes the integral with respect to p over $\mathbb{R}^2$.

Remark 3.3.6. The assumptions of Problem 3.3.5 need some explanations.

1. The assumption $\mathcal{W}^{-1}(W) > 0$ ensures that the quantum logarithm is well-defined. Since $\mathcal{W}^{-1}(W) > 0$ implies that $n_0 > 0$, the latter must be implied as compatibility constraint on n_0.

2. Primarily the conditions (3.49) are of mathematical nature. Recalling that a hermitian matrix is positive definite if and only if its principal minors are positive. Looking at the determinant of $N \coloneqq n_0\sigma_0 + \varepsilon\boldsymbol{n}\cdot\boldsymbol{\sigma}$ ($n_0, \boldsymbol{n}$ from (3.49)), Pauli-algebra yields

$$\det N = \det \begin{pmatrix} n_0 + \varepsilon n_3 & \varepsilon(n_1 - in_2) \\ \varepsilon(n_1 + in_2) & n_0 - \varepsilon n_3 \end{pmatrix} = {n_0}^2 - \varepsilon^2 |\boldsymbol{n}|^2$$

   and hence $\det N > 0$ if and only if $\varepsilon^2|\boldsymbol{n}|^2 < {n_0}^2$. We obtain also

$$\varepsilon^2|\boldsymbol{n}|^2 < {n_0}^2 \implies \varepsilon^2|n_3|^2 < {n_0}^2,$$

   which implies together with $n_0 > 0$ that $0 < \varepsilon n_3 + n_0$. Therefore the conditions (3.49) ensure the assigned matrix is positive definite such that Problem 3.3.6 is well stated.

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3. Let ϱ be the solution to the non dimensional von Neumann equation (3.42) and let $W := \mathcal{W}(\varrho)$ be the corresponding Wigner function and solution to the non dimensional Wigner Boltzmann equation (3.35). The macroscopic density matrix N is then given via the integral of W, i.e. $\langle W \rangle = N$. For now let $n_0, \tilde{n}_1, \tilde{n}_2, \tilde{n}_3$ be the corresponding Pauli-components of N and define $\tilde{\boldsymbol{n}} := (\tilde{n}_1, \tilde{n}_2, \tilde{n}_3)$ such that we can write $N = n_0\sigma_0 + \tilde{\boldsymbol{n}} \cdot \boldsymbol{\sigma}$. If the system is in a well mixed state, we obtain that ${n_0}^2 > \tilde{n}_1^2 + \tilde{n}_2^2 + \tilde{n}_3^2$ and equality holds for pure states (ϱ is the projection one the one-dimensional space spanned by the wave function of the system).

   From now on we will assume, as in Problem 3.3.5, that the spin densities are of order one with respect to ε, which means there exists densities n_1, n_2, n_3 with $\boldsymbol{n} := (n_1, n_2, n_3)$, such that $\tilde{\boldsymbol{n}} = \varepsilon \boldsymbol{n}$. This assumption provides two effects:

   - The condition $\varepsilon^2 |\boldsymbol{n}|^2 < n_0$, ensures that we are in a well mixed state, i.e. $|\tilde{\boldsymbol{n}}|^2 = \varepsilon^2 |\boldsymbol{n}|^2 < |n_0|^2$. The physical meaning of such assumption is that the spin direction of the electron is random and a small polarisation emerges from the average.
   - Our assumption on N will allow us to perform a more practical approximation of the quantum Maxwellian, see Section 3.6, than the more general, see for comparison Section 3.3.3. To avoid confusion we will only use the spin densities $\boldsymbol{n}$, which means that we shall write $N = n_0\sigma_0 + \varepsilon \boldsymbol{n} \cdot \boldsymbol{\sigma}$.

   Quick note here: The assumption affects only the macroscopic density matrix N, which means that W is still of the form $W = w_0\sigma_0 + \boldsymbol{w} \cdot \boldsymbol{\sigma}$ and that $\langle \boldsymbol{w} \rangle = \varepsilon \boldsymbol{n}$.

4. Notice that in the dynamical system the macroscopic densities n_0 and $\boldsymbol{n}$ are also dependent on the space variable x and time variable t. Since the notation is quite heavy we drop for the sake of simplicity the notation of the dependence on t.

■

Notation 3.3.7. *According to the notation introduced above, the integral over $\mathbb{R}^2$ with respect to the momentum p will be denoted from now on as $\langle . \rangle$.*

To show the existence of a solution to Problem 3.3.5 is, already in the 1D case, a very difficult task [MP10, MP11] and would exceed the capacity of this thesis, therefore we assume that the solution exists and show that it must have a particular form. We shall call the solution to Problem 3.3.5 the *quantum Maxwellian* of the system, and denote it as $\mathcal{M}$.

Theorem 3.3.8. *If Problem 3.3.5 has a solution then it is necessarily of the form*

$$\mathcal{M}(x,p) = \mathcal{E}xp \left(-H_\varepsilon(x,p) + \tilde{a}_0(x)\sigma_0 + \varepsilon \left(\sum_{j=1}^{3} a_j(x)\sigma_j \right) \right), \tag{3.51}$$

where $\tilde{a}_0, a_1, a_2, a_3$ are suitable, real, Lagrange multipliers. The function $\mathcal{M}(x,p)$ also fulfills the constraints

$$n_0(x) = \frac{1}{2} \left\langle \operatorname{tr}\left(\mathcal{M}(x,\cdot)\sigma_0\right) \right\rangle, \qquad \varepsilon n_j(x) = \frac{1}{2} \left\langle \operatorname{tr}\left(\mathcal{M}(x,\cdot)\sigma_j\right) \right\rangle, \quad \textit{for } j \in \{1,2,3\}, \tag{3.52}$$

where we recall that $\operatorname{tr}(.)$ *is the matrix trace.*

The proof to this theorem is quite long and will be split up into three parts, but before we prove it, we make some small statements.

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Remark 3.3.9. Notice that $\mathcal{M}$ is also a function time, t, in the dynamical problem, through the quantities $n_0(t,x)$ and $\boldsymbol{n}(t,x)$ To avoid over-notation and to show the dependence on the constraints we will denote the quantum Maxwellian simply with $\mathcal{M}(N)$. Also notice that $\mathcal{M}(N)$ is a hermitian matrix and possesses real Pauli components

$$m_j(N) = \tfrac{1}{2}\operatorname{tr}(\mathcal{M}(N)\sigma_j), \quad \text{for } j \in \{0,1,2,3\}, \qquad \text{where we define } \boldsymbol{m} := (m_1, m_2, m_3).$$

■

We define the hermitian *matrix of Lagrange multipliers*

$$\tilde{A}(x) := \tilde{a}_0(x)\sigma_0 + \varepsilon \boldsymbol{a}(x)\cdot\boldsymbol{\sigma}, \qquad \text{where } \boldsymbol{a}(x) := (a_1(x), a_2(x), a_3(x))^T \tag{3.53}$$

The matrix of Lagrange multipliers $\tilde{A}$ and its Pauli components will also depend in the dynamical problem on the time variable t. Again we will drop this dependence and the dependence on x, and mention it when we think it is important.
Adding the Pauli components of the Hamiltonian H_ε and the Lagrangian multiplier, we introduce a handy notation:

$$-H_\varepsilon(x,p) + \tilde{A}(x) = h_0(x,p)\sigma_0 + \varepsilon \boldsymbol{h}_1(x,p)\cdot\boldsymbol{\sigma}, \tag{3.54}$$

where we define and redefine the following

$$a_0(x) := \tilde{a}_0(x) - V(x), \quad h_0(x,p) := -\frac{|p|^2}{2} + a_0(x), \quad \boldsymbol{h}_1(x,p) := \boldsymbol{a}(x) - \alpha p^\perp. \tag{3.55}$$

As already mentioned it is unknown if a solution to Problem 3.3.5 exists and in which sense it is a solution, and therefore it makes sense to only give a formal proof to Theorem 3.3.8. Doing this proof formally is already an tremendous work and we will see that the appearance of the scaled Planck constant ε in the quantum Maxwellian (3.51) is not clear at all, but can be seen as a more or less direct consequence of our smallness assumption on the polarization of $N = n_0\sigma_0 + \varepsilon\boldsymbol{n}\cdot\boldsymbol{\sigma}$.

3.3.3. Formal Proof of Theorem 3.3.8

This proof will be divided in three parts. First we prove a weaker result, where we show that the Lagrangian multiplier $\tilde{A}$ in the Maxwellian $\mathcal{M}(N)$ has no constant ε in front of the $\boldsymbol{\sigma}$ part.

Theorem 3.3.10. *If Problem 3.3.5 has a solution then it has to be of the form*

$$\mathcal{M}(N) = \mathcal{E}xp\left(-H_\varepsilon(x,p) + \tilde{A}(x)\right) \tag{3.56}$$

where $\tilde{A}(x) = \tilde{a}_0(x)\sigma_0 + \boldsymbol{a}(x)\cdot\boldsymbol{\sigma}$. *The solution also fulfils the constraints*

$$\langle m_0(N)\rangle = n_0, \qquad \langle m_j(N)\rangle = \varepsilon n_j, \quad j \in \{1,2,3\} \tag{3.57}$$

where $\langle . \rangle$ *denotes the integration over* $\mathbb{R}^2$ *with respect to* p.

In the second part we roughly introduce the concept of the semiclassical expansion (details follow in Section 3.6) and calculate the general zeroth order of the quantum Maxwellian. The last part will be used to proof that the Lagrange matrix is actually of the form $\tilde{A}(x) = \tilde{a}_0(x)\sigma_0 + \varepsilon\boldsymbol{a}(x)\cdot\boldsymbol{\sigma}$, by using the constraints $\langle \boldsymbol{m}(N)\rangle = \varepsilon\boldsymbol{n}$. If clear from the context we will drop from now on the dependence on various variables, to avoid over-notation.

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Part One: Proof of Theorem 3.3.10:

This part follows the lines of analogous proofs in literature, see for example [DMR05, DR03] and [BF10]), where we mostly rely on the latter. Let us provisionally define the matrix of Lagrange multipliers

$$\tilde{A}(t,x) = \tilde{a}_0(t,x)\sigma_0 + \boldsymbol{a}(t,x) \cdot \boldsymbol{\sigma}, \tag{3.58}$$

where $\tilde{a}_0, a_1, a_2, a_3$ are real valued functions , therefore $\tilde{A}$ is a hermitian matrix. Consider the functional

$$\mathcal{L}(W,\tilde{A}) := \operatorname{tr}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} (W\mathcal{L}og(W) - W + H_\varepsilon W)\,dxdp - \operatorname{tr}\int_{\mathbb{R}^2} \tilde{A}(x)\,(\langle W\rangle - N)\,dx \tag{3.59}$$

where "tr" is the matrix trace. We note that $\mathcal{L}$ is composed of a free-energy part

$$\mathcal{E}(W) = \operatorname{tr}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} (W\mathcal{L}og(W) - W + H_\varepsilon W)\,dxdp, \tag{3.60}$$

and a Lagrange multiplier part, coming from the constraints

$$\operatorname{tr}\int_{\mathbb{R}^2} \tilde{A}(x)\,(\langle W\rangle - N)\,dx = 2\int_{\mathbb{R}^2} [\tilde{a}_0(\langle w_0\rangle - n_0) + \boldsymbol{a}\cdot(\langle \boldsymbol{w}\rangle - \varepsilon\boldsymbol{n})]\,dx.$$

By standard variational methods, the constrained minimization Problem 3.3.5 is equivalent to the saddle point problem for the functional (3.59), which means that the constrained minimizer $\mathcal{M}(N)$ must satisfy

$$\mathcal{E}(\mathcal{M}(N)) = \min_W \max_{\tilde{A}} \mathcal{L}(W,\tilde{A}) = \max_{\tilde{A}} \min_W \mathcal{L}(W,\tilde{A}). \tag{3.61}$$

To avoid misunderstanding in the upcoming notation we stress the fact that "Tr" denotes the operator trace and "tr" the matrix trace and that δ_ν denotes the Gâteaux derivative at the point ν. We now cite [BF10] page 304, where we decided to substitute the operator S with ϱ.

Lemma 3.3.11. *Let ϱ be a density operator. Putting $f(\varrho) = \varrho\ln(\varrho) - \varrho$, the Gâteaux derivative δ_ϱ of $\varrho \mapsto \operatorname{Tr}\{f(\varrho)\}$ at the point ϱ is given by*

$$\delta_\varrho \operatorname{Tr}\{f\}(\xi) = \operatorname{Tr}\{f'(\varrho)\xi\} = \operatorname{Tr}\{\ln(\varrho)\xi\}, \tag{3.62}$$

for all perturbation ξ of the density operator.

Proof. We refer to [DR03] Lemma 3.3, where the proof is in the appendix, and mention that the notation is changed to $f \widehat{=} H$, $\xi \widehat{=} \delta\varrho$ and the operator $\delta_\varrho \operatorname{Tr}\{f\} \widehat{=} \frac{\delta H}{\delta \varrho}$. □

From the correspondence $W \mapsto \varrho_W$ between Wigner functions and density operators, and using the scaled identities (3.44)-(3.45)

$$\operatorname{Tr}\{\varrho_W\} = \frac{1}{(2\pi\varepsilon)^2}\operatorname{tr}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} W\;dxdp, \qquad \operatorname{Tr}\{\varrho_{W_1}\varrho_{W_2}\} = \frac{1}{(2\pi\varepsilon)^2}\operatorname{tr}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} W_1W_2\;dxdp,$$

it is straightforward to prove the following lemma, which is a rephrasing of Lemma 3.3.11 in terms of Wigner functions. We recall that our Wigner functions are matrix-valued, and so the products have to be understood as matrix-products.

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Lemma 3.3.12. *Putting $f(W) = W\mathcal{L}og(W) - W$, the Gâteaux derivative of the functional*

$$\mathfrak{F}(W) = \operatorname{tr} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} f(W) dx dp,$$

evaluated at W_0, is given by

$$\delta_{W_0} \mathfrak{F}(\xi) = \operatorname{tr} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} f'(W_0)\xi dx dp = \operatorname{tr} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \mathcal{L}og(W_0)\xi dx dp, \tag{3.63}$$

for all perturbation ξ of the Wigner matrix.

Proof. We obtain with Lemma 3.3.11 and $\mathcal{W}^{-1}(\mathcal{L}og(W)) = \ln \varrho_W$ the following

$$\begin{aligned}\delta_{W_0} \mathfrak{F}(\xi) &= \delta_{W_0} \left(\operatorname{tr} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} W\mathcal{L}og(W) - W dx dp \right)(\xi) = \delta_{W_0} ((2\pi\varepsilon)^2 \operatorname{Tr}\{\varrho_W \ln(\varrho_W) - \varrho_W\})(\xi) \\ &= (2\pi\varepsilon)^2 \operatorname{Tr}\{(\ln \varrho_{W_0})\xi\} = \operatorname{tr} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \mathcal{L}og(W_0)\xi dx dp.\end{aligned}$$

□

We now prove that the minimizer has necessarily the form of a quantum exponential, which would pe the first part of proving Theorem 3.3.10.

Lemma 3.3.13. *A necessary condition for $\mathcal{M}(N)$ to be solution to the unconstrained minimization problem*

$$\mathcal{L}(\mathcal{M}(N), \tilde{A}) = \min_W \mathcal{L}(W, \tilde{A}) \tag{3.64}$$

is that it is of the form

$$\mathcal{M}(N) = \mathcal{E}xp\left(-H_\varepsilon + \tilde{A}\right). \tag{3.65}$$

Proof. Let $\tilde{A}$ be fixed, and define for symbols W the functional

$$\mathcal{K}(W, \tilde{A}) := \operatorname{tr} \int_{\mathbb{R}^2} \tilde{A}(x) \langle W(x, \cdot) \rangle dx = 2 \int_{\mathbb{R}^2} (\tilde{a}_0 \langle w_0 \rangle + \boldsymbol{a} \cdot \langle \boldsymbol{w} \rangle) dx,$$

Since $\tilde{A}$ and N are independent of W, we have clearly

$$\delta_W \operatorname{tr} \int_{\mathbb{R}^2} \tilde{A} N dx = 0.$$

With the above we can rewrite the Gâteuax derivative of $\mathcal{L}$ at the point W as

$$\delta_W \mathcal{L} = \delta_W \mathcal{E} - \delta_W \mathcal{K},$$

and therefore the Euler-Lagrange equation associated to the unconstrained minimization problem (3.64) is given by

$$\delta_W \mathcal{E} - \delta_W \mathcal{K} = 0. \tag{3.66}$$

From Lemma 3.3.12 and the linearity of $\operatorname{tr} \int \int H_\varepsilon W \, dx dp$ we obtain

$$\delta_W \mathcal{E}(\xi) = \operatorname{tr} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} [\mathcal{L}og(W(x,p))\xi(x,p) + H_\varepsilon(x,p)\xi(x,p)] \, dx dp.$$

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By linearity, we immediately obtain for the functional $\mathcal{K}$

$$\delta_W \mathcal{K}(\xi) = \operatorname{tr} \int_{\mathbb{R}^2} \tilde{A} \langle \xi \rangle \, dx$$

Therefore the Euler Lagrange (3.66) becomes

$$\operatorname{tr} \left[\int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \mathcal{L}og(W(x,p))\xi(x,p) + H_\varepsilon(x,p)\xi(x,p) dx dp - \int_{\mathbb{R}^2} \tilde{A} \langle \xi \rangle \, dx \right] = 0, \tag{3.67}$$

for all perturbations ξ. The arbitrariness of ξ implies that the solution W has to be of the form $\mathcal{M}(N)$ as in (3.65).

□

With the preparation so far, we are able now to prove Theorem 3.3.10 and bring the first part to a conclusion.

Proof of Theorem 3.3.10. Provided Problem 3.3.5 has a solution $\mathcal{G}$, we show that $\mathcal{G} = \mathcal{M}(N)$ and that it fulfills the constrains (3.57). As mentioned in the beginning of this subsection, that problem is equivalent to the saddle point problem for the functional $\mathcal{L}$, recalling (3.61). Therefore if there exists a solution $\mathcal{G}$, there must also exist $\tilde{A}_0$ such that

$$\mathcal{L}(\mathcal{G}, \tilde{A}_0) = \max_{\tilde{A}} \min_{W} \mathcal{L}(W, \tilde{A}).$$

From Lemma 3.3.13 we deduce that for any given $\tilde{A}$, the solution $\mathcal{M}(N)$ to the minimization problem (3.64) has to be of the form $\mathcal{M}(N) = \mathcal{E}xp(-H_\varepsilon + \tilde{A})$ and fulfills

$$\mathcal{L}(\mathcal{M}(N), \tilde{A}) = \min_{W} \mathcal{L}(W, \tilde{A}).$$

Therefore $\mathcal{G}$ has to be of the same form as $\mathcal{M}(N)$ and hence the solution to the saddle point problem (3.61) is given by $(\mathcal{M}(N), \tilde{A}_0)$. The last remaining statement to prove of Theorem 3.3.10 is, that $\mathcal{M}(N) = m_0(N)\sigma_0 + \boldsymbol{m}(N) \cdot \boldsymbol{\sigma}$ also fulfills the constraints $\langle m_0(N) \rangle = n_0$ and $\langle \boldsymbol{m}(N) \rangle = \varepsilon \boldsymbol{n}$. Knowing that $(\mathcal{M}(N), \tilde{A}_0)$ is a solution to (3.61), we have that $\tilde{A}_0$ solves the maximization problem

$$\mathcal{L}(\mathcal{M}(N), \tilde{A}_0) = \max_{\tilde{A}} \mathcal{L}(\mathcal{M}(N), \tilde{A}). \tag{3.68}$$

and solves therefore the belonging Euler-Lagrange equation

$$\delta_{\tilde{A}_0}(\mathcal{L}(\mathcal{M}(N), .)) = 0. \tag{3.69}$$

Since $\mathcal{M}(N)$ is dependent on $\tilde{A}$, we denote it with $\mathcal{M}(N, \tilde{A})$ for the rest of the proof. The Gâteuax derivative at the point $\tilde{A}_0$ of $\mathcal{L}$ is then given by

$$\delta_{\tilde{A}_0} \mathcal{L} = \delta_W \mathcal{L}|_{(\mathcal{M}(N,\tilde{A}_0),\tilde{A}_0)}(\delta_{\tilde{A}} \mathcal{M}|_{\tilde{A}_0}) + \delta_{\tilde{A}} \mathcal{L}|_{(\mathcal{M}(N,\tilde{A}_0),\tilde{A}_0)}.$$

$\mathcal{M}(N)$ being a minimizer of (3.66) we have that $\delta_W \mathcal{L}|_{(\mathcal{M}(N,\tilde{A}_0),\tilde{A}_0)} = 0$. Since $\mathcal{L}$ is linear with respect to (the Pauli components of) $\tilde{A}$ and $\mathcal{E}$ is independent of $\tilde{A}$, we immediately obtain for perturbations $\boldsymbol{\xi} = \sum_{j=0}^{3} \xi_j \sigma_j$:

$$\begin{aligned}
\delta_{\tilde{A}} \mathcal{L}|_{(\mathcal{M}(N,\tilde{A}_0),\tilde{A}_0)}(\boldsymbol{\xi}) &= \delta_{\tilde{A}} \left(\mathcal{E} - \mathcal{K} \right) |_{(\mathcal{M}(N,\tilde{A}_0),\tilde{A}_0)}(\boldsymbol{\xi}) + \delta_{\tilde{A}} \left(\operatorname{tr} \int_{\mathbb{R}^2} \tilde{A} N \right) \Big|_{(\mathcal{M}(N,\tilde{A}_0),\tilde{A}_0)} (\boldsymbol{\xi}) \\
&= \operatorname{tr} \int_{\mathbb{R}^2} \left(N - \left\langle \mathcal{M}(N, \tilde{A}_0) \right\rangle \right) \boldsymbol{\xi} dx \\
&= 2 \int_{\mathbb{R}^2} \left(n_0 - \left\langle m_0(N, \tilde{A}_0) \right\rangle \right) \xi_0 + 2 \sum_{j=1}^{3} \left(\varepsilon n_j - \left\langle m_j(N, \tilde{A}_0) \right\rangle \right) \xi_j dx
\end{aligned}$$

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Since $\delta_{\tilde{A}_0}\mathcal{L}(\boldsymbol{\xi})$ must equal zero for all perturbations $\boldsymbol{\xi}$, we conclude that $\mathcal{M}(N, \tilde{A}_0)$ must satisfy the constraints (3.57). □

Part Two: A General Zeroth Order Approximation of $\mathcal{M}(N)$:

The Maxwellian is a quantum object, which is hard to describe explicitly. Therefore we assume that there exists a power series, the so called *semiclassical expansion*, such that

$$\mathcal{M}(N) = \sum_{k=0}^{\infty} \varepsilon^k \mathcal{M}^{(k)}(N), \tag{3.70}$$

where $\mathcal{M}^{(k)}(N)$ depends implicitly on the density matrix N and is called the $k-th$ order with respect to the scaled Planck constant ε . In principle the existence of such a power series, such as (3.70) (or earlier (3.21)), is the concept of the semiclassical expansion. More motivation is given in Section (3.6). Furthermore assume that the matrix of Lagrange multipliers also has such an expansion:

$$\tilde{A}(x) = \sum_{k=0}^{\infty} \varepsilon^k \tilde{A}^{(k)}(x), \qquad \text{with } \tilde{A}^{(k)}(x) = \tilde{a}_0^{(k)}(x)\sigma_0 + \boldsymbol{a}^{(k)}(x) \cdot \boldsymbol{\sigma}. \tag{3.71}$$

From the previous subsection (Theorem 3.3.10) we obtained that

$$(3.56): \qquad \mathcal{M}(N) = \mathcal{E}xp\left(-H_\varepsilon(x,p) + \tilde{A}(x)\right)$$

At the moment interesting for us, is the zeroth order of the quantum Maxwellian. We will see that it depends only on the zeroth order of the Lagrange multipliers instead of all orders. Since ε is usually smaller than one, the dominant order of the above expansions is the zeroth order, consequently we will call it the *leading order*. Motivation and details for the *semiclassical expansion*, also regarding the quantum Maxwellian, will follow later in Section 3.6.

Lemma 3.3.14. *Let $\mathcal{M}(N) = \mathcal{E}xp(-H_\varepsilon + \tilde{A})$ be a solution to Problem 3.3.5 and $\tilde{A} = \tilde{a}_0\sigma_0 + \boldsymbol{a} \cdot \boldsymbol{\sigma}$ be the matrix of Lagrange multipliers. Furthermore let $\tilde{A}^{(0)} = \tilde{a}_0^{(0)}\sigma_0 + \boldsymbol{a}^{(0)} \cdot \boldsymbol{\sigma}$ be the leading order of the semiclassical expansion of $\tilde{A}$ with respect to ε. Then the leading order of the quantum Maxwellian is given by*

$$\mathcal{M}(N)^{(0)} = e^{h_0^{(0)}} \left(\cosh\left(\left|\boldsymbol{a}^{(0)}\right|\right)\sigma_0 + \sinh\left(\left|\boldsymbol{a}^{(0)}\right|\right) \frac{\boldsymbol{a}^{(0)}}{\left|\boldsymbol{a}^{(0)}\right|} \cdot \boldsymbol{\sigma}\right) \tag{3.72}$$

where $h_0^{(0)} := -|p|^2/2 - a_0^{(0)}(x)$ and $a_0^{(0)}(x) := \tilde{a}_0^{(0)}(x) - V(x)$. Note that, by continuity, we can assume that

$$\mathcal{M}(N)^{(0)} = \exp\left(h_0^{(0)}\right),$$

if $\boldsymbol{a}^{(0)} = 0$.

Proof. Let us introduce the following function

$$g(\beta) = \mathcal{E}xp(\beta(-H_\varepsilon + \tilde{A})), \qquad \beta \in \mathbb{R}_0^+, \tag{3.73}$$

We immediately deduce $g(1) = \mathcal{M}(N)$ and thanks to function calculus and the properties of the Wigner transformation, we have

$$\begin{aligned}\partial_\beta g(\beta) = \partial_\beta \mathcal{W}(\varrho_{eq}(\beta)) = \ & \mathcal{W}(\partial_\beta \varrho_{eq}(\beta)) = \ \mathcal{W}((-\mathcal{H}_\varepsilon + \tilde{A})\exp(\beta(-\mathcal{H}_\varepsilon + \tilde{A})) \\ = \mathcal{W}(-\mathcal{H}_\varepsilon + \tilde{A}) \# \mathcal{W}(\exp(\beta(-\mathcal{H}_\varepsilon + \tilde{A}))) = \ & (-H_\varepsilon + \tilde{A}) \# \mathcal{E}xp(\beta(-H_\varepsilon + \tilde{A})) \\ = (-H_\varepsilon + \tilde{A}) \# g(\beta) &\end{aligned}$$

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Introducing the semiclassical expansion $g(\beta) = \sum_{k=0}^{\infty} \varepsilon^k g^{(k)}(\beta)$ on the left hand side, using the Pauli components of H_ε (3.55) and the semiclassical expansion of the Moyal product (see Lemma 3.2.20) on the right side, yields

$$\sum_{k=0}^{\infty} \varepsilon^k \partial_\beta g^{(k)}(\beta) = \sum_{k=0}^{\infty} \varepsilon^k \left(h_0\sigma_0 + \boldsymbol{h}_1 \cdot \boldsymbol{\sigma}\right) \#_{(k)} g^{(k)}(\beta). \tag{3.74}$$

Since we are only interested in the leading orders we can simplify the above. Let us recall the structure of $\boldsymbol{h}_1 = \boldsymbol{a} + \varepsilon \alpha p^\perp$ and the semiclassical expansion of the Lagrange multipliers (3.71), then we introduce the zeroth orders

$$h_0^{(0)} := -\frac{|p|^2}{2} + a_0^{(0)}, \qquad \boldsymbol{h}_1^{(0)} := \boldsymbol{a}^{(0)}.$$

Notice that the term $\varepsilon\alpha p^\perp$ does not give any contribution to the leading order with respect to ε, hence the above definition makes sense. Using these and the previous equation (3.74), we obtain by comparing the leading orders

$$\partial_\beta g^{(0)}(\beta) = \left(h_0^{(0)}\sigma_0 + \boldsymbol{a}^{(0)}\boldsymbol{\sigma}\right) \# g^{(0)}(\beta)$$

The zeroth order of the Moyal product coincides with the standard product, and the fact that $g(0) = \sigma_0$ (the exponential operator is the identity operator for $\beta = 0$ and therefore $\mathcal{E}xp(0) = \sigma_0$), which provides the ordinary differential equation

$$\partial_\beta g^{(0)}(\beta) = \left(h_0^{(0)}\sigma_0 + \boldsymbol{a}^{(0)} \cdot \boldsymbol{\sigma}\right) g^{(0)}(\beta), \quad g^{(0)}(0) = \sigma_0. \tag{3.75}$$

From here we could calculate directly the ODE above, which is standard, but still plenty of work, and therefore postponed to the Appendix B.3. We want to take the more indirect but shorter route here. If we set

$$g^{(0)}(\beta) = \exp\left(\beta h_0^{(0)}\right) f(\beta), \tag{3.76}$$

then it is readily seen that the unknown matrix $f(\beta)$ satisfies

$$\partial_\beta f(\beta) = \boldsymbol{a}^{(0)} \cdot \boldsymbol{\sigma} f(\beta), \qquad f(0) = \sigma_0.$$

The solution to this ODE is the matrix exponential

$$f(\beta) = \exp(\beta\, \boldsymbol{a}^{(0)} \cdot \boldsymbol{\sigma}) = \sum_{k=0}^{\infty} \frac{\beta^k}{k!} (\boldsymbol{a}^{(0)} \cdot \boldsymbol{\sigma})^k.$$

Recalling that

$$\boldsymbol{a}^{(0)} \cdot \boldsymbol{\sigma} = \begin{pmatrix} a_3^{(0)} & a_1^{(0)} - i a_2^{(0)} \\ a_1^{(0)} + i a_2^{(0)} & -a_3^{(0)} \end{pmatrix},$$

it can be easily seen by a direct calculation that

$$(\boldsymbol{a}^{(0)} \cdot \boldsymbol{\sigma})^{2k} = \left|\boldsymbol{a}^{(0)}\right|^{2k} \sigma_0, \qquad (\boldsymbol{a}^{(0)} \cdot \boldsymbol{\sigma})^{2k+1} = \left|\boldsymbol{a}^{(0)}\right|^{2k} \boldsymbol{a}^{(0)} \cdot \boldsymbol{\sigma},$$

for $k \in \mathbb{N}$. Then, $f(\beta) = \sigma_0$, if $\left|\boldsymbol{a}^{(0)}\right| = 0$, and if $\left|\boldsymbol{a}^{(0)}\right| \neq 0$

$$\begin{aligned} f(\beta) &= \sum_{k=0}^{\infty} \frac{\left(\beta\left|\boldsymbol{a}^{(0)}\right|\right)^{2k}}{(2k)!} \sigma_0 + \sum_{k=0}^{\infty} \frac{\left(\beta\left|\boldsymbol{a}^{(0)}\right|\right)^{2k+1}}{(2k+1)!} \frac{\boldsymbol{a}^{(0)}}{|\boldsymbol{a}^{(0)}|} \cdot \boldsymbol{\sigma} \\ &= \cosh\left(\beta\left|\boldsymbol{a}^{(0)}\right|\right) \sigma_0 + \sinh\left(\beta\left|\boldsymbol{a}^{(0)}\right|\right) \frac{\boldsymbol{a}^{(0)}}{|\boldsymbol{a}^{(0)}|} \cdot \boldsymbol{\sigma}, \end{aligned}$$

Substituting in (3.76) and recalling that $\mathcal{M}^{(0)}(N) = g^{(0)}(1)$, we obtain (3.72). □

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Part Three: The Final Form

To finish the proof of Theorem 3.3.8, we have to show that the zeroth order of the matrix $\tilde{A}$ only depends on $\tilde{a}_0$. We state this in the upcoming Proposition.

Proposition 3.3.15. *Let $\mathcal{M}(N)$ be a solution to Problem 3.3.5 and be of the form*

$$\mathcal{M}(N) = \mathcal{E}xp(-H_\varepsilon(x,p) + \tilde{A}(x)).$$

Then, the leading order of the Lagrange multiplier $\tilde{A}$ is $\tilde{A}^{(0)} = \tilde{a}_0(x)\sigma_0$.

Proof. Recalling our assumption $N = n_0\sigma_0 + \varepsilon \boldsymbol{n}\cdot\boldsymbol{\sigma}$, we have that the leading order of N is $N^{(0)} = n_0^{(0)}\sigma_0$. From Theorem 3.3.10 we know that the quantum Maxwellian satisfies the constraints (3.57), which at leading order read as follows

$$\left\langle \mathcal{M}_0^{(0)}(N)\right\rangle = n_0^{(0)}, \qquad \left\langle \boldsymbol{\mathcal{m}}^{(0)}(N)\right\rangle = 0. \tag{3.77}$$

Assume now that $\boldsymbol{a}^{(0)} \neq 0$, then from Lemma 3.3.14 we know that

$$\boldsymbol{\mathcal{m}}^{(0)}(N) = e^{h_0^{(0)}} \sinh\left(\left|\boldsymbol{a}^{(0)}\right|\right) \frac{\boldsymbol{a}^{(0)}}{\left|\boldsymbol{a}^{(0)}\right|}\cdot\boldsymbol{\sigma}.$$

Since $\left\langle \boldsymbol{\mathcal{m}}^{(0)}(N)\right\rangle$ has to be zero, this is equivalent to $\left|\left\langle \boldsymbol{\mathcal{m}}^{(0)}(N)\right\rangle\right| = 0$ and therefore

$$\left|\left\langle \boldsymbol{\mathcal{m}}^{(0)}(N)\right\rangle\right| = \left|\left\langle e^{h_0^{(0)}}\right\rangle \sinh\left(\left|\boldsymbol{a}^{(0)}\right|\right)\frac{\boldsymbol{a}^{(0)}}{\left|\boldsymbol{a}^{(0)}\right|}\right| = \left|\left\langle e^{h_0^{(0)}}\right\rangle \sinh\left(\left|\boldsymbol{a}^{(0)}\right|\right)\right| = 0.$$

Since $\left\langle e^{h_0^{(0)}}\right\rangle = 2\pi \exp\left(a_0^{(0)}\right) \neq 0$, we necessarily have

$$\boldsymbol{a}^{(0)}(x) = 0, \qquad \forall x\in\mathbb{R}^2.$$

□

3.3.4. The Collision Operator

The definition of the equilibrium state via entropy maximization allows us to adopt a relatively simple way to add collisions in the transport model (3.35). Similar as in Section 1.3 and in Chapter 2, we introduce a relaxation-time (BGK-like) collision operator of the form

$$\mathcal{Q}(W) = \frac{1}{t_c}(\mathcal{M}(\langle W\rangle) - W), \tag{3.78}$$

where t_c is the typical collision time of the system, which is for the sake of simplicity assumed to be constant. We recall that $\langle W\rangle$ denotes the integral of W over $\mathbb{R}^2$ with respect to the momentum p. Additionally we recall that our density matrix N is given as exactly that integral, i.e.

$$N = \langle W\rangle\,, \text{ where } n_0 = \langle w_0\rangle\,, \text{ and } \varepsilon\boldsymbol{n} = \langle \boldsymbol{w}\rangle\,.$$

Since our goal is to derive a diffusive model for N, we only need very general properties of the collision operator, above all the conservation of the particle number and spin, and,

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consequently, of the densities n_k, $k = 0,1,2,3$. Our relaxation-time operator provides it because

$$N = \langle W \rangle = \left\langle \mathcal{M}(\langle W \rangle) \right\rangle, \tag{3.79}$$

which of course implies

$$\langle \mathcal{Q}(W) \rangle = 0. \tag{3.80}$$

We then add the collision operator (3.78) to the non-dimensional Wigner Boltzmann equation (3.35) and obtain

$$\frac{t_E}{t_0}\partial_t W + \mathcal{T}W = \mathcal{Q}(W), \tag{3.81}$$

which completes our quantum transport model.

Remark 3.3.16. It may seem strange to add the collision term so late to the equation, but we decided to go this path to keep it as simple as possible. We could already add the collision operator in the von Neumann equation (3.2) (see [BM10]), and then go along the same path we followed, with that additional term, which would result in the same equation (3.81). ■

3.4. Time Scaling

The standard procedure for the diffusive regime would be to define the diffusive time scale (for details check Section 1.3, where the typical collision time would be much smaller than the energy time scale and the system would be observed longer than the energy time scale

$$\tau = \frac{t_c}{t_E} \ll 1, \qquad \frac{t_E}{t_0} = \tau, \quad \text{such that } t_0 = \frac{t_E^2}{t_c}.$$

This leads to the diffusive scaled Wigner Boltzmann equation (compare with Section 1.3)

$$\tau^2 \partial_t W + \tau \mathcal{T} W = \mathcal{M}(N) - W. \tag{3.82}$$

From here the common path to obtain a macroscopic model would be the *Chapman Enskog expansion*, which we introduced in Section 2.3.1. In our quantum setting, there are two major obstacles that will not appear in the standard case. First the transport term $\mathcal{T}$ is more difficult to handle, due the quantum quantities, like the quantum Maxwellian and the pseudo differential operator. The other obstacle occurs later in the expansion, which is easier to understand if we follow the three steps introduces in Section 2.3.1 and stumble over that difficulty.

1. Let W_τ be a solution to (3.82) and assume the existence of two functions W_0, U_τ such that
$$W_\tau = W_0 + \tau U_\tau.$$
Letting τ formally going to 0 in (3.82) shows that $W_0 = \mathcal{M}(N)$.

2. Dividing equation (3.82) through τ and pass to the formal limit of τ going to 0, we obtain that
$$U := \lim_{\tau \to 0} U_\tau = -\mathcal{T}\mathcal{M}(N).$$

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3. Last step is to turn to the momentum equation, which is (3.82) integrated

$$\partial_t \langle W_\tau \rangle + \frac{1}{\tau} \left\langle \mathcal{T}\mathcal{M}(N) \right\rangle + \langle \mathcal{T} U_\tau \rangle = 0, \tag{3.83}$$

and pass finally to the limit $\tau \to 0$ to obtain the diffusive equation.

We see here that Step 3 is only possible if the term $\tau^{-1} \left\langle \mathcal{T}\mathcal{M}(N) \right\rangle$ also converges to zero. Until now the standard argument has been that the term in front of τ^{-1} (in our case $\mathcal{T}\mathcal{M}(N)$) is odd in p and therefore the integral over it vanishes leading to an equation of the form

$$\partial_t N - \left\langle \mathcal{T}\mathcal{T}\mathcal{M}(N) \right\rangle = 0, \tag{3.84}$$

where $\left\langle \mathcal{T}\mathcal{T}\mathcal{M}(N) \right\rangle$ represents the diffusive part. This would fit into the expected form of the Chapman Enskog procedure. We state our first observation.

Proposition 3.4.1. *Let W be the solution to the WBE* (3.82)*, where $\mathcal{M}(N)$ is the quantum Maxwellian of the system, given by (3.51), $\tilde{A}(x)$ is the matrix of Lagrange multiplier, defined in (3.53) let $\mathcal{N}$ the moment operator (in our case $\mathcal{N}(.) = \langle . \rangle$). Then, $\mathcal{N}(\mathcal{T}\mathcal{M}(N)) = 0$ if and only if $\mathcal{N}([\tilde{A}, \mathcal{M}(N)]_\#) = 0$. In our particular setting if $\tilde{A}$ commutes with $N = \mathcal{N}(W)$.*

Proof. We recall that the hamiltonian part of the WBE is the Wigner transform of the von Neumann equation (3.2), and then

$$\mathcal{T}W = -\frac{1}{\mathrm{i}\varepsilon}[H_\varepsilon, W]_\#,$$

where H_ε is the scaled Hamiltonian (3.39) and $[H_\varepsilon, W]_\# := H_\varepsilon \# W - W \# H_\varepsilon$. From Theorem 3.3.8 we know that the quantum Maxwellian has to be of the form $\mathcal{M}(N) = \mathcal{E}xp(-H_\varepsilon + \tilde{A})$, which is an operator exponentiation in the Wigner picture. By functional calculus we know that any operator commutes with its exponentiation (like with any other of its functions), and this implies

$$\left(-H_\varepsilon + \tilde{A}\right) \# \mathcal{M}(N) - \mathcal{M}(N) \# \left(-H_\varepsilon + \tilde{A}\right) = 0.$$

This leads us to

$$-\mathrm{i}\varepsilon \mathcal{T}\mathcal{M}(N) = [H_\varepsilon, \mathcal{M}(N)]_\# = -[-H_\varepsilon + \tilde{A}, \mathcal{M}(N)]_\# + [\tilde{A}, \mathcal{M}(N)]_\# = [\tilde{A}, \mathcal{M}(N)]_\#, \tag{3.85}$$

which proves the first statement. Using identity (3.20), which gives us $\langle \tilde{A} \# W \rangle = \langle \tilde{A} W \rangle$, and also $\langle W \# \tilde{A} \rangle = \langle W \tilde{A} \rangle$, yields

$$-\mathrm{i}\varepsilon \left\langle \mathcal{T}\mathcal{M}(N) \right\rangle = \left\langle [\tilde{A}, \mathcal{M}(N)] \right\rangle = \left[\tilde{A}, \left\langle \mathcal{M}(N) \right\rangle\right] = [\tilde{A}, N],$$

which immediately proves the second statement. □

Remark 3.4.2. Proposition 3.4.1 applies in general to models where a given set of densities is fixed and it helps us to understand why in other studies the condition $\left\langle \mathcal{T}\mathcal{M}(N) \right\rangle \neq 0$ was never met. For example in Ref. [BM10] the focus is on the spin-up and spin-down densities $n_\pm := \langle w_0 \pm w_3 \rangle$. Since they worked mostly in the von Neumann picture, we reformulate their definitions. Let therefore ϱ be the solution to the von Neumann equation (3.2) and $W = \mathcal{W}(\varrho)$ the corresponding Wigner function (also solution to the WBE). The following moment operators are used in [BM10]

$$\mathcal{N}_1(\varrho) := \langle w_{11} \rangle, \qquad \mathcal{N}_2(\varrho) := \langle w_{22} \rangle,$$

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and let us define

$$\mathcal{N}_\pm(W) := \langle (1/2)\,\mathrm{tr}(W\sigma_0) \pm (1/2)\,\mathrm{tr}(W\sigma_3)\rangle\,,$$

such that

$$\mathcal{N}_1 = \mathcal{N}_+ \circ \mathcal{W}, \qquad \mathcal{N}_2 = \mathcal{N}_- \circ \mathcal{W}$$

Since only the densities n_+ and n_- are conserved in [BM10], the quantum Maxwellian $\tilde{\mathcal{M}}$ from [BM10] depends on a matrix of given densities N such that

$$\mathcal{N}_1(\tilde{\mathcal{M}}) = N_{11}, \qquad \mathcal{N}_2(\tilde{\mathcal{M}}) = N_{22}.$$

Therefore only two constraints in the quantum maximum entropy principle (QMEP) are needed, leading to matrix of Lagrange multipliers $\tilde{A}$ that is diagonal. Clearly, in such case we get again with identity (3.20) that

$$\mathcal{N}_1([\tilde{A}, \tilde{\mathcal{M}}]) = \mathcal{N}_+([\tilde{A}, \mathcal{W}(\tilde{\mathcal{M}})]_\#) = \tilde{A}_{11}N_{11} - N_{11}\tilde{A}_{11} = 0,$$
$$\mathcal{N}_2([\tilde{A}, \tilde{\mathcal{M}}]) = \mathcal{N}_-([\tilde{A}, \mathcal{W}(\tilde{\mathcal{M}})]_\#) = \tilde{A}_{22}N_{22} - N_{22}\tilde{A}_{22} = 0.$$

As another example, in the semiclassical full-spin model introduced in Ref. [EH14] the equilibrium state is of the form $cN\exp(-|p|^2/2)$ (where N is the full matrix of densities, exp is the classical exponential, and c is a normalization factor) and the moment operator coincides with ours. This means that $N = \exp(\tilde{A})$ and, therefore, $\tilde{A}N = N\tilde{A}$. ■

When, as in our case, $\langle \mathcal{T}\mathcal{M}(N)\rangle \neq 0$, the Chapman-Enskog procedure is inconsistent with the diffusive scaling, which has a huge impact on our work and stays in contrast to all previous existing derivations. Therefore we have to consider hydrodynamic scaling (which is suitable for local equilibria with no-vanishing current). However, we stress that the collisions we considering do not conserve the current: the residual current at equilibrium is of quantum mechanical nature (and in fact such current is of order ε^2, see (3.97) and (3.143)) As mentioned in Section 1.3, in the hydrodynamic regime we choose the reference time t_0 equal to the energy time scale t_E (which means that it is of order τ with respect to the diffusive t_0)

$$\tau = \frac{t_c}{t_E} \ll 1, \qquad t_0 = t_E.$$

Applying this to equation (3.81) gives us the hydrodynamic scaled Wigner Boltzmann (HWB) equation

$$\tau\partial_t W + \tau\mathcal{T}W = \mathcal{M}(N) - W, \tag{3.86}$$

that is

$$\tau\partial_t w_0 + \tau\Big((\nabla_x w_0)p + \alpha\varepsilon\nabla_x^\perp \cdot \boldsymbol{w} - \Theta_\varepsilon[V]w_0\Big) = \mathcal{m}_0(N) - w_0, \tag{3.87}$$

$$\tau\partial_t \boldsymbol{w} + \tau\Big((\nabla_x \boldsymbol{w})p + \alpha\varepsilon\nabla_x^\perp w_0 - \Theta_\varepsilon[V]\boldsymbol{w} - 2\alpha p^\perp \times \boldsymbol{w}\Big) = \boldsymbol{\mathcal{m}}(N) - \boldsymbol{w}. \tag{3.88}$$

3.5. The Full Quantum Model

The first derived model is the "*full quantum model*", which is correct to all orders in the scaled Planck constant ε. It provides quantum drift-diffusion equations for the macroscopic density n_0 and the spin densities n_1, n_2, n_3. When we were talking about semiclassical parameters , we meant the scaled Planck constant. It is also possible to use the Knudsen number τ as semiclassical parameter.

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Main Theorem 3.5.1 (Full Quantum Model)**.** *Let W be the solution to the Wigner Boltzmann equation* (3.86)*, $N = \langle W \rangle$ with $N = n_0\sigma_0 + \varepsilon \boldsymbol{n} \cdot \boldsymbol{\sigma}$, $\mathcal{M}(N)$ the quantum Maxwellian given in (3.51), $\tilde{A} = \tilde{a}_0\sigma_0 + \varepsilon \boldsymbol{a} \cdot \boldsymbol{\sigma}$ the matrix of Lagrange multipliers, and $J_j := \langle p\mathfrak{m}_j(N) \rangle$ the matrix of the first momentum. Then, at first order in τ, the Pauli components of N solve the following equations:*

$$\partial_t n_0 = \tau \operatorname{div}\left(n_0 \nabla a_0 + n_0 \nabla V + \varepsilon^2 \left(\boldsymbol{n} \cdot (\nabla \boldsymbol{a})\right)\right) + 2\tau\alpha\varepsilon^2 \left((\nabla^\perp) \cdot (\boldsymbol{n} \times \boldsymbol{a})\right), \tag{3.89}$$

$$\begin{aligned} \partial_t \boldsymbol{n} = &- 2(\boldsymbol{n} \times \boldsymbol{a}) + \tau \operatorname{div}\left(n_0 \nabla \boldsymbol{a} + \boldsymbol{n} \nabla a_0 + \boldsymbol{n} \nabla V + \frac{2}{\varepsilon}(J^T \times \boldsymbol{a})\right) \\ &- 2\tau\alpha \left(n_0(\nabla^\perp \times \boldsymbol{a}) + \nabla^\perp(a_0 + V) \times \boldsymbol{n} - \frac{2}{\varepsilon}\left(\boldsymbol{a}\left\langle p^\perp \cdot \boldsymbol{\mathfrak{m}}(N)\right\rangle + J^T \boldsymbol{a}^\perp\right)\right) \\ &- 2\tau \left(2\varepsilon(\boldsymbol{n} \times \boldsymbol{a}) \times \boldsymbol{a} - \boldsymbol{n} \times \partial_t^{(0)} \boldsymbol{a}\right) \end{aligned} \tag{3.90}$$

where $a_0 := \tilde{a}_0 - V$, and $\partial_t^{(0)}$ means that the time-derivatives of n_0 and $\boldsymbol{n}$ are given by the zeroth-order equations $\partial_t^{(0)} n_0 = 0$ and $\partial_t^{(0)} \boldsymbol{n} = -2(\boldsymbol{n} \times \boldsymbol{a})$, and recall that the planar gradient is defined as $\nabla := (\partial_{x_1}, \partial_{x_2}, 0)$.

The proof for Main Theorem 3.5.1 is postponed to the next section, since we need some preparation. Also there we introduce how we use τ as semiclassical parameter.

Remark 3.5.2. The Lagrange multipliers a_0 and $\boldsymbol{a}$ are non-local functions of the densities n_0 and $\boldsymbol{n}$, via the constraint $\langle \mathcal{M}(N) \rangle = N = \langle W \rangle$. Then, the system (3.89)-(3.90) is formally closed. However, this relation is very implicit and strongly non-local. In literature numerical methods have been proposed for solving problems of this kind in the scalar [GM05] and bipolar [BMNP15] cases. ∎

3.5.1. Derivation of the Full Quantum Model

To obtain the model equations (3.89)-(3.90) we are going to apply a Chapman-Enskog method, to the Wigner-Boltzmann equation in hydrodynamic scaling (HWBE from now on). Recall

$$\tau \partial_t W + \tau \mathcal{T} W = \mathcal{M}(N) - W, \tag{3.91}$$

and assume that there exists a function G, that depends on τ, such that

$$W = \mathcal{M}(N) + \tau G.$$

and G is of order one with respect to τ. This is already similar to the Chapman-Enskog ansatz in Section 2.3.1, but we will not pass to the limit $\tau \to 0$. Since the transport operator $\mathcal{T}$ is linear we compute from the HWBE (3.91) that

$$\begin{aligned} G = -\frac{1}{\tau}\left(\mathcal{M}(N) - W\right) &= - \partial_t W - \mathcal{T} W = -\partial_t \mathcal{M}(N) - \mathcal{T}\mathcal{M}(N) - \tau\left(\partial_t G + \mathcal{T} G\right) \\ &= - \partial_t \mathcal{M}(N) - \mathcal{T}\mathcal{M}(N) + \mathcal{O}(\tau). \end{aligned}$$

Integrating (3.91) with respect to p, and taking into account that $\langle W \rangle = N$ and that $\langle \mathcal{M}(N) - W \rangle = 0$, yields

$$\begin{aligned} \partial_t N &= - \langle \mathcal{T} W \rangle = - \left\langle \mathcal{T}\mathcal{M}(N) \right\rangle - \tau \langle \mathcal{T} G \rangle \\ &= - \left\langle \mathcal{T}\mathcal{M}(N) \right\rangle + \tau \left\langle \mathcal{T}\mathcal{T}\mathcal{M}(N) \right\rangle + \left\langle \mathcal{T}\partial_t \mathcal{M}(N) \right\rangle + \mathcal{O}(\tau^2). \end{aligned} \tag{3.92}$$

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which, when explicitly computed, yields the full quantum model (3.89)-(3.90). Since we are interested in a diffusive equation, it second order terms with respect to τ can be disregarded. The reader should notice that the above equation $\partial_t \mathcal{M}(N)$ depends through the chain rule on $\partial_t N$ (however, because of the non-local dependence of $\mathcal{M}(N)$ on N, the chain rule must be interpreted in functional sense): this will allow us to replace approximate, at first-order in τ, $\partial_t N$ with $\partial_t^{(0)} N$. The latter is given by (3.95), making the equation self-consistent.

Remark 3.5.3. Another method, which yields the same result is coming from a more physical point of view and was introduced in [Cer69]. We mention this here, because we used that method also in [BHJ]. This method differs a bit to the one we introduced in Section 2.3.1, since we similarly will expand the HWBE semiclassical in time. Therefore assume that the solution W has an expansion of the form

$$W(x,p) = \sum_{k=0}^{\infty} \tau^k W^{(k)}(x,p). \tag{3.93}$$

Dividing the HWBE by τ and integrating it with respect to p (recalling that $\langle \mathcal{M}(N) - W \rangle = 0$), we obtain

$$\partial_t N = -\langle \mathcal{T} W \rangle . \tag{3.94}$$

We get directly the semiclassical expansion of the time derivative of N from the above, using the fact that the transport operator $\mathcal{T}$ is linear,

$$\partial_t N = \sum_{k=0}^{\infty} \tau \partial_t^{(k)} N, \qquad \text{where } \partial_t^{(k)} N = -\left\langle \mathcal{T} W^{(k)} \right\rangle . \tag{3.95}$$

We remark that, in the spirit of the Chapman-Enskog approach, it is only the equation for N that is expanded, and not N itself, which is an $\mathcal{O}(1)$ quantity with respect to τ. This means that we assume that the semiclassical expansion of N is just the leading order, i.e.

$$N = \sum_{k=0}^{\infty} \tau^k N_\tau^{(k)} = N_\tau^{(0)},$$

$N_\tau^{(k)}$ is the k-th order with respect to τ and equals zero for all $k \geq 1$. Inserting the expansion (3.93) into the HWBE (3.91) and letting formally τ go to zero gives us

$$W^{(0)} = \mathcal{M}(N).$$

Substituting $W^{(0)}$ with $\mathcal{M}(N)$ in the expansion (3.93) and comparing the first order of τ in equation (3.91) gives also the first order of W with respect to τ which is

$$\tau W^{(1)} = -\tau \partial_t \mathcal{M}(N) - \tau \mathcal{T} \mathcal{M}(N)$$

Putting these results in (3.94) we obtain the equation for N

$$\partial_t N = -\left\langle \mathcal{T} \mathcal{M}(N) \right\rangle + \tau \left\langle \mathcal{T} \mathcal{T} \mathcal{M}(N) \right\rangle + \tau \left\langle \mathcal{T} \partial_t \mathcal{M}(N) \right\rangle + \mathcal{O}(\tau^2)$$

■

Remark 3.5.4. As discussed in Section 3.4, $\langle \mathcal{T} \mathcal{M}(N) \rangle$ is the zeroth-order current, that vanishes in other models, and $\langle \mathcal{T} \mathcal{T} \mathcal{M}(N) \rangle$ is the diffusive part. The term $\langle \mathcal{T} \partial_t \mathcal{M}(N) \rangle$ is a new term, which typically arises from the Chapman-Enskog procedure in hydrodynamic scaling [Cer69]. ■

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To get the desired model we need now to calculate every term occurring in the right side of (3.92). Therefore we recall the definitions of the odd and even Moyal product

$$(3.25): \qquad f_1\#_{(odd)}f_2 = \frac{1}{2}(f_1\#f_2 - f_2\#f_1), \qquad f_1\#_{(even)}f_2 = \frac{1}{2}(f_1\#f_2 + f_2\#f_1).$$

Furthermore using the lowercase "#" under a mathematical operation means that the products in that operations are replaced by the Moyal product. The next proposition will have all the needed tools to obtain the final equations, where some of them are just scaled versions of previous statements.

Proposition 3.5.5. *Let f and ξ be two arbitrary scalar valued symbols, such that f only depends on x, i.e. $f(x,p) = f(x)$, and let $\Theta_\varepsilon[f]$ be the pseudo differential operator defined in Definition 3.2.26. Then we have for $j \in \{1,2\}$ the following identities:*

1. $2f\#_{(odd)}\xi = i\varepsilon\Theta[f](\xi)$,
2. $p_j(f\#\xi) = f\#(p_j\xi) + (\varepsilon/2i)(\partial_{x_j}f)\xi$,
3. $p_j(\xi\#f) = (p_j\xi)\#f - (\varepsilon/2i)(\partial_{x_j}f)\xi$,
4. $\langle\Theta_\varepsilon[f](\xi)\rangle = 0$,
5. $\langle p_j\Theta_\varepsilon[f](\xi)\rangle = -(\partial_{x_j}f)\langle\xi\rangle$,
6. $\langle f\#_{(even)}\xi\rangle = f\langle\xi\rangle$,
7. $\langle p_j(f\#_{(even)}\xi)\rangle = f\langle p_j\xi\rangle$,

where we recall that $\langle.\rangle$ denotes the integration over $p \in \mathbb{R}^2$.

Proof. We want to mention that for the points 4-7, the proofs can be found in the literature, but we will prove these points in a, for us, more elegant way. Our idea is to use the first three points 1-3, to prove the other points, This differs to the common procedure, where the Fourier transformation and the δ-distribution are used as tool.

1. This follows directly from Lemma 3.2.27 by using the scaled versions.
2. The key idea is to use the semiclassical expansion of the Moyal product, see Lemma 3.2.20. Due to the fact that f only depends on the spatial variable x, the expansion reduces to

$$f\#\xi = \sum_{k=0}^{\infty}\varepsilon^k\frac{1}{(2\mathrm{i})^k}\sum_{|r|=k}\frac{(-1)^{|r|}}{r!}\partial_x^r f\,\partial_p^r\xi$$

Since $\partial_p^r p_j$ vanishes for $|r| > 1$ we have with the product rule that

$$f\#_{(k)}(p_j\xi) = p_j(f\#_{(k)}\xi), \qquad \text{for } j \in \{1,2\},\ \forall k > 1,$$

and hence

$$\begin{aligned} f\#(p_j\xi) &= p_j f\xi - \frac{\varepsilon}{2\mathrm{i}}(\partial_{x_j}f)\xi - \frac{\varepsilon}{2\mathrm{i}}(\nabla_x f\cdot\nabla_p\xi) + p_j\sum_{k=2}^{\infty}\varepsilon^k f\#_{(k)}\xi \\ &= p_j(f\#\xi) - \frac{\varepsilon}{2\mathrm{i}}(\partial_{x_j}f)\xi. \end{aligned}$$

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3. This is pretty similar to the previous point where we point out that

$$\xi\#_{(k)}f = \frac{1}{(2\mathrm{i})^k}\sum_{|s|=k}\frac{1}{s!}\partial_p^s\xi\,\partial_x^s f, \qquad (p_j\xi)\#_{(k)}f = \frac{1}{(2\mathrm{i})^k}\sum_{|s|=k}\frac{1}{s!}\partial_p^s(p_j\xi)\,\partial_x^s f,$$

and hence

$$\begin{aligned}(p_j\xi)\#f &= p_j\xi f + \frac{\varepsilon}{2\mathrm{i}}\xi\partial_{x_j}f + \frac{\varepsilon}{2\mathrm{i}}(\nabla_p\xi\cdot\nabla_x f) + p_j\sum_{k=2}^{\infty}\varepsilon^k\xi\#_{(k)}f \\ &= p_j(\xi\#f) + \frac{\varepsilon}{2\mathrm{i}}\xi\partial_{x_j}f.\end{aligned}$$

4. By using the first point and the integral identity for the Moyal product $\langle f\#g\rangle = f\langle g\rangle$ (see (3.18) in Proposition 3.2.17), we have

$$\langle\Theta_\varepsilon[f](\xi)\rangle = \frac{2}{\mathrm{i}\varepsilon}\left\langle f\#_{(odd)}\xi\right\rangle = \frac{1}{\mathrm{i}\varepsilon}\left(\langle f\#\xi\rangle - \langle\xi\#f\rangle\right) = \frac{1}{\mathrm{i}\varepsilon}\left(f\langle\xi\rangle - \langle\xi\rangle f\right) = 0.$$

5. From the first three points we get

$$\langle p_j\Theta_\varepsilon[f](\xi)\rangle = \frac{2}{\mathrm{i}\varepsilon}\left\langle p_j(f\#_{(odd)}\xi)\right\rangle = \frac{1}{\mathrm{i}\varepsilon}\left\langle\frac{\varepsilon}{\mathrm{i}}(\partial_{x_j}f)\xi\right\rangle = -(\partial_{x_j}f)\langle\xi\rangle\,.$$

6. The first point and Proposition 3.2.17 provide

$$\left\langle f\#_{(even)}\xi\right\rangle = \frac{1}{2}\langle f\#\xi + \xi\#f\rangle = \frac{1}{2}\left(\langle f\#\xi\rangle + \langle\xi\#f\rangle\right) = \frac{1}{2}(f\langle\xi\rangle + \langle\xi\rangle f) = f\langle\xi\rangle\,.$$

7. Again using the first three points, the integral identity for the Moyal product (see (3.18) as used for point 4) and the previous point 6, yields

$$\left\langle p_j(f\#_{(even)}\xi)\right\rangle = \frac{1}{2}\langle f\#(p_j\xi) + (p_j\xi)\#f\rangle = \left\langle f\#_{(even)}(p_j\xi)\right\rangle = f\langle p_j\xi\rangle\,.$$

□

Proof of Main Theorem 3.5.1:

Recalling our so far derived equation, where we omit from now on to write the dependence on N to keep the notation as simple as possible,

$$\partial_t N = -\left\langle\mathcal{T}\mathcal{M}\right\rangle + \tau\left\langle\mathcal{T}\mathcal{T}\mathcal{M}\right\rangle + \tau\left\langle\mathcal{T}\partial_t\mathcal{M}\right\rangle. \tag{3.96}$$

Let us start with with the first term at the right-hand side of (3.96). We have seen in Proposition 3.4.1 that $\mathrm{i}\varepsilon\langle\mathcal{T}\mathcal{M}\rangle = -[\tilde{A}, N]$. Using this, the representations $N = n_0\sigma_0 + \varepsilon\boldsymbol{n}\cdot\boldsymbol{\sigma}$, $\tilde{A} = \tilde{a}_0\sigma_0 + \varepsilon\boldsymbol{a}\cdot\boldsymbol{\sigma}$, and the Pauli algebra (see (3.8)), we obtain

$$\begin{aligned}\left\langle\mathcal{T}\mathcal{M}\right\rangle &= \frac{1}{\mathrm{i}\varepsilon}\left((n_0\sigma_0 + \varepsilon\boldsymbol{n}\cdot\boldsymbol{\sigma})(\tilde{a}_0\sigma_0 + \varepsilon\boldsymbol{a}\cdot\boldsymbol{\sigma}) - (\tilde{a}_0\sigma_0 + \varepsilon\boldsymbol{a}\cdot\boldsymbol{\sigma})(n_0\sigma_0 + \varepsilon\boldsymbol{n}\cdot\boldsymbol{\sigma})\right) \\ &= \frac{1}{\mathrm{i}\varepsilon}\Big((\varepsilon n_0\boldsymbol{a} + \varepsilon\tilde{a}_0\boldsymbol{n} + \mathrm{i}\varepsilon^2(\boldsymbol{n}\times\boldsymbol{a})) - \varepsilon(\tilde{a}_0\boldsymbol{n} + \varepsilon n_0\boldsymbol{a} + \mathrm{i}\varepsilon^2(\boldsymbol{a}\times\boldsymbol{n}))\Big) \\ &= 2\varepsilon(\boldsymbol{n}\times\boldsymbol{a})\cdot\boldsymbol{\sigma}.\end{aligned} \tag{3.97}$$

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Passing to the second term, $\langle \mathcal{T}\mathcal{T}\mathcal{M}\rangle$, we first compute $\mathcal{T}\mathcal{M}$ by using the representation $-\mathrm{i}\varepsilon\mathcal{T}\mathcal{M} = [\tilde{A},\mathcal{M}]_\#$ (see (3.85)). Notice that $f\#_{(odd)}\xi = -(\xi\#_{(odd)}f)$ for two scalar valued symbols. This combined with Proposition 3.5.5 and the decomposition $\mathcal{M} = m_0\sigma_0 + \boldsymbol{m}\cdot\boldsymbol{\sigma}$ provides

$$\begin{aligned}\mathcal{T}\mathcal{M} =& \frac{1}{\mathrm{i}\varepsilon}\left(\mathcal{M}\#\tilde{A} - \tilde{A}\#\mathcal{M}\right)\\ =&\frac{2}{\mathrm{i}\varepsilon}\left(m_0\#_{(odd)}\tilde{a}_0 + \varepsilon\sum_{j=1}^3 m_j\#_{(odd)}a_j\right)\sigma_0 + \frac{2}{\mathrm{i}\varepsilon}\left(\varepsilon m_0\#_{(odd)}\boldsymbol{a} + \boldsymbol{m}\#_{(odd)}\tilde{a}_0 + \mathrm{i}\varepsilon\,\boldsymbol{m}\times_{\#_{(even)}}\boldsymbol{a}\right)\cdot\boldsymbol{\sigma}\\ =&\left(-\Theta_\varepsilon[\tilde{a}_0](m_0) - \varepsilon\sum_{j=1}^3\Theta_\varepsilon[a_j](m_j)\right)\sigma_0 + \left(-\varepsilon\Theta_\varepsilon[\boldsymbol{a}](m_0) - \Theta_\varepsilon[\tilde{a}_0](\boldsymbol{m}) + 2\,\boldsymbol{m}\times_{\#_{(even)}}\boldsymbol{a}\right)\cdot\boldsymbol{\sigma}.\end{aligned}$$

Next, to calculate $\mathcal{T}\mathcal{T}\mathcal{M}$ we use the above Pauli representation of $\mathcal{T}\mathcal{M} = (\mathcal{T}\mathcal{M})_0\sigma_0 + \boldsymbol{\mathcal{T}\mathcal{M}}\cdot\boldsymbol{\sigma}$ and the definition of the transport operator $\mathcal{T}$ (see (3.36)), which gives us

$$\begin{aligned}\mathcal{T}\mathcal{T}\mathcal{M} =&\Big(p\cdot\nabla_x(\mathcal{T}\mathcal{M})_0 + \alpha\varepsilon(\nabla_x^\perp)\cdot\boldsymbol{\mathcal{T}\mathcal{M}} - \Theta_\varepsilon[V](\mathcal{T}\mathcal{M})_0\Big)\sigma_0\\ &+\Big(p\cdot\nabla_x\boldsymbol{\mathcal{T}\mathcal{M}} + \alpha\varepsilon\nabla_x^\perp(\mathcal{T}\mathcal{M})_0 - 2\alpha p^\perp\times\boldsymbol{\mathcal{T}\mathcal{M}} - \Theta_\varepsilon[V]\boldsymbol{\mathcal{T}\mathcal{M}}\Big)\cdot\boldsymbol{\sigma}.\end{aligned}$$

We now take the integral with respect to p. By using Proposition 3.5.5, and recalling that $a_0 = \tilde{a}_0 - V$, we obtain for the zeroth-component

$$\Big\langle(\mathcal{T}\mathcal{T}\mathcal{M})_0\Big\rangle = -\int_{\mathbb{R}^2} p\cdot\nabla_x\left(\Theta_\varepsilon[\tilde{a}_0](m_0) + \varepsilon\sum_{j=1}^3\Theta_\varepsilon[a_j](m_j)\right)dp \tag{3.98}$$

$$+\int_{\mathbb{R}^2}\alpha\varepsilon(\nabla_x^\perp)\cdot\Big(-\varepsilon\Theta_\varepsilon[\boldsymbol{a}](m_0) - \Theta_\varepsilon[\tilde{a}_0](\boldsymbol{m}) + 2(\boldsymbol{m}\times_{\#_{(even)}}\boldsymbol{a})\Big)\,dp \tag{3.99}$$

$$+\int_{\mathbb{R}^2}\Theta_\varepsilon[V]\left(\Theta_\varepsilon[\tilde{a}_0](m_0) + \varepsilon\sum_{j=1}^3\Theta_\varepsilon[a_j](m_j)\right)dp. \tag{3.100}$$

The integrals (3.98) to (3.100) will be treated separately. Using that $\tilde{a}_0 = a_0 + V$ combined with Proposition 3.5.5, yields

$$\begin{aligned}-(3.98) =& \left\langle\sum_{k=1}^2 p_k\partial_{x_k}(\Theta_\varepsilon[\tilde{a}_0](m_0)) + \sum_{j=1}^3\varepsilon p_k\partial_{x_k}(\Theta_\varepsilon[a_j](m_j))\right\rangle\\ =&\sum_{k=1}^2\sum_{j=1}^3\partial_{x_k}\langle p_k\Theta_\varepsilon[\tilde{a}_0](m_0)\rangle + \varepsilon\partial_{x_k}\langle p_k\Theta_\varepsilon[a_j](m_j)\rangle\\ =&\sum_{k=1}^2\sum_{j=1}^3 -\partial_{x_k}((\partial_{x_k}\tilde{a}_0)\langle m_0\rangle) - \varepsilon\partial_{x_k}((\partial_{x_k}a_j)\langle m_j\rangle)\\ =&\sum_{k=1}^2\sum_{j=1}^3 -\partial_{x_k}(n_0\partial_{x_k}a_0 + n_0\partial_{x_k}V) - \varepsilon\partial_{x_k}((\partial_{x_k}a_j)\varepsilon n_j)\\ =&-\nabla_x\cdot\Big(n_0\nabla_x a_0 + n_0\nabla_x V + \varepsilon^2(\boldsymbol{n}\cdot(\nabla_x\boldsymbol{a}))\Big).\end{aligned}$$

The expression $\nabla_x\cdot(\boldsymbol{n}\cdot(\nabla_x\boldsymbol{a}))$ is equal to $\sum_{k=1}^2\partial_{x_k}(\boldsymbol{n}\cdot\partial_{x_k}\boldsymbol{a})$. For the next integral (3.99) we mainly use Proposition 3.5.5:

$$\begin{aligned}(3.99) =&\alpha\varepsilon(\nabla_x^\perp)\cdot\langle-\varepsilon\Theta_\varepsilon[\boldsymbol{a}](m_0) - \Theta_\varepsilon[\tilde{a}_0](\boldsymbol{m})\rangle + \alpha\varepsilon(\nabla_x^\perp)\cdot\Big\langle\boldsymbol{m}\times_{\#_{(even)}}\boldsymbol{a}\Big\rangle = \boldsymbol{m}\times_{\#_{(even)}}\boldsymbol{a}\\ =&\alpha\varepsilon^2((\nabla_x^\perp)\cdot(\boldsymbol{n}\times\boldsymbol{a}))\end{aligned}$$

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In the last integral (3.100) we can interpret $\Theta_\varepsilon[\tilde{a}_0](\mathcal{m}_0) + \varepsilon \sum_{j=1}^3 \Theta_\varepsilon[a_j](\mathcal{m}_j)$ as scalar valued symbol that depends on x and p. Hence we obtain, again thanks to Proposition 3.5.5, that (3.100)= 0. Adding (3.98) and (3.99) together leads us to

$$\left\langle (\mathcal{TTM})_0 \right\rangle = \nabla_x \cdot \left(n_0 \nabla_x a_0 + n_0 \nabla_x V + \varepsilon^2 \boldsymbol{n} \cdot (\nabla_x \boldsymbol{a}) \right) + 2\alpha\varepsilon^2 \left((\nabla^\perp) \cdot (\boldsymbol{n} \times \boldsymbol{a}) \right).$$

For the $\boldsymbol{\sigma}$-components we obtain

$$\begin{aligned}
\left\langle \boldsymbol{\mathcal{TTM}} \right\rangle = & \int_{\mathbb{R}^2} p \cdot \nabla_x \left(-\varepsilon \Theta_\varepsilon[\boldsymbol{a}](\mathcal{m}_0) - \Theta_\varepsilon[\tilde{a}_0](\boldsymbol{\mathcal{m}}) + 2(\boldsymbol{\mathcal{m}} \times_{\#_{(even)}} \boldsymbol{a}) \right) dp & (3.101)\\
& - \int_{\mathbb{R}^2} \alpha\varepsilon(\nabla_x^\perp) \Big(\Theta_\varepsilon[\tilde{a}_0](\mathcal{m}_0) + \varepsilon \sum_{j=1}^3 \Theta_\varepsilon[a_j](\mathcal{m}_j) \Big) dp & (3.102)\\
& - \int_{\mathbb{R}^2} 2\alpha(p^\perp) \times \left(-\varepsilon \Theta_\varepsilon[\boldsymbol{a}](\mathcal{m}_0) - \Theta_\varepsilon[\tilde{a}_0](\boldsymbol{\mathcal{m}}) + 2(\boldsymbol{\mathcal{m}} \times_{\#_{(even)}} \boldsymbol{a}) \right) dp & (3.103)\\
& + \int_{\mathbb{R}^2} \Theta_\varepsilon[V] \left(\varepsilon \Theta_\varepsilon[\boldsymbol{a}](\mathcal{m}_0) + \Theta_\varepsilon[\tilde{a}_0](\boldsymbol{\mathcal{m}}) + 2(\boldsymbol{\mathcal{m}} \times_{\#_{(even)}} \boldsymbol{a}) \right) dp. & (3.104)
\end{aligned}$$

As we did it before we will calculate (3.101)-(3.104) separately, where the main tool will be again Proposition 3.5.5. For the first integral we get

$$\begin{aligned}
(3.101) &= \sum_{k=1}^2 \partial_{x_k} \left(\varepsilon \left\langle -p_k \Theta_\varepsilon[\boldsymbol{a}](\mathcal{m}_0) \right\rangle - \left\langle p_k \Theta_\varepsilon[\tilde{a}_0](\boldsymbol{\mathcal{m}}) \right\rangle + 2 \left\langle p_k (\boldsymbol{\mathcal{m}} \times_{\#_{(even)}} \boldsymbol{a}) \right\rangle \right)\\
&= \sum_{k=1}^2 \partial_{x_k} \left(\varepsilon n_0 \partial_{x_k} \boldsymbol{a} + (\partial_{x_k} \tilde{a}_0) \varepsilon \boldsymbol{n} + 2 \left\langle p_k \boldsymbol{\mathcal{m}} \right\rangle \times \boldsymbol{a} \right)\\
&= \varepsilon \nabla_x \cdot (n_0 \nabla_x \boldsymbol{a} + (\nabla_x a_0) \boldsymbol{n} + (\nabla_x V) \boldsymbol{n}) + 2 \nabla_x \cdot (J^T \times \boldsymbol{a}),
\end{aligned}$$

where $(J^T)_k = \langle p_k \boldsymbol{\mathcal{m}} \rangle$, the cross product in $(J^T \times \boldsymbol{a})$ is to understand column wise and $\nabla_x \cdot (J^T \times \boldsymbol{a}) = \sum_{j=1}^2 \partial_{x_j}((J^T)_j \times \boldsymbol{a})$. The next integral is dealt with quickly, since

$$(3.102) = \alpha\varepsilon(\nabla_x^\perp) \left(\langle \Theta_\varepsilon[\tilde{a}_0](\mathcal{m}_0) \rangle + \varepsilon \sum_{j=1}^3 \langle \Theta_\varepsilon[a_j](\mathcal{m}_j) \rangle \right) = 0.$$

For the third integral we mention that the cross product refers always to the vector parts, hence we obtain

$$\begin{aligned}
-(3.103) =& 2\alpha \left(-\varepsilon \left\langle p^\perp \times \Theta_\varepsilon[\boldsymbol{a}](\mathcal{m}_0) \right\rangle - \left\langle p^\perp \times \Theta_\varepsilon[\tilde{a}_0](\boldsymbol{\mathcal{m}}) \right\rangle + 2 \left\langle p^\perp \times (\boldsymbol{\mathcal{m}} \times_{\#_{(even)}} \boldsymbol{a}) \right\rangle \right)\\
=& 2\alpha \left(\varepsilon n_0 \nabla_x^\perp \times \boldsymbol{a} + \nabla_x^\perp \tilde{a}_0 \times \varepsilon \boldsymbol{n} + 2 \left\langle p^\perp \times (\boldsymbol{\mathcal{m}} \times_{\#_{(even)}} \boldsymbol{a}) \right\rangle \right)
\end{aligned}$$

The term where we build the cross product twice needs comparatively extra treatment. First we use the Graßmann-identity $\boldsymbol{v}_1 \times (\boldsymbol{v}_2 \times \boldsymbol{v}_3) = (\boldsymbol{v}_1 \cdot \boldsymbol{v}_3)\boldsymbol{v}_2 - (\boldsymbol{v}_1 \cdot \boldsymbol{v}_2)\boldsymbol{v}_3$ for any vectors $\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3 \in \mathbb{R}^3$, where we need to be careful with the Moyal product. In particular we have

$$\begin{aligned}
\left\langle p^\perp \times (\boldsymbol{\mathcal{m}} \times_{\#_{(even)}} \boldsymbol{a}) \right\rangle =& \left\langle p_2 (a_1 \#_{(even)} \boldsymbol{\mathcal{m}}) - p_1 (a_2 \#_{(even)} \boldsymbol{\mathcal{m}}) \right\rangle\\
& - \left\langle p_2 (\mathcal{m}_1 \#_{(even)} \boldsymbol{a}) - p_1 (\mathcal{m}_2 \#_{(even)} \boldsymbol{a}) \right\rangle\\
=& (a_1 \langle p_2 \boldsymbol{\mathcal{m}} \rangle - a_2 \langle p_1 \boldsymbol{\mathcal{m}} \rangle) - (\langle p_2 \mathcal{m}_1 \rangle \boldsymbol{a} - \langle p_1 \mathcal{m}_2 \rangle \boldsymbol{a})\\
=& - J^T \boldsymbol{a}^\perp - \left\langle p^\perp \cdot \boldsymbol{\mathcal{m}} \right\rangle \boldsymbol{a}
\end{aligned}$$

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Substituting this into the previous result yields

$$(3.103) = -2\varepsilon\alpha\left(n_0\nabla_x^\perp \times \boldsymbol{a} + \nabla_x^\perp(a_0+V)\times\boldsymbol{n}\right) + 4\alpha\left(\left\langle p^\perp\cdot\boldsymbol{\mathfrak{m}}\right\rangle\boldsymbol{a} + J^T\boldsymbol{a}^\perp\right).$$

In (3.104) we integrate the pseudo differential applied to some symbol with respect to the momentum and hence (3.104) = 0. Adding (3.101) and (3.103) gives us

$$\begin{aligned}\left\langle\mathcal{T}\mathcal{T}\mathcal{M}\right\rangle =& \varepsilon\nabla_x\cdot(n_0\nabla_x\boldsymbol{a} + (\nabla_x a_0)\boldsymbol{n} + (\nabla_x V)\boldsymbol{n}) + 2\nabla_x\cdot\left(J^T\times\boldsymbol{a}\right)\\ &- 2\alpha\varepsilon\left(n_0(\nabla_x^\perp\times\boldsymbol{a}) + \nabla_x^\perp(a_0+V)\times\boldsymbol{n}\right) + 4\alpha\left(\boldsymbol{a}\left\langle p^\perp\cdot\boldsymbol{\mathfrak{m}}\right\rangle + J^T\boldsymbol{a}^\perp\right).\end{aligned}$$

We now turn to the last term $\langle\mathcal{T}\partial_t\mathcal{M}\rangle$. Using (3.97) and the linearity of $\mathcal{T}$, we have that

$$\left\langle\mathcal{T}\partial_t\mathcal{M}\right\rangle = \partial_t\left\langle\mathcal{T}\mathcal{M}\right\rangle = 2\varepsilon(\partial_t\boldsymbol{n}\times\boldsymbol{a} + \boldsymbol{n}\times\partial_t\boldsymbol{a})\cdot\boldsymbol{\sigma}.$$

The time derivatives appearing here have to be discussed. Since we are approximating at first-order in τ and the above term is already at first order, we are interested here in only the zeroth order of the time derivative of the density. Recalling the expansion (3.95), $\partial_t^{(k)}N = -\langle\mathcal{T}W^{(k)}\rangle$, we have from (3.97) that $\partial_t^{(0)}\boldsymbol{n} = -2\varepsilon(\boldsymbol{n}\times\boldsymbol{a})$. As already remarked, the time dependence of each a_j for $j\in\{0,1,2,3\}$ comes from the macroscopic densities n_0, n_1, n_2, n_3, since the Lagrange multipliers depend non-locally from the densities through the constraint $\langle\mathcal{M}(N)\rangle = N$. Hence, we can write

$$\partial_t\boldsymbol{a} = \sum_{i=0}^{3}\frac{\delta\boldsymbol{a}}{\delta n_i}\partial_t n_i \approx \sum_{i=0}^{3}\frac{\delta\boldsymbol{a}}{\delta n_i}\partial_t^{(0)}n_i + \mathcal{O}(\tau) = -2\varepsilon\sum_{i=1}^{3}\frac{\delta\boldsymbol{a}}{\delta n_i}(\boldsymbol{n}\times\boldsymbol{a})_i + \mathcal{O}(\tau),$$

where we stress the fact that the derivative of a_j with respect to n_i is a functional derivative. The right hand side is already the expansion in τ and therefore we can write

$$\partial_t^{(0)}\boldsymbol{a} = -2\varepsilon\sum_{i=1}^{3}\frac{\partial\boldsymbol{a}}{\partial n_i}(\boldsymbol{n}\times\boldsymbol{a})_i.$$

Together we have for the very last term

$$\left\langle\mathcal{T}\partial_t\mathcal{M}\right\rangle = -2\varepsilon(2\varepsilon(\boldsymbol{n}\times\boldsymbol{a})\times\boldsymbol{a} - \boldsymbol{n}\times\partial_t^{(0)}\boldsymbol{a})\cdot\boldsymbol{\sigma} + \mathcal{O}(\tau).$$

It remains to compare the Pauli-components on both sides in our starting equation (3.96). Recalling the structure of the macroscopic density $N = n_0\sigma_0 + \varepsilon\boldsymbol{n}\cdot\boldsymbol{\sigma}$, we have

$$\begin{aligned}\partial_t n_0\sigma_0 + \varepsilon\partial_t\boldsymbol{n}\cdot\boldsymbol{\sigma} =& -2\varepsilon(\boldsymbol{n}\times\boldsymbol{a})\cdot\boldsymbol{\sigma}\\ &+\tau\left(\nabla_x\cdot\left(n_0\nabla_x a_0 + n_0\nabla_x V + \varepsilon^2\boldsymbol{n}\cdot(\nabla_x\boldsymbol{a})\right) + 2\alpha\varepsilon^2\left(\nabla_x^\perp\cdot(\boldsymbol{n}\times\boldsymbol{a})\right)\right)\sigma_0\\ &+\tau\varepsilon\nabla_x\cdot\left(n_0\nabla_x\boldsymbol{a} + (\nabla_x a_0)\boldsymbol{n} + (\nabla_x V)\boldsymbol{n} + 2J^T\times\boldsymbol{a}\right)\cdot\boldsymbol{\sigma}\\ &-2\alpha\varepsilon\tau\left(n_0(\nabla_x^\perp\times\boldsymbol{a}) + \nabla_x^\perp(a_0+V)\times\boldsymbol{n}\right)\cdot\boldsymbol{\sigma}\\ &+4\tau\alpha\left(\boldsymbol{a}\left\langle p^\perp\cdot\boldsymbol{\mathfrak{m}}\right\rangle + J^T\boldsymbol{a}^\perp\right)\cdot\boldsymbol{\sigma}\\ &-2\tau\varepsilon(2\varepsilon(\boldsymbol{n}\times\boldsymbol{a})\times\boldsymbol{a} - \boldsymbol{n}\times\partial_t^{(0)}\boldsymbol{a})\cdot\boldsymbol{\sigma},\end{aligned}$$

which gives us (3.89)-(3.90).

□

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Remark 3.5.6. Comparing the obtained results here with our results in [BHJ], we see two differences. The first difference is that in the full quantum model (3.89)-(3.90) the variable ε appears with power one and two, which comes from our smallness assumption that the spin components are of order ε (see Remark 3.3.6).
The second difference is, that the term $4\tau\alpha(\boldsymbol{a}\langle p^{\perp} \cdot \boldsymbol{\mathcal{m}}\rangle + J^T\boldsymbol{a}^{\perp})$ from the above calculations differs slightly from the term $4\alpha\varepsilon^{-1}\langle p^{\perp} \times (\boldsymbol{a} \times \boldsymbol{\mathcal{m}})\rangle$ obtained in [BHJ] (see formula (24)). These two terms actually coincide, since using the Graßmann identity, as in the proof before, yields

$$\boldsymbol{a}\left\langle p^{\perp} \cdot \boldsymbol{\mathcal{m}}\right\rangle + J^T\boldsymbol{a}^{\perp} = -\left\langle p^{\perp} \times (\boldsymbol{\mathcal{m}} \times \boldsymbol{a})\right\rangle = \left\langle p^{\perp} \times (\boldsymbol{a} \times \boldsymbol{\mathcal{m}})\right\rangle.$$

The representation we chose here, will come more handy in the upcoming calculations. ■

3.6. The Semiclassical Full Spin Model

What does semiclassical mean? Since this expression already dropped several times we want to take the time and motivate the idea behind it. Quantum objects are complicated and are hard to understand. Classical physics behaves differently than quantum physics and hence it feels quite unnatural to work in the quantum setting. A good example for this would be the quantum Maxwellian $\mathcal{M}(N)$ defined in (3.3.8). We see that this operator has no explicit form due to the dependence on the matrix of Lagrange multipliers and the combination with the Wigner-Weyl formalism. Its classical counterpart, the Maxwellian from Maxwell-Boltzmann statistics, is better explored, since it is the exponential applied to some function depending on the momentum (see for example [EH14], [JÖ9]).
The idea to understand a quantum object better, is to compare it with some kind of "*classical counterpart*" and add approximated quantum effects, which leads us to the term "*semiclassical*". Since we want to look at the system on a "macroscopic" scale, quantum effects are expected to be small. The scaled Planck constant ε (or in the unscaled setting $\hbar$) represents these quantum effects, which implies that it is small ($\varepsilon \sim \mathcal{O}(10^{-2})$) and together with the assumption that the dependence on ε is regular, leads to the "semiclassical expansion" as a power series in epsilon. To give more insight, assume that $\mathfrak{A}$ is a quantum object and let ε be the scaled Planck constant (see (3.32)). Then we expect that it is possible to express $\mathfrak{A}$ as

$$\mathfrak{A} = \sum_{k=0}^{\infty} \varepsilon^k \mathfrak{A}^{(k)},$$

where $\mathfrak{A}^{(k)}$ could be interpreted as the $k-$th zoom factor into the quantum level and in particular the zeroth zoom factor $\mathfrak{A}$ represents then the classical level.

The concept was already in some sense introduced with Lemma 3.2.20. We see now that the leading orders in the expansion usually can be interpreted in terms of classical physics. For example the zeroth order of the Moyal product is just the "*standard multiplication*", i.e for two symbols f, g we have $f\#_{(0)}g = fg$. Comparatively more tangible is maybe the pseudo differential $\Theta_\varepsilon[V](f)$ of a symbol f. We have shown in Lemma 3.2.27 (now in the scaled version), that $\Theta_\varepsilon[V](f) = \frac{1}{i\varepsilon}V\#_{(odd)}f$, and therefore the zeroth order (the "*classical counterpart*", see i.e. (1.6) or (1.7)), is given by

$$(\Theta_\varepsilon[V](f))^{(0)} = \frac{1}{i\varepsilon}V\#_{(1)}f = \nabla_x V \cdot \nabla_p f.$$

which coincides with the potential part from the classical Boltzmann picture.
The difficulty with the semiclassical approach is that there exists no standard procedure and deriving it is highly technical. Our goal of this section is to derive the semiclassical approximation for the change in time of the macroscopic density matrix N.

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3.6.1. The Model Equations for N:

As already remarked, the full quantum model (3.89)-(3.90) is a very involved and non-local problem. On the other hand, in most applications, we expect the semiclassical parameter ε to be small [BM10]. Moreover, we see from Lemma 3.2.20 that the Moyal product becomes local if its semiclassical expansion is truncated at some order. Then, it is natural to approximate the equations (3.89)-(3.90) by assuming the semiclassical parameter ε to be small. This is typically done in quantum drift-diffusion and quantum hydrodynamics models [BM10, DR03, DMR05, JÖ9], where it turns out that interesting terms, such as the Bohm potential, appear in the semiclassical expansion already at second-order in ε.

In the present case, the semiclassical expansion leads to a proliferation of terms, already at lower orders, and therefore, in order to end up with a reasonably compact model, we decided to neglect terms that are more than second order in ε and α. In fact, in usual applications, ε and α could be both small (e.g. of order $\mathcal{O}(10^{-2})$, see Ref. [KNAT02] for detailed values of all physical quantities and Table I in Ref. [BM10] for the calculated non-dimensional variables), which makes reasonable a second order approximation with respect to both parameters. The model we get is summarized in the following theorem.

Main Theorem 3.6.1 (Semiclassical model). *Let $N = n_0\sigma_0 + \varepsilon\boldsymbol{n}\cdot\boldsymbol{\sigma}$ be the solution to the non-local quantum spin drift diffusion model* (3.89)-(3.90) *from Theorem 3.5.1. Then, neglecting terms of order $\varepsilon^k\alpha^l$, with $k,l\in\mathbb{N}$ and $k+l>2$, N formally satisfies the following semiclassical drift diffusion equations:*

$$\partial_t n_0 = \tau \operatorname{div}\left(\nabla n_0 + n_0\nabla V - \frac{\varepsilon^2}{6} n_0 \nabla\left(\frac{\Delta\sqrt{n_0}}{\sqrt{n_0}}\right)\right) \tag{3.105}$$

$$\begin{aligned}\partial_t \boldsymbol{n} =& \tau \operatorname{div}(\nabla\boldsymbol{n} + \boldsymbol{n}\nabla V) - 2\tau\alpha(2\nabla^\perp + \nabla V^\perp)\times\boldsymbol{n} - 4\tau\alpha^2(2\boldsymbol{n} + (\boldsymbol{n}^\perp)^\perp) \\ &+ \frac{\varepsilon^2}{6}\frac{\boldsymbol{n}}{n_0}\times\mathcal{B}(N) + \tau\frac{\varepsilon^2}{12}\operatorname{div}\Big(\boldsymbol{n}\mathcal{A}(N) - \nabla(\Delta\boldsymbol{n}) + (\nabla\boldsymbol{n})\mathcal{C}(N) + \mathcal{B}(N)\nabla n_0 + \mathcal{D}(N)\Big) \\ &+ \tau\frac{\varepsilon^2}{3}\boldsymbol{n}\times\left(\frac{\boldsymbol{n}}{n_0}\times\mathcal{B}(N) - \mathcal{B}(N)\right),\end{aligned} \tag{3.106}$$

where we recall that the planar gradient is defined as $\nabla := (\partial_{x_1}, \partial_{x_2}, 0)$, and we define

$$\begin{aligned}\mathcal{A}(N) &:= 2\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0} - 4\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0} - \frac{\nabla n_0}{n_0}\frac{\Delta n_0}{n_0} - \frac{\nabla n_0}{n_0}\frac{(\nabla\otimes\nabla)n_0}{n_0}, \\ \mathcal{B}(N) &:= \frac{\Delta\boldsymbol{n}}{n_0} - \frac{\nabla\boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0}, \\ \mathcal{C}(N) &:= \left(\frac{\Delta n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2 + 4\left|\frac{\boldsymbol{n}}{n_0}\right|^2\right)\sigma_0 + \frac{\nabla\otimes\nabla n_0}{n_0}, \\ \mathcal{D}(N) &:= \frac{(\nabla n_0(\nabla\otimes\nabla))}{n_0}\boldsymbol{n} - \left(\nabla\boldsymbol{n}\cdot\frac{\nabla n_0}{n_0}\right)\frac{\nabla n_0}{n_0},\end{aligned}$$

where $(\nabla n_0(\nabla\otimes\nabla\boldsymbol{n}))_j = \nabla n_0(\nabla\otimes\nabla n_j)$ for $j\in\{1,2,3\}$.

Note that the equation for n_0 is the usual quantum drift-diffusion equation, also obtained in Refs. [BF10, DMR05, JÖ9] and others, and this is decoupled from the equation for $\boldsymbol{n}$.

To obtain the semiclassical model we need to expand the quantum Maxwellian $\mathcal{M}(N)$ and the matrix of Lagrange multipliers $\tilde{A}$ in powers of the semiclassical parameter ε, assumed now to be small. These expansions, truncated at the desired order will provide approximations of the non-local terms in the full quantum model (3.89)-(3.90), yielding the approximated, local model (3.105)-(3.106). These calculations will be provided in the next two sections.

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3.6.2. Semiclassical Expansion of the Quantum Maxwellian

This topic was already broached in Section 3.3.3 and will be now treated more in detail as promised. First let us recall some definitions and then we state our result, which we want to prove for this section.

$$h_0(x,p) = \left(-\frac{|p|^2}{2} + a_0\right), \qquad a_0(x) = \tilde{a}_0(x) - V(x), \qquad \boldsymbol{h}_1(x,p) = (\boldsymbol{a} - \alpha p^{\perp}).$$

Theorem 3.6.2 ((Semiclassical Expansion - Quantum Maxwellian))**.** *Let $\mathcal{M}(N) = m_0(N)\sigma_0 + \boldsymbol{m}(N)\cdot\boldsymbol{\sigma}$ be the solution to the QMEP (Problem 3.3.5), given by the expression* (3.51)*. Then the quantum Maxwellian can be expressed by*

$$\begin{aligned}\mathcal{M}(N) =& \exp(h_0)\sigma_0 + \varepsilon\exp(h_0)\boldsymbol{h}_1\cdot\boldsymbol{\sigma}\\ &+ \varepsilon^2\frac{1}{8}\exp(h_0)\left(\Delta a_0 + \frac{1}{3}\left(|\nabla a_0|^2 - p^T(\nabla\otimes\nabla a_0)p\right) + 4|\boldsymbol{h}_1|^2\right)\sigma_0\\ &+ \varepsilon^3\frac{1}{24}\exp(h_0)\Big[\left(3\Delta a_0 + |\nabla a_0|^2 - p^T(\nabla\otimes\nabla a_0)p + 4|\boldsymbol{h}_1|^2\right)\boldsymbol{h}_1 +\\ &+ 3\Delta\boldsymbol{a} - 12\alpha\nabla^{\perp}\times\boldsymbol{a} + \left(2\nabla\boldsymbol{a}\cdot\nabla a_0 - p^T(\nabla\otimes\nabla\boldsymbol{a})p + 2\alpha\nabla^{\perp}(\nabla a_0\cdot p)\right)\\ &+ 4\left((\nabla\boldsymbol{a})p - \alpha(\nabla a_0)^{\perp}\right)\times\boldsymbol{h}_1\Big]\cdot\boldsymbol{\sigma} + \mathcal{O}(\varepsilon^4),\end{aligned}$$

where the Lagrange multiplier a_j for $j\in\{0,1,2,3\}$ are dependent on N and recall that the planar gradient is defined as $\nabla := (\partial_{x_1}, \partial_{x_2}, 0)$.

Before we proof the above we want to give some remarks. We mentioned that we are only interested in an expansion of our model up to the second order with respect to ε, so why do we expand here up to the third order? The reason is the appearance of the term $\varepsilon^{-1}(J^T\times\boldsymbol{a})$ in the non-local model (3.89)-(3.90), since J is dependent on $\boldsymbol{m}$. Next we observe that the leading order of the quantum Maxwellian looks familiar to the classical Maxwellian, which we expected from the start. As last fact we see another consequence of our smallness assumption on the spin polarization (see Remark 3.3.6). In the first four orders, the even ones only contribute to the σ_0-component and the odd ones consist only of $\boldsymbol{\sigma}$-components. The upcoming calculations will clarify that this happens because of the smallness assumption and will show that the special structure of N reduces the work tremendously.

Let us take a closer look on the quantum Maxwellian itself. Theorem 3.3.8 proved the particular form of $\mathcal{M}(N)$, where we already were in the non dimensional setting (recall our scaling from Section 3.2.6). Recall the quantities $E_0 = k_B T_0$ (the reference energy), the unscaled Hamiltonian $E_0 H_\varepsilon = H$ (see Example 3.2.31) and $\tilde{A}$, which is the matrix of Lagrange multiplier appearing in $\mathcal{M}(N)$. Using this, we rewrite the scaled quantum Maxwellian in the sense that

$$\mathcal{M}(N) = \mathcal{E}xp\left(\frac{1}{E_0}\left(H + E_0\tilde{A}\right)\right).$$

Defining the quantity $\beta(T) := (k_B T)^{-1}$, T representing the variable temperature, we can express the above also as

$$\mathcal{M}(N) = \mathcal{E}xp\left(\beta(T_0)\left(H + E_0\tilde{A}\right)\right).$$

The quantity β is well defined for every temperature $T > 0$, we have $\beta(T)\in\mathbb{R}^+$ and $\beta(T)$ converges for T to infinity towards zero. Additionally we see that the newly introduced

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variable has again units, hence we need to scale it. The reference unit for $\beta(T)$ is $\beta_0 = (E_0)^{-1}$, which implies that the corresponding non-dimensional parameter is given by $\tilde{\beta} := \beta/\beta_0$. Scaling $\beta \to \beta_0\tilde{\beta}$ provides then

$$\widetilde{\mathcal{M}(N)}(\tilde{\beta}) := \mathcal{M}(N)(\beta_0\tilde{\beta}) = \mathcal{E}xp\left(\beta_0\tilde{\beta}\left(H + E_0\tilde{A}\right)\right) = \mathcal{E}xp\left(\tilde{\beta}\left(H_\varepsilon + \tilde{A}\right)\right).$$

Due to the choice of the reference energy E_0 as the thermal one, we have constant temperature $T = T_0$, yielding

$$\tilde{\beta}(T_0) = \frac{\beta(T_0)}{\beta_0} = \frac{1}{k_B T_0} E_0 = 1.$$

This leads us back to our quantum Maxwellian

$$\widetilde{\mathcal{M}(N)}(\tilde{\beta}(T_0)) = \widetilde{\mathcal{M}(N)}(1) = \mathcal{E}xp\left(\left(H_\varepsilon + \tilde{A}\right)\right) = \mathcal{M}(N).$$

Motivated from the above we define the *general quantum Maxwellian*

$$g(\beta) := \mathcal{E}xp\left(\beta\left(H_\varepsilon + \tilde{A}\right)\right) \qquad \beta \in \mathbb{R}_0^+. \tag{3.107}$$

The reader should notice, that $g(1) = \mathcal{M}(N)$, and that $g(\beta)$ is still a function of time, space and momentum, but for simplicity we drop the regarding notation. The above function $g(\beta)$ already appeared in the proof of Theorem 3.3.8, see (3.73), and there we derived the differential equation

$$\partial_\beta g(\beta) = (-H_\varepsilon + \tilde{A})\#\mathcal{E}xp\left(\beta\left(H_\varepsilon + \tilde{A}\right)\right), \tag{3.108}$$

with the initial condition

$$g(0) = \sigma_0,$$

which corresponds to the fact that the exponential operator is the identity operator for $\beta = 0$.

Proof of Theorem 3.6.2:

The main idea is to use equation (3.108) and the semiclassical expansion of the Moyal product (see Lemma 3.2.20), to obtain the semiclassical orders of g and then use the relation $g(1) = \mathcal{M}(N)$. First let us rewrite (3.108) in a more compact form, with the variables introduced in the beginning of the section:

$$\partial_\beta g(\beta) = (h_0\sigma_0 + \varepsilon\boldsymbol{h}_1 \cdot \boldsymbol{\sigma})\#g(\beta), \qquad g(0) = \sigma_0. \tag{3.109}$$

Using the approach of the semiclassical expansion $g(\beta) = \sum_{k=0}^{\infty}\varepsilon^k g^{(k)}(\beta)$ and the semiclassical representation of the Moyal product from Lemma 3.2.20 in the differential equation (3.109), we obtain

$$\sum_{k=0}^{\infty}\varepsilon^k\partial_\beta g^{(k)}(\beta) = \sum_{l=0}^{\infty}\varepsilon^l(h_0\sigma_0 + \varepsilon\boldsymbol{h}_1\cdot\boldsymbol{\sigma})\#_{(l)}\left(\sum_{k=0}^{\infty}\varepsilon^k g^{(k)}(\beta)\right).$$

Comparing the orders of ε leads us to the formula for $g^{(k)}$:

$$\partial_\beta g^{(k)}(\beta) = \sum_{l=0}^{k} h_0\sigma_0\#_{(l)}g^{(k-l)}(\beta) + \sum_{l=0}^{k-1}(\boldsymbol{h}_1\cdot\boldsymbol{\sigma})\#_{(l)}g^{(k-1-l)}(\beta), \qquad \forall k,l \in \mathbb{N}_0. \tag{3.110}$$

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Since the zero order Moyal product is just multiplication between matrices, we obtain for every $k \in \mathbb{N}$ an ODE, with the noise that depends on $g^{(l)}, l < k$ and with the initial condition $g(0) = \sigma_0$. This initiates for all orders the initial conditions, which means that $g^{(0)}(0) = \sigma_0$ and $g^{(k)}(0) = 0$ for all $k > 0$. For example we obtain for $k = 0$ the simple ODE:

$$\partial_\beta g^{(0)}(\beta) = h_0 g^{(0)}(\beta), \quad g^{(0)}(0) = \sigma_0,$$

with the solution

$$g^{(0)}(\beta) = \exp\left(\beta h_0\right)\sigma_0. \tag{3.111}$$

This gives us also the zeroth order of $\mathcal{M}(N)$, since $g^{(0)}(1) = \mathcal{M}^{(0)}(N)$. For $k > 1$ we have always to solve a differential equation of the form

$$\partial_\beta g^{(k)}(\beta) = h_0\sigma_0 g^{(k)} + \sum_{l=0}^{k-1} h_0\sigma_0 \#_{(l)} g^{(k-l)} + (\boldsymbol{h}_1 \cdot \boldsymbol{\sigma})\#_{(l)} g^{(k-1-l)}, \quad g^{(k)}(0) = 0. \tag{3.112}$$

Formula (3.112) shows us that we have to proceed iteratively to determine $g^{(k)}(\beta)$. The exhausting part is to calculate the different Moyal products occurring in (3.112), since none of these terms appear twice. After evaluating these terms, we have to solve a simple ODE, which is simply done by applying Duhamel's formula, and is therefore postponed to the Appendix B.3. To help us out, with the Moyal product - terms, we add the notations

$$H_0 = h_0\sigma_0, \qquad H_1 = \boldsymbol{h}_1 \cdot \boldsymbol{\sigma}$$

(h_0 and $\boldsymbol{h}_1$ being given by (3.55)) and, if clear from the context, we omit writing the dependence of g on β. The upcoming Lemma will be used to shorten some of the forthcoming calculations and is readily proven by applying the chain rule. We recall that the k-th order Moyal product $\#_{(k)}$ is defined in (3.22), which coincides with the scaled version in (3.38).

Lemma 3.6.3. *Let ζ, ξ be two symbols and and if ξ is in particular a function of ζ, i.e. $\xi(x,p) = \xi(\zeta(x,p))$, then we have that $\zeta \#_{(1)} \xi = 0$.*

Proof. Since ξ is a function depended of ζ, we have that $\partial_{xj}\xi(\zeta) = \xi' \partial_{xj}\zeta$, and that $\partial_{pj}\xi(\zeta) = \xi'\partial_{pj}\zeta$, therefore we obtain

$$\nabla_p\zeta\nabla_x\xi(\zeta) - \nabla_x\zeta\nabla_p\xi(\zeta) = \xi'(\nabla_p\zeta\nabla_x\zeta - \nabla_x\zeta\nabla_p\zeta) = 0.$$

□

The derivation of $g^{(0)}$ was already discussed before, see formula (3.111), and even more detailed in Section 3.3.3. To keep the notation as simple as possible we will identify the zero order with its σ_0-component:

$$g^{(0)} \equiv \exp(\beta h_0). \tag{3.113}$$

The calculated derivatives of h_0 and $g^{(0)}$ that will be needed for the rest of the proof are calculated in the Appendix B.2.

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Order one of $g(\beta)$

Formula (3.112) gives us here

$$\partial_\beta g^{(1)} = H_0 g^{(1)} + h_0 \#_{(1)} g^{(0)} \sigma_0 + g^{(0)} \boldsymbol{h}_1 \cdot \boldsymbol{\sigma}$$

Using Lemma 3.6.3 we deduce immediately that $h_0 \#_{(1)} g^{(0)} = 0$, and we obtain the initial value problem

$$\partial_\beta g^{(1)}(\beta) = H_0 g^{(1)}(\beta) + g^{(0)} \boldsymbol{h}_1 \cdot \boldsymbol{\sigma}, \qquad g^{(1)}(0) = 0, \tag{3.114}$$

having the solution (see Appendix B.3)

$$g^{(1)}(\beta) = \beta \exp(\beta h_0) \boldsymbol{h}_1 \cdot \boldsymbol{\sigma}, \tag{3.115}$$

Order two of $g(\beta)$

Formula (3.112) gives us here

$$\partial_\beta g^{(2)} = H_0 \#_{(0)} g^{(2)} + H_0 \#_{(1)} g^{(1)} + H_0 \#_{(2)} g^{(0)} + H_1 \#_{(0)} g^{(1)} + H_1 \#_{(1)} g^{(0)}$$

The first term $H_0 \#_{(0)} g^{(2)}(\beta)$ is the one that contains the unknown, while the others are known from the preceding orders. For the j-th Pauli component (for $j \in \{1,2,3\}$) of the second term we can write

$$\begin{aligned}
2\mathrm{i} h_0 \#_{(1)} g_j^{(1)} &= \nabla_p h_0 \nabla_x (\beta g^{(0)} (a_j - \alpha p_j^\perp)) - \nabla_x h_0 \nabla_p (\beta g^{(0)} (a_j - \alpha p_j^\perp)) \\
&= (-p) \beta g^{(0)} \nabla_x a_j - \nabla_x a_0 (\nabla_p p_j^\perp) \alpha \beta g^{(0)} \\
&= \nabla_x (\boldsymbol{h}_1)_j \nabla_p g^{(0)}(\beta) - \nabla_p (\boldsymbol{h}_1)_j \nabla_x g^{(0)}(\beta) \\
&= -2\mathrm{i} (\boldsymbol{h}_1)_j \#_{(1)} g^{(0)}.
\end{aligned}$$

Therefore the terms $H_0 \#_{(1)} g^{(1)}$ and $H_1 \#_{(1)} g^{(0)}$ cancel out. For the remaining terms we only have the σ_0-component. Since $\partial_x^r \partial_p^s h_0$ equals zero for $|r|, |s| \geq 1$, we obtain

$$\begin{aligned}
h_0 \#_{(2)} g_0^{(0)} &= -\frac{1}{4} \sum_{|r|+|s|=2} \frac{(-1)^{|r|}}{r! s!} \partial_x^r \partial_p^s h_0 \ \partial_p^r \partial_x^s g^{(0)} \\
&= -\frac{1}{8} \sum_{i,k=1}^{2} \partial_{x_i} \partial_{x_k} h_0 \ \partial_{p_i} \partial_{p_k} g^{(0)} - \delta_{ik} \partial_{x_i} \partial_{x_k} g^{(0)} \\
&= -\frac{1}{8} \sum_{i,k=1}^{2} \partial_{x_i} \partial_{x_k} a_0 \beta g^{(0)} (-\delta_{ik} + \beta p_i p_k) - \delta_{ik} \beta g^{(0)} (\partial_{x_i} \partial_{x_k} a_0 + \beta (\partial_{x_i} a_0)(\partial_{x_k} a_0)) \\
&= \frac{\beta}{8} g^{(0)} \left[2\Delta a_0 - \beta \Big(p^T (\nabla \otimes \nabla a_0) p - |\nabla a_0|^2 \Big) \right].
\end{aligned}$$

The last remaining term is $H_1 \#_{(0)} g^{(1)}(\beta)$, where the zero-order Moyal product is just the ordinary multiplication. We stress furthermore that we are multiplying two hermitian matrices, where one of them is a multiple of H_1 and therefore

$$H_1 \#_{(0)} g^{(1)} = (\boldsymbol{h}_1 \cdot \boldsymbol{\sigma})(\beta g^{(0)} \boldsymbol{h}_1 \cdot \boldsymbol{\sigma}) = \beta g^{(0)} |\boldsymbol{h}_1|^2 \sigma_0$$

The above leads us now to the ODE

$$\partial_\beta g^{(2)}(\beta) = H_0 g^{(2)}(\beta) + \beta g^{(0)} \left[\left(\frac{1}{4} \Delta a_0 - \frac{\beta}{8} \Big(p^T (\nabla \otimes \nabla a_0) p - |\nabla a_0|^2 \Big) \right) + |\boldsymbol{h}_1|^2 \right] \sigma_0,$$

with initial value $g^{(2)}(0) = 0$. The solution is then given by (see Appendix B.3.2)

$$g^{(2)}(\beta) = \frac{\beta^2}{8} \exp(\beta h_0) \left(\Delta a_0 + \frac{\beta}{3} \Big(|\nabla a_0|^2 - p^T (\nabla \otimes \nabla a_0) p \Big) + 4 |\boldsymbol{h}_1|^2 \right) \sigma_0, \tag{3.116}$$

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Order three of $g(\beta)$

Formula (3.112) gives us here

$$\partial_\beta g^{(3)} = H_0 g^{(3)} + H_0 \#_{(1)} g^{(2)} + H_0 \#_{(2)} g^{(1)} + H_0 \#_{(3)} g^{(0)} + H_1 g^{(2)} + H_1 \#_{(1)} g^{(1)} + H_1 \#_{(2)} g^{(0)}. \tag{3.117}$$

Skipping the first term on the right-side, containing the unknown, let us consider the second term, which only contributes to the σ_0 component. To facilitate the calculations we write $g^{(2)} = \lambda_1 \lambda_2 \sigma_0$, where

$$\lambda_1 := \frac{\beta^2}{8} g^{(0)}, \qquad \lambda_2 := \Delta a_0 + \frac{\beta}{3}\Big(|\nabla a_0|^2 - p^T(\nabla \otimes \nabla a_0)p\Big) + 4|\boldsymbol{h}_1|^2. \tag{3.118}$$

We see that λ_1 is a function of h_0, hence we deduce with the product rule from Lemma 3.6.3

$$\begin{aligned} 2\mathrm{i} h_0 \#_{(1)} g^{(2)} &= 2\mathrm{i}(h_0 \#_{(1)} \lambda_1)\lambda_2 \sigma_0 + 2\mathrm{i}\lambda_1 (h_0 \#_{(1)} \lambda_2)\sigma_0 = 2\mathrm{i}\lambda_1 (h_0 \#_{(1)} \lambda_2)\sigma_0 \\ &= \frac{\beta^2}{8} g^{(0)} \left[\frac{\beta}{3} p \cdot \nabla_x (p^T(\nabla_x \otimes \nabla_x a_0)p) - p \cdot \nabla_x(\Delta_x a_0) + 8(\alpha(\nabla_x^\perp a_0) - (\nabla_x \boldsymbol{a})p) \cdot \boldsymbol{h}_1\right] \sigma_0. \end{aligned}$$

The last equality is not so fast calculated and is therefore postponed to the Appendix B.3.3. Since the next term $H_0 \#_{(2)} g^{(1)}$ reduces to $h_0 \#_{(2)} \boldsymbol{g}^{(1)} \cdot \boldsymbol{\sigma}$, we have to calculate $h_0 \#_{(2)} \boldsymbol{g}^{(1)}$. Using again the fact that $\partial_x^r \partial_p^s h_0$ equals zero for $|r|, |s| \geq 1$ and $\partial_{p_i}\partial_{p_k} h_0 = -\delta_{ik}$, we have

$$\begin{aligned} h_0 \#_{(2)} \boldsymbol{g}^{(1)} &= -\frac{1}{4} \sum_{|r|+|s|=2} \frac{(-1)^{|r|}}{r!s!} \partial_x^r \partial_p^s h_0 \, \partial_p^r \partial_x^s \boldsymbol{g}^{(1)} \\ &= -\frac{1}{8} \sum_{i,k=1}^{2} \partial_{x_i}\partial_{x_k} h_0 \, \partial_{p_i}\partial_{p_k} \boldsymbol{g}^{(1)} + \frac{1}{8} \sum_{k=1}^{2} \partial_{x_k}^2 \boldsymbol{g}^{(1)}, \end{aligned}$$

where the derivatives of $\boldsymbol{g}^{(1)}$ are given by

$$\begin{aligned} \partial_{p_k} \boldsymbol{g}^{(1)} &= -\beta \exp(\beta h_0) \left(\beta p_k \boldsymbol{h}_1 + \alpha \partial_{p_k} p^\perp\right), \\ \partial_{p_i}\partial_{p_k} \boldsymbol{g}^{(1)} &= \beta^2 \exp(\beta h_0) \left((\beta p_i p_k - \delta_{ik}) \boldsymbol{h}_1 + \alpha \left(p_i \partial_{p_k} p^\perp + p_k \partial_{p_i} p^\perp\right)\right), \\ \partial_{x_k} \boldsymbol{g}^{(1)} &= \beta \exp(\beta h_0) \left(\beta(\partial_{x_k} a_0)\boldsymbol{h}_1 + \partial_{x_k} \boldsymbol{a}\right), \\ \partial_{x_k}^2 \boldsymbol{g}^{(1)} &= \beta \exp(\beta h_0) \left(\left(\beta^2(\partial_{x_k} a_0)^2 + \beta \partial_{x_k}^2 a_0\right) \boldsymbol{h}_1 + 2\beta(\partial_{x_k} a_0)\partial_{x_k} \boldsymbol{a} + \partial_{x_k}^2 \boldsymbol{a}\right). \end{aligned}$$

Substituting the derivatives into the previous gives us

$$\begin{aligned} \sum_{i,k=1}^{2} \partial_{x_i}\partial_{x_k} h_0 \, \partial_{p_i}\partial_{p_k} \boldsymbol{g}^{(1)} &= \sum_{i,k=1}^{2} (\partial_{x_i}\partial_{x_k} a_0)\beta^2 g^{(0)} \left[(\beta p_i p_k - \delta_{ik}) \boldsymbol{h}_1 + \alpha \left(p_i \partial_{p_k} p^\perp + p_k \partial_{p_i} p^\perp\right)\right] \\ &= \beta^2 g^{(0)} \left[(\beta p^T (\nabla_x \otimes \nabla_x a_0)p - \Delta a_0)\boldsymbol{h}_1 + 2\alpha p^T((\nabla_x \otimes \nabla_x)a_0)\nabla_p p^\perp\right], \end{aligned}$$

and

$$\begin{aligned} \sum_{i=1}^{2} \partial_{x_i}^2 \boldsymbol{g}^{(1)} &= \sum_{i=1}^{2} \beta g^{(0)} \left[\left(\beta^2(\partial_{x_i} a_0)^2 + \beta \partial_{x_i}^2 a_0\right) \boldsymbol{h}_1 + 2\beta(\partial_{x_i} a_0)\partial_{x_i} \boldsymbol{a} + \partial_{x_i}^2 \boldsymbol{a}\right] \\ &= \beta g^{(0)} \left[\left(\beta^2 |\nabla_x a_0|^2 + \beta \Delta_x a_0\right) \boldsymbol{h}_1 + 2\beta \nabla_x \boldsymbol{a} \cdot \nabla_x a_0 + \Delta_x \boldsymbol{a}\right]. \end{aligned}$$

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Using the identity $p^T(\nabla_x \otimes \nabla_x a_0)\nabla_p p^\perp = -\nabla_x^\perp(\nabla_x a_0 \cdot p)$ (see Appendix B.3.3), we obtain

$$h_0\#_{(2)}\boldsymbol{g}^{(1)} = \frac{\beta}{8}g^{(0)}\Big[\beta\left(2\Delta_x a_0 + \beta\left(|\nabla_x a_0|^2 - p^T(\nabla_x \otimes \nabla_x a_0)p\right)\right)\boldsymbol{h}_1 \\ + 2\beta(\alpha\nabla_x^\perp(\nabla_x a_0 \cdot p) + \nabla_x \boldsymbol{a} \cdot \nabla_x a_0) + \Delta_x \boldsymbol{a}\Big].$$

We calculate the next term $H_0\#_{(3)}g^{(0)}$ which only gives contribution to the σ_0 component, hence can be reduced to $(h_0\#_{(3)}g^{(0)})\sigma_0$. Using $\partial_x^r\partial_p^s h_0 = 0$ for $|s| = 3 - |r|,\ |r| \leq 2$, yields

$$h_0\#_{(3)}g^{(0)} = \left(-\frac{1}{2\mathrm{i}}\right)^3 \sum_{|r|+|s|=3} \frac{(-1)^{|r|}}{r!s!}\partial_x^r\partial_p^s h_0\ \partial_p^r\partial_x^s g^{(0)} = \frac{1}{8\mathrm{i}}\sum_{|r|=3}\left(\frac{1}{r!}\right)\partial_x^r h_0\ \partial_p^r g^{(0)}.$$

For the derivative of h_0 we have $\partial_x^r h_0 = \partial_x^r a_0$, and for the derivatives of $g^{(0)}$ we have

$$\begin{aligned}\partial_{p_k}g^{(0)} =&(-p_k)\beta\exp\left(\beta h_0\right),\\ \partial_{p_i}\partial_{p_k}g^{(0)} =&\beta\exp\left(\beta h_0\right)\left(\beta p_i p_k - \delta_{ik}\right),\\ \partial_{p_i}\partial_{p_k}\partial_{p_l}g^{(0)} =&\beta^2\exp\left(\beta h_0\right)\left(p_i\delta_{kl} + p_l\delta_{ik} + p_k\delta_{il} - \beta p_i p_k p_l\right),\end{aligned}$$

which leads us to (see for comparison Example 3.2.23)

$$\begin{aligned}H_0\#_{(3)}g^{(0)} =&\frac{1}{8\mathrm{i}}\frac{1}{6}\sum_{i=1}^2\sum_{k=1}^2\sum_{l=1}^2\left(\partial_{x_i}\partial_{x_k}\partial_{x_l}a_0\right)\beta^2 g^{(0)}(p_i\delta_{kl} + p_l\delta_{ik} + p_k\delta_{il} - \beta p_i p_k p_l)\\ =&\frac{\beta^2}{16\mathrm{i}}g^{(0)}\left[p\cdot\nabla_x(\Delta_x a_0) - \frac{\beta}{3}p\cdot\nabla_x\left(p^T(\nabla_x\otimes\nabla_x a_0)p\right)\right]\sigma_0.\end{aligned}$$

The fact that we found an imaginary quantity need not worry us, since we will see that this cancels out with the other-σ_0 components.

Next term is just a ordinary multiplication between $\boldsymbol{\sigma}$- and σ_0- components, hence

$$\boldsymbol{h}_1\#_{(0)}g^{(2)} = \frac{\beta^2}{8}g^{(0)}\left(\Delta_x a_0 + \frac{\beta}{3}\left(|\nabla_x a_0|^2 - p^T(\nabla_x\otimes\nabla_x a_0)p\right) + 4|\boldsymbol{h}_1|^2\right)\boldsymbol{h}_1\cdot\boldsymbol{\sigma}.$$

The following term needs a bit more attention, since it is the first time we multiplicate two $\boldsymbol{\sigma}$-components. The Pauli algebra gives us here (see (3.8))

$$H_1\#_{(1)}g^{(1)} = (\boldsymbol{h}_1\cdot\boldsymbol{\sigma})\#_{(1)}\left(\boldsymbol{g}^{(1)}\cdot\boldsymbol{\sigma}\right) = \left(\boldsymbol{h}_1\cdot_{\#_1}\boldsymbol{g}^{(1)}\right)\sigma_0 + \left(\boldsymbol{h}_1\times_{\#_1}\boldsymbol{g}^{(1)}\right)\cdot\mathrm{i}\boldsymbol{\sigma},$$

where we understand $\cdot_{\#_1}$ and $\times_{\#_1}$ as the usual vector operations where the multiplication is replaced by the order-1 Moyal product. Recalling that $g^{(1)}(\beta) = \beta\exp(\beta h_0)\boldsymbol{h}_1\cdot\boldsymbol{\sigma}$ (see (3.115)), we obtain for the first term at the right-hand side, by using Lemma 3.6.3

$$\begin{aligned}2\mathrm{i}\boldsymbol{h}_1\cdot_{\#_1}\boldsymbol{g}^{(1)} =&\left(\nabla_p\boldsymbol{h}_1\cdot\nabla_x(\beta g^{(0)}\boldsymbol{h}_1) - \nabla_x\boldsymbol{h}_1\cdot\nabla_p(\beta g^{(0)}\boldsymbol{h}_1)\right)\\ =&\beta g^{(0)}\left(\nabla_p\boldsymbol{h}_1\cdot\nabla_x\boldsymbol{h}_1 - \nabla_x\boldsymbol{h}_1\cdot\nabla_p\boldsymbol{h}_1\right) + \left(\nabla_p\boldsymbol{h}_1\cdot\nabla_x\beta g^{(0)} - \nabla_x\boldsymbol{h}_1\cdot\nabla_p\beta g^{(0)}\right)\cdot\boldsymbol{h}_1\\ =&\left(\nabla_p\boldsymbol{h}_1\cdot\nabla_x\beta g^{(0)} - \nabla_x\boldsymbol{h}_1\cdot\nabla_p\beta g^{(0)}\right)\cdot\boldsymbol{h}_1\\ =&\left(-\alpha\nabla_p p^\perp\cdot(\beta^2 g^{(0)}\nabla_x a_0) - \nabla_x\boldsymbol{a}\cdot(-p\beta^2 g^{(0)})\right)\\ =&\beta^2 g^{(0)}\left(-\alpha(\nabla_x a_0)^\perp + (\nabla_x\boldsymbol{a})p\right)\cdot\boldsymbol{h}_1.\end{aligned}$$

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The second term obtained from the Pauli algebra is $2\mathrm{i}\boldsymbol{h}_1 \times_{\#_1} \boldsymbol{g}^{(1)} = \nabla_p \boldsymbol{h}_1 \times \nabla_x \boldsymbol{g}^{(1)} - \nabla_x \boldsymbol{h}_1 \times \nabla_p \boldsymbol{g}^{(1)}$, where the cross product refers to the components of $\boldsymbol{h}_1$ and $\boldsymbol{g}^{(1)}$ and not to the gradients, see Appendix B.3.3. We get for this part

$$\begin{aligned}2\mathrm{i}\beta^{-1}\boldsymbol{h}_1 \times_{\#_1} \boldsymbol{g}^{(1)} =& \nabla_p \boldsymbol{h}_1 \times (\nabla_x g^{(0)} \boldsymbol{h}_1) - \nabla_x \boldsymbol{h}_1 \times (\nabla_p g^{(0)} \boldsymbol{h}_1)\\ =& \nabla_p \boldsymbol{h}_1 \times ((\nabla_x g^{(0)})\boldsymbol{h}_1 + g^{(0)}\nabla_x \boldsymbol{h}_1) - \nabla_x \boldsymbol{h}_1 \times ((\nabla_p g^{(0)})\boldsymbol{h}_1 + g^{(0)}\nabla_p \boldsymbol{h}_1)\\ =& (\nabla_p \boldsymbol{h}_1 \nabla_x g^{(0)} - \nabla_x \boldsymbol{h}_1 \nabla_p g^{(0)}) \times \boldsymbol{h}_1 + 2g^{(0)}\nabla_p \boldsymbol{h}_1 \times \nabla_x \boldsymbol{h}_1\\ =& g^{(0)}\left(\beta(-\alpha(\nabla_x a_0)^\perp + (\nabla_x \boldsymbol{a})p) \times \boldsymbol{h}_1 - 2\alpha(\nabla_x^\perp \times \boldsymbol{a})\right).\end{aligned}$$

Therefore,

$$\begin{aligned}H_1\#_{(1)}g^{(1)} = \beta g^{(0)}\Bigg[&\frac{1}{2\mathrm{i}}\left(\beta((\nabla_x \boldsymbol{a})p - \alpha(\nabla_x a_0)^\perp)\cdot \boldsymbol{h}_1\right)\sigma_0\\ &+\frac{1}{2}\left(\beta((\nabla_x \boldsymbol{a})p - \alpha(\nabla_x a_0)^\perp) \times \boldsymbol{h}_1 - 2\alpha(\nabla_x^\perp \times \boldsymbol{a})\right)\cdot \boldsymbol{\sigma}\Bigg].\end{aligned}$$

The last term of (3.117), i.e. $H_1\#_{(2)}g^{(0)}$, will only give a contribution to the $\boldsymbol{\sigma}$-components, and we have again that $\partial_p^r\partial_x^s \boldsymbol{h}_1 = 0$ for $|r| \geq 2$ and also for $|r| \geq 1 \wedge |s| \geq 1$. Here the Moyal product of the Pauli components is to understand as $(\boldsymbol{h}_1\#_{(2)}g^{(0)})_j = (\boldsymbol{h}_1)_j\#_{(2)}g^{(0)}$ and we obtain

$$\begin{aligned}\boldsymbol{h}_1\#_{(2)}g^{(0)} =& -\frac{1}{8}\sum_{k=1}^{2}\sum_{l=1}^{2}\partial_{x_k}\partial_{x_l}\boldsymbol{h}_1\partial_{p_k}\partial_{p_l}g^{(0)}\\ =& -\frac{1}{8}\sum_{k=1}^{2}\sum_{l=1}^{2}(\partial_{x_k}\partial_{x_l}\boldsymbol{a})\beta g^{(0)}\left(p_k p_l \beta - \delta_{kl}\right)\\ =& -\frac{1}{8}\beta g^{(0)}\left(\beta p^T(\nabla_x \otimes \nabla_x \boldsymbol{a})p - \Delta_x \boldsymbol{a}\right).\end{aligned}$$

By substituting in (3.117) all the explicitly computed terms, we see that all the σ_0-components cancel themselves out. Since only derivatives with respect to x remain, we drop the notation again and obtain the ODE

$$\begin{aligned}\partial_\beta g^{(3)} =& H_0 g^{(3)} + \frac{\beta}{8}g^{(0)}\Bigg[\beta\left(3\Delta a_0 + \frac{4}{3}\beta\left(|\nabla a_0|^2 - p^T(\nabla\otimes\nabla a_0)p\right) + 4|\boldsymbol{h}_1|^2\right)\boldsymbol{h}_1\\ &+ 2\Delta \boldsymbol{a} - 8\alpha(\nabla^\perp \times \boldsymbol{a}) + \beta\left(2\nabla \boldsymbol{a}\cdot\nabla a_0 - p^T(\nabla\otimes\nabla \boldsymbol{a})p + 2\alpha\nabla^\perp(\nabla a_0 \cdot p)\right)\\ &+ 4\beta(\nabla \boldsymbol{a} p - \alpha(\nabla a_0)^\perp) \times \boldsymbol{h}_1\Bigg]\cdot\boldsymbol{\sigma},\end{aligned}$$

with initial datum $g^{(3)}(0) = 0$. Solving the ODE (see Appendix B.3.3) yields

$$\begin{aligned}g^{(3)}(\beta) =& \frac{\beta^2}{24}\exp(\beta h_0)\Bigg[\left(3\beta\Delta a_0 + \beta^2(|\nabla a_0|^2 - p^T(\nabla\otimes\nabla a_0)p) + 4\beta|\boldsymbol{h}_1|^2\right)\boldsymbol{h}_1\\ &+ 3\Delta\boldsymbol{a} - 12\alpha(\nabla^\perp)\times\boldsymbol{a} + \beta\Big(2\nabla\boldsymbol{a}\cdot\nabla a_0 - p^T(\nabla\otimes\nabla\boldsymbol{a})p + 2\alpha(\nabla^\perp)(\nabla a_0\cdot p)\Big)\\ &+ 4\beta\Big((\nabla\boldsymbol{a})p - \alpha(\nabla a_0)^\perp\Big)\times\boldsymbol{h}_1\Bigg]\cdot\boldsymbol{\sigma}.\end{aligned} \tag{3.119}$$

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Adding the orders (3.111),(3.115), (3.116) and (3.119) we obtain the semiclassical expansion of $g(\beta)$ up to the third order

$$\begin{aligned}
g(\beta) =& \exp(\beta h_0)\sigma_0 + \varepsilon\beta\exp(\beta h_0)\boldsymbol{h}_1\cdot\boldsymbol{\sigma} + \\
&+ \varepsilon^2\frac{\beta^2}{8}\exp(\beta h_0)\left(\Delta a_0 + \frac{\beta}{3}\Big(|\nabla a_0|^2 - p^T(\nabla\otimes\nabla a_0)p\Big) + 4|\boldsymbol{h}_1|^2\right)\sigma_0 + \\
&+ \varepsilon^3\frac{\beta^2}{24}\exp(\beta h_0)\Bigg[\Big(3\beta\Delta a_0 + \beta^2(|\nabla a_0|^2 - p^T(\nabla\otimes\nabla a_0)p) + 4\beta|\boldsymbol{h}_1|^2\Big)\boldsymbol{h}_1 \\
&\quad + 3\Delta\boldsymbol{a} - 12\alpha(\nabla^\perp)\times\boldsymbol{a} + \beta\Big(2\nabla\boldsymbol{a}\cdot\nabla a_0 - p^T(\nabla\otimes\nabla\boldsymbol{a})p + 2\alpha(\nabla^\perp)(\nabla a_0\cdot p)\Big) \\
&\quad + 4\beta\Big((\nabla\boldsymbol{a})p - \alpha(\nabla a_0)^\perp\Big)\times\boldsymbol{h}_1\Bigg]\cdot\boldsymbol{\sigma} + \mathcal{O}(\varepsilon^4).
\end{aligned}$$

Setting in the above $\beta = 1$ we obtain the semiclassical expansion of $\mathcal{M}(N)$ up to the third order.

□

3.6.3. Semiclassical Expansion of the Lagrange Multiplier

In the previous section we derived the semiclassical expansion of the quantum Maxwellian, but we did hide an important fact. We expanded $\mathcal{M}$ (dropping from now on the dependence on N, for the sake of simplicity) under the consideration that $\mathcal{M}$ is an explicit function of the semiclassical parameter ε, which is equivalent to assuming that the Lagrange multipliers are of order 1 (or that the Lagrange multipliers are not quantum objects). In fact we have seen in Section 3.3.3 that a_0 and $\boldsymbol{a}$ also have a semiclassical expansion, and that for example the zeroth order of the quantum Maxwellian depends only on the zeroth order of a_0. This means that $\mathcal{M}$ also depends on ε through its dependence on $\tilde{A}$. In order to stress this fact we provisionally write the quantum Maxwellian as a function of ε and $\tilde{A}(\varepsilon)$, i.e. $\mathcal{M}(\varepsilon, \tilde{A}(\varepsilon))$. With the Taylor expansion at $\epsilon = 0$ we obtain at first hand the *semiclassical expansion of the Lagrange multipliers*

$$a_j(\varepsilon) = \sum_{k=0}^{\infty}\varepsilon^k a_j^{(k)}, \qquad \text{where } a_j^{(k)} = \frac{1}{k!}\frac{\partial^k a_j}{\partial\varepsilon^k}\bigg|_{\varepsilon=0}, \qquad \text{for } j\in\{0,1,2,3\} \tag{3.120}$$

where we recall that $a_0 = \tilde{a}_0 - V$, and at second hand we obtain the complete expansion of the quantum Maxwellian

$$\mathcal{M}(\varepsilon) = \sum_{k=0}^{\infty}\varepsilon^k\mathcal{M}^{(k)}, \qquad \text{where } \mathcal{M}^{(k)} = \frac{1}{k!}\frac{d^k}{d\varepsilon^k}\mathcal{M}(\varepsilon,\tilde{A}(\varepsilon))\bigg|_{\varepsilon=0}.$$

The previous work was not in vain, since the relation between the general quantum Maxwellian $g(\beta)$ (see (3.107)) and $\mathcal{M}$ is still important. We have that the explicit dependence on ε of $\mathcal{M}$ comes from the semiclassical expansion of g, which means that

$$\frac{\partial^m\mathcal{M}}{\partial\varepsilon^m}\bigg|_{\varepsilon=0} = \frac{\partial^m g(1)}{\partial\varepsilon^m}\bigg|_{\varepsilon=0} = m!g^{(m)}(1),$$

where $g^{(m)}$ is the m-th order of the semiclassical expansion $g(\beta) = \sum_{m=0}^{\infty}\varepsilon^m g^{(m)}(\beta)$ we calculated in Section 3.6.2. Since the Pauli representatives are unique, we identify the matrix

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$\tilde{A}(\varepsilon)$ with the four dimensional vector $(a_0(\varepsilon), a_1(\varepsilon), a_2(\varepsilon), a_3(\varepsilon))$ and obtain for the first four orders the equations (detailed calculations in the Appendix B.4.1)

$$\mathcal{M}^{(0)} = \mathcal{M}\big|_{\varepsilon=0}, \tag{3.121}$$

$$\mathcal{M}^{(1)} = \frac{\partial \mathcal{M}}{\partial \varepsilon}\bigg|_{\varepsilon=0} + \sum_{j=0}^{3} \frac{\partial \mathcal{M}}{\partial a_j}\bigg|_{\varepsilon=0} a_j^{(1)}, \tag{3.122}$$

$$\begin{aligned}2\mathcal{M}^{(2)} =& \frac{\partial^2 \mathcal{M}}{\partial \varepsilon^2}\bigg|_{\varepsilon=0} + \sum_{j=0}^{3} 2\frac{\partial^2 \mathcal{M}}{\partial \varepsilon \partial a_j}\bigg|_{\varepsilon=0} a_j^{(1)} \\ &+ \sum_{j=0}^{3}\sum_{k=0}^{3} \frac{\partial^2 \mathcal{M}}{\partial a_j \partial a_k}\bigg|_{\varepsilon=0} a_j^{(1)} a_k^{(1)} + 2\frac{\partial \mathcal{M}}{\partial a_j}\bigg|_{\varepsilon=0} a_j^{(2)},\end{aligned} \tag{3.123}$$

$$\begin{aligned}6\mathcal{M}^{(3)} =& \frac{\partial^3 \mathcal{M}}{\partial \varepsilon^3}\bigg|_{\varepsilon=0} + \sum_{j=0}^{3} 3\frac{\partial^3 \mathcal{M}}{\partial \varepsilon^2 \partial a_j}\bigg|_{\varepsilon=0} a_j^{(1)} + 6\frac{\partial^2 \mathcal{M}}{\partial \varepsilon \partial a_j}\bigg|_{\varepsilon=0} a_j^{(2)} + 6\frac{\partial \mathcal{M}}{\partial a_j}\bigg|_{\varepsilon=0} a_j^{(3)} \\ &+ \sum_{j=0}^{3}\sum_{k=0}^{3} 3\frac{\partial^3 \mathcal{M}}{\partial \varepsilon \partial a_j \partial a_k}\bigg|_{\varepsilon=0} a_j^{(1)} a_k^{(1)} + \frac{\partial^2 \mathcal{M}}{\partial a_j \partial a_k}\bigg|_{\varepsilon=0} \left(4a_j^{(2)} a_k^{(1)} + 2a_k^{(2)} a_j^{(1)}\right) \\ &+ \sum_{j=0}^{3}\sum_{k=0}^{3}\sum_{i=0}^{3} \frac{\partial^3 \mathcal{M}}{\partial a_j \partial a_k \partial a_i}\bigg|_{\varepsilon=0} a_j^{(1)} a_k^{(1)} a_i^{(1)},\end{aligned} \tag{3.124}$$

How do we now obtain from the above the various orders of our Lagrange multipliers? The answer is the constraint $\langle \mathcal{M} \rangle = n_0\sigma_0 + \varepsilon \boldsymbol{n} \cdot \boldsymbol{\sigma}$ given in Problem 3.3.5, which gives us through comparison of the the orders of ε the following four equations

$$1. \left\langle \mathcal{M}^{(0)} \right\rangle = n_0\sigma_0, \qquad 2. \left\langle \mathcal{M}^{(1)} \right\rangle = \boldsymbol{n} \cdot \boldsymbol{\sigma}, \qquad 3. \left\langle \mathcal{M}^{(2)} \right\rangle = 0, \qquad 4. \left\langle \mathcal{M}^{(3)} \right\rangle = 0. \tag{3.125}$$

With the above it will be possible to evaluate the orders of a_0 and $\boldsymbol{a}$, and write them as functions of ε and N. Before we do that, let us state a basic result from measure theory.

Proposition 3.6.4. *Let $u \in \mathbb{R}$, then*

$$\int_{\mathbb{R}} e^{\frac{-u^2}{2}} du = \sqrt{2\pi}, \qquad \int_{\mathbb{R}} u e^{\frac{-u^2}{2}} du = 0, \qquad \int_{\mathbb{R}} u^2 e^{\frac{-u^2}{2}} du = \sqrt{2\pi}, \qquad \int_{\mathbb{R}} u^3 e^{\frac{-u^2}{2}} du = 0.$$

Proof. The first integrand is a Gaussian density function with expectation value one and variation zero. Since the function $F(A) = \frac{1}{\sqrt{2\pi}} \int_A \exp(-u^2/2) du$ is a probability on $\mathbb{R}$, means that $F(\mathbb{R}) = 1$, we get immediately the first result. That the third integral vanishes, is obtained by partial integration and the first result. In the second and fourth integral, odd functions are integrated over the whole space, and therefore their integrals are zero. □

Theorem 3.6.5. *Let $\tilde{a}_0$ and $\boldsymbol{a}$ be the Lagrange multiplier, given through Theorem 3.3.8, and recall $a_0 = \tilde{a}_0 - V$. Then the semiclassical expansions of the Pauli components are given by:*

$$\begin{aligned} a_0 =& \log\left(\frac{1}{2\pi} n_0\right) - \varepsilon^2 \left(\frac{1}{12}\left(\frac{\Delta n_0}{n_0} - \frac{1}{2}\frac{|\nabla n_0|^2}{{n_0}^2}\right) + \frac{1}{2}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \alpha^2\right) + \mathcal{O}(\varepsilon^4), \\ \boldsymbol{a} =& \frac{1}{n_0}\boldsymbol{n} + \varepsilon^2 \left[\frac{1}{12 n_0}\left(\left(\frac{\Delta n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2 + 4\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + 8\alpha^2\right)\boldsymbol{n} + 4\alpha^2 \left(\boldsymbol{n}^\perp\right)^\perp\right) - \right. \\ & \left. - \frac{1}{12}\left(\frac{\Delta \boldsymbol{n}}{n_0} - \frac{\nabla \boldsymbol{n}}{n_0} \cdot \frac{\nabla n_0}{n_0}\right) + \frac{\alpha}{6 n_0}\left(4\nabla + \frac{\nabla n_0}{n_0}\right)^\perp \times \boldsymbol{n}\right] + \mathcal{O}(\varepsilon^3), \end{aligned}$$

where $\left(\boldsymbol{n}^\perp\right)^\perp = (-n_1, -n_2, 0)^T$ and $\left(4\nabla + \frac{\nabla n_0}{n_0}\right)^\perp = 4\nabla^\perp + \frac{\nabla^\perp n_0}{n_0}$.

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Remark 3.6.6. Again we observe here a consequence of our smallness assumption on the macroscopic density N (see Remark 3.3.6). Apparently the odd orders (up to the third at least) vanish, which makes the calculations less tedious. Furthermore we recall that in Section 3.3.3 the zeroth order of the matrix of Lagrange multiplier was calculated, where we obtained the special structure $\tilde{A} = \tilde{a}_0\sigma_0 + \varepsilon \boldsymbol{a}\cdot\boldsymbol{\sigma}$. So the above semiclassical expansion of $\boldsymbol{a}$ is the right one, but to obtain the m-th order of $\tilde{A}$ we have the relation

$$\tilde{A}^{(0)} = (a_0^{(0)} - V)\sigma_0, \qquad \tilde{A}^{(m)} = {a_0}^{(m)}\sigma_0 + \boldsymbol{a}^{(m-1)}\cdot\boldsymbol{\sigma},\ m \geq 1.$$

■

Proof of Theorem 3.6.5:

As already mentioned we have to combine the constraint equations (3.125) with the relations given in (3.121)-(3.124) to obtain the different orders. From the first equation in (3.125) and (3.121) we get with Proposition 3.6.4

$$n_0 = \left\langle \boldsymbol{m}_0^{(0)}\Big|_{\varepsilon=0} \right\rangle = \left\langle g_0^{(0)}(1)\Big|_{\varepsilon=0} \right\rangle = \left\langle \exp\left(-\frac{|p|^2}{2} + a_0\right) \right\rangle = 2\pi \exp\left(a_0^{(0)}\right),$$

which allows us to identify the leading order Lagrange multiplier by

$$a_0^{(0)} = \log\left(\frac{1}{2\pi} n_0\right).$$

From now on we will denote

$$h_0^{(0)} := -\frac{|p|^2}{2} + a_0^{(0)}, \qquad \boldsymbol{h}_1^{(0)} := \boldsymbol{a}^{(0)} - \alpha p^{\perp}. \tag{3.126}$$

To solve the higher-order constraint equations in (3.125), we shall need the following derivatives of $\mathcal{M}$:

$$\frac{\partial^k \mathcal{M}}{\partial \varepsilon^k}\Big|_{\varepsilon=0} = k!\, g^{(k)}(1)\big|_{\varepsilon=0}, \tag{3.127}$$

$$\frac{\partial \mathcal{M}}{\partial a_j}\Big|_{\varepsilon=0} = \begin{cases} \exp\left(h_0^{(0)}\right)\sigma_0, & \text{for } j=0,\\ 0, & \text{else,}\end{cases} \tag{3.128}$$

$$\frac{\partial^2 \mathcal{M}}{\partial a_j \partial a_k}\Big|_{\varepsilon=0} = \begin{cases} \exp\left(h_0^{(0)}\right)\sigma_0, & \text{for } j=k=0,\\ 0, & \text{else,}\end{cases} \tag{3.129}$$

$$\frac{\partial^2 \mathcal{M}}{\partial \varepsilon \partial a_j}\Big|_{\varepsilon=0} = \begin{cases} \exp\left(h_0^{(0)}\right)\boldsymbol{h}_1^{(0)}\cdot\boldsymbol{\sigma}, & \text{for } j=0,\\ \exp\left(h_0^{(0)}\right)\sigma_j, & \text{else.}\end{cases} \tag{3.130}$$

From the second constraint equation in (3.125) we get again with Proposition 3.6.4

$$\begin{aligned}\boldsymbol{n}\cdot\boldsymbol{\sigma} =& \left\langle \exp\left(h_0^{(0)}\right)\boldsymbol{h}_1^{(0)}\cdot\boldsymbol{\sigma} + \exp\left(h_0^{(0)}\right)a_0^{(1)}\sigma_0 \right\rangle\\ =& \left\langle \exp\left(-\frac{|p|^2}{2} + a_0^{(0)}\right)\boldsymbol{a}^{(0)}\cdot\boldsymbol{\sigma} \right\rangle + \alpha\left\langle \exp\left(-\frac{|p|^2}{2}\right)p^{\perp} \right\rangle \exp\left(a_0^{(0)}\right)\cdot\boldsymbol{\sigma} + n_0 a_0^{(1)}\sigma_0\\ =& n_0\boldsymbol{a}^{(0)}\cdot\boldsymbol{\sigma} + n_0 a_0^{(1)}\sigma_0,\end{aligned}$$

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which, by comparison of the Pauli components, leads to

$$a_0^{(1)} = 0, \qquad \boldsymbol{a}^{(0)} = \frac{1}{n_0}\boldsymbol{n}. \tag{3.131}$$

For the next orders we look at the third equation of (3.125) and obtain with (3.123), the derivatives (3.127)-(3.130) and the already calculated orders that

$$\begin{aligned} 0 &= \left\langle \frac{\partial^2 \mathcal{M}}{\partial \varepsilon^2}\bigg|_{\varepsilon=0} + \sum_{j=0}^{3} 2\frac{\partial^2 \mathcal{M}}{\partial \varepsilon \partial a_j}\bigg|_{\varepsilon=0} a_j^{(1)} + \sum_{j=0}^{3}\sum_{k=0}^{3} \frac{\partial^2 \mathcal{M}}{\partial a_j \partial a_k}\bigg|_{\varepsilon=0} a_j^{(1)} a_k^{(1)} + 2\frac{\partial \mathcal{M}}{\partial a_j}\bigg|_{\varepsilon=0} a_j^{(2)} \right\rangle \\ &= \left\langle 2g^{(2)}(1)\Big|_{\varepsilon=0} + 2\exp\left(h_0^{(0)}\right)\left(\sum_{j=1}^{3} a_j^{(1)}\sigma_j\right) + 2\exp\left(h_0^{(0)}\right) a_0^{(2)}\sigma_0 \right\rangle. \end{aligned}$$

Since $g^{(2)}$ only consists of a σ_0-component, the only Paul components regarding $\boldsymbol{\sigma}$ appearing on the right hand side are $\boldsymbol{a}^{(1)}$, hence we can deduce

$$\boldsymbol{a}^{(1)} = \mathbf{0}.$$

So what we obtain from the above is that

$$a_0^{(2)} = -\frac{1}{n_0}\left\langle g_0^{(2)}(1)\Big|_{\varepsilon=0} \right\rangle$$

The right hand side can be integrated with basic techniques and is therefore put into the Appendix B.4.2. The result is then

$$a_0^{(2)} = -\frac{1}{12}\Delta \log(n_0) - \frac{1}{24}|\nabla \log(n_0)|^2 - \frac{1}{2}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 - \alpha^2, \tag{3.132}$$

or after resolving the derivatives of the logarithm (see also Appendix B.4.2)

$$a_0^{(2)} = -\frac{1}{12}\left(\frac{\Delta n_0}{n_0} - \frac{1}{2}\frac{|\nabla n_0|^2}{{n_0}^2}\right) - \frac{1}{2}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 - \alpha^2.$$

For the last needed orders, $\boldsymbol{a}^{(2)}$ and $a_0^{(3)}$, we need the last constraint equation given in (3.125). Looking at (3.124), the equation reduces drastically, due to the fact that the first orders of a_0 and $\boldsymbol{a}$ vanish, and hence we have to solve

$$0 = \left\langle \frac{1}{6}\frac{\partial^3 \mathcal{M}}{\partial \varepsilon^3}\bigg|_{\varepsilon=0} + \sum_{j=0}^{3} \frac{\partial^2 \mathcal{M}}{\partial \varepsilon \partial a_j}\bigg|_{\varepsilon=0} a_j^{(2)} + \frac{\partial \mathcal{M}}{\partial a_0}\bigg|_{\varepsilon=0} a_0^{(3)} \right\rangle \tag{3.133}$$

The first two terms have only the spinorial part while the third one has only the trace part (see (3.119) and eqs. (3.127)–(3.130)), which immediately leads to

$$a_0^{(3)} = 0. \tag{3.134}$$

What remains is given by

$$0 = \left\langle \boldsymbol{g}^{(3)}(1)\Big|_{\varepsilon=0} + a_0^{(2)}\exp\left(h_0^{(0)}\right)\boldsymbol{h}_1^{(0)} + \exp\left(h_0^{(0)}\right)\boldsymbol{a}^{(2)} \right\rangle \cdot \boldsymbol{\sigma} \tag{3.135}$$

$$= \left\langle \boldsymbol{g}^{(3)}(1)\Big|_{\varepsilon=0} \right\rangle \cdot \boldsymbol{\sigma} + a_0^{(2)}\boldsymbol{n}\cdot\boldsymbol{\sigma} + n_0\boldsymbol{a}^{(2)}\cdot\boldsymbol{\sigma}, \tag{3.136}$$

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and therefore for the last needed component we have to calculate

$$\boldsymbol{a}^{(2)} = -\frac{1}{n_0}\left\langle \boldsymbol{g}^{(3)}(1)\Big|_{\varepsilon=0}\right\rangle - \frac{1}{n_0}a_0^{(2)}\boldsymbol{n}.$$

The computations are cumbersome, but straightforward and are therefore put into the Appendix B.4.3. The result for the integral is

$$\left\langle \boldsymbol{g}^{(3)}(1)\Big|_{\varepsilon=0}\right\rangle = \frac{n_0}{12}\left(\left[\Delta a_0^{(0)} + \frac{1}{2}\left|\nabla a_0^{(0)}\right|^2 + 2\left(\left|\boldsymbol{a}^{(0)}\right|^2 + 2\alpha^2\right)\right]\boldsymbol{a}^{(0)} - 4\alpha^2\left(\boldsymbol{a}^{(0)\perp}\right)^\perp\right)$$
$$+ \frac{n_0}{12}\left(\Delta\boldsymbol{a}^{(0)} + \nabla\boldsymbol{a}^{(0)}\cdot\nabla a_0^{(0)} - \alpha\left(8\nabla + 2\nabla a_0^{(0)}\right)^\perp \times \boldsymbol{a}^{(0)}\right), \quad (3.137)$$

where $(\boldsymbol{a}^{(0)\perp})^\perp = (-a_1^{(0)}, -a_2^{(0)}, 0)^T$ and

$$\left(8\nabla + 2\nabla a_0^{(0)}\right)^\perp \times \boldsymbol{a}^{(0)} = 8\nabla^\perp \times \boldsymbol{a}^{(0)} + 2(\nabla a_0^{(0)})^\perp \times \boldsymbol{a}^{(0)}.$$

Moreover, since $\boldsymbol{a}^{(0)} = \frac{1}{n_0}\boldsymbol{n}$, we have

$$\nabla\boldsymbol{a}^{(0)} = \frac{1}{n_0}\left(\nabla\boldsymbol{n} - \frac{1}{n_0}\boldsymbol{n}\nabla n_0\right),$$
$$\Delta\boldsymbol{a}^{(0)} = \frac{1}{n_0}\left(\Delta\boldsymbol{n} - \frac{2}{n_0}\nabla\boldsymbol{n}\cdot\nabla n_0 - \frac{1}{n_0}\Delta n_0\boldsymbol{n} + 2\left|\frac{\nabla n_0}{n_0}\right|^2\boldsymbol{n}\right).$$

Substituting the known orders, the integral of $g^{(3)}(1)$ and the above derivatives into the equation for $\boldsymbol{a}^{(2)}$ (see (3.137) and for the detailed calculations Appendix B.4.3) yields

$$\boldsymbol{a}^{(2)} = \frac{1}{12n_0}\left(\left(\frac{\Delta n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2 + 4\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + 8\alpha^2\right)\boldsymbol{n} + 4\alpha^2\left(\boldsymbol{n}^\perp\right)^\perp\right)$$
$$- \frac{1}{12}\left(\frac{\Delta\boldsymbol{n}}{n_0} - \frac{\nabla\boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0}\right) + \frac{\alpha}{6n_0}\left(4\nabla + \frac{\nabla n_0}{n_0}\right)^\perp \times \boldsymbol{n}, \quad (3.138)$$

where $(\boldsymbol{n}^\perp)^\perp = (-n_1, -n_2, 0)^T$ and $\left(4\nabla + \frac{\nabla n_0}{n_0}\right)^\perp = 4\nabla^\perp + \frac{\nabla^\perp n_0}{n_0}$.

□

3.6.4. Derivation of the Semiclassical Model (Proof of Main Theorem 3.6.1)

Before substituting the semiclassical expansions of $\mathcal{M}$, a_0 and $\boldsymbol{a}$ into the full quantum model (3.89)-(3.90), we recall (see Theorem 3.6.1) that we will only expand up to the order $\mathcal{O}(\alpha^k\varepsilon^l)$ with $k, l \in \mathbb{N}$, $k+l \leq 2$. Hence it will be enough to work with already approximated versions of the last calculated orders of g (eq. (3.119)) and $\boldsymbol{a}$ (eq. (3.138)), namely

$$g^{(3)}(1) = \frac{1}{24}\exp(h_0)\Bigg[\left(3\Delta a_0 + (|\nabla a_0|^2 - p^T(\nabla\otimes\nabla a_0)p) + 4\left|\boldsymbol{a} - \alpha p^\perp\right|^2\right)\boldsymbol{a} \quad (3.139)$$
$$+ 3\Delta\boldsymbol{a} + 2\nabla\boldsymbol{a}\cdot\nabla a_0 - p^T(\nabla\otimes\nabla\boldsymbol{a})p + 4\Big((\nabla\boldsymbol{a})p\Big)\times\boldsymbol{a}\Bigg] + \mathcal{O}(\alpha),$$

$$\boldsymbol{a}^{(2)} = \left(\frac{1}{3}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \frac{1}{12}\frac{\Delta n_0}{n_0} - \frac{1}{12}\left|\frac{\nabla n_0}{n_0}\right|^2\right)\frac{\boldsymbol{n}}{n_0} - \frac{1}{12}\frac{\Delta\boldsymbol{n}}{n_0} + \frac{1}{12}\frac{\nabla\boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0} + \mathcal{O}(\alpha). \quad (3.140)$$

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The reason why we did this not earlier was for the sake of completeness. If the reader is interested in a more detailed model we invite to calculate it with the full orders.
Now, we substitute all calculated expansions into the full quantum model (3.89)-(3.90) and disregard the terms where the product of the powers of α and ε exceeds two.

The semiclassical equation for n_0:

Beginning from the first quantity, which would be the charge density, we derive its semiclassical equation. Recall the non-local equation for n_0 (3.89):

$$\partial_t n_0 = \tau \operatorname{div}\left(n_0 \nabla a_0 + n_0 \nabla V + \varepsilon^2 \left(\boldsymbol{n} \cdot (\nabla \boldsymbol{a})\right)\right) + 2\tau\alpha\varepsilon^2 \left((\nabla^\perp) \cdot (\boldsymbol{n} \times \boldsymbol{a})\right).$$

The order of the last term is already out of our interest and can be therefore disregarded. Hence we need only to determine the gradient of a_0 and $\boldsymbol{a}$. Taking a closer look onto the first one we get

$$\begin{aligned}\nabla a_0 =& \nabla(a_0^{(0)} + \varepsilon^2 a_0^{(2)} + \mathcal{O}(\varepsilon^3)) \\ =& \nabla \left(\log\left(\frac{1}{2\pi} n_0\right) - \varepsilon^2 \left(\frac{1}{12}\left(\frac{\Delta n_0}{n_0} - \frac{1}{2}\frac{|\nabla n_0|^2}{{n_0}^2}\right) + \frac{1}{2}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \alpha^2\right)\right) + \mathcal{O}(\varepsilon^3) \\ =& \frac{\nabla n_0}{n_0} - \varepsilon^2 \nabla \left(\frac{1}{12}\left(\frac{\Delta n_0}{n_0} - \frac{1}{2}\frac{|\nabla n_0|^2}{{n_0}^2}\right) + \frac{1}{2}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \alpha^2\right) + \mathcal{O}(\varepsilon^3).\end{aligned}$$

Before we take the gradient we rewrite one particular term of $a_0^{(2)}$, namely

$$\frac{\Delta n_0}{n_0} - \frac{1}{2}\frac{|\nabla n_0|^2}{{n_0}^2} = 2\left(\frac{\Delta\sqrt{n_0}}{\sqrt{n_0}}\right). \tag{3.141}$$

This term is called the *Bohm potential* and is quite of interest among physicists and one of the reasons why the semiclassical expansion is mostly expanded up to the second order. For more details on this topic we refer to [Boh52a, Boh52b, DMR05, DT09, Jü09]. Since the Bohm potential is already in a "nice form" we pass to the next term:

$$\nabla\left(\frac{|\boldsymbol{n}|^2}{|n_0|^2}\right) = \frac{1}{|n_0|^4}(2|n_0|^2 \boldsymbol{n} \cdot \nabla \boldsymbol{n} - 2|\boldsymbol{n}|^2 n_0 \nabla n_0) = 2\left(\frac{1}{{n_0}^2}\boldsymbol{n}\cdot\nabla\boldsymbol{n} - \frac{|\boldsymbol{n}|^2}{{n_0}^3}\nabla n_0\right),$$

where we understand $(\boldsymbol{n} \cdot \nabla \boldsymbol{n})_j = \boldsymbol{n} \cdot \partial_{x_j} \boldsymbol{n}$. So we obtain

$$n_0 \nabla a_0 = \nabla n_0 - \varepsilon^2 \left(\frac{1}{6} n_0 \nabla \left(\frac{\Delta\sqrt{n_0}}{\sqrt{n_0}}\right) + \frac{1}{n_0}\boldsymbol{n}\cdot\nabla\boldsymbol{n} - \frac{|\boldsymbol{n}|^2}{{n_0}^2}\nabla n_0\right) + \mathcal{O}(\varepsilon^3).$$

For $\nabla \boldsymbol{a}$ we only need the zeroth order, since it is already multiplied with ε^2. Here we get:

$$\nabla \boldsymbol{a} = \nabla(\boldsymbol{a}^{(0)} + \mathcal{O}(\varepsilon^2)) = \nabla\left(\frac{\boldsymbol{n}}{n_0}\right) + \mathcal{O}(\varepsilon^2) = \frac{1}{n_0}\nabla\boldsymbol{n} - \frac{1}{{n_0}^2}\boldsymbol{n}\nabla n_0 + \mathcal{O}(\varepsilon^2).$$

Let us point out that $\nabla \boldsymbol{n}$ and $\boldsymbol{n}\nabla n_0$ are matrices with the rows ∇n_j and $n_j \nabla n_0$ respectively, for $j \in \{1,2,3\}$. Hence we obtain for the last term

$$\boldsymbol{n}\cdot\nabla\boldsymbol{a} = \sum_{j=1}^{3}\frac{n_j}{n_0}\nabla n_j - \frac{n_j^2}{{n_0}^2}\nabla n_0 + \mathcal{O}(\varepsilon^2) = \frac{1}{n_0}\boldsymbol{n}\cdot\nabla\boldsymbol{n} - \frac{|\boldsymbol{n}|^2}{{n_0}^2}\nabla n_0 + \mathcal{O}(\varepsilon^2).$$

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Substituting the results into the non-local equation for n_0 we get

$$\begin{aligned}\partial_t n_0 =& \tau \operatorname{div}\Big(n_0\nabla a_0 + n_0\nabla V + \varepsilon^2\left(\boldsymbol{n}\cdot(\nabla\boldsymbol{a})\right)\Big) + \mathcal{O}(\alpha\varepsilon^2)\\ =&\tau \operatorname{div}\left(n_0\nabla n_0 - \varepsilon^2\left(\frac{1}{6}n_0\nabla\left(\frac{\Delta\sqrt{n_0}}{\sqrt{n_0}}\right) + \frac{1}{n_0}\boldsymbol{n}\cdot\nabla\boldsymbol{n} - \frac{|\boldsymbol{n}|^2}{n_0{}^2}\nabla n_0\right)\right.\\ &\left.+n_0\nabla V + \varepsilon^2\left(\frac{1}{n_0}\boldsymbol{n}\cdot\nabla\boldsymbol{n} - \frac{|\boldsymbol{n}|^2}{n_0{}^2}\nabla n_0\right)\right) + \mathcal{O}(\varepsilon^3)\\ =&\tau \operatorname{div}\left(n_0\nabla n_0 + n_0\nabla V - \frac{\varepsilon^2}{6}n_0\nabla\left(\frac{\Delta\sqrt{n_0}}{\sqrt{n_0}}\right)\right) + \mathcal{O}(\varepsilon^3),\end{aligned}$$

where we also used that α is of the same order as ε.

The Semiclassical Equations for the Spin Components:

We now derive the semiclassical equation (3.106) for the "spin part" $\boldsymbol{n}$, by substituting the semiclassical approximations of $\mathcal{M}$, a_0 and $\boldsymbol{a}$ in the full quantum model (3.90), that we recall here for convenience:

$$\begin{aligned}\partial_t\boldsymbol{n} =& -2(\boldsymbol{n}\times\boldsymbol{a}) + \tau\operatorname{div}\left(n_0\nabla\boldsymbol{a} + \boldsymbol{n}\nabla a_0 + \boldsymbol{n}\nabla V + \frac{2}{\varepsilon}(J^T\times\boldsymbol{a})\right)\\ &-2\tau\alpha\left(n_0(\nabla^\perp\times\boldsymbol{a}) + \nabla^\perp(a_0+V)\times\boldsymbol{n} - \frac{2}{\varepsilon}\left(\boldsymbol{a}\left\langle p^\perp\cdot\boldsymbol{m}\right\rangle + J^T\boldsymbol{a}^\perp\right)\right)\\ &-2\tau\left(2\varepsilon(\boldsymbol{n}\times\boldsymbol{a})\times\boldsymbol{a} - \boldsymbol{n}\times\partial_t^{(0)}\boldsymbol{a}\right).\end{aligned} \tag{3.142}$$

And to have everything at one point we recall also the semiclassical expansions, where we use the approximated versions of the last orders (3.139) -(3.140) introduced in the beginning of the proof:

$$\begin{aligned}\mathcal{M}(N) =& \exp(h_0)\sigma_0 + \varepsilon\exp(h_0)\boldsymbol{h}_1\cdot\boldsymbol{\sigma}\\ &+\frac{\varepsilon^2}{8}\exp(h_0)\left(\Delta a_0 + \frac{1}{3}\Big(|\nabla a_0|^2 - p^T(\nabla\otimes\nabla a_0)p\Big) + 4|\boldsymbol{h}_1|^2\right)\sigma_0\\ &+\frac{\varepsilon^3}{24}\exp(h_0)\Bigg[\left(3\Delta a_0 + (|\nabla a_0|^2 - p^T(\nabla\otimes\nabla a_0)p) + 4\left|\boldsymbol{a}-\alpha p^\perp\right|^2\right)\boldsymbol{a}\\ &\qquad + 3\Delta\boldsymbol{a} + 2\nabla\boldsymbol{a}\cdot\nabla a_0 - p^T(\nabla\otimes\nabla\boldsymbol{a})p + 4\Big((\nabla\boldsymbol{a})p\Big)\times\boldsymbol{a}\Bigg]\cdot\boldsymbol{\sigma} + \mathcal{O}(\varepsilon^4),\end{aligned}$$

and

$$\begin{aligned}a_0 =& \log\left(\frac{1}{2\pi}n_0\right) - \varepsilon^2\left(\frac{1}{12}\left(\frac{\Delta n_0}{n_0} - \frac{1}{2}\frac{|\nabla n_0|^2}{n_0{}^2}\right) + \frac{1}{2}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \alpha^2\right) + \mathcal{O}(\varepsilon^4),\\ \boldsymbol{a} =& \frac{1}{n_0}\boldsymbol{n} + \varepsilon^2\left(\left(\frac{1}{3}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \frac{1}{12}\frac{\Delta n_0}{n_0} - \frac{1}{12}\left|\frac{\nabla n_0}{n_0}\right|^2\right)\frac{\boldsymbol{n}}{n_0} - \frac{1}{12}\frac{\Delta\boldsymbol{n}}{n_0} + \frac{1}{12}\frac{\nabla\boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0}\right) + \mathcal{O}(\varepsilon^3).\end{aligned}$$

Next we recall the already calculated derivatives from various orders (for the calculations see Appendix B.4.2 and Appendix B.4.3)

$$\begin{aligned}\nabla a_0^{(0)} =& \frac{\nabla n_0}{n_0}, & \nabla\boldsymbol{a}^{(0)} =& \frac{1}{n_0{}^2}\left(n_0\nabla\boldsymbol{n} - \boldsymbol{n}\nabla n_0\right),\\ \Delta a_0^{(0)} =& \frac{\Delta n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2, & \Delta\boldsymbol{a}^{(0)} =& \frac{1}{n_0}\left(\Delta\boldsymbol{n} - \frac{2}{n_0}\nabla\boldsymbol{n}\cdot\nabla n_0 - \frac{1}{n_0}\Delta n_0\boldsymbol{n} + 2\left|\frac{\nabla n_0}{n_0}\right|^2\boldsymbol{n}\right).\end{aligned}$$

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Let us for the start calculate the remaining derivatives that are needed for our substitution, where we put the lengthy but straightforward calculations into Appendix B.4.4. They are given by

$$\nabla a_0^{(2)} = -\frac{1}{12}\left(\frac{\nabla(\Delta n_0)}{n_0} - \frac{\nabla n_0}{n_0}\frac{\Delta n_0}{n_0} - \frac{\nabla n_0}{n_0}\frac{(\nabla\otimes\nabla)n_0}{n_0} + \left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right) - \left(\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0} - \left|\frac{\boldsymbol{n}}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right),$$

$$\begin{aligned}\nabla\boldsymbol{a}^{(2)} = &\frac{\boldsymbol{n}}{n_0}\left(\frac{2}{3}\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0} - \left|\frac{\boldsymbol{n}}{n_0}\right|^2\frac{\nabla n_0}{n_0} + \frac{1}{12}\frac{\nabla(\Delta n_0)}{n_0} - \frac{1}{6}\frac{\nabla n_0}{n_0}\frac{\Delta n_0}{n_0} - \frac{1}{6}\frac{\nabla n_0}{n_0}\frac{(\nabla\otimes\nabla)n_0}{n_0}\right)\\ &+\frac{\boldsymbol{n}}{n_0}\left(\frac{1}{4}\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right) + \frac{1}{12}\frac{\nabla\boldsymbol{n}}{n_0}\left(\frac{(\nabla\otimes\nabla)n_0}{n_0} + \left(4\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \frac{\Delta n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2\right)\sigma_0\right)\\ &+\frac{1}{12}\left(\frac{\Delta\boldsymbol{n}}{n_0} - 2\left(\frac{\nabla\boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0}\right)\right)\frac{\nabla n_0}{n_0} + \frac{1}{12}\frac{\nabla n_0}{n_0}\frac{(\nabla\otimes\nabla)\boldsymbol{n}}{n_0} - \frac{1}{12}\frac{\nabla(\Delta\boldsymbol{n})}{n_0},\end{aligned}$$

where $((\nabla n_0(\nabla\otimes\nabla))\boldsymbol{n})_j = \nabla n_0(\nabla\otimes\nabla)n_j$, and $\nabla\boldsymbol{a}^{(2)}$ is a 3×3 matrix, where the last column equals zero.

With the above derivations we are able to substitute everything in the equation for the spin components (3.90). Due to the multilinearity of the cross product we are able to split the first term into two parts.

$$\boldsymbol{n}\times\boldsymbol{a} = \boldsymbol{n}\times\boldsymbol{a}^{(0)} + \varepsilon^2\boldsymbol{n}\times\boldsymbol{a}^{(2)} + \mathcal{O}(\varepsilon^3)$$

Both terms $\boldsymbol{a}^{(0)}$ and $\boldsymbol{a}^{(2)}$ have at least one term, multiplied with $\boldsymbol{n}$ and therefore the cross product with those vanish. We obtain

$$-2\boldsymbol{n}\times\boldsymbol{a} = \frac{\varepsilon^2}{6}\frac{\boldsymbol{n}}{n_0}\times\left(\frac{\Delta\boldsymbol{n}}{n_0} - \frac{\nabla\boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0}\right) + \mathcal{O}(\varepsilon^3). \tag{3.143}$$

Next term we look at is $\operatorname{div}(n_0\nabla\boldsymbol{a}+\boldsymbol{n}\nabla a_0+\boldsymbol{n}\nabla V)$, where we will not evaluate the divergence. Since we have already everything at hand that we need, we obtain

$$\begin{aligned}n_0\nabla\boldsymbol{a} + \boldsymbol{n}\nabla a_0 = &\, n_0\nabla\left(\boldsymbol{a}^{(0)} + \varepsilon^2\boldsymbol{a}^{(2)}\right) + \boldsymbol{n}\left(\nabla a_0^{(0)} + \varepsilon^2\nabla a_0^{(2)}\right) + \mathcal{O}(\varepsilon^3) =\\ = &\,\nabla\boldsymbol{n} - \boldsymbol{n}\frac{\nabla n_0}{n_0} + \boldsymbol{n}\frac{\nabla n_0}{n_0}\\ &+\frac{\varepsilon^2}{12}\boldsymbol{n}\left(8\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0} - 12\left|\frac{\boldsymbol{n}}{n_0}\right|^2\frac{\nabla n_0}{n_0} + \frac{\nabla(\Delta n_0)}{n_0} - 2\frac{\nabla n_0}{n_0}\frac{\Delta n_0}{n_0} - 2\frac{\nabla n_0}{n_0}\frac{(\nabla\otimes\nabla)n_0}{n_0}\right)\\ &+\varepsilon^2\boldsymbol{n}\left(\frac{1}{4}\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right) + \frac{\varepsilon^2}{12}\nabla\boldsymbol{n}\left(\frac{(\nabla\otimes\nabla)n_0}{n_0} + \left(4\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \frac{\Delta n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2\right)\sigma_0\right)\\ &+\frac{\varepsilon^2}{12}\left(\left(\Delta\boldsymbol{n} - 2\left(\nabla\boldsymbol{n}\cdot\frac{\nabla n_0}{n_0}\right)\right)\frac{\nabla n_0}{n_0} + \frac{\nabla n_0(\nabla\otimes\nabla)}{n_0}(\boldsymbol{n}) - \nabla(\Delta\boldsymbol{n})\right)\\ &-\frac{\varepsilon^2}{12}\boldsymbol{n}\left(\frac{\nabla(\Delta n_0)}{n_0} - \frac{\nabla n_0}{n_0}\frac{\Delta n_0}{n_0} - \frac{\nabla n_0}{n_0}\frac{(\nabla\otimes\nabla)n_0}{n_0} + \left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right)\\ &-\varepsilon^2\boldsymbol{n}\left(\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0} - \left|\frac{\boldsymbol{n}}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right) + \mathcal{O}(\varepsilon^3)\end{aligned}$$

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Summarizing yields

$$\begin{aligned} n_0\nabla \boldsymbol{a} + \boldsymbol{n}\nabla a_0 =& \nabla \boldsymbol{n} + \frac{\varepsilon^2}{12}\boldsymbol{n}\left(2\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0} - 4\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla \boldsymbol{n}}{n_0} - \frac{\nabla n_0}{n_0}\frac{\Delta n_0}{n_0} - \frac{\nabla n_0}{n_0}\frac{(\nabla\otimes\nabla)n_0}{n_0}\right) \\ & - \frac{\varepsilon^2}{12}\nabla(\Delta \boldsymbol{n}) + \frac{\varepsilon^2}{12}\nabla\boldsymbol{n}\left(\frac{(\nabla\otimes\nabla)n_0}{n_0} + \left(4\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \frac{\Delta n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2\right)\sigma_0\right) \\ & + \frac{\varepsilon^2}{12}\left(\left(\Delta\boldsymbol{n} - 2\left(\nabla\boldsymbol{n}\cdot\frac{\nabla n_0}{n_0}\right)\right)\frac{\nabla n_0}{n_0} + \frac{(\nabla n_0(\nabla\otimes\nabla))}{n_0}\boldsymbol{n}\right) + \mathcal{O}(\varepsilon^3). \end{aligned}$$

For better understanding of the last line, $\nabla\boldsymbol{n}\frac{(\nabla\otimes\nabla)n_0}{n_0}$ is a simple matrix-matrix multiplication and for $j\in\{1,2,3\}$ we have

$$\begin{aligned} (\Delta\boldsymbol{n}\nabla n_0 + (\nabla\boldsymbol{n}\cdot\nabla n_0)\nabla n_0 + (\nabla n_0(\nabla\otimes\nabla))\boldsymbol{n})_j = \\ = \Delta n_j\nabla n_0 + (\nabla n_j\cdot\nabla n_0)\nabla n_0 + \nabla n_0(\nabla\otimes\nabla)n_j. \end{aligned} \tag{3.144}$$

Since we cannot simplify it any further, we leave the upper expression as it is for now and continue with the next term, namely $\operatorname{div}\left(\frac{1}{\varepsilon}J^T\times\boldsymbol{a}\right)$. Recall that $J^T = \langle p_1\boldsymbol{m}|p_2\boldsymbol{m}|0\rangle$ is a 3×3 matrix and that the cross product is to understand as

$$J^T\times\boldsymbol{a} = \left(\langle p_1\boldsymbol{m}\rangle\times\boldsymbol{a}\mid \langle p_2\boldsymbol{m}\rangle\times\boldsymbol{a}\mid 0\right).$$

Further recall that $\boldsymbol{m} = \varepsilon\boldsymbol{m}^{(1)} + \varepsilon^3\boldsymbol{m}^{(3)} + \mathcal{O}(\varepsilon^4)$ and since $J^T\times\boldsymbol{a}$ is multiplied by ε^{-1} we have to expand $J^T\times\boldsymbol{a}$ up to order three:

$$\frac{1}{\varepsilon}\langle p_k\boldsymbol{m}\rangle\times\boldsymbol{a} = \left\langle p_k\boldsymbol{m}^{(1)}\right\rangle\times\boldsymbol{a}^{(0)} + \varepsilon^2\left\langle p_k\boldsymbol{m}^{(1)}\right\rangle\times\boldsymbol{a}^{(2)} + \varepsilon^2\left\langle p_k\boldsymbol{m}^{(3)}\right\rangle\times\boldsymbol{a}^{(0)} + \mathcal{O}(\varepsilon^3), \qquad \text{for } k\in\{1,2\}.$$

The factors $\boldsymbol{m}^{(1)}$ and $\boldsymbol{m}^{(3)}$ are both dependent on a_0 and $\boldsymbol{a}$. Difficulties arise from the term $\exp(h_0)$ and can be solved by using the Taylor expansion of the exponential ($\exp(x) = 1 + x + \mathcal{O}(x^2)$), in the sense that

$$\begin{aligned} \exp(a_0) =& \exp\left(a_0^{(0)} + \varepsilon^2 a_0^{(2)} + \mathcal{O}(\varepsilon^3)\right) = \frac{n_0}{2\pi}\exp\left(\varepsilon^2 a_0^{(2)} + \mathcal{O}(\varepsilon^3)\right) \\ =& \frac{n_0}{2\pi}\left(1 + \varepsilon^2 a_0^{(2)} + \mathcal{O}(\varepsilon^3)\right). \end{aligned} \tag{3.145}$$

Using the integral values of Proposition 3.6.4 and the above expansion (3.145), we obtain

$$\begin{aligned} \left\langle p_k\boldsymbol{m}^{(1)}\right\rangle =& \langle p_k\exp(h_0)(\boldsymbol{h}_1)\rangle = \exp(a_0)\left\langle p_k\exp\left(-\frac{|p|^2}{2}\right)\left(-\alpha p^\perp\right)\right\rangle \\ =& \begin{cases} \alpha n_0\boldsymbol{e}_2 + \mathcal{O}(\alpha\varepsilon^2) & k=1, \\ -\alpha n_0\boldsymbol{e}_1 + \mathcal{O}(\alpha\varepsilon^2) & k=2, \end{cases} \end{aligned} \tag{3.146}$$

$$\left(J^T\right)^{(1)} = \alpha n_0\left(\boldsymbol{e}_2| - \boldsymbol{e}_1|0\right) + \mathcal{O}(\alpha\varepsilon^2). \tag{3.147}$$

With the previous calculations we get for our first two expressions of $\frac{1}{\varepsilon}J^T\times\boldsymbol{a}$:

$$\begin{aligned} \left\langle p^T\boldsymbol{m}^{(1)}\right\rangle\times\boldsymbol{a}^{(0)} &= \alpha n_0\left(\boldsymbol{e}_2| - \boldsymbol{e}_1|0\right)\times\frac{1}{n_0}\boldsymbol{n} = \alpha\begin{pmatrix} n_3 & 0 & 0 \\ 0 & n_3 & 0 \\ -n_1 & -n_2 & 0\end{pmatrix} + \mathcal{O}(\alpha\varepsilon^2), \\ \varepsilon^2\left\langle p^T\boldsymbol{m}^{(1)}\right\rangle\times\boldsymbol{a}^{(2)} &= \alpha\varepsilon^2 n_0\left(\boldsymbol{e}_2| - \boldsymbol{e}_1|0\right)\times\boldsymbol{a}^{(2)} = \mathcal{O}(\alpha\varepsilon^2). \end{aligned}$$

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Taking a closer look on the last term in the semi classical expansion of $J^T \times \boldsymbol{a}$ and using again that all odd terms with respect to p vanish, we have

$$\left\langle p_k \mathfrak{m}^{(3)} \right\rangle = \frac{1}{24} \left\langle p_k \exp\left(h_0\right) \left(\Big(4|\boldsymbol{h}_1|^2 - p^T(\nabla \otimes \nabla a_0)p \Big) \boldsymbol{a} - p^T(\nabla \otimes \nabla \boldsymbol{a})p + 4\Big((\nabla \boldsymbol{a})p \Big) \times \boldsymbol{a} \right) \right\rangle. \tag{3.148}$$

The integrals $\left\langle p_k \exp(h_0) p^T(\nabla \otimes \nabla a_0) p \boldsymbol{a} \right\rangle$ and $\left\langle p_k \exp(h_0) p^T(\nabla \otimes \nabla \boldsymbol{a}) p \right\rangle$ equal zero, because in each line exists at least one expression, that is odd with respect to either p_1 or p_2 . Therefore the above (3.148) reduces to

$$\left\langle p_k \mathfrak{m}^{(3)} \right\rangle = \frac{1}{6} \left\langle p_k \exp\left(h_0\right) \left(|\boldsymbol{h}_1|^2 \boldsymbol{a} + \Big((\nabla \boldsymbol{a})p \Big) \times \boldsymbol{a} \right) \right\rangle.$$

Recalling that we are already at second order with respect to ε, we lay our focus on the zero orders with respect to ε and α in the next calculations, and obtain

$$\begin{aligned} \left\langle p_k \exp\left(h_0\right) |\boldsymbol{h}_1|^2 \right\rangle \boldsymbol{a}^{(0)} &= \left\langle p_k \exp\left(h_0\right) \left(|\boldsymbol{a}|^2 + \alpha^2 \left|p^\perp\right|^2 - 2\alpha(\boldsymbol{a} \cdot p^\perp) \right) \right\rangle \boldsymbol{a}^{(0)} \\ &= \mathcal{O}(\alpha), \end{aligned}$$

The term $(\nabla \boldsymbol{a})p$ is a matrix-vector multiplication, where p multiplies with the gradient, hence

$$\begin{aligned} (\nabla \boldsymbol{a})p \times \boldsymbol{a} &= \left(\nabla \boldsymbol{a}^{(0)} \right) p \times \boldsymbol{a}^{(0)} + \mathcal{O}(\varepsilon^2) \\ &= \left(\nabla \left(\frac{1}{n_0} \boldsymbol{n} \right) p \right) \times \frac{1}{n_0} \boldsymbol{n} + \mathcal{O}(\varepsilon^2) \\ &= \left(\frac{1}{n_0} (\nabla \boldsymbol{n})p - \frac{1}{{n_0}^2} (\nabla n_0 \cdot p) \boldsymbol{n} \right) \times \frac{1}{n_0} \boldsymbol{n} \\ &= \frac{1}{{n_0}^2} (\nabla \boldsymbol{n} p) \times \boldsymbol{n}. \end{aligned}$$

This and (3.145) gives us

$$\begin{aligned} \left\langle p_k \exp\left(h_0\right) \left(\nabla \boldsymbol{a}^{(0)} p \right) \right\rangle \times \boldsymbol{a}^{(0)} &= \exp(a_0) \left\langle p_k \exp\left(-\frac{|p|^2}{2} \right) \left(\frac{1}{n_0} (\nabla \boldsymbol{n} p) \right) \right\rangle \times \frac{\boldsymbol{n}}{n_0} \\ &= \frac{1}{n_0} \partial_{x_k} \boldsymbol{n} \times \boldsymbol{n}. \end{aligned}$$

Therefore we obtain for the last term in (3.148):

$$\varepsilon^2 \left\langle p^T \mathfrak{m}^{(3)} \right\rangle \times \boldsymbol{a}^{(0)} = \varepsilon^2 \frac{1}{6 n_0} \nabla \boldsymbol{n} \times \boldsymbol{n} + \mathcal{O}(\alpha \varepsilon^2).$$

In total we get

$$\frac{1}{\varepsilon} J^T \times \boldsymbol{a} = \alpha \begin{pmatrix} n_3 & 0 & 0 \\ 0 & n_3 & 0 \\ -n_1 & -n_2 & 0 \end{pmatrix} + \varepsilon^2 \frac{1}{6 n_0} \nabla \boldsymbol{n} \times \boldsymbol{n} + \mathcal{O}(\alpha \varepsilon^2 + \varepsilon^3).$$

Since we take the divergence of the above, and the latter has a nicer form, we evaluate the divergence and obtain with using the product rule for the cross product

$$\operatorname{div} \left(\frac{1}{\varepsilon} J^T \times \boldsymbol{a} \right) = -\alpha (\nabla^\perp) \times \boldsymbol{n} + \frac{\varepsilon^2}{6} \left(\frac{\Delta \boldsymbol{n}}{n_0} - \frac{\nabla n_0}{n_0} \cdot \frac{\nabla \boldsymbol{n}}{n_0} \right) \times \boldsymbol{n} + \mathcal{O}(\alpha \varepsilon^2 + \varepsilon^3).$$

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Next term to resolve is $-2\tau\alpha(n_0(\nabla^\perp \times \boldsymbol{a}) + \nabla^\perp(a_0 + V) \times \boldsymbol{n})$. Since this term is of order one with respect to α, we only need to expand it until the first order with respect to ε. Therefore, up to an error $\mathcal{O}(\alpha\varepsilon^2)$ we approximate it with

$$
\begin{aligned}
&-2\tau\alpha\left(n_0\left(\nabla^\perp \times \boldsymbol{a}^{(0)}\right) + \nabla^\perp\left(a_0^{(0)} + V\right) \times \boldsymbol{n}\right) = \\
&\quad = -2\tau\alpha\left(\left(\nabla^\perp - \frac{\nabla^\perp n_0}{n_0}\right) \times \boldsymbol{n} + \left(\frac{\nabla^\perp n_0}{n_0} + \nabla^\perp V\right) \times \boldsymbol{n}\right) = -2\tau\alpha(\nabla^\perp + \nabla V^\perp) \times \boldsymbol{n}.
\end{aligned}
$$

For the last term in line two of the spin equation (3.142) we use that $p^\perp \cdot \boldsymbol{h}_1 = p^\perp \cdot \boldsymbol{a} - \alpha|p^\perp|^2$ and that $J^T \boldsymbol{a}^\perp = -\varepsilon\alpha(\boldsymbol{n}^\perp)^\perp + \mathcal{O}(\alpha\varepsilon^2)$, see formula (3.147). This yields together with (3.145)

$$
\begin{aligned}
4\tau\frac{\alpha}{\varepsilon}\left(\boldsymbol{a}\left\langle p^\perp \cdot \boldsymbol{m}\right\rangle + J^T\boldsymbol{a}^\perp\right) &= 4\tau\frac{\alpha}{\varepsilon}\left(\frac{\boldsymbol{n}}{n_0}\left\langle\varepsilon\exp\left(h_0\right)p^\perp \cdot \boldsymbol{h}_1\right\rangle - \varepsilon\alpha(\boldsymbol{n}^\perp)^\perp\right) + \mathcal{O}(\alpha\varepsilon^2) \\
&= 4\tau\alpha^2\left(-\frac{\boldsymbol{n}}{n_0}\exp(a_0)\left\langle\exp\left(-\frac{|p|^2}{2}\right)\left|p^\perp\right|^2\right\rangle - (\boldsymbol{n}^\perp)^\perp\right) + \mathcal{O}(\alpha\varepsilon^2) \\
&= -4\tau\alpha^2\left(2\boldsymbol{n} + (\boldsymbol{n}^\perp)^\perp\right) + \mathcal{O}(\alpha\varepsilon^2).
\end{aligned}
$$

We now focus our attention on the expansion of the last terms of eq. (3.90),

$$
-2\varepsilon(\boldsymbol{n} \times \boldsymbol{a}) \times \boldsymbol{a} + \boldsymbol{n} \times \partial_t^{(0)}\boldsymbol{a},
$$

where the unusual operator $\partial_t^{(0)}$ appears. Recalling that $\boldsymbol{a}^{(0)} = \frac{1}{n_0}\boldsymbol{n}$, and since the cross product of two parallel vectors vanish, we observe for the first term

$$
\varepsilon\boldsymbol{n} \times \boldsymbol{a} = \varepsilon\frac{1}{n_0}\boldsymbol{n} \times \boldsymbol{n} + \mathcal{O}(\varepsilon^3) = \mathcal{O}(\varepsilon^3). \tag{3.149}
$$

The second term needs slightly more treatment. We first approximate it at relevant orders:

$$
\partial_t^{(0)}\boldsymbol{a} = \partial_t^{(0)}\boldsymbol{a}^{(0)} + \varepsilon^2\partial_t^{(0)}\boldsymbol{a}^{(2)} + \mathcal{O}(\varepsilon^3).
$$

Starting with the zero-order we have to calculate

$$
\partial_t^{(0)}\boldsymbol{a}^{(0)} = \partial_t^{(0)}\left(\frac{1}{n_0}\boldsymbol{n}\right) = \frac{1}{n_0}\partial_t^{(0)}\boldsymbol{n} - \frac{1}{{n_0}^2}\boldsymbol{n}\,\partial_t^{(0)}n_0.
$$

We see in the full quantum model, namely eq. (3.90), that the zero-order time derivative of n_0 equals zero and $\partial_t^{(0)}\boldsymbol{n} = -2(\boldsymbol{n} \times \boldsymbol{a})$. Hence

$$
\begin{aligned}
\partial_t^{(0)}\boldsymbol{a}^{(0)} &= \frac{1}{n_0}\partial_t^{(0)}\boldsymbol{n} = -\frac{2}{n_0}(\boldsymbol{n} \times \boldsymbol{a}) = -\frac{2}{n_0}(\boldsymbol{n} \times \boldsymbol{a}^{(0)}) - \varepsilon^2\frac{2}{n_0}(\boldsymbol{n} \times \boldsymbol{a}^{(2)}) + \mathcal{O}(\varepsilon^3) \\
&= -\frac{2}{{n_0}^2}(\boldsymbol{n} \times \boldsymbol{n}) - \varepsilon^2\frac{2}{n_0}(\boldsymbol{n} \times \boldsymbol{a}^{(2)}) + \mathcal{O}(\varepsilon^3) = -\varepsilon^2\frac{2}{n_0}(\boldsymbol{n} \times \boldsymbol{a}^{(2)}) + \mathcal{O}(\varepsilon^3).
\end{aligned}
$$

Recalling that $\boldsymbol{a}^{(2)}$ is given by (3.138), it will be convenient to define

$$
f(n_0, \boldsymbol{n}) := \left(\frac{1}{3}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \frac{1}{12}\frac{\Delta n_0}{n_0} - \frac{1}{12}\left|\frac{\nabla n_0}{n_0}\right|^2\right),
$$

so that

$$
\boldsymbol{a}^{(2)} = f(n_0, \boldsymbol{n})\frac{\boldsymbol{n}}{n_0} - \frac{1}{12}\frac{\Delta\boldsymbol{n}}{n_0} + \frac{1}{12}\frac{\nabla\boldsymbol{n}}{n_0} \cdot \frac{\nabla n_0}{n_0}. \tag{3.150}
$$

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Observe that the function f takes values in $\mathbb{R}$, and the vector $f(n_0, \boldsymbol{n})\boldsymbol{n}$ is parallel to $\boldsymbol{n}$, which gives us that $\boldsymbol{n} \times (f(n_0, \boldsymbol{n})\boldsymbol{n}) = 0$. Using this and the form (3.150), yields

$$\partial_t^{(0)} \boldsymbol{a}^{(0)} = -\varepsilon^2 \frac{2}{n_0}(\boldsymbol{n} \times \boldsymbol{a}^{(2)}) + \mathcal{O}(\varepsilon^3) = \varepsilon^2 \frac{1}{6n_0}\left(\boldsymbol{n} \times \left(\frac{\Delta \boldsymbol{n}}{n_0} - \frac{\nabla \boldsymbol{n}}{n_0} \cdot \frac{\nabla n_0}{n_0}\right)\right) + \mathcal{O}(\varepsilon^3)$$

Lastly, we have to calculate $\partial_t^{(0)} \boldsymbol{a}^{(2)}$. Using the product rule and again the fact that $\partial_t^{(0)} n_0 = 0$ we can write

$$\partial_t^{(0)} \boldsymbol{a}^{(2)} = \left(\partial_t^{(0)} f(n_0, \boldsymbol{n})\right) \frac{\boldsymbol{n}}{n_0} + f(n_0, \boldsymbol{n}) \frac{1}{n_0} \partial_t^{(0)} \boldsymbol{n} - \frac{1}{12} \partial_t^{(0)} \left(\frac{\Delta \boldsymbol{n}}{n_0} - \frac{\nabla \boldsymbol{n}}{n_0} \cdot \frac{\nabla n_0}{n_0}\right) \tag{3.151}$$

Eventually we shall only need $\boldsymbol{n} \times \partial_t^{(0)} \boldsymbol{a}^{(2)}$ and it is not necessary to calculate the derivative of f on the right-hand side, because the term $(\partial_t^{(0)} f(n_0, \boldsymbol{n}))\boldsymbol{n}$ is parallel to $\boldsymbol{n}$ and therefore vanishes after evaluating the cross product. Since $\partial_t^{(0)} \boldsymbol{a}^{(2)}$ is already a second-order term, all occurring orders higher than zero in the above expression can be disregarded. In particular,

$$\partial_t^{(0)} \boldsymbol{n} = -2(\boldsymbol{n} \times \boldsymbol{a}) = -2(\boldsymbol{n} \times \boldsymbol{a}^{(0)}) + \mathcal{O}(\varepsilon^2) = -2\frac{1}{n_0}(\boldsymbol{n} \times \boldsymbol{n}) + \mathcal{O}(\varepsilon^2) = \mathcal{O}(\varepsilon^2)$$

and therefore the second term at the right-hand side of (3.151) can be disregarded. So, the only non-negligible contribution can only come from the last term. Using again $\partial_t^{(0)} n_0 = 0$ and $\partial_t^{(0)} \boldsymbol{n} = -2(\boldsymbol{n} \times \boldsymbol{a})$, we obtain for such term

$$\begin{aligned}\partial_t^{(0)} \left(\frac{\Delta \boldsymbol{n}}{n_0} - \frac{\nabla \boldsymbol{n}}{n_0} \cdot \frac{\nabla n_0}{n_0}\right) &= \frac{1}{n_0}(\Delta \partial_t^{(0)} \boldsymbol{n}) - \frac{1}{n_0} \nabla \partial_t^{(0)} \boldsymbol{n} - (\Delta \boldsymbol{n} - \nabla \boldsymbol{n} + n_0 \nabla - \nabla n_0) \frac{\partial_t^{(0)} n_0}{{n_0}^2} \\ &= -\frac{2}{n_0} \Delta \left(\boldsymbol{n} \times \boldsymbol{a}^{(0)}\right) + \frac{2}{n_0} \nabla \left(\boldsymbol{n} \times \boldsymbol{a}^{(0)}\right) + \mathcal{O}(\varepsilon^2) = \mathcal{O}(\varepsilon^2).\end{aligned}$$

Hence

$$\partial_t^{(0)} \boldsymbol{a}^{(2)} = \left(\partial_t^{(0)} f(n_0, \boldsymbol{n})\right) \frac{\boldsymbol{n}}{n_0} + \mathcal{O}(\varepsilon^2),$$

yielding finally into

$$\begin{aligned}\boldsymbol{n} \times \partial_t^{(0)} \boldsymbol{a} &= \boldsymbol{n} \times \partial_t^{(0)} \boldsymbol{a}^{(0)} + \varepsilon^2 \left(\boldsymbol{n} \times \partial_t^{(0)} \boldsymbol{a}^{(2)}\right) + \mathcal{O}(\varepsilon^3) \\ &= \varepsilon^2 \frac{1}{6n_0} \boldsymbol{n} \times \left(\boldsymbol{n} \times \left(\frac{\Delta \boldsymbol{n}}{n_0} - \frac{\nabla \boldsymbol{n}}{n_0} \cdot \frac{\nabla n_0}{n_0}\right)\right) + \mathcal{O}(\varepsilon^3).\end{aligned} \tag{3.152}$$

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Substituting all obtained approximations into the full spin equation (3.142) and then summarizing them, yields

$$\begin{aligned}
\partial_t \boldsymbol{n} =& \frac{\varepsilon^2}{6}\frac{\boldsymbol{n}}{n_0} \times \left(\frac{\Delta \boldsymbol{n}}{n_0} - \frac{\nabla \boldsymbol{n}}{n_0} \cdot \frac{\nabla n_0}{n_0}\right) + \tau \operatorname{div}(\nabla \boldsymbol{n} + \boldsymbol{n}\nabla V) \\
&+ \tau \frac{\varepsilon^2}{12} \operatorname{div}\left(\boldsymbol{n}\left(2\left|\frac{\nabla n_0}{n_0}\right|^2 \frac{\nabla n_0}{n_0} - 4\frac{\boldsymbol{n}}{n_0} \cdot \frac{\nabla \boldsymbol{n}}{n_0} - \frac{\nabla n_0}{n_0}\frac{\Delta n_0}{n_0} - \frac{\nabla n_0}{n_0}\frac{(\nabla \otimes \nabla) n_0}{n_0}\right) - \nabla(\Delta \boldsymbol{n})\right) \\
&+ \tau \frac{\varepsilon^2}{12} \operatorname{div}\left(\nabla \boldsymbol{n}\left(\frac{(\nabla \otimes \nabla) n_0}{n_0} + \left(4\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \frac{\Delta n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2\right)\sigma_0\right)\right) \\
&+ \tau \frac{\varepsilon^2}{12} \operatorname{div}\left(\left(\Delta \boldsymbol{n} - 2\left(\nabla \boldsymbol{n} \cdot \frac{\nabla n_0}{n_0}\right)\right)\frac{\nabla n_0}{n_0} + \frac{(\nabla n_0(\nabla \otimes \nabla))}{n_0}\boldsymbol{n}\right) \\
&- 2\tau\alpha(\nabla^\perp) \times \boldsymbol{n} + \tau\frac{\varepsilon^2}{3}\left(\frac{\Delta \boldsymbol{n}}{n_0} - \frac{\nabla n_0}{n_0} \cdot \frac{\nabla \boldsymbol{n}}{n_0}\right) \times \boldsymbol{n} \\
&- 2\tau\alpha(\nabla^\perp + \nabla^\perp V) \times \boldsymbol{n} - 4\tau\alpha^2(2\boldsymbol{n} + (\boldsymbol{n}^\perp)^\perp) \\
&+ \tau\frac{\varepsilon^2}{3}\frac{\boldsymbol{n}}{n_0} \times \left(\boldsymbol{n} \times \left(\frac{\Delta \boldsymbol{n}}{n_0} - \frac{\nabla \boldsymbol{n}}{n_0} \cdot \frac{\nabla n_0}{n_0}\right)\right) + \mathcal{O}(\alpha\varepsilon^2 + \varepsilon^3) \\
=& \tau \operatorname{div}(\nabla \boldsymbol{n} + \boldsymbol{n}\nabla V) - 2\tau\alpha(2\nabla^\perp + \nabla V^\perp) \times \boldsymbol{n} - 4\tau\alpha^2(2\boldsymbol{n} + (\boldsymbol{n}^\perp)^\perp) + \frac{\varepsilon^2}{6}\frac{\boldsymbol{n}}{n_0} \times \mathcal{B}(N) \\
&+ \tau\frac{\varepsilon^2}{12} \operatorname{div}\left(\boldsymbol{n}\mathcal{A}(N) - \nabla(\Delta \boldsymbol{n}) + \nabla \boldsymbol{n}\mathcal{C}(N) + \mathcal{B}(N)\nabla n_0 + \mathcal{D}(N)\right) \\
&+ \tau\frac{\varepsilon^2}{3}\boldsymbol{n} \times \left(\frac{\boldsymbol{n}}{n_0} \times \mathcal{B}(N) - \mathcal{B}(N)\right) + \mathcal{O}(\alpha\varepsilon^2 + \varepsilon^3)
\end{aligned}$$

where

$$\begin{aligned}
\mathcal{A}(N) &:= 2\left|\frac{\nabla n_0}{n_0}\right|^2 \frac{\nabla n_0}{n_0} - 4\frac{\boldsymbol{n}}{n_0} \cdot \frac{\nabla \boldsymbol{n}}{n_0} - \frac{\nabla n_0}{n_0}\frac{\Delta n_0}{n_0} - \frac{\nabla n_0}{n_0}\frac{(\nabla \otimes \nabla) n_0}{n_0} \\
\mathcal{B}(N) &:= \frac{\Delta \boldsymbol{n}}{n_0} - \frac{\nabla \boldsymbol{n}}{n_0} \cdot \frac{\nabla n_0}{n_0} \\
\mathcal{C}(N) &:= \left(\frac{\Delta n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2 + 4\left|\frac{\boldsymbol{n}}{n_0}\right|^2\right)\sigma_0 + \frac{\nabla \otimes \nabla n_0}{n_0} \\
\mathcal{D}(N) &:= \frac{(\nabla n_0(\nabla \otimes \nabla))}{n_0}\boldsymbol{n} - \left(\nabla \boldsymbol{n} \cdot \frac{\nabla n_0}{n_0}\right)\frac{\nabla n_0}{n_0}
\end{aligned}$$

and Main Theorem 3.6.1 is therefore proved.

□

The spin model (3.105)-(3.106) obtained in Main Theorem 3.6.1 is for us the nicest and the most vivid form of the equations. For the interested reader we also did the work to resolve the divergence in the second line of (3.106) from Main Theorem 3.6.1. The calculations are tedious and the result does not give more insight than the model obtained in Main Theorem 3.6.1, and is therefore put into the Appendix B.5. A bit more interesting could be the single component equations, but we also decided to put them just into the Appendix B.6.

3.7. Conclusion & Comparison with other Models

The first fact that is interesting to see, is that the the semiclassical model (3.105) - (3.106) is semi coupled and at the leading orders regarding to ε, like when $\varepsilon \to 0$, we even have a

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decoupled system. First we want to focus on the spin equations (3.106) and present under certain conditions that we can get an explicit expression for the spin density n_3. Looking on the leading order with respect to ε we have

$$\partial_t \boldsymbol{n} = \tau \operatorname{div}(\nabla \boldsymbol{n} + \boldsymbol{n}\nabla V) - 2\tau\alpha(2\nabla^\perp + \nabla V^\perp) \times \boldsymbol{n} - 4\tau\alpha^2(2\boldsymbol{n} + (\boldsymbol{n}^\perp)^\perp) \tag{3.153}$$

After rescaling equation (3.153) in time to a diffusive timescale, we obtain the same equation as in [BHJ], hence our model also coincides with the work of El Hajj [EH14].
Furthermore if we consider for sake of simplicity, that the densities n_1, n_2 are constant with respect to time and space, we obtain out of equation (3.153) the following equations

$$0 = 2\partial_{x_1} n_3 + \partial_{x_1} V n_3 - 2\alpha n_1, \tag{3.154}$$
$$0 = 2\partial_{x_2} n_3 + \partial_{x_2} V n_3 - 2\alpha n_2, \tag{3.155}$$
$$\partial_t n_3 = \tau(\operatorname{div}(\nabla n_3 + n_3 \nabla V)) - 2\tau\alpha(\nabla V \cdot \boldsymbol{n}) - 8\tau\alpha^2 n_3. \tag{3.156}$$

Recall that the planar gradient is given by $\nabla = (\partial_{x_1}, \partial_{x_2}, 0)$ and therefore $\nabla V \cdot \boldsymbol{n} = n_1\partial_{x_1} V + n_2 \partial_{x_2} V$. From the first two equations (3.154) - (3.155) we obtain an equation for the gradient of n_3, namely

$$\nabla n_3 = -\frac{1}{2} n_3 \nabla V - \alpha(\boldsymbol{n}^\perp)^\perp. \tag{3.157}$$

Assuming in this particular case, for sake of simplicity, that ∇V is a constant force F, we can substitute the equation (3.157) into the equation for the time derivative of n_3, (3.156), and obtain with a second substitution the following

$$\begin{aligned}
\partial_t n_3 =& \tau(\operatorname{div}(\nabla n_3 + \nabla V n_3)) - 2\tau\alpha(\nabla V \cdot \boldsymbol{n}) - 8\tau\alpha^2 n_3 \\
=& \tau\left(\operatorname{div}\left(2^{-1} n_3 \nabla V - \alpha(\boldsymbol{n}^\perp)^\perp\right)\right) - 2\tau\alpha(\nabla V \cdot \boldsymbol{n}) - 8\tau\alpha^2 n_3 \\
=& \tau\left(2^{-1}\nabla n_3 \cdot \nabla V\right) - 2\tau\alpha(\nabla V \cdot \boldsymbol{n}) - 8\tau\alpha^2 n_3 \\
=& \tau\left(-4^{-1} n_3 |\nabla V|^2 - 2^{-1}\alpha(\boldsymbol{n}^\perp)^\perp \cdot \nabla V\right) - 2\tau\alpha(\nabla V \cdot \boldsymbol{n}) - 8\tau\alpha^2 n_3 \\
=& -\tau\left(\left|\frac{F}{2}\right|^2 + 8\alpha^2\right) n_3 - \tau\alpha\left(\frac{1}{2}(\boldsymbol{n}^\perp)^\perp + 2\boldsymbol{n}\right) \cdot F,
\end{aligned}$$

which is now simply an ODE with the solution

$$n_3(t,x) = C \exp\left(-\tau\left(\left|\frac{F}{2}\right|^2 + 8\alpha^2\right) t\right) + \frac{\alpha}{2} \frac{\left((\boldsymbol{n}^\perp)^\perp + 4\boldsymbol{n}\right) \cdot F}{\left|\frac{F}{2}\right|^2 + 8\alpha^2}.$$

The reader should notice that the last component of F is zero and that $(\boldsymbol{n}^\perp)^\perp$ does only depend on n_1, n_2, which were assumed to be constant, therefore the term that is added to the exponential depends only on the space variable and is independent of time. Looking at the long time behaviour of the solution we obtain the convergence to a steady state which relies on the potential energy

$$\lim_{t\to\infty} n_3(t,x) = -\frac{3\alpha}{2} \frac{n_1 F_1 + n_2 F_2}{\left|\frac{F}{2}\right|^2 + 8\alpha^2}.$$

At last we want to show that our model can be really seen as a generalization of other models. As mentioned in the beginning of this section we already had a comparison with

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the model of El Hajj [EH14]. Since other models are mostly in diffusive time regime and are focused on the spin up and spin down densities (usually defined as $\tilde{n}_\pm := \tilde{n_0} \pm \tilde{n}_3$), we define the spin up and spin down densities as $n_\pm := n_0 \pm \varepsilon n_3$ and will rescale properly. Our second reference model from the start comes from [BM10], where a model for the spin up and spin down densities was considered. To compare our model with the one derived in Theorem 2 from [BM10], we need to set in our model n_1 and n_2 equal zero. Therefore the respective equations from our semiclassical model (3.105)-(3.106) are given by

$$\partial_t n_0 = \tau \operatorname{div}(\nabla n_0 + n_0 \nabla V) - \tau \frac{\varepsilon^2}{6} \operatorname{div}\left(n_0 \nabla \left(\frac{\Delta \sqrt{n_0}}{\sqrt{n_0}} \right) \right), \tag{3.158}$$

$$\partial_t n_3 = \tau \operatorname{div}(\nabla n_3 + n_3 \nabla V) - 8\tau\alpha^2 n_3 + \mathcal{O}(\varepsilon^2). \tag{3.159}$$

where we only took the leading order equation of n_3 with respect to ε and set $n_1 = n_2 = 0$. Rescaling the above into a diffusive regime, where collisions are still assumed to act on a time-scale much shorter than t_E. The system is observed on a time-scale much larger than $t_0 = t_E$. Assuming that the relaxation time equals the collision time, e.g. $t_p = t_c$ (t_p is the constant used in [BM10]) and looking at a larger reference time $t_0 = t_E^2/t_c$, see Section 3.4, we get the diffusive scaled equations (notice that τ cancels in the equations)

$$\partial_t n_0 = \operatorname{div}(\nabla n_0 + n_0 \nabla V) - \frac{\varepsilon^2}{6} \operatorname{div}\left(n_0 \nabla \left(\frac{\Delta \sqrt{n_0}}{\sqrt{n_0}} \right) \right), \tag{3.160}$$

$$\partial_t n_3 = \operatorname{div}(\nabla n_3 + n_3 \nabla V) - 8\alpha^2 n_3 + \mathcal{O}(\varepsilon^2). \tag{3.161}$$

As first consequence of this we see that equation (3.160) is the typical semiclassical quantum model for the charge density, compare for example [BF10], [DMR05], [Jö9].

Next adding (3.160) to (3.161), subtracting (3.161) from (3.160), and using also the identities $n_0 = \frac{1}{2}(n_+ + n_-)$ and $n_3 = \frac{1}{2\varepsilon}(n_+ - n_-)$, leads us to the spin up and spin down equations,

$$\partial_t n_+ - \operatorname{div}(\nabla n_+ + n_+ \nabla V) + \frac{\varepsilon^2}{6} \operatorname{div}\left(n_0 \nabla \left(\frac{\Delta \sqrt{n_0}}{\sqrt{n_0}} \right) \right) = 4\alpha^2 (n_- - n_+), \tag{3.162}$$

$$\partial_t n_- - \operatorname{div}(\nabla n_- + n_- \nabla V) + \frac{\varepsilon^2}{6} \operatorname{div}\left(n_0 \nabla \left(\frac{\Delta \sqrt{n_0}}{\sqrt{n_0}} \right) \right) = 4\alpha^2 (n_+ - n_-). \tag{3.163}$$

With the general binomial formula we have, since $n_0 = n_\pm \mp \varepsilon n_3$, that

$$\sqrt{n_0} = \sqrt{n_\pm} \sqrt{1 \mp \varepsilon \frac{n_3}{n_\pm}} = \sqrt{n_\pm} \left(1 \mp \sum_{k=1}^{\infty} \frac{1}{2^k} \varepsilon^k \left(\frac{n_3}{n_\pm} \right)^k \right) = \sqrt{n_\pm} + \mathcal{O}(\varepsilon),$$

and therefore we obtain

$$\partial_t n_+ - \operatorname{div}(\nabla n_+ + n_+ \nabla V) + \frac{\varepsilon^2}{6} \operatorname{div}\left(n_+ \nabla \left(\frac{\Delta \sqrt{n_+}}{\sqrt{n_+}} \right) \right) = 4\alpha^2 (n_- - n_+), \tag{3.164}$$

$$\partial_t n_- - \operatorname{div}(\nabla n_- + n_- \nabla V) + \frac{\varepsilon^2}{6} \operatorname{div}\left(n_- \nabla \left(\frac{\Delta \sqrt{n_-}}{\sqrt{n_-}} \right) \right) = 4\alpha^2 (n_+ - n_-). \tag{3.165}$$

We see that the model equations (3.164)-(3.165) coincide with the derived equations for the same quantities in [BM10] Theorem 2.

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4. Large-Time Asymptotics for a Matrix Spin Drift-Diffusion Model

As last chapter we present some long time behaviour of spin in a bounded domain, under the assumption that on the boundary the average spin is zero. This means we expect that if we "add" all spins together they cancel themself out. As an example we could say that if we let time pass to infinity we await that half of the electrons have spin up and the other half has spin down. This is not very precise, but gives a rough idea what we are looking for.

4.1. The Setting

As we have seen in the previous chapter, the derivation of a spin model takes a lot of effort. Since the full quantum model (3.89)-(3.90) is highly non local, it is difficult to deal with. To study the long time behaviour of that model would exceed the purpose of this work. Also the semiclassical approximation (3.105)-(3.106) is too connected to proceed at that level. The most suitable, for our purpose, would be either the model appearing in [EH14] or the model derived in [PN11]. In these papers the macroscopic models where derived from the *spinor Boltzmann equation* (copied from [PN11] and also called generalized matrix Boltzmann equation)

$$\partial_t F + \frac{1}{\hbar}(\nabla_k h_0 \cdot \nabla_x F - \nabla_x h_0 \cdot \nabla_k F) + \frac{i}{\hbar}[F, \boldsymbol{h} \cdot \boldsymbol{\sigma}] = \frac{1}{\tau_c}\mathcal{Q}_{ij}(F) + \frac{1}{\tau_{sf}}\mathcal{Q}_{sf}(F),$$

where k denotes the momentum, $\mathfrak{H} = h_0\sigma_0 + \boldsymbol{h} \cdot \boldsymbol{\sigma}$ is the Hamiltonian of the system, $\hbar$ the Planck constant, $\mathcal{Q}_{ij}$ is a spin conserving collision operator and $\mathcal{Q}_{sf}$ denotes the effect *spin flip* happing also sometimes during collisions. For explicit depiction, further details and the derivation of the macroscopic model (4.1)-(4.2) we suggest to read [PN11].

One of the tools to obtain the exponential decay will be the study of the relative free energy, which is from the idea similar to the relative entropy presented in Definition 2.4.2. The proof of the long time behaviour is therefore similar, though very different from the one we did already, where details will be provided later. Since this chapter relies on our already published paper [HJ20] the sections and texts will be almost everywhere the same. Let us also stress that the occurring densities (e.g. n_0, $\boldsymbol{n}$) in this chapter are different to the ones appearing in the other chapters, but the overall meaning remains the same (e.g. $\boldsymbol{n}$ still denotes the macroscopic spin densities, hence we keep the notation.

4.1.1. Model Equations

We assume that the dynamics of the (Hermitian) density matrix $N(x,t) \in \mathbb{C}^{2\times 2}$, the current density matrix $J(x,t) \in \mathbb{C}^{2\times 2}$, and the electric potential $V(x,t)$ is given by the (scaled)

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matrix equations

$$\partial_t N - \operatorname{div} J + \mathrm{i}\gamma[N, \boldsymbol{\mu}\cdot\boldsymbol{\sigma}] = \frac{1}{\tau}\left(\frac{1}{2}\operatorname{tr}(N)\sigma_0 - N\right), \tag{4.1}$$

$$J = DP^{-1/2}(\nabla N + N\nabla V)P^{-1/2}, \tag{4.2}$$

$$-\lambda^2\Delta V = \operatorname{tr}(N) - g(x) \quad \text{in } \Omega,\ t > 0, \tag{4.3}$$

where $[A, B] = AB - BA$ is the commutator for matrices A and B. The (scaled) physical parameters are the strength of the pseudo-exchange field $\gamma > 0$, the normalized precession vector $\boldsymbol{\mu} = (\mu_1, \mu_2, \mu_3) \in \mathbb{R}^3$, the spin-flip relaxation time $\tau > 0$, the diffusion constant $D > 0$, the Debye length $\lambda > 0$, and the doping concentration $g(x)$. Equation (4.3) is the Poisson equation for the electric potential [JÜ9]. The precession vector plays the role of the local direction of the magnetization in the ferromagnet, and we assume that it is constant. This assumption is crucial for our analysis. Furthermore, $P = \sigma_0 + p\boldsymbol{\mu}\cdot\boldsymbol{\sigma} = \sigma_0 + p(\mu_1\sigma_1 + \mu_2\sigma_2 + \mu_3\sigma_3)$ is the matrix of spin polarization of the scattering rates, $p \in [0, 1)$ represents the spin polarization, σ_0 is the unit matrix in $\mathbb{R}^{2\times 2}$, and we recall that $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the vector of Pauli matrices, defined by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Recall also that the number i is the complex unit, and $\operatorname{tr}(N)$ denotes the trace of the matrix N. Since the Pauli matrices are traceless, $\operatorname{tr}(N)$ only contains the σ_0-component of N, which is the charge density. The commutator $[N, \boldsymbol{\mu}\cdot\boldsymbol{\sigma}]$ models the precession of the spin polarization. The right-hand side in (4.1) describes the spin-flip relaxation of the spin density to the (spinless) equilibrium state.

Equations (4.1)–(4.3) are solved in the bounded domain $\Omega \subset \mathbb{R}^3$ with time $t > 0$ and are supplemented with the boundary and initial conditions

$$N = \frac{1}{2}n_D\sigma_0,\ V = V_D \quad \text{on } \partial\Omega,\ t > 0, \qquad N(0) = N^0 \quad \text{in } \Omega. \tag{4.4}$$

This means that no spin effects occur on the boundary. For simplicity, we choose time-independent boundary data; see [ZJ13] for boundary data depending on time. Mixed Dirichlet–Neumann boundary conditions may be also considered as long as they allow for $W^{2,q_0}(\Omega)$ elliptic regularity results, which restricts the geometry of $\partial\Omega$. Therefore, we have chosen pure Dirichlet boundary data as in [JNS15].

The density matrix N can be expressed in terms of the Pauli matrix according to $N = \frac{1}{2}n_0\sigma_0 + \boldsymbol{n}\cdot\boldsymbol{\sigma}$ and $\boldsymbol{n} = (n_1, n_2, n_3)$ is called the spin-vector density. Model (4.1)–(4.2), written in the four variables $n_0, \ldots, n_3$, is a cross-diffusion system with the constant diffusion matrix

$$\frac{D}{1-p^2}\begin{pmatrix} 1 & -p\boldsymbol{\mu}^\top \\ -p\boldsymbol{\mu} & \eta\mathbb{I} + (1-\eta)\boldsymbol{\mu}\otimes\boldsymbol{\mu} \end{pmatrix} \in \mathbb{R}^{4\times 4},$$

where $\mathbb{I}$ is the unit matrix in $\mathbb{R}^{3\times 3}$. Although this matrix is symmetric and positive definite, the strong coupling complicates the analysis of system (4.1)–(4.2), because maximum principle arguments and other standard tools cannot be (easily) applied.

The spin polarization matrix couples the charge and spin components of the electrons. If $p \neq 0$ we obtain by comparison of coefficients of the matrix σ_0 in (4.1), see also [PN11],

$$\partial_t n_0 - D_p \operatorname{div} j_0 = 0, \quad j_0 = \nabla n_0 + n_0\nabla V - 2p(\nabla\boldsymbol{n} + \boldsymbol{n}\nabla V)\cdot\boldsymbol{\mu}, \quad -\lambda^2\Delta V = n_0 - g(x), \tag{4.5}$$

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where $D_p = D/(1-p^2)$.
If $p = 0$, we recover the classical Van-Roosbroeck drift-diffusion equations for the electron charge density n_0 [Mar86, Roo50],

$$\partial_t n_0 - D \operatorname{div} j_0 = 0, \quad j_0 = \nabla n_0 + n_0 \nabla V, \quad -\lambda^2 \Delta V = n_0 - g(x), \tag{4.6}$$

The boundary conditions are $n_0 = n_D$ and $V = V_D$ on $\partial\Omega$ and the initial condition is $n_0(0) = n_0^0$ in Ω, where $N^0 = \frac{1}{2} n_0^0 \sigma_0 + \boldsymbol{n}^0 \cdot \boldsymbol{\sigma}$. Another special case is given by the two-component spin drift-diffusion model. The spin-up and spin-down densities $n_\pm = \frac{1}{2} n_0 \pm \boldsymbol{n} \cdot \boldsymbol{\mu}$, respectively, satisfy the equations

$$\partial_t n_+ - \operatorname{div}\left(D_+(\nabla n_+ + n_+ \nabla V)\right) = \frac{1}{2\tau}(n_- - n_+), \tag{4.7}$$

$$\partial_t n_- - \operatorname{div}\left(D_-(\nabla n_- + n_- \nabla V)\right) = \frac{1}{2\tau}(n_+ - n_-), \tag{4.8}$$

$$n_\pm = \frac{n_D}{2}, \quad V = V_D \quad \text{on } \partial\Omega, \quad n_\pm(0) = \frac{1}{2} n_0^0 \pm \boldsymbol{n}^0 \cdot \boldsymbol{\mu} \quad \text{in } \Omega, \tag{4.9}$$

where $D_\pm = D/(1 \pm p)$. These equations are weakly coupled through the relaxation term.

As already mentioned model (4.1)–(4.2) was derived in [PN11] from a matrix Boltzmann equation in the diffusion limit. The scattering operator in the Boltzmann model is assumed to consist of a dominant collision operator from the Stone model and a spin-flip relaxation operator. When the scattering rate in the Stone model is smooth and invariant under isometric transformations, the diffusion D can be identified with a positive number [Pou91, Prop. 1].

Remark 4.1.1. The reader may has noticed the appearance of the factor 1/2 in front of some quantities, especially in $N = (1/2)n_0 + \boldsymbol{n} \cdot \boldsymbol{\sigma}$. This comes from the fact that we use here a slightly different definition (e.g $n_0 = \operatorname{tr}(N)$) in comparison to the previous chapter (in Chapter 3 we used $n_0 = (1/2)\operatorname{tr}(N)$). ■

4.1.2. State of the Art

The first result on the global existence of solutions to the Van-Roosbroeck equations (4.6) (for electrons and positively charged holes) was proved by Mock [Moc74]. He showed in [Moc75] that the solution decays exponentially fast to the equilibrium state provided that the initial data is sufficiently close to the equilibrium. These results were generalized under physically more realistic assumptions on the boundary by Gajewski [Gaj85] and Gajewski and Gröger [GG86, GG89]. Further large-time asymptotics can be found in [AMT00] for the whole-space problem and in [BAMV04], where the diffusion constant was replaced by a diffusion matrix. Moreover, in [DFW08], the stability of the solutions in Wasserstein spaces was investigated.

Convergence rates of the whole-space solutions to their self-similar profile were investigated intensively in the literature. In [BP00], the relative free energy allowed the authors to prove the self-similar asymptotics in the $L^1(\mathbb{R}^d)$ norm. The results were improved in [KK08], showing optimal $L^p(\mathbb{R}^d)$ decay estimates. The asymptotic profile to drift-diffusion-Poisson equations with fractional diffusion was analyzed in [OY09, Yam12].

Concerning drift-diffusion models for the spin-polarized electron transport, there are only few mathematical results. The stationary two-component drift-diffusion model (4.7)–(4.8) was analyzed in [GG10], while the transient equations were investigated in [Gli08]. In particular, Glitzky proved in [Gli08] the exponential decay to equilibrium. An existence analysis for a diffusion model for the spin accumulation with fixed electron current but non-constant magnetization was proved in [PG10] in one space dimension and in [GCW07, GCW15] for three space dimensions.

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Also quantum spin diffusion models have been considered. For instance, in [ZJ13], the large-time asymptotics for a simple spin drift-diffusion system for quantum electron transport in graphene was studied. A more general quantum spin drift-diffusion model was derived in [BM10], with numerical experiments in [BMNP15]. Numerical simulations for diffusion models for the spin accumulation, coupled with the Landau–Lifshitz–Gilbert equation, can be found in [CAS15, RAH+16]. For spin transport models in superlattices, we refer, for instance, to [BBA10].

The existence of global weak solutions to the matrix spin drift-diffusion model (4.1)–(4.4) was shown in [JNS15] with constant precession vector and in [Zam14] with non-constant precession vector but assuming velocity saturation. Under the condition that the (thermal) equilibrium density is sufficiently small, the exponential decay to equilibrium was proved in [Zam14]. An implicit Euler finite-volume scheme that preserves some of the features of the continuous model was analyzed in [CHJS16]. The numerical results of [CHJS16] indicate that the relative free energy is decaying with exponential rate, but no analytical proof was given.

4.1.3. The Steady State and the Stationary Equations

As in the paper [HJ20], we prove in this thesis that the solution $(N(t), V(t))$ to (4.1)–(4.4) converges exponentially fast to a steady state $(\frac{1}{2}n_\infty\sigma_0, V_\infty)$, solving the stationary spinless drift-diffusion-Poisson equations

$$\operatorname{div}(\nabla n_\infty + n_\infty \nabla V_\infty) = 0, \quad -\lambda^2\Delta V_\infty = n_\infty - g(x) \quad \text{in } \Omega, \tag{4.10}$$

$$n_\infty = n_D, \quad V_\infty = V_D \quad \text{on } \partial\Omega \tag{4.11}$$

under the condition that the boundary data is close to the (thermal) equilibrium state, defined by $\log n_D + V_D = 0$ on $\partial\Omega$. Compared to [Zam14], where $\|n_\infty\|_{L^\infty(\Omega)} \ll 1$ is needed, our smallness assumption is physically reasonable; see the discussion below Main Theorem 4.2.1.

The existence of weak solutions to the stationary drift-diffusion problem with data close to the equilibrium state (especially satisfying the assumptions in the upcoming Main Theorem 4.2.1) is well known; see [Mar86, Theorem 3.2.1]. The solution satisfies n_∞, $V_\infty \in H^1(\Omega) \cap L^\infty(\Omega)$ and

$$0 < m_\infty \le n_\infty \le M_\infty \quad \text{in } \Omega \tag{4.12}$$

for some m_∞, $M_\infty > 0$. Note that we cannot expect uniqueness of weak solutions in general, since there are devices (thyristors) that allow for multiple physical stationary solutions. However, uniqueness can be expected for data sufficiently close to the (thermal) equilibrium state [Ala95, Moc82]. We call a solution to (4.10)–(4.11) a (thermal) equilibrium state if the electrochemical potential $\phi_\infty := \log n_\infty + V_\infty$ vanishes in Ω. This state needs the compatibility condition $\phi_D := \log n_D + V_D = 0$ on $\partial\Omega$.

The following lemma provides some a priori estimates for (n_∞, V_∞) and shows that the current density $J_\infty := n_\infty\nabla\phi_\infty$ is arbitrarily small in the $L^\infty(\Omega)$ norm if the boundary data is sufficiently close to the equilibrium state $\phi_D = 0$ in the $W^{2,q_0}(\Omega)$ sense.

Lemma 4.1.2 (A priori estimates)**.** *Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with $\partial\Omega \in C^{1,1}$ and let $0 < m_* < 1$, $\lambda > 0$. Furthermore, let the data satisfies $g \in L^\infty(\Omega)$, $g \ge 0$ in Ω, and*

$$n_D,\ V_D \in W^{2,q_0}(\Omega), \quad n_D \ge m_* > 0 \text{ on } \partial\Omega,$$

Define $\phi_D := \log n_D + V_D$, then there exists a constant $C_\infty > 0$ independent of (n_∞, V_∞) such that

$$\|\nabla\phi_\infty\|_{L^\infty(\Omega)} \le C_\infty \|\phi_D\|_{W^{2,q_0}(\Omega)}.$$

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Proof. Since $n_\infty - g(x) \in L^\infty(\Omega)$, elliptic regularity yields $V_\infty \in W^{2,q_0}(\Omega)$, and the $W^{2,q_0}(\Omega)$ norm of V_∞ depends on M_∞, $\|V_D\|_{W^{2,q_0}(\Omega)}$, and $\|g\|_{L^\infty(\Omega)}$. Using the test function $n_\infty - n_D$ in the weak formulation of the first equation in (4.10), we find that

$$\begin{aligned}\int_\Omega |\nabla(n_\infty - n_D)|^2 dx &= -\int_\Omega \nabla n_D \cdot \nabla(n_\infty - n_D)dx - \int_\Omega n_\infty \nabla V_\infty \cdot \nabla(n_\infty - n_D)dx \\ &\le (\|\nabla n_D\|_{L^2(\Omega)} + M_\infty \|\nabla V_\infty\|_{L^2(\Omega)})\|\nabla(n_\infty - n_D)\|_{L^2(\Omega)}.\end{aligned}$$

This implies that

$$\begin{aligned}\|\nabla n_\infty\|_{L^2(\Omega)} &\le 2\|\nabla n_D\|_{L^2(\Omega)} + M_\infty\|\nabla V_\infty\|_{L^2(\Omega)} \\ &\le C(1 + \|\nabla n_D\|_{L^2(\Omega)} + \|\nabla V_D\|_{L^2(\Omega)}).\end{aligned}$$

Since $q_0 > 3$, we have $W^{2,q_0}(\Omega) \hookrightarrow W^{1,\infty}(\Omega)$. Thus, $b := \nabla V_\infty \in L^\infty(\Omega)$ and elliptic regularity for

$$\Delta n_\infty + b \cdot \nabla n_\infty = \lambda^{-2} n_\infty(n_\infty - g(x)) \in L^\infty(\Omega)$$

shows that $n_\infty \in W^{2,q_0}(\Omega)$ with an a priori bound depending on the norms $\|n_D\|_{W^{2,q_0}(\Omega)}$ and $\|n_\infty\|_{H^1(\Omega)}$. Summarizing,

$$\|n_\infty\|_{W^{2,q_0}(\Omega)} + \|V_\infty\|_{W^{2,q_0}(\Omega)} \le C.$$

It holds that $W^{2,q_0}(\Omega) \hookrightarrow C^{0,\alpha}(\overline{\Omega})$ for all $0 < \alpha < 1$. Hence, $n_\infty \in C^{0,\alpha}(\overline{\Omega})$. The first equation in (4.10) can be formulated as

$$\operatorname{div}\big(n_\infty \nabla(\phi_\infty - \phi_D)\big) = -\operatorname{div}(n_\infty \nabla \phi_D) \in L^{q_0}(\Omega),$$

which shows that, by elliptic regularity again,

$$\|\phi_\infty - \phi_D\|_{W^{2,q_0}(\Omega)} \le C(m_\infty, M_\infty)\|\phi_D\|_{W^{2,q_0}(\Omega)}$$

and, in view of the continuous embedding $W^{2,q_0}(\Omega) \hookrightarrow W^{1,\infty}(\Omega)$,

$$\|\nabla\phi_\infty\|_{L^\infty(\Omega)} \le C\|\phi_\infty\|_{W^{2,q_0}(\Omega)} \le C\|\phi_D\|_{W^{2,q_0}(\Omega)}.$$

This finishes the proof. □

4.2. Long Time Behaviour of the Full Spin Matrix N

Our main result is as follows.

Main Theorem 4.2.1 (Exponential time decay)**.** *Let $T > 0$ and let $\Omega \subset \mathbb{R}^3$ be a bounded domain with $\partial\Omega \in C^{1,1}$. Furthermore, let $0 < m_* < 1$, $\lambda > 0$, $\gamma > 0$, $D > 0$, $0 \le p < 1$, $q_0 > 3$, and $\boldsymbol{\mu} \in \mathbb{R}^3$ with $|\boldsymbol{\mu}| = 1$. The data satisfies $g \in L^\infty(\Omega)$, $g \ge 0$ in Ω, and*

$$\begin{aligned}&n_D,\ V_D \in W^{2,q_0}(\Omega), \quad n_D \ge m_* > 0 \text{ on } \partial\Omega, \\ &n_0^0,\ \boldsymbol{n}^0 \cdot \boldsymbol{\mu} \in L^\infty(\Omega), \quad \frac{1}{2}n_0^0 \pm \boldsymbol{n}^0 \cdot \boldsymbol{\mu} \ge \frac{m_*}{2} > 0.\end{aligned}$$

Let $\phi_D := \log n_D + V_D$. Then there exist $\kappa > 0$, $C_0 > 0$, and $\delta > 0$ such that if $\|\phi_D\|_{W^{2,q_0}(\Omega)} \le \delta$,

$$\|n_\pm(t) - \tfrac{1}{2}n_\infty\|_{L^2(\Omega)} + \|V(t) - V_\infty\|_{H^1(\Omega)} \le C_0 e^{-\kappa t}, \quad t > 0,$$

where $n_\pm$ are solutions to (4.7)–(4.9) and (n_∞, V_∞) is the weak solution to (4.10)–(4.11). Furthermore, there exists $\tau_0 > 0$ such that if $0 < \tau \le \tau_0$ then

$$\|N(t) - \tfrac{1}{2}n_\infty\sigma_0\|_{L^2(\Omega;\mathbb{C}^{2\times 2})} \le C_0^* e^{-\kappa^* t}, \quad t > 0,$$

and C_0, $C_0^* > 0$ depend on the initial relative free energy $H(0)$ (see (4.14) below).

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The smallness condition on ϕ_D means that the system is close to equilibrium, as $\phi_D = 0$ characterizes the (thermal) equilibrium state. Since the stationary drift-diffusion equations (4.10) may possess multiple solutions if ϕ_D is large in a certain sense [Ala95, Moc75], the condition on ϕ_D is not surprising. The smallness condition on the relaxation time, however, seems to be purely technical. It is needed to estimate the drift part when we derive $L^2(\Omega)$ bounds for the perpendicular component of $\boldsymbol{n}$. If an entropy structure exists for the equation for $\boldsymbol{n}$, we expect that this condition can be avoided but currently, such a structure is not clear; see [JNS15, Remarks 3.1–3.2]. If the initial spin-vector density is parallel to the precession vector, we are able to remove the smallness condition on τ; see Remark 4.2.9. We show in Remark 4.2.10 that, independently of the initial spin-vector density, the smallness condition is satisfied in a certain physical regime.

The analysis of the asymptotic behavior of the solutions to the Van-Roosbroeck drift-diffusion system (4.6) and the two-component system (4.7)–(4.8) is based on the observation that the relative free energy, consisting of the internal and electric energies, is a Lyapunov functional along the solutions and that the energy dissipation can be bounded from below in terms of the relative free energy itself. The strong coupling of (4.1)-(4.2) prohibits this approach. Indeed, it is shown in [JNS15, Section 3] that the relative free energy associated to (4.1)-(4.2), consisting of the von Neumann energy and the electric energy, is nonincreasing in time only in very particular cases.

Our idea is the observation that the matrix system (4.1)–(4.2) can be reformulated as drift-diffusion-type equations in terms of certain projections of the density matrix relative to the precession vector. This idea was already used in [JNS15] for the existence analysis. The reformulation removes the cross-diffusion terms, which allows us to apply the techniques of Gajewski and Gröger [GG89] used for the Van-Roosbroeck model. This idea only works if the precession vector $\boldsymbol{\mu}$ is constant. A non-constant vector $\boldsymbol{\mu}$ (solving the Landau–Lifshitz–Gilbert equation) was considered in [ZJ16], but this spin model is simplified and no large-time asymptotics was proved.

More precisely, we decompose the density matrix $N = \frac{1}{2}n_0\sigma_0 + \boldsymbol{n}\cdot\boldsymbol{\sigma}$ and $N^0 = \frac{1}{2}n_0^0\sigma_0 + \boldsymbol{n}^0\cdot\boldsymbol{\sigma}$. Then the spin-up and spin-down densities $n_\pm = \frac{1}{2}n_0 \pm \boldsymbol{n}\cdot\boldsymbol{\mu}$ solve (4.7)–(4.9). The information on $n_\pm$ is not sufficient to recover the density matrix. Therefore, we also consider the perpendicular component of $\boldsymbol{n}$ with respect to $\boldsymbol{\mu}$, $\boldsymbol{n}_\perp = \boldsymbol{n} - (\boldsymbol{n}\cdot\boldsymbol{\mu})\boldsymbol{\mu}$, which solves

$$\partial_t \boldsymbol{n}_\perp - \operatorname{div}\left(\frac{D}{\eta}(\nabla \boldsymbol{n}_\perp + \boldsymbol{n}_\perp \nabla V)\right) - 2\gamma(\boldsymbol{n}_\perp \times \boldsymbol{\mu}) = -\frac{\boldsymbol{n}_\perp}{\tau}, \tag{4.13}$$

where $\eta = \sqrt{1-p^2}$, with the boundary and initial conditions $\boldsymbol{n}_\perp = 0$ on $\partial\Omega$ and $\boldsymbol{n}_\perp = \boldsymbol{n}^0 - (\boldsymbol{n}^0\cdot\boldsymbol{\mu})\boldsymbol{\mu}$. The density matrix can be reconstructed from $(n_+, n_-, \boldsymbol{n}_\perp)$ by setting $n_0 = n_+ + n_-$ and $\boldsymbol{n} = \boldsymbol{n}_\perp + (\boldsymbol{n}\cdot\boldsymbol{\mu})\boldsymbol{\mu} = \boldsymbol{n}_\perp + \frac{1}{2}(n_+ - n_-)\boldsymbol{\mu}$.

A key element of the proof is the derivation of a uniform positive lower bound for $n_\pm$. This is shown by using the De Giorgi–Moser iteration method inspired by the proof of [GG89, Lemma 3.6]. More precisely, we choose the test functions $e^t w_\pm^{q-1}/n_\pm$ in (4.7) and (4.8), respectively, where $w_\pm = -\min\{0, \log n_\pm + m\}$ with $m > 0$, $q \in \mathbb{N}$, and pass to the limit $q \to \infty$, leading to $\|w_\pm(t)\|_{L^\infty(\Omega)} \le K$ and consequently to the desired bound $w_\pm(t) \ge e^{-m-K}$ in Ω. Second, we calculate the time derivative of the free energy

$$H(t) = \int_\Omega \left(h(n_+|n_\infty) + h(n_-|n_\infty) + \frac{\lambda^2}{2}|\nabla(V - V_\infty)|^2\right)(t)dx, \tag{4.14}$$

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where $h(n_\pm|n_\infty) = n_\pm \log(2n_\pm/n_\infty) - n_\pm + \frac{1}{2}n_\infty$, leading to the free energy inequality

$$\frac{dH}{dt} + C_1 \int_\Omega (n_+|\nabla(\phi_+ - \phi_D)|^2 + n_-|\nabla(\phi_- - \phi_D)|^2) \\ \leq C_2 \|\nabla \phi_D\|^2_{L^\infty(\Omega)} \int_\Omega ((n_+ - \tfrac{1}{2}n_\infty)^2 + (n_- - \tfrac{1}{2}n_\infty)^2)dx, \tag{4.15}$$

where $\phi_\pm = \log n_\pm + V$ are the electrochemical potentials and $C_1 > 0$ and $C_2 > 0$ are some constants independent of the solution and independent of time. The right-hand side can be estimated, up to a factor, by the free energy H times $\|\nabla\phi_D\|^2_{L^\infty(\Omega)}$. Furthermore, using the time-uniform positive lower bound for $n_\pm$, the energy dissipation (the second term on the left-hand side of (4.15)) is bounded from below by H, up to a factor. Therefore, if $\|\nabla\phi_D\|_{L^\infty(\Omega)} \leq \delta$, (4.15) becomes, for some time-independent constants $C_3 > 0$ and $C_4 > 0$,

$$\frac{dH}{dt} + (C_3 - C_4\delta^2)H \leq 0.$$

Choosing $\delta^2 < C_3/C_4$, the Gronwall inequality implies the exponential decay with respect to the free energy and, as a consequence, in the $L^2(\Omega)$ norm of $n_\pm - n_\infty$ with rate $\kappa := C_3 - C_4\delta^2 > 0$.

Third, we prove the time decay of $\boldsymbol{n}_\perp$. Since we are not aware of an entropy structure for (4.13), we rely on $L^2(\Omega)$ estimates. This means that we use the test function $\boldsymbol{n}_\perp$ in the weak formulation of (4.13) such that the term $(\boldsymbol{n}_\perp \times \boldsymbol{\mu}) \cdot \boldsymbol{n}_\perp$ vanishes. However, in order to handle the term coming from the doping concentration, we need a smallness condition on the relaxation time $\tau > 0$. Such a condition is not needed in the Van-Rooosbroeck model.

Remark 4.2.2. We see a surprising behaviour of the spin in our particular setting. It seems that it converges in the same amount to either the upwards- or either the downwards direction (whatever now up and down means), due to the fact that the average spin is zero on the boundary. So the spin seems to adapt to the behaviour on the boundary, which is indeed an interesting fact. ■

The path to the exponential decay is organized as follows. The stationary equations were already studied in Section 4.1.3. In Section 4.2.1, we prove the lower and upper uniform bounds for $n_\pm$, the entropy inequality, and some bounds for the free energy and energy dissipation. Theorem 4.2.1 is proved in Section 4.2.2. In the appendix, we prove a uniform L^∞ bound for any function that satisfies an iterative inequality using the De Giorgi–Moser method.

4.2.1. Uniform Estimates

In this section, we prove some a priori estimates that are uniform in time. A uniform upper bound for $n_\pm$ was already shown in [JNS15, Theorem 1.1]. For the convenience of the reader, we present the proof.

Lemma 4.2.3 (Uniform upper bound for $n_\pm$)**.** *Introduce*

$$M = \max\left\{\frac{1}{2}\sup_{\partial\Omega} n_D, \sup_\Omega\left(\frac{1}{2}n_0^0 + |\boldsymbol{n}^0 \cdot \boldsymbol{\mu}|\right), \sup_\Omega g\right\}.$$

Then

$$n_\pm(t) \leq M \quad \textit{in } \Omega,\ t > 0.$$

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Proof. We use the test functions $(n_+ - M)^+$ in (4.7) and $(n_- - M)^+$ in (4.8), where $z^+ = \max\{0, z\}$, and add both equations. Observing that $(n_\pm - M)^+ = 0$ on $\partial\Omega$ and $(n_\pm(0) - M)^+ = 0$ in Ω, we find after standard manipulations that

$$\begin{aligned}
\frac{1}{2}\int_\Omega &(|(n_+(t) - M)^+|^2 + |(n_-(t) - M)^+|^2)dx \\
&+ \int_0^t\int_\Omega (D_+|\nabla(n_+ - M)^+|^2 + D_-|\nabla(n_- - M)^+|^2)dxds \\
&= -\frac{1}{2\tau}\int_0^t\int_\Omega (n_+ - n_-)((n_+ - M)^+ - (n_- - M)^+)dxds \\
&- D_+\int_0^t\int_\Omega (n_+ - M)^+\nabla V \cdot \nabla(n_+ - M)^+ dxds \\
&- D_-\int_0^t\int_\Omega (n_- - M)^+\nabla V \cdot \nabla(n_- - M)^+ dxds \\
&- D_+M\int_0^t\int_\Omega \nabla V \cdot \nabla(n_+ - M)^+ dxds - D_-M\int_0^t\int_\Omega \nabla V \cdot \nabla(n_- - M)^+ dxds.
\end{aligned}$$

Since $z \mapsto (z - M)^+$ is monotone, the first integral on the right-hand side is nonnegative. Then, writing $(n_\pm - M)\nabla V \cdot \nabla(n_\pm - M)^+ = \nabla V \cdot \frac{1}{2}\nabla[(n_\pm - M)^+]^2$, integrating by parts, and using the Poisson equation leads to

$$\begin{aligned}
\frac{1}{2}\int_\Omega &(|(n_+(t) - M)^+|^2 + |(n_-(t) - M)^+|^2)dx \\
&+ \int_0^t\int_\Omega (D_+|\nabla(n_+ - M)^+|^2 + D_-|\nabla(n_- - M)^+|^2)dxds \\
&\le -\frac{D_+}{2\lambda^2}\int_0^t\int_\Omega |(n_+ - M)^+|^2(n_+ + n_- - g(x))dxds \\
&- \frac{D_-}{2\lambda^2}\int_0^t\int_\Omega |(n_- - M)^+|^2(n_+ + n_- - g(x))dxds \\
&- \frac{D_+M}{\lambda^2}\int_0^t\int_\Omega (n_+ - M)^+(n_+ + n_- - g(x))dxds \\
&- \frac{D_-M}{\lambda^2}\int_0^t\int_\Omega (n_- - M)^+(n_+ + n_- - g(x))dxds.
\end{aligned}$$

As $M \ge \|g\|_{L^\infty(\Omega)}$ and we integrate only over $\{n_\pm > M\}$, we have $n_+ + n_- - g(x) \ge 0$ on this set. Therefore, all integrals on the right-hand side are nonnegative, and we conclude that

$$\begin{aligned}
\frac{1}{2}\int_\Omega &(|(n_+(t) - M)^+|^2 + |(n_-(t) - M)^+|^2)dx \\
&+ \int_0^t\int_\Omega (D_+|\nabla(n_+ - M)^+|^2 + D_-|\nabla(n_- - M)^+|^2)dxds \le 0.
\end{aligned}$$

This shows that $(n_\pm(t) - M)^+ = 0$ and hence $n_\pm(t) \le M$ in Ω, $t > 0$.

□

Lemma 4.2.4 (Uniform positive lower bound for $n_\pm$)**.** *There exists $m > 0$ such that for all $t > 0$,*

$$n_\pm(t) \ge m > 0 \quad \text{in } \Omega.$$

Proof. We show first that $n_\pm$ is strictly positive with a lower bound that depends on time. For this, we use the test functions $(n_\pm - m^*(t))^- = \min\{0, n_\pm - m^*(t)\}$, where $m^*(t) = m_0e^{-\mu t}$,

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$\mu = 2\lambda^{-2}D_-M$, and

$$m_0 = \min\left\{\inf_{\partial\Omega}\frac{n_D}{2}, \inf_{\Omega}\left(\frac{1}{2}n_0^0 + \boldsymbol{n}^0\cdot\boldsymbol{\mu}\right)\right\} > 0,$$

in (4.7), (4.8), respectively, and add both equations. Proceeding similarly as in the proof of Lemma 4.2.3, we obtain

$$\begin{aligned}
&\frac{1}{2}\int_\Omega ((n_+ - m^*)^-(t)^2 + (n_- - m^*)^-(t)^2)dx \\
&\quad + D_+\int_0^t\int_\Omega |\nabla(n_+ - m^*)^-|^2 dxds + D_-\int_0^t\int_\Omega |\nabla(n_- - m^*)^-|^2 dxds \\
&= -\frac{1}{2\tau}\int_0^t\int_\Omega (n_+ - n_-)((n_+ - m^*)^- - (n_- - m^*)^-)dxds \\
&\quad - \frac{D_+}{2}\int_0^t\int_\Omega \nabla[(n_+ - m^*)^-]^2\cdot\nabla V dxds - \frac{D_-}{2}\int_0^t\int_\Omega \nabla[(n_- - m^*)^-]^2\cdot\nabla V dxds \\
&\quad - D_+\int_0^t m^*(s)\int_\Omega \nabla(n_+ - m^*)^-\cdot\nabla V dxds \\
&\quad - D_-\int_0^t m^*(s)\int_\Omega \nabla(n_- - m^*)^-\cdot\nabla V dxds \\
&\quad + \mu\int_0^t m^*(s)\int_\Omega ((n_+ - m^*)^- + (n_- - m^*)^-)dxds.
\end{aligned}$$

The first term on the right-hand side is nonpositive since $z \mapsto (z - m^*)^-$ is monotone. For the remaining terms, we use the Poisson equation and the estimate $n_0 = n_+ + n_- \le 2M$:

$$\begin{aligned}
&\frac{1}{2}\int_\Omega ((n_+ - m^*)^-(t)^2 + (n_- - m^*)^-(t)^2)dx \\
&\le -\frac{D_+}{2\lambda^2}\int_0^t\int_\Omega |(n_+ - m^*)^-|^2(n_0 - g(x))dxds \\
&\quad - \frac{D_-}{2\lambda^2}\int_0^t\int_\Omega |(n_- - m^*)^-|^2(n_0 - g(x))dxds \\
&\quad - \frac{D_+}{\lambda^2}\int_0^t m^*(s)\int_\Omega (n_+ - m^*)^-(n_0 - g(x))dxds \\
&\quad - \frac{D_-}{\lambda^2}\int_0^t m^*(s)\int_\Omega (n_- - m^*)^-(n_0 - g(x))dxds \\
&\quad + \mu\int_0^t m^*(s)\int_\Omega ((n_+ - m^*)^- + (n_- - m^*)^-)dxds \\
&\le \frac{D_-}{2\lambda^2}\|g\|_{L^\infty(\Omega)}\int_0^t\int_\Omega (|(n_+ - m^*)^-|^2 + |(n_- - m^*)^-|^2)dxds \\
&\quad - \frac{D_+}{\lambda^2}\int_0^t m^*(s)\int_\Omega (n_+ - m^*)^-\left(2M - \frac{\lambda^2}{D_+}\mu\right)dxds \\
&\quad - \frac{D_-}{\lambda^2}\int_0^t m^*(s)\int_\Omega (n_- - m^*)^-\left(2M - \frac{\lambda^2}{D_-}\mu\right)dxds \\
&\le \frac{D_-}{2\lambda^2}\|g\|_{L^\infty(\Omega)}\int_0^t\int_\Omega (|(n_+ - m^*)^-|^2 + |(n_- - m^*)^-|^2)dxds.
\end{aligned}$$

In the last inequality, we used $2M - \lambda^2 D_\pm^{-1}\mu \le 0$. By Gronwall's lemma, this shows that $n_\pm \ge m^*(t) > 0$ in Ω.

In the second step, we prove that $n_\pm$ is strictly positive uniformly in time. The idea is to use the Di Giorgi–Moser iteration method similarly as in the proof of Lemma 3.6 in [GG89].

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We set $w_\pm = -(\log n_\pm + m)^- \in L^2(0,T;H^1(\Omega))$ and take the test function $e^t w_\pm^{q-1}/n_\pm$ in (4.7), (4.8), respectively, where $0 < -\log(m_*/2) < m < 1$ and $q \in \mathbb{N}, q \geq 2$. Because of the previous step, which ensures that $n_\pm > 0$, this test function is well defined. Moreover, $\log(n_D/2) + m \geq \log(m_*/2) + m \geq 0$ and $\log(n_0^0/2 \pm \boldsymbol{n}^0 \cdot \boldsymbol{\mu}) + m \geq \log(m_*/2) + m \geq 0$ such that $w_\pm = 0$ on $\partial\Omega$ and $w_\pm(0) = 0$ in Ω. Formally, we compute $\partial_t(e^t w_\pm^q) - e^t w_\pm^q = -qe^t w_\pm^{q-1} n_\pm^{-1} \partial_t n_\pm$. Therefore, integrating this identity formally over Ω and $(0,t)$ and using (4.7)–(4.8),

$$\begin{aligned}
&\int_\Omega e^t(w_+^q(t) + w_-^q(t))dx - \int_0^t \int_\Omega e^s(w_+^q + w_-^q)dxds \\
&\quad = -q\int_0^t e^s\left(\left\langle \partial_t n_+, \frac{w_+^{q-1}}{n_+}\right\rangle + \left\langle \partial_t n_-, \frac{w_-^{q-1}}{n_-}\right\rangle\right)ds \\
&\quad = \frac{q}{2\tau}\int_0^t e^s\int_\Omega (n_+ - n_-)\left(\frac{w_+^{q-1}}{n_+} - \frac{w_-^{q-1}}{n_-}\right)dxds \\
&\qquad - D_+ q\int_0^t e^s\int_\Omega (\nabla n_+ + n_+\nabla V)\cdot((q-1)w_+^{q-2} + w_+^{q-1})\frac{\nabla n_+}{n_+^2}dxds \\
&\qquad - D_- q\int_0^t e^s\int_\Omega (\nabla n_- + n_-\nabla V)\cdot((q-1)w_-^{q-2} + w_-^{q-1})\frac{\nabla n_-}{n_-^2}dxds,
\end{aligned}$$

where $\langle\cdot,\cdot\rangle$ is the duality product of $H^{-1}(\Omega)$ and $H_0^1(\Omega)$. The computation can be made rigorous by a density argument; see [Jü95, (5.18)] for a similar statement. Since $z \mapsto (-(\log z + m)^-)^{q-1}/z$ is nonincreasing for $z > 0$, the first term on the right-hand side is nonpositive, giving

$$\begin{aligned}
&\int_\Omega e^t(w_+^q(t) + w_-^q(t))dx - \int_0^t \int_\Omega e^s(w_+^q + w_-^q)dxds \\
&\quad \leq -D_+ q\int_0^t e^s\int_\Omega ((q-1)w_+^{q-2} + w_+^{q-1})(|\nabla w_+|^2 - \nabla V\cdot\nabla w_+)dxds \\
&\qquad - D_- q\int_0^t e^s\int_\Omega ((q-1)w_-^{q-2} + w_-^{q-1})(|\nabla w_-|^2 - \nabla V\cdot\nabla w_-)dxds.
\end{aligned}$$

Taking into account the Poisson equation and the inequalities $D_+ \leq D_-$, $w_\pm \geq 0$, and $n_0 \leq 2M$, this becomes

$$\begin{aligned}
&\int_\Omega e^t(w_+^q(t) + w_-^q(t))dx - \int_0^t \int_\Omega e^s(w_+^q + w_-^q)dxds \\
&\qquad + \frac{4D_+(q-1)}{q}\int_0^t e^s\int_\Omega (|\nabla w_+^{q/2}|^2 + |\nabla w_-^{q/2}|^2)dxds \\
&\qquad + \frac{4D_+ q}{(q+1)^2}\int_0^t e^s\int_\Omega (|\nabla w_+^{(q+1)/2}|^2 + |\nabla w_-^{(q+1)/2}|^2)dxds \\
&\quad \leq \frac{D_+ q}{\lambda^2}\int_0^t e^s\int_\Omega \left(w_+^{q-1} + \frac{1}{q}w_+^q\right)(n_0 - g(x))dxds \\
&\qquad + \frac{D_- q}{\lambda^2}\int_0^t e^s\int_\Omega \left(w_-^{q-1} + \frac{1}{q}w_-^q\right)(n_0 - g(x))dxds \\
&\quad \leq \frac{2D_+ M}{\lambda^2}\int_0^t e^s\int_\Omega (qw_+^{q-1} + w_+^q)dxds + \frac{2D_- M}{\lambda^2}\int_0^t e^s\int_\Omega (qw_-^{q-1} + w_-^q)dxds \\
&\quad \leq \frac{2D_- Mq}{\lambda^2}\int_0^t e^s\int_\Omega (w_+^q + w_-^q)dxds + \frac{4D_- M}{\lambda^2}\int_0^t e^s\int_\Omega dxds. \qquad (4.16)
\end{aligned}$$

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In the last inequality, we used Young's inequality: $qw_\pm^{q-1} \le (q-1)w_\pm^q + 1$. We infer that

$$\int_\Omega e^t(w_+^q(t) + w_-^q(t))dx + K_0 \int_0^t \int_\Omega e^s(|\nabla w_+^{q/2}|^2 + |\nabla w_-^{q/2}|^2)dxds$$
$$\le K_1 q \int_0^t \int_\Omega e^s(w_+^q + w_-^q)dxds + K_2 e^t$$

for some constants K_0, K_1, $K_2 > 0$ which are independent of q and time.

Lemma C.1.1 in the appendix shows that $w_\pm$ is bounded in L^∞ with a constant which depends on the $L^\infty(0,T;L^1(\Omega))$ norm of $w_\pm$. Therefore, it remains to estimate $w_\pm$ in this norm. To this end, we take $q = 2$ in (4.16):

$$\int_\Omega e^t(w_+^2(t) + w_-^2(t))dx - \int_0^t e^s \int_\Omega (w_+^2 + w_-^2)dxds$$
$$+ \frac{8}{9}D_+ \int_0^t e^s \int_\Omega (|\nabla w_+^{3/2}|^2 + |\nabla w_-^{3/2}|^2)dxds$$
$$\le \frac{4D_-M}{\lambda^2} \int_0^t e^s \int_\Omega (w_+^2 + w_-^2)dxds + \frac{4D_-M}{\lambda^2} \int_0^t e^s \int_\Omega dxds.$$

By the Poincaré inequality, for some constants $C_i > 0$, we obtain

$$\int_\Omega e^t(w_+^2(t) + w_-^2(t))dx \le \int_0^t e^s \int_\Omega \big(-C_1(w_+^3 + w_-^3) + C_2(w_+^2 + w_-^2)\big)dxds + C_3 e^t.$$

Since $f(x) = -C_1x^3 + C_2x^2 = (-C_1x + C_2)x^2$ has a maximum $\widetilde{C}_4 > 0$ for $x \ge 0$, we can estimate the right-hand side by $e^t(\widetilde{C}_4 \operatorname{meas}(\Omega) + C_3)$. Division by e^t leads to

$$\int_\Omega (w_+^2(t) + w_-^2(t))dx \le C_4 := \widetilde{C}_4 \operatorname{meas}(\Omega) + C_3,$$

which does not depend on time. In particular, this shows that $w_\pm$ is bounded in $L^\infty(0,T;$ $L^1(\Omega))$ uniformly in time. Thus, by Lemma C.1.1, $\|w_\pm(t)\|_{L^\infty(\Omega)} \le K$ for some constant $K > 0$ and $n_\pm(t) \ge \exp(-K - m)$ in Ω, $t > 0$. This finishes the proof. □

Remark 4.2.5. The factor e^t is necessary to derive time-uniform bounds. Indeed, without this factor, the last term on the right-hand side of (4.16) becomes $4D_-M\lambda^{-2} \int_0^t \int_\Omega dsdx$ which is unbounded as $t \to \infty$. ■

We introduce the relative free energy

$$H(t) = \int_\Omega \Big(h(n_+|n_\infty) + h(n_-|n_\infty) + \frac{\lambda^2}{2}|\nabla(V - V_\infty)|^2\Big)(t)dx,$$

where $h(n_\pm|n_\infty) = n_\pm \log(2n_\pm/n_\infty) - n_\pm + \frac{1}{2}n_\infty$, and the electrochemical potentials $\phi_\pm = \log n_\pm + V$.

Lemma 4.2.6 (Relative free energy estimate)**.** *It holds that*

$$\frac{dH}{dt} \le -\frac{D_+}{2} \int_\Omega (n_+|\nabla(\phi_+ - \phi_\infty)|^2 + n_-|\nabla(\phi_- - \phi_\infty)|^2)dx$$
$$+ \frac{D_-}{2} \int_\Omega ((n_+ - \tfrac{1}{2}n_\infty)^2 + (n_- - \tfrac{1}{2}n_\infty)^2)|\nabla\phi_\infty|^2 dx$$
$$- \frac{1}{8\tau} \int_\Omega (\sqrt{n_+} - \sqrt{n_-})^2 dx.$$

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Proof. Using the Poisson equation and the definitions $\phi_\pm = \log n_\pm + V$ and $\phi_\infty = \log n_\infty + V_\infty$, it follows that

$$\begin{aligned}\frac{dH}{dt} &= \left\langle \partial_t n_+, \log\frac{2n_+}{n_\infty}\right\rangle + \left\langle \partial_t n_-, \log\frac{2n_-}{n_\infty}\right\rangle - \lambda^2\langle \partial_t \Delta(V-V_\infty), V-V_\infty\rangle \\ &= \left\langle \partial_t n_+, \log\frac{n_+}{n_\infty} + \log 2\right\rangle + \left\langle \partial_t n_-, \log\frac{n_-}{n_\infty} + \log 2\right\rangle + \langle \partial_t(n_+ + n_-), V-V_\infty\rangle \\ &= \langle \partial_t n_+, \phi_+ - \phi_\infty + \log 2\rangle + \langle \partial_t n_-, \phi_- - \phi_\infty + \log 2\rangle \end{aligned} \tag{4.17}$$

This can be made rigorous similarly as in [Jü95, formula (5.18)], together with the techniques in [Eva10, Theorem 3, p. 287].

Next, we subtract $\frac{1}{2}D_\pm\times$(4.10) from (4.7) and (4.8), respectively:

$$\begin{aligned}\partial_t n_+ - D_+ \operatorname{div}\left(n_+\nabla(\phi_+ - \phi_\infty) + (n_+ - \tfrac{1}{2}n_\infty)\nabla\phi_\infty\right) &= -\frac{1}{2\tau}(n_+ - n_-), \\ \partial_t n_- - D_- \operatorname{div}\left(n_-\nabla(\phi_- - \phi_\infty) + (n_- - \tfrac{1}{2}n_\infty)\nabla\phi_\infty\right) &= -\frac{1}{2\tau}(n_- - n_+).\end{aligned}$$

Inserting these equations into (4.17), we find that

$$\begin{aligned}\frac{dH}{dt} = &-D_+\int_\Omega n_+|\nabla(\phi_+ - \phi_\infty)|^2 dx - D_-\int_\Omega n_-|\nabla(\phi_- - \phi_\infty)|^2 dx \\ &- D_+\int_\Omega (n_+ - \tfrac{1}{2}n_\infty)\nabla\phi_\infty\cdot\nabla(\phi_+ - \phi_\infty)dx \\ &- D_-\int_\Omega (n_- - \tfrac{1}{2}n_\infty)\nabla\phi_\infty\cdot\nabla(\phi_- - \phi_\infty)dx \\ &- \frac{1}{2\tau}\int_\Omega (n_+ - n_-)(\log n_+ - \log n_-)dx.\end{aligned}$$

We use the elementary inequality

$$(y-z)(\log y - \log z) \ge \frac{1}{4}\left(\sqrt{y} - \sqrt{z}\right)^2 \quad \text{for } y, z > 0 \tag{4.18}$$

to estimate the last term. Then the Young inequality and the lower bound $n_\pm \ge m$ lead to

$$\begin{aligned}\frac{dH}{dt} \le &-\frac{D_+}{2}\int_\Omega n_+|\nabla(\phi_+ - \phi_\infty)|^2 dx - \frac{D_-}{2}\int_\Omega n_-|\nabla(\phi_- - \phi_\infty)|^2 dx \\ &+ \frac{D_+}{2m}\int_\Omega (n_+ - \tfrac{1}{2}n_\infty)^2|\nabla\phi_\infty|^2 dx + \frac{D_-}{2m}\int_\Omega (n_- - \tfrac{1}{2}n_\infty)^2|\nabla\phi_\infty|^2 dx \\ &- \frac{1}{8\tau}\int_\Omega \left(\sqrt{n_+} - \sqrt{n_-}\right)^2 dx,\end{aligned}$$

finishing the proof. □

Lemma 4.2.7 (Lower bound for the chemical potentials)**.** *It holds that*

$$\begin{aligned}&\|\nabla(\phi_+ - \phi_\infty)\|^2_{L^2(\Omega)} + \|\nabla(\phi_- - \phi_\infty)\|^2_{L^2(\Omega)} \\ &\quad \ge C\left(\|n_+ - \tfrac{1}{2}n_\infty\|^2_{L^2(\Omega)} + \|n_- - \tfrac{1}{2}n_\infty\|^2_{L^2(\Omega)} + \|\nabla(V - V_\infty)\|^2_{L^2(\Omega)}\right),\end{aligned}$$

where $C > 0$ depends only on M, M_∞, λ, and Ω.

Recall that M is the upper bound for $n_\pm$ (see Lemma 4.2.3) and M_∞ is the upper bound for n_∞ (see (4.12)).

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Proof. It holds that $\phi_\pm - \phi_\infty + \log 2 = 0$ on $\partial\Omega$. Thus, the Young and Poincaré inequalities yield for any $\varepsilon > 0$,

$$\begin{aligned}\int_\Omega (n_\pm - \tfrac{1}{2}n_\infty)(\phi_\pm - \phi_\infty + \log 2)dx &\le \varepsilon \|n_\pm - \tfrac{1}{2}n_\infty\|^2_{L^2(\Omega)} + C(\varepsilon)\|\phi_\pm - \phi_\infty + \log 2\|^2_{L^2(\Omega)} \\ &\le \varepsilon \|n_\pm - \tfrac{1}{2}n_\infty\|^2_{L^2(\Omega)} + C(\varepsilon,\Omega)\|\nabla(\phi_\pm - \phi_\infty)\|^2_{L^2(\Omega)}.\end{aligned} \tag{4.19}$$

Inserting the definitions of $\phi_\pm$ and ϕ_∞, taking into account the Poisson equation $-\lambda^2\Delta(V - V_\infty) = n_0 - n_\infty$ and inequality (4.18), and finally using the bounds $m \le n_\pm \le M$ and $m_\infty \le n_\infty \le M_\infty$, we obtain

$$\begin{aligned}&\int_\Omega (n_+ - \tfrac{1}{2}n_\infty)(\phi_+ - \phi_\infty + \log 2)dx + \int_\Omega (n_- - \tfrac{1}{2}n_\infty)(\phi_- - \phi_\infty + \log 2)dx \\ &= \int_\Omega (n_+ - \tfrac{1}{2}n_\infty)(\log n_+ - \log(\tfrac{1}{2}n_\infty))dx + \int_\Omega (n_- - \tfrac{1}{2}n_\infty)(\log n_- - \log(\tfrac{1}{2}n_\infty))dx \\ &\quad + \int_\Omega (n_0 - n_\infty)(V - V_\infty)dx \\ &\ge \frac{1}{4}\int_\Omega \left(\sqrt{n_+} - \sqrt{\tfrac{1}{2}n_\infty}\right)^2 dx + \frac{1}{4}\int_\Omega \left(\sqrt{n_-} - \sqrt{\tfrac{1}{2}n_\infty}\right)^2 dx + \lambda^2\int_\Omega |\nabla(V - V_\infty)|^2 dx \\ &= \frac{1}{4}\int_\Omega \frac{(n_+ - n_\infty/2)^2}{(\sqrt{n_+} + \sqrt{n_\infty/2})^2}dx + \frac{1}{4}\int_\Omega \frac{(n_- - n_\infty/2)^2}{(\sqrt{n_-} + \sqrt{n_\infty/2})^2}dx + \lambda^2\int_\Omega |\nabla(V - V_\infty)|^2 dx \\ &\ge C_2\int_\Omega (n_+ - \tfrac{1}{2}n_\infty)^2 dx + C_2\int_\Omega (n_- - \tfrac{1}{2}n_\infty)^2 dx + \lambda^2\int_\Omega |\nabla(V - V_\infty)|^2 dx,\end{aligned}$$

where $C_2 = \frac{1}{4}(\sqrt{M} + \sqrt{M_\infty/2})^{-2}$. Combining this estimate with (4.19) and taking $\varepsilon < C_1$, we conclude the proof. □

Lemma 4.2.8 (Bounds for the relative free energy)**.** *There exist constants C_ϕ, $C_H > 0$ independent of the solution and time such that*

$$\begin{aligned}H &\le C_\phi(\|\nabla(\phi_+ - \phi_\infty)\|^2_{L^2(\Omega)} + \|\nabla(\phi_- - \phi_\infty)\|^2_{L^2(\Omega)}), \\ H &\ge C_H(\|n_+ - \tfrac{1}{2}n_\infty\|^2_{L^2(\Omega)} + \|n_- - \tfrac{1}{2}n_\infty\|^2_{L^2(\Omega)}).\end{aligned}$$

Proof. Set $f(y) = y\log(y/z) - y + z$ for some fixed $z > 0$. A Taylor expansion shows that

$$y\log\frac{y}{z} - y + z = f(y) = f(z) + f'(z)(y-z) + \frac{1}{2}f''(\xi)(y-z)^2 = \frac{(y-z)^2}{2\xi},$$

where ξ is between y and z. Consequently, since $n_\pm \ge m$ and $n_\infty \ge m_\infty$,

$$n_\pm \log\frac{2n_\pm}{n_\infty} - n_\pm + \frac{1}{2}n_\infty \le \frac{1}{2C_1}(n_\pm - \tfrac{1}{2}n_\infty)^2,$$

where $C_1 = \min\{m, m_\infty/2\}$, and, using Lemma 4.2.7, we find that

$$\begin{aligned}H &\le \max\left\{\frac{1}{2C_1}, \frac{\lambda^2}{2}\right\}(\|n_+ - \tfrac{1}{2}n_\infty\|^2_{L^2(\Omega)} + \|n_- - \tfrac{1}{2}n_\infty\|^2_{L^2(\Omega)} + \|\nabla(V - V_\infty)\|^2_{L^2(\Omega)}) \\ &\le \max\left\{\frac{1}{2C_1}, \frac{\lambda^2}{2}\right\}C(\|\nabla(\phi_+ - \phi_\infty)\|^2_{L^2(\Omega)} + \|\nabla(\phi_- - \phi_\infty)\|^2_{L^2(\Omega)}).\end{aligned}$$

For the second estimate, we use

$$n_\pm \log\frac{2n_\pm}{n_\infty} - n_\pm + \frac{1}{2}n_\infty \ge \frac{(n_\pm - \frac{1}{2}n_\infty)^2}{2C_2}, \quad \text{where } 2C_2 = \max\{M, M_\infty/2\},$$

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to conclude that

$$H \geq \frac{1}{2C_2}\int_\Omega \big((n_+ - \tfrac12 n_\infty)^2 + (n_- - \tfrac12 n_\infty)^2\big)dx.$$

This finishes the proof. □

4.2.2. Proof of Main Theorem 4.2.1

The starting point is the free-energy inequality in Lemma 4.2.6. We need to estimate the integral containing $\nabla\phi_\infty$. In view of Lemmas 4.1.2 and 4.2.8,

$$\begin{aligned}\int_\Omega (n_\pm - \tfrac12 n_\infty)^2|\nabla\phi_\infty|^2dx &\leq \|\nabla\phi_\infty\|^2_{L^\infty(\Omega)}\|n_\pm - \tfrac12 n_\infty\|^2_{L^2(\Omega)} \\ &\leq C_\infty^2\|\phi_D\|^2_{W^{2,q_0}(\Omega)}\|n_\pm - \tfrac12 n_\infty\|^2_{L^2(\Omega)} \leq C_\infty^2 C_H^{-1}\|\phi_D\|^2_{W^{2,q_0}(\Omega)}H. \end{aligned}\tag{4.20}$$

By the lower bound of $n_\pm$ and Lemma 4.2.7, the free-energy inequality in Lemma 4.2.6 becomes

$$\frac{dH}{dt} + \left(\frac{D_+m}{2C_\phi} - \frac{D_-C_\infty^2}{C_H}\|\phi_D\|^2_{W^{2,q_0}(\Omega)}\right)H + \frac{1}{8\tau}\|\sqrt{n_+} - \sqrt{n_-}\|^2_{L^2(\Omega)} \leq 0.$$

Let $\delta > 0$ satisfy $2\kappa := D_+m/(2C_\phi) - D_-(C_\infty^2/C_H)\delta^2 > 0$ and choose n_D and V_D such that$\|\phi_D\|_{W^{2,q_0}(\Omega)} \leq \delta$. Then Gronwall's lemma implies that $H(t) \leq H(0)\exp(-2\kappa t)$ for $t > 0$. By Lemma 4.2.8,

$$\|n_+(t) - \tfrac12 n_\infty\|_{L^2(\Omega)} + \|n_-(t) - \tfrac12 n_\infty\|_{L^2(\Omega)} \leq C_H^{-1/2}H(0)^{1/2}e^{-\kappa t}, \quad t > 0.$$

The $H^1(\Omega)$ elliptic estimate for the Poisson problem $-\lambda^2\Delta(V - V_\infty) = (n_+ - \frac12 n_\infty) + (n_- - \frac12 n_\infty)$ in Ω, $V - V_\infty = 0$ on $\partial\Omega$ gives

$$\|V(t) - V_\infty\|_{H^1(\Omega)} \leq C\|n_+(t) - \tfrac12 n_\infty\|_{L^2(\Omega)} + C\|n_-(t) - \tfrac12 n_\infty\|_{L^2(\Omega)} \leq Ce^{-\kappa t},$$

which proves the first estimate. For the second result, recall that we can decompose $N(t)$ as $N(t) = \frac12(n_+ + n_-)\sigma_0 + (\boldsymbol{n}_\perp + \frac12(n_+ - n_-)\boldsymbol{\mu})\cdot\boldsymbol{\sigma}$. We use $\boldsymbol{n}_\perp$ as a test function in (4.13):

$$\begin{aligned}\frac12\frac{d}{dt}\int_\Omega |\boldsymbol{n}_\perp|^2dx &+ \frac{D}{\eta}\int_\Omega |\nabla\boldsymbol{n}_\perp|^2dx + \frac{1}{\tau}\int_\Omega |\boldsymbol{n}_\perp|^2dx \\ &= -\frac{D}{2\eta}\int_\Omega \nabla|\boldsymbol{n}_\perp|^2\cdot\nabla V dx = -\frac{D}{2\eta\lambda^2}\int_\Omega |\boldsymbol{n}_\perp|^2(n_0 - g(x))dx \\ &\leq \frac{D}{2\eta\lambda^2}\|g\|_{L^\infty(\Omega)}\int_\Omega |\boldsymbol{n}_\perp|^2dx.\end{aligned}$$

Thus, if $\tau \leq 2\eta\lambda^2/(D\|g\|_{L^\infty(\Omega)})$, the Poincaré inequality shows that

$$\frac{d}{dt}\int_\Omega |\boldsymbol{n}_\perp|^2dx + 2C(D,\eta,\Omega)\int_\Omega |\boldsymbol{n}_\perp|^2dx \leq 0.$$

By Gronwall's lemma,

$$\|\boldsymbol{n}_\perp(t)\|_{L^2(\Omega)} \leq \|\boldsymbol{n}_\perp(0)\|_{L^2(\Omega)}e^{-C(D,\eta,\Omega)t}, \quad t > 0.$$

Therefore, we find that

$$\begin{aligned}\|N(t) - \tfrac12 n_\infty\sigma_0\|_{L^2(\Omega;\mathbb{C}^{2\times2})} &\leq \|(\tfrac12(n_+ - \tfrac12 n_\infty) + \tfrac12(n_- - \tfrac12 n_\infty))\sigma_0\|_{L^2(\Omega;\mathbb{C}^{2\times2})} \\ &\quad + \|\boldsymbol{n}_\perp + \tfrac12(n_+ - n_-)\boldsymbol{\mu})\cdot\boldsymbol{\sigma}\|_{L^2(\Omega;\mathbb{C}^{2\times2})} \\ &\leq C_H^{-1/2}H(0)^{1/2}e^{-\kappa t} + \|\boldsymbol{n}_\perp(0)\|_{L^2(\Omega)}e^{-C(D,\eta,\Omega)t} \leq C_0^*e^{-\kappa^* t},\end{aligned}$$

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where $C_0^* = \max(2C_H^{-1/2}H(0)^{1/2}, \|\boldsymbol{n}_\perp(0)\|_{L^2(\Omega)})$ and $\kappa^* = \min(\kappa, C(D,\eta,\Omega)t)$. This concludes the proof of Theorem 4.2.1.

□

Remark 4.2.9. Let $\boldsymbol{\mu} = (0,0,1)^\top$ and $\boldsymbol{n}^0 = (0,0,n_3^0)$. Then the components n_1 and n_2 of the spin-vector density satisfy the equation

$$\partial_t n_i = \operatorname{div}\left(\frac{D}{\eta^2}(\nabla n_i + n_i \nabla V)\right), \quad i = 1, 2,$$

with boundary conditions $n_i = 0$ on $\partial\Omega$ and initial conditions $n_i(0) = 0$ in Ω. The unique solution is given by $n_i(t) = 0$ for all $t > 0$ and $i = 1, 2$. Since $\boldsymbol{n} = \boldsymbol{n}_\perp + (\boldsymbol{n}\cdot\boldsymbol{\mu})\boldsymbol{\mu} = \boldsymbol{n}_\perp + n_3\boldsymbol{\mu}$, the perpendicular component vanishes, $\boldsymbol{n}_\perp(t) = 0$. We conclude that the dynamics of the system is completely determined by $n_\pm$, and the proof of Theorem 4.2.1 gives the exponential decay without any condition on τ. In particular, the density matrix $N(t) = \frac{1}{2}(n_+ + n_-)\sigma_0 + \frac{1}{2}(n_+ - n_-)\sigma_3$ converges exponentially fast towards $\frac{1}{2}n_\infty\sigma_0$ as $t \to \infty$. ■

Remark 4.2.10. We discuss the physical relevance of the smallness condition of the scaled relaxation time $\tau \le 2\eta\lambda^2/(D\|g\|_{L^\infty(\Omega)})$. In scaled variables, we may assume that $D = 1$ and $\|g\|_{L^\infty(\Omega)} = 1$. The scaled Debye length is given by $\lambda^2 = \varepsilon_s U_T/(qL^2g^*) = 2.7\cdot 10^{-1}$, where the physical parameters are explained in Table 4.1. We have assumed that the semiconductor material is lowly doped. The scaled relaxation time is $\tau = \tau_0/t^*$, where the typical time is defined by $t^* = L^2/(\mu_0 U_T) = 1.5\cdot 10^{-11}\,\mathrm{s}$. The spin-flip relaxation time is assumed to be $\tau_0 = 1\,\mathrm{ps}$. This value is realistic in GaAs quantum wells at temperature $T = 50\,\mathrm{K}$; see [BF92, Figure 1]. It follows that $\tau = 6\cdot 10^{-2}$. Thus, the inequality $\tau \le 2\eta\lambda^2/(D\|g\|_{L^\infty(\Omega)})$ is satisfied if $\eta \ge 0.11$ or $p \le 0.99$. This covers almost the full range of $p \in [0,1)$. ■

Parameter	physical meaning	numerical value
q	elementary charge	$1.6\cdot 10^{-19}$ As
ε_s	permittivity constant	10^{-12} As/(Vcm)
μ_0	(low field) mobility constant	$1.5\cdot 10^3$ cm^2/(Vs)
U_T	thermal voltage at $T = 50\,\mathrm{K}$	$4.3\cdot 10^{-3}$ V
g^*	maximal doping concentration	10^{15}/cm^3
τ_0	spin-flip relaxation time	10^{-12} s
L	length of the device	10^{-5} cm

Table 4.1.: Physical parameters.

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Appendices

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A. Addendum Effective Energy Transport Model

A.1. Compact Embedding of $\mathrm{H}^s(\mathbb{T}^d)$ in $\mathrm{L}^2(\mathbb{T}^d)$

We add here the proof for Proposition 2.3.17, where we prove that the space $\mathrm{H}^s(\mathbb{T}^d)$, given through Definition 2.3.9, embeds compactly into $\mathrm{L}^2(\mathbb{T}^d)$. A similar compactness result is given in [Amb20], which is slightly more specific than ours. If we would replace $\mathbb{T}^d$ with $\mathbb{R}^d$, the compact embedding $\mathrm{H}^s(\mathbb{R}^d) \subset\subset \mathrm{L}^2(\mathbb{R}^d)$ is proven in [DPV12].
Since we do not prove the equivalence to the fractional Sobolev space, we did not find in literature a fitting result, hence we prove it on our own. The proof relies on basic functional analysis, which can be found for example in [Rud91].

Proposition A.1.1. *For all $s \in (0,1)$ the embedding $\mathrm{H}^s(\mathbb{T}^d) \hookrightarrow \mathrm{L}^2(\mathbb{T}^d)$ is compact for all dimensions $d \in \mathbb{N}$ (not.: $\mathrm{H}^s(\mathbb{T}^d) \subset\subset \mathrm{L}^2(\mathbb{T}^d)$).*

Proof. Fix $s \in (0,1)$, and notice that the embedding

$$\iota : \mathrm{H}^s(\mathbb{T}^d) \to \mathrm{L}^2(\mathbb{T}^d), \quad g \mapsto g$$

is linear and continuous, hence bounded. Therefore it is enough to show that ι is a compact operator. Define the family $(\iota_N)_{N\in\mathbb{N}}$ of operators

$$\iota_N : \mathrm{H}^s(\mathbb{T}^d) \to \mathrm{L}^2(\mathbb{T}^d), \quad g \mapsto \sum_{\substack{l\in\mathbb{Z}^d \\ |l|\leq N}} \mathfrak{F}_x\left(g\right)(l)\; e^{2\pi i l\cdot x},$$

where $\mathfrak{F}_x\left(.\right)$ denotes the Fourier transformation on the torus (see Definition 2.3.7) and $\mathfrak{F}^{-1}$ its inverse. Since $g \in \mathrm{L}^2(\mathbb{T}^d)$ we have (for details see [Gra08] Proposition 3.1.16)

$$g(x) = \mathfrak{F}^{-1}(\mathfrak{F}_x\left(g\right))(x) \coloneqq \sum_{l\in\mathbb{Z}^d} \mathfrak{F}_x\left(g\right)(l)\; e^{2\pi i l\cdot x} \qquad \text{for a.e. } x \in \mathbb{T}^d.$$

From that and Plancherel's identity (see (2.43)) we deduce for all $g \in \mathrm{H}^s(\mathbb{T}^d)$

$$\begin{aligned} \|(\iota - \iota_N)(g)\|^2_{\mathrm{L}^2(\mathbb{T}^d)} &= \Big\| \sum_{l\in\mathbb{Z}^d, |l|>N} \mathfrak{F}_x\left(g\right)(l)\; e^{2\pi i l\cdot x}\Big\|^2_{\mathrm{L}^2(\mathbb{T}^d)} = \left\|\mathfrak{F}^{-1}\left(\mathfrak{F}_x\left(g\right) \mathbb{1}_{|l|>N}\right)\right\|^2_{\mathrm{L}^2(\mathbb{T}^d)} = \\ &= \sum_{l\in\mathbb{Z}^d, |l|>N} |\mathfrak{F}_x\left(g\right)(l)|^2 \leq \frac{1}{|N|^{2s}} \sum_{l\in\mathbb{Z}^d, |l|>N} |l|^{2s} |\mathfrak{F}_x\left(g\right)(l)|^2 \leq \\ &\leq \frac{1}{|N|^{2s}} \|g\|^2_{\mathrm{H}^s(\mathbb{T}^d)} \end{aligned}$$

Hence we obtain the convergence

$$\lim_{N\to\infty} \sup_{\substack{g\in\mathrm{H}^s(\mathbb{T}^d) \\ \|g\|_{\mathrm{H}^s(\mathbb{T}^d)}=1}} \|(\iota - \iota_N)(g)\|_{\mathrm{L}^2(\mathbb{T}^d)} \leq \lim_{N\to\infty} \frac{1}{N^s} = 0,$$

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which gives us that ι_N convergences towards ι with respect to the operator norm.
Second step is to show that ι_N is a compact operator for all $N \in \mathbb{N}$. To prove this we will see that the range of each ι_N has finite dimension. Obviously we have

$$\mathfrak{F}_x\left(\iota_N(g)\right)(l) = \begin{cases} \mathfrak{F}_x(g)(l), & \text{for } |l| \leq N, \\ 0 & \text{for } |l| > N. \end{cases}$$

Define the cardinality $\tilde{N} := \#\left\{l \in \mathbb{Z}^d : |l| \leq N\right\}$ and the subspace of ℓ^2 with finite non zero entries

$$\ell^2_N(\mathbb{Z}^d) := \operatorname{span}\left\{(a_l)_{l\in\mathbb{Z}^d} \in \ell^2(\mathbb{Z}^d) : a_l = 0 \ \forall |l| > N\right\}.$$

Clearly $\dim \ell^2_N(\mathbb{Z}^d) = \tilde{N}$ and we see also that $\mathfrak{F}_x\left(\iota_N(\mathrm{H}^s(\mathbb{T}^d))\right) \subseteq \ell^2_N(\mathbb{Z}^d)$. Since $\mathfrak{F}_x(.)$ is an injective isometry from $\mathrm{L}^2(\mathbb{T}^d)$ to $\ell^2(\mathbb{Z}^d)$ (consequence of Plancherel's identity), we have that $\dim \mathfrak{F}_x\left(\iota_N(\mathrm{H}^s(\mathbb{T}^d))\right) \leq \tilde{N}$. From basic functional analysis we know that bounded operators with finite range are compact and that the space of compact operators is a closed subspace of the bounded operators with respect to the operator norm (see [Rud91] Theorem 4.18). Hence ι_N is compact for all $N \in \mathbb{N}$ and since ι is the limit of $(\iota_N)_{N\in\mathbb{N}}$ we finally conclude that for all $s \in (0,1)$ the embedding $\iota : \mathrm{H}^s(\mathbb{T}^d) \to \mathrm{L}^2(\mathbb{T}^d)$ is compact. □

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B. Addendum Spin Drift Diffusion

B.1. Calculations for the General Zeroth Order of the Maxwellian

This section is devoted to the calculations for the ODE (3.75):

$$\partial_\beta g^{(0)}(\beta) = \left(h_0^{(0)}\sigma_0 + \boldsymbol{a}^{(0)} \cdot \boldsymbol{\sigma}\right) \#_{(0)} g^{(0)}(\beta), \qquad g^{(0)}(0) = \sigma_0. \tag{B.1}$$

where we recall $h_0^{(0)} = -\frac{1}{2}|p|^2 + a_0{}^{(0)}$, $a_0{}^{(0)}(x) = \tilde{a}_0^{(0)}(x) - V(x)$ and $\#_{(0)}$ equals the normal product (see Lemma (3.2.20)). If we write (3.75) explicit, we have

$$\partial_\beta \begin{pmatrix} g_{11}^{(0)}(\beta) & g_{12}^{(0)}(\beta) \\ g_{21}^{(0)}(\beta) & g_{22}^{(0)}(\beta) \end{pmatrix} = \begin{pmatrix} h_0^{(0)} + a_3^{(0)} & a_1^{(0)} - \mathrm{i}a_2^{(0)} \\ a_1^{(0)} + \mathrm{i}a_2^{(0)} & h_0^{(0)} - a_3^{(0)} \end{pmatrix} \begin{pmatrix} g_{11}^{(0)}(\beta) & g_{12}^{(0)}(\beta) \\ g_{21}^{(0)}(\beta) & g_{22}^{(0)}(\beta) \end{pmatrix},$$

with the starting condition

$$\begin{pmatrix} g_{11}^{(0)}(0) & g_{12}^{(0)}(0) \\ g_{21}^{(0)}(0) & g_{22}^{(0)}(0) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

If $\boldsymbol{a}^{(0)}(x)$ would be constant zero, the differential equation would reduce to a single one of the form

$$\partial_\beta g^{(0)}(\beta) = \left(h_0^{(0)} + a_0{}^{(0)}\right) g^{(0)}(\beta)$$

with the solution

$$g^{(0)}(\beta) = \exp\left(\beta\left(h_0^{(0)} + a_0{}^{(0)}\right)\right)\sigma_0.$$

The next important case is that when $a_1^{(0)}(x) = 0 = a_2^{(0)}(x)$ for some $x \in \mathbb{R}^3$. The differential equation to solve would be

$$\partial_\beta \begin{pmatrix} g_{11}^{(0)}(\beta) & g_{12}^{(0)}(\beta) \\ g_{21}^{(0)}(\beta) & g_{22}^{(0)}(\beta) \end{pmatrix} = \begin{pmatrix} \left(h_0^{(0)} + a_3^{(0)}\right) g_{11}^{(0)}(\beta) & \left(h_0^{(0)} + a_3^{(0)}\right) g_{12}^{(0)}(\beta) \\ \left(h_0^{(0)} - a_3^{(0)}\right) g_{21}^{(0)}(\beta) & \left(h_0^{(0)} - a_3^{(0)}\right) g_{22}^{(0)}(\beta) \end{pmatrix},$$
$$\begin{pmatrix} g_{11}^{(0)}(0) & g_{12}^{(0)}(0) \\ g_{21}^{(0)}(0) & g_{22}^{(0)}(0) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Here we obtain the solution

$$g^{(0)}(\beta) = \begin{pmatrix} \exp\left(\beta\left(h_0^{(0)} + a_3^{(0)}\right)\right) & 0 \\ 0 & \exp\left(\beta\left(h_0^{(0)} - a_3^{(0)}\right)\right) \end{pmatrix} \tag{B.2}$$

Last we solve the equation (3.75) for each x and p, where we assume that $a_1^{(0)}(x) \neq 0 \neq a_2^{(0)}(x)$. This leads us to solving two linear differential equations of the form

$$\dot{y}_1(\beta) = By_1(\beta) \qquad \text{with } y_1(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{B.3}$$

$$\dot{y}_2(\beta) = By_2(\beta) \qquad \text{with } y_2(0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{B.4}$$

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where $y_1,\ y_2$ are functions of $\beta \in \mathbb{R}_0^+$ with two components and where $B := h_0^{(0)}\sigma_0 + \boldsymbol{a}^{(0)} \cdot \boldsymbol{\sigma}$ is a 2×2 matrix. Equations (B.3) and (B.4) represent the equations for the columns $g_{.1}^{(0)}(\beta)$ and $g_{.2}^{(0)}(\beta)$ respectively. We will not give all calculations but we go through the most important steps. The eigenvalues of B are

$$\lambda_{1,2} = h_0^{(0)} \pm \left|\boldsymbol{a}^{(0)}\right|.$$

The belonging eigenvectors have the following equations

$$\underbrace{\begin{pmatrix} a_3^{(0)} - \left|\boldsymbol{a}^{(0)}\right| & a_1^{(0)} - \mathrm{i}a_2^{(0)} \\ a_1^{(0)} + \mathrm{i}a_2^{(0)} & -a_3^{(0)} - \left|\boldsymbol{a}^{(0)}\right| \end{pmatrix}}_{=B-\lambda_1 Id} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = 0,$$
$$\underbrace{\begin{pmatrix} a_3^{(0)} + \left|\boldsymbol{a}^{(0)}\right| & a_1^{(0)} - \mathrm{i}a_2^{(0)} \\ a_1^{(0)} + \mathrm{i}a_2^{(0)} & -a_3^{(0)} + \left|\boldsymbol{a}^{(0)}\right| \end{pmatrix}}_{=B-\lambda_2 Id} \begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix} = 0. \tag{B.5}$$

For equation (B.3) we look at the second line, which provides the condition

$$v_2 = -\frac{a_1^{(0)} + \mathrm{i}a_2^{(0)}}{-a_3^{(0)} - |\boldsymbol{a}^{(0)}|} v_1, \qquad \gamma_2 = -\frac{a_1^{(0)} + \mathrm{i}a_2^{(0)}}{-a_3^{(0)} + |\boldsymbol{a}^{(0)}|} \gamma_1$$

Then we choose for equation (B.3) the following eigenvectors

$$\boldsymbol{v} = \begin{pmatrix} \frac{a_3^{(0)} + |\boldsymbol{a}^{(0)}|}{a_1^{(0)} + \mathrm{i}a_2^{(0)}} \\ 1 \end{pmatrix}, \qquad \boldsymbol{\gamma} = \begin{pmatrix} \frac{a_3^{(0)} - |\boldsymbol{a}^{(0)}|}{a_1^{(0)} + \mathrm{i}a_2^{(0)}} \\ 1 \end{pmatrix},$$

and obtain the general solution

$$y_1(\beta) = C_{11} \exp\left(\beta\left(h_0^{(0)} + \left|\boldsymbol{a}^{(0)}\right|\right)\right) \boldsymbol{v} + C_{21} \exp\left(\beta\left(h_0^{(0)} - \left|\boldsymbol{a}^{(0)}\right|\right)\right) \boldsymbol{\gamma}.$$

With the starting condition of (B.3) we obtain as solution for the ODE (B.3)

$$g_{.1}^{(0)}(\beta) = y_1(\beta) = \frac{e^{\beta\left(h_0^{(0)}\right)}}{2|\boldsymbol{a}^{(0)}|} \begin{pmatrix} e^{\beta|\boldsymbol{a}^{(0)}|}\left(a_3^{(0)} + \left|\boldsymbol{a}^{(0)}\right|\right) - e^{-\beta|\boldsymbol{a}^{(0)}|}\left(a_3^{(0)} - \left|\boldsymbol{a}^{(0)}\right|\right) \\ \left(e^{\beta|\boldsymbol{a}^{(0)}|} - e^{-\beta|\boldsymbol{a}^{(0)}|}\right)\left(a_1^{(0)} + \mathrm{i}a_2^{(0)}\right) \end{pmatrix}.$$

For the second differential equation (B.4) we choose different eigenvectors $\tilde{\boldsymbol{v}}, \tilde{\boldsymbol{\gamma}}$ of the solution space, to simplify the calculations. Looking in (B.5) at the first line, we obtain the relations

$$\tilde{v}_2 = \frac{-a_3^{(0)} + \left|\boldsymbol{a}^{(0)}\right|}{a_1^{(0)} - \mathrm{i}a_2^{(0)}} \tilde{v}_1, \qquad \tilde{\gamma}_2 = \frac{-a_3^{(0)} - \left|\boldsymbol{a}^{(0)}\right|}{a_1^{(0)} - \mathrm{i}a_2^{(0)}} \tilde{\gamma}_1$$

The new chosen eigenvectors are

$$\tilde{\boldsymbol{v}} = \begin{pmatrix} 1 \\ \frac{-a_3^{(0)} + |\boldsymbol{a}^{(0)}|}{a_1^{(0)} - \mathrm{i}a_2^{(0)}} \end{pmatrix}, \qquad \tilde{\boldsymbol{\gamma}} = \begin{pmatrix} 1 \\ \frac{-a_3^{(0)} - |\boldsymbol{a}^{(0)}|}{a_1^{(0)} - \mathrm{i}a_2^{(0)}} \end{pmatrix},$$

leading us to the general solution of (B.4):

$$y_2(\beta) = C_{12} \exp\left(\beta\left(h_0^{(0)} + \left|\boldsymbol{a}^{(0)}\right|\right)\right) \tilde{\boldsymbol{v}} + C_{22} \exp\left(\beta\left(h_0^{(0)} - \left|\boldsymbol{a}^{(0)}\right|\right)\right) \tilde{\boldsymbol{\gamma}}.$$

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The starting condition of (B.4) provides us the solution of (B.4)

$$g^{(0)}_{.2}(\beta) = y_2(\beta) = \frac{e^{\beta\left(h_0^{(0)}\right)}}{2|\boldsymbol{a}^{(0)}|}\begin{pmatrix} \left(e^{\beta|\boldsymbol{a}^{(0)}|} - e^{-\beta|\boldsymbol{a}^{(0)}|}\right)\left(a_1^{(0)} - \mathrm{i}a_2^{(0)}\right) \\ e^{\beta|\boldsymbol{a}^{(0)}|}\left(\left|\boldsymbol{a}^{(0)}\right| - a_3^{(0)}\right) + e^{-\beta|\boldsymbol{a}^{(0)}|}\left(a_3^{(0)} + \left|\boldsymbol{a}^{(0)}\right|\right)\end{pmatrix}.$$

Recalling the identities $\cosh(x) = \frac{1}{2}(\exp(x)+\exp(-x))$, $\sinh(x) = \frac{1}{2}(\exp(x)-\exp(-x))$, and introducing the short notation $e^{\pm} := e^{\pm\beta|\boldsymbol{a}^{(0)}|}$, leads us to the zero order of $g(\beta)$:

$$\begin{aligned} g^{(0)}(\beta) =& \frac{e^{\beta\left(h_0^{(0)}\right)}}{2|\boldsymbol{a}^{(0)}|}\begin{pmatrix} \left|\boldsymbol{a}^{(0)}\right|(e^+ + e^-) + a_3^{(0)}(e^+ - e^-) & (e^+ - e^-)(a_1^{(0)} - \mathrm{i}a_2^{(0)}) \\ (e^+ - e^-)(a_1^{(0)} + \mathrm{i}a_2^{(0)}) & \left|\boldsymbol{a}^{(0)}\right|(e^+ + e^-) - a_3^{(0)}(e^+ - e^-)\end{pmatrix} \\ =& e^{\beta\left(h_0^{(0)}\right)}\left(\cosh\left(\beta\left|\boldsymbol{a}^{(0)}\right|\right)\sigma_0 + \sinh\left(\beta\left|\boldsymbol{a}^{(0)}\right|\right)\frac{\boldsymbol{a}^{(0)}}{|\boldsymbol{a}^{(0)}|}\cdot\boldsymbol{\sigma}\right) \end{aligned} \tag{B.6}$$

Since $\mathcal{M}(N) = g(1)$, we obtain the zero order of $\mathcal{M}(N)$

$$\mathcal{M}^{(0)}(N) = e^{\left(h_0^{(0)}\right)}\left(\cosh\left(\left|\boldsymbol{a}^{(0)}\right|\right)\sigma_0 + \sinh\left(\left|\boldsymbol{a}^{(0)}\right|\right)\frac{\boldsymbol{a}^{(0)}}{|\boldsymbol{a}^{(0)}|}\cdot\boldsymbol{\sigma}\right),$$

Remark B.1.1. If we take a closer look on $g^{(0)}(\beta)$, we see that if we let $\boldsymbol{a}^{(0)}$ go to zero we have that, since $\sinh(x)/x$ converges to one for x going to zero,

$$\lim_{\boldsymbol{a}^{(0)}\to 0} g^{(0)}(\beta) = e^{\beta\left(h_0^{(0)}\right)}\sigma_0.$$

Also if we let $a_1^{(0)}, a_2^{(0)} \to 0$ in (B.6) we see that $g^{(0)}(\beta)$ converges to the same solution as in (B.2). ■

B.2. Needed derivatives of $g^{(0)}$

For the sake of completeness we give here the derivatives we need for the calculations, starting with h_0:

$$\partial_{x_k} h_0 = \partial_{x_k}\left(-\frac{|p|}{2}^2 + a_0\right) = \partial_{x_k} a_0, \qquad \partial_{p_k} h_0 = \partial_{p_k}\left(-\frac{|p|}{2}^2 + a_0\right) = -p_k,$$

$$\partial_{x_j}\partial_{x_k} h_0 = \partial_{x_j}\partial_{x_k}\left(-\frac{|p|}{2}^2 + a_0\right) = \partial_{x_j}\partial_{x_k} a_0, \qquad \partial_{x_j}\partial_{p_k} h_0 = \partial_{x_j}\partial_{p_k}\left(-\frac{|p|}{2}^2 + a_0\right) = 0,$$

$$\partial_{p_j}\partial_{p_k} h_0 = \partial_{p_j}\partial_{p_k}\left(-\frac{|p|}{2}^2 + a_0\right) = -\delta_{jk} \qquad \partial_{p_j}\partial_{x_k} h_0 = \partial_{p_j}\partial_{x_k}\left(-\frac{|p|}{2}^2 + a_0\right) = 0.$$

Recall that $g^{(0)} = \exp(\beta h_0)\sigma_0$, we have that $g_0^{(0)} = \exp(\beta h_0)$, then we get for the x-derivatives of $g_0^{(0)}$:

$$\begin{aligned} \partial_{x_k} g_0^{(0)}(\beta) &= \beta(\partial_{x_k} a_0)\exp(\beta h_0) \\ \partial_{x_j}\partial_{x_k} g_0^{(0)}(\beta) &= \partial_{x_j}(\beta(\partial_{x_k} a_0)\exp(\beta h_0)) \\ &= \beta(\partial_{x_j}\partial_{x_k} a_0)\exp(\beta h_0) + \beta^2(\partial_{x_j} a_0)(\partial_{x_k} a_0)\exp(\beta h_0) \\ &= \beta\exp(\beta h_0)(\partial_{x_j}\partial_{x_k} a_0 + \beta(\partial_{x_j} a_0)(\partial_{x_k} a_0)). \end{aligned}$$

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The derivatives for $g_0^{(0)}(\beta)$ with respect to the momentum p are given by:

$$\begin{aligned}
\partial_{p_k} g_0^{(0)}(\beta) =& (-p_k)\beta \exp(\beta h_0) \\
\partial_{p_j}\partial_{p_k} g_0^{(0)}(\beta) =& -\delta_{jk}\beta \exp(\beta h_0) + p_j p_k \beta^2 \exp(\beta h_0) \\
=& \beta \exp(\beta h_0)(\beta p_j p_k - \delta_{jk}) \\
\partial_{p_i}\partial_{p_j}\partial_{p_k} g^{(0)}(\beta) =& (-p_i)\beta^2 \exp(\beta h_0)(\beta p_j p_k - \delta_{jk}) + \beta \exp(\beta h_0)(\beta \delta_{ij} p_k + \beta p_j \delta_{ik}) \\
=& \beta^2 \exp(\beta h_0)(p_i \delta_{jk} + p_k \delta_{ij} + p_j \delta_{ik} - \beta p_i p_j p_k)
\end{aligned}$$

B.3. Calculations and Solving the ODEs for the Orders of $g(\beta)$

This part of the appendix is devoted to solve the ODEs appearing in the proof of Theorem 3.6.2. First we state a well known formula, without the proof.

Theorem B.3.1 (Duhamels formula)**.** *Let u, ζ, ξ be three functions from $\mathbb{R}$ to $\mathbb{R}$ sufficiently smooth. Then we have for the following differential equation*

$$u' = \zeta u + \xi,$$

the following solution

$$u = C \exp\left(\int_0^\beta \zeta(s) ds\right) + \int_0^\beta \exp\left(\int_s^\beta \zeta(\tau) d\tau\right) \xi(s) ds.$$

Recall the definitions:

$$h_0 = \left(-\frac{|p|^2}{2} + a_0\right), \qquad a_0 = \tilde{a}_0 - V, \qquad \boldsymbol{h}_1 = (\boldsymbol{a} - \alpha p^\perp), \qquad H_0 = h_0 \sigma_0, \qquad H_1 = \boldsymbol{h}_1 \cdot \boldsymbol{\sigma}.$$

B.3.1. The ODE for the first order

We want to solve

$$\partial_\beta g^{(1)}(\beta) = H_0 g^{(1)}(\beta) + g^{(0)} \boldsymbol{h}_1 \cdot \boldsymbol{\sigma}, \qquad g^{(1)}(0) = 0,$$

With Duhamel's formula we obtain

$$\begin{aligned}
g^{(1)}(\beta) =& C \exp(\beta h_0) + \int_0^\beta \exp((\beta - s) h_0) \exp(s h_0) \boldsymbol{h}_1 ds \\
=& C \exp(\beta h_0) + \int_0^\beta \exp(\beta h_0) \boldsymbol{h}_1 ds.
\end{aligned}$$

Since our initial condition demands that $g^{(1)}(0) = 0$ we have that C has to be zero and therefore:

$$g^{(1)}(\beta) = \beta \exp\left(\beta\left(-\frac{|p|^2}{2} + a_0\right)\right)\left(\boldsymbol{a} - \alpha p^\perp\right) \cdot \boldsymbol{\sigma}.$$

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B.3.2. The ODE for the Second Order

Next ODE is to solve is

$$\partial_\beta g^{(2)}(\beta) = H_0 g^{(2)}(\beta) + \beta g^{(0)} \left[\left(\frac{1}{4}\Delta a_0 - \frac{\beta}{8}\Big(p^T(\nabla \otimes \nabla a_0)p - |\nabla a_0|^2\Big)\right) + |\boldsymbol{h}_1|^2 \right] \sigma_0,$$
$$g^{(2)}(0) = 0$$

which means that we have four equations to solve. The ODEs corresponding to the off diagonal, have the simple solutions

$$(g^{(2)}(\beta))_{12} = C \exp(\beta h_0) = (g^{(2)}(\beta))_{21}.$$

The initial value $g^{(2)}(0) = 0$ implies that the constant C has to be zero and hence

$$(g^{(2)}(\beta))_{12} = 0 = (g^{(2)}(\beta))_{21}.$$

For the diagonal terms of $g^{(2)}(\beta)$ we apply Duhamel's formula (see Theorem B.3.1). Both equations are equal, hence have the same solution:

$$\begin{aligned}(g^{(2)}(\beta))_{jj} =& C\exp(\beta h_0) + \int_0^\beta \exp((\beta - s)h_0)\, s \exp(sh_0) \cdot \\ & \cdot \left(\frac{1}{4}\Delta a_0 + \frac{s}{8}\Big(|\nabla a_0|^2 - p^T(\nabla \otimes \nabla a_0)p\Big) + |\boldsymbol{h}_1|^2\right) ds \\ =& C\exp(\beta h_0) + \exp(\beta h_0)\int_0^\beta s\left(\frac{1}{4}\Delta a_0 + \frac{s}{8}\Big(|\nabla a_0|^2 - p^T(\nabla \otimes \nabla a_0)p\Big) + |\boldsymbol{h}_1|^2\right) ds \\ =& \exp(\beta h_0)\left(C + \frac{\beta^2}{2}\left(\frac{1}{4}\Delta a_0 + \frac{\beta}{12}\Big(|\nabla a_0|^2 - p^T(\nabla \otimes \nabla a_0)p\Big) + |\boldsymbol{h}_1|^2\right)\right)\end{aligned}$$

The initial condition is $(g^{(2)}(0))_{jj} = 0$ provides again that C has to be zero. Therefore we obtain for the second order term the following expression:

$$g^{(2)}(\beta) = \frac{\beta^2}{8}\exp\left(\beta\left(-\frac{|p|^2}{2} + a_0\right)\right)\left(\Delta a_0 + \frac{\beta}{3}\Big(|\nabla a_0|^2 - p^T(\nabla \otimes \nabla a_0)p\Big) + 4\Big|\boldsymbol{a} - \alpha p^\perp\Big|^2\right)\sigma_0.$$

B.3.3. Calculations for the Third Order

Here we add some calculations, that are basic, to give slightly more insight what happens in between. We mark with small boxes to which term we add calculations. In addition we mention that a vector valued function $\boldsymbol{f}$, with dependence on the space variable x, multiplied with $\nabla_p p^\perp$ is the same as crossing $\boldsymbol{f}$ with the third canonical basis vector of $\mathbb{R}^2$, meaning $(\nabla_p p^\perp)\boldsymbol{f} = \boldsymbol{f}^\perp$ and $\boldsymbol{f}^T(\nabla_p p^\perp) = (\nabla_p p^\perp)^T \boldsymbol{f} = -\boldsymbol{f}^\perp$

$\boxed{h_0 \#_{(2)} g^{(1)}(\beta):}$

First we give here the calculations for $h_0 \#_{(1)} \lambda_2$, where we defined λ_2 in the Proof of Theorem 3.6.2

$$\lambda_2 := \Delta a_0 + \frac{\beta}{3}\Big(|\nabla a_0|^2 - p^T(\nabla \otimes \nabla a_0)p\Big) + 4|\boldsymbol{h}_1|^2.$$

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Starting with the x derivative we have

$$\begin{aligned}
\partial_{x_i}|\nabla_x a_0|^2 &= \partial_{x_i}\sum_{j=1}^{3}(\partial_{x_j}a_0)^2 = \sum_{j=1}^{3}2\partial_{x_j}a_0(\partial_{x_i}\partial_{x_j}a_0) = 2(\nabla_x a_0(\nabla_x\otimes\nabla_x a_0))_i,\\
\nabla_x|\nabla_x a_0|^2 &= 2(\nabla_x a_0(\nabla_x\otimes\nabla_x a_0)),\\
\partial_{x_i}\left|\boldsymbol{a}-\alpha p^\perp\right|^2 &= \partial_{x_i}((a_1-\alpha p_2)^2+(a_2+\alpha p_1)^2+a_3^2)\\
&= \partial_{x_i}(a_1^2+a_2^2+a_3^2-2\alpha(p_2a_1-p_1a_2)+\alpha^2(p_1^2+p_2^2))\\
&= 2(a_1\partial_{x_i}a_1+a_2\partial_{x_i}a_2+a_3\partial_{x_i}a_3-2\alpha(p_2\partial_{x_i}a_1-p_1\partial_{x_i}a_2))\\
&= 2\boldsymbol{a}\cdot\partial_{x_i}\boldsymbol{a}-2\alpha p^\perp\cdot\partial_{x_i}\boldsymbol{a}\\
&= 2(\boldsymbol{a}-\alpha p^\perp)\cdot\partial_{x_i}\boldsymbol{a}\\
\nabla_x|\boldsymbol{h}_1|^2 &= 2(\boldsymbol{a}-\alpha p^\perp)^T\nabla_x\boldsymbol{a} = 2(\nabla_x\boldsymbol{a})^T(\boldsymbol{a}-\alpha p^\perp).
\end{aligned}$$

Therefore we have for λ_2 the following gradient with respect to x

$$\nabla_x\lambda_2 = \nabla_x(\Delta_x a_0)+\frac{\beta}{3}(2(\nabla_x a_0)(\nabla_x\otimes\nabla_x a_0)-\nabla_x(p^T(\nabla_x\otimes\nabla_x a_0)p)+8(\nabla_x\boldsymbol{a})^T\boldsymbol{h}_1.$$

For the derivatives with respect to p we prepare:

$$\begin{aligned}
\partial_{p_i}(p^T(\nabla_x\otimes\nabla_x a_0)p) &= \partial_{p_i}\sum_{j=1}^{2}\sum_{k=1}^{2}\partial_{x_j}\partial_{x_k}a_0p_jp_k = \sum_{j,k=1}^{2}\partial_{x_k}\partial_{x_j}a_0\delta_{ij}p_k+\partial_{x_j}\partial_{x_k}a_0\delta_{ik}p_j\\
&= \sum_{k=1}^{2}\partial_{x_j}\partial_{x_i}a_0p_k+\sum_{j=1}^{2}\partial_{x_i}\partial_{x_j}a_0p_j = 2\sum_{j=1}^{2}\partial_{x_j}\partial_{x_i}a_0p_i,\\
&= 2\partial_{x_i}(\nabla_x a_0\cdot p),\\
\nabla_p(p^T(\nabla_x\otimes\nabla_x a_0)p) &= 2((\nabla_x\otimes\nabla_x)a_0)p,\\
\partial_{p_i}\left(\left|\boldsymbol{a}-\alpha p^\perp\right|^2\right) &= \partial_{p_i}(a_1^2+a_2^2+a_3^2-2\alpha(p_2a_1-p_1a_2)+\alpha^2(p_1^2+p_2^2))\\
&= -2\alpha(\delta_{i2}a_1-\delta_{i1}a_2)+\alpha^2 2p_i,\\
\nabla_p\left(|\boldsymbol{h}_1|^2\right) &= 2\alpha(\alpha p+\boldsymbol{a}^\perp) = 2\alpha(\alpha(\boldsymbol{e}_3\times p)\times\boldsymbol{e}_3+\boldsymbol{a}\times\boldsymbol{e}_3)\\
&= 2\alpha(\alpha(\boldsymbol{e}_3\times p)+\boldsymbol{a})\times\boldsymbol{e}_3 = 2\alpha(-\alpha(p\times\boldsymbol{e}_3)+\boldsymbol{a})\times\boldsymbol{e}_3\\
&= 2\alpha(\boldsymbol{a}-\alpha p^\perp)\times\boldsymbol{e}_3 = 2\alpha(\nabla_p p^\perp)(\boldsymbol{a}-\alpha p^\perp).
\end{aligned}$$

and therefore we obtain

$$\nabla_p\lambda_2 = -\frac{2\beta}{3}((\nabla_x\otimes\nabla_x)a_0)p+8\alpha(\nabla_p p^\perp)\boldsymbol{h}_1.$$

Since the matrix $(\nabla_x\otimes\nabla_x)a_0$ is symmetric we have that

$$p\cdot((\nabla_x a_0)(\nabla_x\otimes\nabla_x a_0)) = (\nabla_x a_0)(\nabla_x\otimes\nabla_x a_0)p,$$

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which leads us to

$$\begin{aligned}
&\nabla_p h_0 \cdot \nabla_x \lambda_2 - \nabla_x h_0 \cdot \nabla_p \lambda_2 = \\
&\quad = - p \cdot \left(\nabla_x(\Delta_x a_0) + \frac{\beta}{3}(2(\nabla_x a_0)(\nabla_x \otimes \nabla_x a_0) - \nabla_x(p^T(\nabla_x \otimes \nabla_x a_0)p)) + 8(\nabla_x \boldsymbol{a})^T \boldsymbol{h}_1 \right) \\
&\qquad - (\nabla_x a_0) \cdot \left(-\frac{2\beta}{3}((\nabla_x \otimes \nabla_x) a_0) p + 8\alpha(\nabla_p p^\perp) \boldsymbol{h}_1 \right) \\
&\quad = \frac{\beta}{3} p \cdot \nabla_x(p^T(\nabla_x \otimes \nabla_x a_0)p) - p \cdot \nabla_x(\Delta_x a_0) - 8p \cdot (\nabla_x \boldsymbol{a})^T \boldsymbol{h}_1 - 8\alpha \nabla_x a_0 \cdot (\nabla_p p^\perp) \boldsymbol{h}_1 \\
&\quad = \frac{\beta}{3} p \cdot \nabla_x(p^T(\nabla_x \otimes \nabla_x a_0)p) - p \cdot \nabla_x(\Delta_x a_0) - 8(\nabla_x \boldsymbol{a}) p \cdot \boldsymbol{h}_1 + 8\alpha(\nabla_x a_0 \times \boldsymbol{e}_3) \cdot \boldsymbol{h}_1 \\
&\quad = \frac{\beta}{3} p \cdot \nabla_x(p^T(\nabla_x \otimes \nabla_x a_0)p) - p \cdot \nabla_x(\Delta_x a_0) + 8(\alpha(\nabla_x^\perp a_0) - (\nabla_x \boldsymbol{a})p) \cdot \boldsymbol{h}_1 .
\end{aligned}$$

The final result is then

$$\begin{aligned}
&h_0 \#_{(1)} g^{(2)} = \frac{1}{2\mathrm{i}} \frac{\beta^2}{8} g^{(0)} \left(\nabla_p h_0 \cdot \nabla_x \lambda_2 - \nabla_x h_0 \cdot \nabla_p \lambda_2 \right) \sigma_0 = \\
&= \frac{\beta^2}{16\mathrm{i}} \exp(\beta h_0) \left[\frac{\beta}{3} p \cdot \nabla_x(p^T(\nabla_x \otimes \nabla_x a_0)p) - p \cdot \nabla_x(\Delta_x a_0) - 8(\alpha(\nabla_x^\perp a_0) + (\nabla_x \boldsymbol{a})p) \cdot \boldsymbol{h}_1 \right] \sigma_0 .
\end{aligned}$$

$p^T(\nabla_x \otimes \nabla_x a_0)\nabla_p p^\perp = -\nabla_x^\perp(\nabla_x a_0 \cdot p)$:

With the behaviour of $\nabla_p p^\perp$ mentioned in the beginning we get

$$p^T(\nabla_x \otimes \nabla_x a_0)\nabla_p p^\perp = - \left((\nabla_x \otimes \nabla_x a_0)p\right) \times \boldsymbol{e}_3 = -\nabla_x^\perp(\nabla_x a_0 \cdot p).$$

$2\mathrm{i}\boldsymbol{h}_1 \times_{\#_1} \boldsymbol{g}^{(1)} = \nabla_p \boldsymbol{h}_1 \times \nabla_x \boldsymbol{g}^{(1)} - \nabla_x \boldsymbol{h}_1 \times \nabla_p \boldsymbol{g}^{(1)}$:

$$\begin{aligned}
&\left(\boldsymbol{h}_1 \times_{\#_{(1)}} \boldsymbol{g}^{(1)} \right) = \\
&= \frac{1}{2\mathrm{i}} \begin{pmatrix} \nabla_p(h_1)_2 \cdot \nabla_x g_3^{(1)} - \nabla_x(h_1)_2 \cdot \nabla_p g_3^{(1)} - \nabla_p(h_1)_3 \cdot \nabla_x g_2^{(1)} + \nabla_x(h_1)_3 \cdot \nabla_p g_2^{(1)} \\ -[\nabla_p(h_1)_1 \cdot \nabla_x g_3^{(1)} - \nabla_x(h_1)_1 \cdot \nabla_p g_3^{(1)} - \nabla_p(h_1)_3 \cdot \nabla_x g_1^{(1)} + \nabla_x(h_1)_3 \cdot \nabla_p g_1^{(1)}] \\ \nabla_p(h_1)_1 \cdot \nabla_x g_2^{(1)} - \nabla_x(h_1)_1 \cdot \nabla_p g_2^{(1)} - \nabla_p(h_1)_2 \cdot \nabla_x g_1^{(1)} + \nabla_x(h_1)_2 \cdot \nabla_p g_1^{(1)} \end{pmatrix} \\
&= \frac{1}{2\mathrm{i}} \begin{pmatrix} \nabla_p(h_1)_2 \cdot \nabla_x g_3^{(1)} - \nabla_p(h_1)_3 \cdot \nabla_x g_2^{(1)} + \nabla_x(h_1)_3 \cdot \nabla_p g_2^{(1)} - \nabla_x(h_1)_2 \cdot \nabla_p g_3^{(1)} \\ -[\nabla_p(h_1)_1 \cdot \nabla_x g_3^{(1)} - \nabla_p(h_1)_3 \cdot \nabla_x g_1^{(1)} + \nabla_x(h_1)_3 \cdot \nabla_p g_1^{(1)} - \nabla_x(h_1)_1 \cdot \nabla_p g_3^{(1)}] \\ \nabla_p(h_1)_1 \cdot \nabla_x g_2^{(1)} - \nabla_p(h_1)_2 \cdot \nabla_x g_1^{(1)} + \nabla_x(h_1)_2 \cdot \nabla_p g_1^{(1)} - \nabla_x(h_1)_1 \cdot \nabla_p g_2^{(1)} \end{pmatrix} \\
&= \frac{1}{2\mathrm{i}} \left(\nabla_p \boldsymbol{h}_1 \times . \nabla_x \boldsymbol{g}^{(1)} - \nabla_x \boldsymbol{h}_1 \times . \nabla_p \boldsymbol{g}^{(1)} \right).
\end{aligned}$$

The notation $\times .$ just specifies that the cross product multiplication is actually the euclidean scalar product, which was dropped in the proof of Theorem 3.6.2.

Substituting the terms to obtain the ODE:

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$$\begin{aligned}
\partial_\beta g^{(3)} =& H_0 g^{(3)} + H_0 \#_{(1)} g^{(2)} + H_0 \#_{(2)} g^{(1)} + H_0 \#_{(3)} g^{(0)} + H_1 g^{(2)} + H_1 \#_{(1)} g^{(1)} + H_1 \#_{(2)} g^{(0)} \\
=& H_0 g^{(3)} + \\
&+ \frac{\beta^2}{16\mathrm{i}} g^{(0)} \left[\frac{\beta}{3} p \cdot \nabla_x (p^T (\nabla_x \otimes \nabla_x a_0) p) - p \cdot \nabla_x (\Delta_x a_0) + 8(\alpha(\nabla_x^\perp a_0) - (\nabla_x \boldsymbol{a}) p) \cdot \boldsymbol{h}_1 \right] \sigma_0 \\
&+ \frac{\beta^2}{8} g^{(0)} \left[\left(2\Delta_x a_0 + \beta \left(|\nabla_x a_0|^2 - p^T (\nabla_x \otimes \nabla_x a_0) p \right) \right) \boldsymbol{h}_1 \right] \cdot \boldsymbol{\sigma} \\
&+ \frac{\beta}{8} g^{(0)} \left[2\beta(\alpha \nabla_x^\perp (\nabla_x a_0 \cdot p) + \nabla_x \boldsymbol{a} \cdot \nabla_x a_0) + \Delta_x \boldsymbol{a} \right] \cdot \boldsymbol{\sigma} \\
&+ \frac{\beta^2}{16\mathrm{i}} g^{(0)} \left[p \cdot \nabla_x (\Delta_x a_0) - \frac{\beta}{3} p \cdot \nabla_x \left(p^T (\nabla_x \otimes \nabla_x a_0) p \right) \right] \sigma_0 \\
&+ \frac{\beta}{8}^2 g^{(0)} \left[\Delta_x a_0 + \frac{\beta}{3} \left(|\nabla_x a_0|^2 - p (\nabla_x \otimes \nabla_x a_0) p \right) + 4 |\boldsymbol{h}_1|^2 \right] \boldsymbol{h}_1 \cdot \boldsymbol{\sigma} \\
&+ \frac{\beta}{2\mathrm{i}} \left[\left(\beta ((\nabla_x \boldsymbol{a}) p - \alpha (\nabla_x a_0)^\perp) \cdot \boldsymbol{h}_1 \right) \right] \sigma_0 \\
&+ \frac{\beta}{2} g^{(0)} \left[\beta \left((\nabla_x \boldsymbol{a}) p - \alpha (\nabla_x a_0)^\perp \right) \times \boldsymbol{h}_1 - 2\alpha (\nabla_x^\perp \times \boldsymbol{a}) \right] \cdot \boldsymbol{\sigma} \\
&- \frac{1}{8} \beta g^{(0)} \left[\beta p^T (\nabla_x \otimes \nabla_x \boldsymbol{a}) p - \Delta_x \boldsymbol{a} \right] \cdot \boldsymbol{\sigma} = \\
=& H_0 g^{(3)} + \frac{\beta}{8} g^{(0)} \left[\beta \left(3\Delta_x a_0 + \frac{4}{3} \beta \left(|\nabla_x a_0|^2 - p^T (\nabla_x \otimes \nabla_x a_0) p \right) + 4 |\boldsymbol{h}_1|^2 \right) \boldsymbol{h}_1 + \right. \\
&+ 2\Delta_x \boldsymbol{a} - 8\alpha (\nabla_x^\perp \times \boldsymbol{a}) + \beta \left(2\nabla_x \boldsymbol{a} \cdot \nabla_x a_0 - p^T (\nabla_x \otimes \nabla_x \boldsymbol{a}) p + 2\alpha \nabla_x^\perp (\nabla_x a_0 \cdot p) \right) + \\
&\left. + 4\beta \left((\nabla_x \boldsymbol{a}) p - \alpha (\nabla_x a_0)^\perp \right) \times \boldsymbol{h}_1 \right] \cdot \boldsymbol{\sigma}
\end{aligned}$$

Solving the ODE:

Recalling the initial condition is $g^{(3)}(0) = 0$, we want to solve the above differential equation. An immediate consequence is, after comparing the Pauli components, that the zero component has to be zero, i.e.

$$g_0^{(3)} = 0.$$

For the $\boldsymbol{\sigma}$ components we can apply Duhamel's formular (Theorem B.3.1) simultaneously and therefore

$$\begin{aligned}
\boldsymbol{g}^{(3)}(\beta) =& C \exp(\beta h_0) + \int_0^\beta \exp((\beta - s) h_0) \exp(s h_0) \cdot \\
&\cdot \frac{s}{8} \left[s \left(3\Delta_x a_0 + \frac{4s}{3} (|\nabla_x a_0|^2 - p^T (\nabla \otimes \nabla a_0) p) + 4 |\boldsymbol{h}_1|^2 \right) \boldsymbol{h}_1 + \right. \\
&\quad + 2\Delta_x \boldsymbol{a} - 8\alpha (\nabla_x^\perp \times \boldsymbol{a}) + s \left(2\nabla_x \boldsymbol{a} \nabla_x a_0 - p^T (\nabla_x \otimes \nabla_x \boldsymbol{a}) p + 2\alpha \nabla_x^\perp (\nabla_x a_0 \cdot p) \right) + \\
&\quad \left. + 4s \left((\nabla_x \boldsymbol{a}) p - \alpha (\nabla_x a_0)^\perp \right) \times \boldsymbol{h}_1 \right] ds.
\end{aligned}$$

With the starting condition $g^{(3)}(0) = 0$ we have that the constant C equals zero and therefore

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we obtain as result, after simple integration,

$$\begin{aligned}g^{(3)}(\beta) =&\frac{\beta^2}{24}\exp\left(\beta h_0\right)\Big[\Big(3\beta\Delta a_0 + \beta^2(|\nabla a_0|^2 - p^T(\nabla\otimes\nabla a_0)p) + 4\beta|\boldsymbol{h}_1|^2\Big)\boldsymbol{h}_1\\ &+ 3\Delta\boldsymbol{a} - 12\alpha(\nabla^\perp\times\boldsymbol{a}) + \beta\Big(2\nabla\boldsymbol{a}\cdot\nabla a_0 - p^T(\nabla\otimes\nabla\boldsymbol{a})p + 2\alpha(\nabla^\perp)(\nabla a_0\cdot p)\Big)\\ &+ 4\beta\Big((\nabla\boldsymbol{a})p - \alpha(\nabla a_0)^\perp\Big)\times\boldsymbol{h}_1\Big]\cdot\boldsymbol{\sigma}.\end{aligned}$$

B.4. Calculations for the Semiclassical Expansion of the Lagrange Multipliers

B.4.1. The Total Derivatives of $\mathcal{M}$ with respect to ε

To obtain the equaions (3.121)-(3.124) we need to calculate the total derivatives of the quantum Maxwellian. It is just applying the chainrule and to save time for the reader, we do it here.

$$\begin{aligned}\frac{d\mathcal{M}}{d\varepsilon} =&\frac{\partial\mathcal{M}}{\partial\varepsilon} + \sum_{j=0}^{3}\frac{\partial\mathcal{M}}{\partial a_j}\frac{\partial a_j}{\partial\varepsilon},\\ \frac{d^2\mathcal{M}}{d\varepsilon^2} =&\frac{d}{d\varepsilon}\left(\frac{\partial\mathcal{M}}{\partial\varepsilon} + \sum_{j=0}^{3}\frac{\partial\mathcal{M}}{\partial a_j}\frac{\partial a_j}{\partial\varepsilon}\right)\\ =&\frac{\partial^2\mathcal{M}}{\partial\varepsilon^2} + 2\sum_{j=0}^{3}\frac{\partial^2\mathcal{M}}{\partial\varepsilon\partial a_j}\frac{\partial a_j}{\partial\varepsilon} + \sum_{j=0}^{3}\sum_{k=0}^{3}\frac{\partial^2\mathcal{M}}{\partial a_j\partial a_k}\frac{\partial a_j}{\partial\varepsilon}\frac{\partial a_k}{\partial\varepsilon} + \frac{\partial\mathcal{M}}{\partial a_j}\frac{\partial^2 a_j}{\partial\varepsilon^2},\\ \frac{d^3\mathcal{M}}{d\varepsilon^3} =&\frac{d}{d\varepsilon}\left(\frac{\partial^2\mathcal{M}}{\partial\varepsilon^2} + 2\sum_{j=0}^{3}\frac{\partial^2\mathcal{M}}{\partial\varepsilon\partial a_j}\frac{\partial a_j}{\partial\varepsilon} + \sum_{j=0}^{3}\sum_{k=0}^{3}\frac{\partial^2\mathcal{M}}{\partial a_j\partial a_k}\frac{\partial a_j}{\partial\varepsilon}\frac{\partial a_k}{\partial\varepsilon} + \frac{\partial\mathcal{M}}{\partial a_j}\frac{\partial^2 a_j}{\partial\varepsilon^2}\right)\\ =&\frac{\partial^3\mathcal{M}}{\partial\varepsilon^3} + \sum_{j=0}^{3}\frac{\partial^3\mathcal{M}}{\partial\varepsilon^2\partial a_j}\frac{\partial a_j}{\partial\varepsilon} + 2\sum_{j=0}^{3}\frac{\partial^3\mathcal{M}}{\partial\varepsilon^2\partial a_j}\frac{\partial a_j}{\partial\varepsilon} + 2\sum_{j=0}^{3}\sum_{k=0}^{3}\frac{\partial^2\mathcal{M}}{\partial\varepsilon\partial a_j}\frac{\partial^2 a_j}{\partial\varepsilon^2} + \frac{\partial^3\mathcal{M}}{\partial\varepsilon\partial a_j\partial a_k}\frac{\partial a_j}{\partial\varepsilon}\frac{\partial a_k}{\partial\varepsilon}\\ &+ \sum_{k=0}^{3}\sum_{j=0}^{3}\frac{\partial^2\mathcal{M}}{\partial a_j\partial\varepsilon}\frac{\partial^2 a_j}{\partial\varepsilon^2} + \frac{\partial\mathcal{M}}{\partial a_j}\frac{\partial^3 a_j}{\partial\varepsilon^3} + \frac{\partial^2\mathcal{M}}{\partial a_j\partial a_k}\frac{\partial a_k}{\partial\varepsilon}\frac{\partial^2 a_j}{\partial\varepsilon^2}\\ &+ \sum_{j=0}^{3}\sum_{k=0}^{3}\frac{\partial^3\mathcal{M}}{\partial a_j\partial a_k\partial\varepsilon}\frac{\partial a_j}{\partial\varepsilon}\frac{\partial a_k}{\partial\varepsilon} + \frac{\partial^2\mathcal{M}}{\partial a_j\partial a_k}\left(\frac{\partial^2 a_j}{\partial\varepsilon^2}\frac{\partial a_k}{\partial\varepsilon} + \frac{\partial^2 a_k}{\partial\varepsilon^2}\frac{\partial a_j}{\partial\varepsilon}\right)\\ &+ \sum_{j=0}^{3}\sum_{k=0}^{3}\sum_{i=0}^{3}\frac{\partial^3\mathcal{M}}{\partial a_j\partial a_k\partial a_i}\frac{\partial a_j}{\partial\varepsilon}\frac{\partial a_k}{\partial\varepsilon}\frac{\partial a_i}{\partial\varepsilon}\\ =&\frac{\partial^3\mathcal{M}}{\partial\varepsilon^3} + 3\sum_{j=0}^{3}\frac{\partial^3\mathcal{M}}{\partial\varepsilon^2\partial a_j}\frac{\partial a_j}{\partial\varepsilon} + 3\sum_{j=0}^{3}\frac{\partial^2\mathcal{M}}{\partial\varepsilon\partial a_j}\frac{\partial^2 a_j}{\partial\varepsilon^2} + 3\sum_{j=0}^{3}\sum_{k=0}^{3}\frac{\partial^3\mathcal{M}}{\partial\varepsilon\partial a_j\partial a_k}\frac{\partial a_j}{\partial\varepsilon}\frac{\partial a_k}{\partial\varepsilon}\\ &+ \sum_{j=0}^{3}\frac{\partial\mathcal{M}}{\partial a_j}\frac{\partial^3 a_j}{\partial\varepsilon^3} + \sum_{j=0}^{3}\sum_{k=0}^{3}\frac{\partial^2\mathcal{M}}{\partial a_j\partial a_k}\left(2\frac{\partial^2 a_j}{\partial\varepsilon^2}\frac{\partial a_k}{\partial\varepsilon} + \frac{\partial^2 a_k}{\partial\varepsilon^2}\frac{\partial a_j}{\partial\varepsilon}\right)\\ &+ \sum_{j=0}^{3}\sum_{k=0}^{3}\sum_{i=0}^{3}\frac{\partial^3\mathcal{M}}{\partial a_j\partial a_k\partial a_i}\frac{\partial a_j}{\partial\varepsilon}\frac{\partial a_k}{\partial\varepsilon}\frac{\partial a_i}{\partial\varepsilon}.\end{aligned}$$

Now we need to evaluate these derivatives at $\varepsilon = 0$ and by replacing the partial derivatives of a_j with the respective order (see (3.120)) we obtain the desired equations.

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B.4.2. Calculations for $a_0^{(2)}$

In this section we want to calculate the second order of a_0 where we have derived in the proof of Theorem 3.6.5 that

$$a_0^{(2)} = -\frac{1}{n_0}\left\langle g_0^{(2)}(1)\Big|_{\varepsilon=0}\right\rangle. \tag{B.7}$$

We recall the already calculated orders

$$a_0^{(0)} = \log\left(\frac{n_0}{2\pi}\right),\ a_0^{(1)} = 0,\ \boldsymbol{a}^{(0)} = \frac{\boldsymbol{n}}{n_0},\ \boldsymbol{a}^{(1)} = \boldsymbol{0},\ h_0^{(0)} = -\frac{|p|^2}{2} + a_0^{(0)},\ \boldsymbol{h}_1^{(0)} = \boldsymbol{a}^{(0)} + \alpha p^\perp$$

Looking at the integral in (B.7) we get with Proposition 3.6.4 and that $\langle \exp(h_0^{(0)})\rangle = n_0$:

$$\begin{aligned}\left\langle g_0^{(2)}(1)\Big|_{\varepsilon=0}\right\rangle =&\left\langle \frac{1}{8}\exp\left(h_0^{(0)}\right)\left(\Delta a_0^{(0)} + \frac{1}{3}\left(\left|\nabla a_0^{(0)}\right|^2 - p^T\left(\nabla\otimes\nabla a_0^{(0)}\right)p\right) + 4\left|\boldsymbol{h}_1^{(0)}\right|^2\right)\right\rangle\\ =&\frac{1}{8}\left(n_0\left(\Delta a_0^{(0)} + \frac{1}{3}\left|\nabla a_0^{(0)}\right|^2\right) + \left\langle \exp\left(h_0^{(0)}\right)\left(4\left|\boldsymbol{h}_1^{(0)}\right|^2 - \frac{1}{3}p(\nabla\otimes\nabla a_0^{(0)})p\right)\right\rangle\right).\end{aligned}$$

We integrate the last two terms on the right hand side. Notice in the upcoming calculations that $\exp(h_0)$ is even in p and so multiplying it with p_j makes it odd. Therefore $\langle \exp(h_0)p_jp_k\rangle$ equals zero if $j\neq k$ and that $\langle \exp(h_0^{(0)})p_j^2\rangle = \exp(a_0^{(0)})2\pi = n_0$ for $j\in\{1,2\}$. We get

$$\begin{aligned}\left\langle \exp\left(h_0^{(0)}\right)p^T\left(\nabla\otimes\nabla a_0^{(0)}\right)p\right\rangle =& \sum_{j,k=1}^{2}\left\langle \exp\left(h_0^{(0)}\right)\partial_{x_j}\partial_{x_k}a_0^{(0)}\,p_jp_k\right\rangle = \sum_{j=1}^{2}\left\langle \exp\left(h_0^{(0)}\right)\partial_{x_j}^2 a_0^{(0)}p_j^2\right\rangle\\ =&\sum_{j=1}^{2}\exp\left(a_0^{(0)}\right)\partial_{x_j}^2 a_0^{(0)}\left\langle \exp\left(-|p|^2/2\right)p_j^2\right\rangle = \frac{1}{2\pi}n_0\sum_{j=1}^{3}\partial_{x_j}^2 a_0^{(0)}2\pi\\ =&n_0\Delta a_0^{(0)}.\end{aligned}$$

For the second integral, with similar argumentations we get

$$\begin{aligned}\left\langle \exp\left(h_0^{(0)}\right)\left|\boldsymbol{h}_1^{(0)}\right|^2\right\rangle =&\left\langle \exp\left(h_0^{(0)}\right)\left(\left|\boldsymbol{a}^{(0)}\right|^2 + \alpha^2\left|p^\perp\right|^2 - 2\alpha p_2 a_1^{(0)} + 2\alpha p_1 a_2^{(0)}\right)\right\rangle\\ =&\frac{1}{2\pi}n_0\left(2\pi\left|\boldsymbol{a}^{(0)}\right|^2 + 4\pi\alpha^2\right) = n_0\left(\left|\boldsymbol{a}^{(0)}\right|^2 + 2\alpha^2\right).\end{aligned}$$

Substituting our results and the various orders into (B.7), and using the fact that the derivative of the logarithm can also be rewritten as $\partial_{x_j}\log(n_0/2\pi) = \partial_{x_j}\log(n_0)$, provides

$$\begin{aligned}a_0^{(2)} =& -\frac{1}{8n_0}\left(n_0\left(\Delta a_0^{(0)} + \frac{1}{3}\left|\nabla a_0^{(0)}\right|^2\right) + 4n_0\left(\left|\boldsymbol{a}^{(0)}\right|^2 + 2\alpha^2\right) - \frac{1}{3}n_0\Delta a_0^{(0)}\right)\\ =& -\frac{1}{12}\Delta a_0^{(0)} - \frac{1}{24}\left|\nabla a_0^{(0)}\right|^2 - \frac{1}{2}\left|\boldsymbol{a}^{(0)}\right|^2 - \alpha^2\\ =& -\frac{1}{12}\Delta\log(n_0) - \frac{1}{24}|\nabla\log(n_0)|^2 - \frac{1}{2}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 - \alpha^2.\end{aligned}$$

Additionally we add the needed derivatives of $\log(n_0)$ for $j\in\{1,2\}$ to obtain a more handy form of $a_0^{(2)}$:

$$\begin{aligned}\partial_{x_j}\log(n_0) =&\frac{1}{n_0}\partial_{x_j}n_0,\quad \partial_{x_j}\left(\partial_{x_j}\log(n_0)\right) = \partial_{x_j}\left(\frac{1}{n_0}\partial_{x_j}n_0\right) = \frac{1}{n_0^2}\left((\partial_{x_j}^2 n_0)n_0 - \left(\partial_{x_j}n_0\right)^2\right),\\ \nabla\log(n_0) =&\frac{\nabla n_0}{n_0},\qquad \Delta\log(n_0) = \frac{\Delta n_0}{n_0} - \frac{|\nabla n_0|^2}{n_0^2},\end{aligned}$$

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and hence

$$a_0^{(2)} = -\frac{1}{12}\left(\frac{\Delta n_0}{n_0} - \frac{|\nabla n_0|^2}{{n_0}^2}\right) - \frac{1}{24}\left|\frac{\nabla n_0}{n_0}\right|^2 - \frac{1}{2}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 - \alpha^2$$
$$= -\frac{1}{12}\left(\frac{\Delta n_0}{n_0} - \frac{1}{2}\frac{|\nabla n_0|^2}{{n_0}^2}\right) - \frac{1}{2}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 - \alpha^2.$$

B.4.3. Calculations for $\boldsymbol{a}^{(2)}$

Starting point here is the equation

$$\boldsymbol{a}^{(2)} = -\frac{1}{n_0}\left\langle \boldsymbol{g}^{(3)}(1)\Big|_{\varepsilon=0}\right\rangle - \frac{1}{n_0} a_0^{(2)} \boldsymbol{n}. \tag{B.8}$$

The integral on the right hand side is given by

$$\left\langle \boldsymbol{g}^{(3)}(1)\Big|_{\varepsilon=0}\right\rangle = \frac{1}{24}\Big\langle \exp\left(h_0^{(0)}\right)\Big[\Big(3\Delta a_0^{(0)} + \left|\nabla a_0^{(0)}\right|^2 - p^T(\nabla\otimes\nabla a_0^{(0)})p + 4\left|\boldsymbol{h}_1^{(0)}\right|^2\Big)\boldsymbol{h}_1^{(0)} +$$
$$+ 2\nabla \boldsymbol{a}^{(0)}\cdot\nabla a_0^{(0)} - p^T(\nabla\otimes\nabla\boldsymbol{a}^{(0)})p + 2\alpha\nabla^\perp(\nabla a_0^{(0)}\cdot p)$$
$$+ 3\Delta\boldsymbol{a}^{(0)} - 12\alpha\nabla^\perp\times\boldsymbol{a}^{(0)} + 4\Big((\nabla\boldsymbol{a}^{(0)})p - \alpha(\nabla a_0^{(0)})^\perp\Big)\times\boldsymbol{h}_1^{(0)}\Big]\Big\rangle$$
$$= \frac{n_0}{24}\left(\left(3\Delta a_0^{(0)} + \left|\nabla a_0^{(0)}\right|^2\right)\boldsymbol{a}^{(0)} + 2\nabla\boldsymbol{a}^{(0)}\cdot\nabla a_0^{(0)} + 3\Delta\boldsymbol{a}^{(0)} - 12\alpha\nabla^\perp\times\boldsymbol{a}^{(0)}\right)$$
$$+ \frac{1}{24}\Big\langle \exp\left(h_0^{(0)}\right)\Big[\Big(-p^T(\nabla\otimes\nabla a_0^{(0)})p + 4\left|\boldsymbol{h}_1^{(0)}\right|^2\Big)\boldsymbol{h}_1^{(0)} - p^T(\nabla\otimes\nabla\boldsymbol{a}^{(0)})p$$
$$+ 2\alpha\nabla^\perp(\nabla a_0^{(0)}\cdot p) + 4\Big(\left(\nabla\boldsymbol{a}^{(0)}\right)p - \alpha\left(\nabla a_0^{(0)}\right)^\perp\Big)\times\boldsymbol{h}_1^{(0)}\Big]\Big\rangle.$$

In the previous Section (see Appendix B.4.2) we already dealt with some integrals of the same kind and additionally with Proposition 3.6.4 we deduce that

$$\left\langle \exp\left(h_0^{(0)}\right)\left(p^T\left(\nabla\otimes\nabla a_0^{(0)}\right)p\right)\boldsymbol{h}_1^{(0)}\right\rangle = \left\langle \exp\left(h_0^{(0)}\right)\left(p^T(\nabla\otimes\nabla a_0^{(0)})p\right)\right\rangle\boldsymbol{a}^{(0)}$$
$$+ \alpha\left\langle \exp\left(h_0^{(0)}\right)\left(p^T(\nabla\otimes\nabla a_0^{(0)})p\right)p^\perp\right\rangle$$
$$= n_0\left(\Delta a_0^{(0)}\right)\boldsymbol{a}^{(0)},$$

and

$$\left\langle \exp\left(h_0^{(0)}\right)\left(\left|\boldsymbol{h}_1^{(0)}\right|^2\right)\boldsymbol{h}_1^{(0)}\right\rangle = \left\langle \exp\left(h_0^{(0)}\right)\left(\left|\boldsymbol{h}_1^{(0)}\right|^2\right)\right\rangle\boldsymbol{a}^{(0)} - \alpha\left\langle \exp\left(h_0^{(0)}\right)\left(\left|\boldsymbol{h}_1^{(0)}\right|^2\right)p^\perp\right\rangle$$
$$= n_0\left(\left|\boldsymbol{a}^{(0)}\right|^2 + 2\alpha^2\right)\boldsymbol{a}^{(0)} + 2\alpha^2\left\langle \exp\left(h_0^{(0)}\right)\left(\boldsymbol{a}^{(0)}\cdot p^\perp\right)p^\perp\right\rangle$$
$$= n_0\left(\left|\boldsymbol{a}^{(0)}\right|^2 + 2\alpha^2\right)\boldsymbol{a}^{(0)} - 2\alpha^2 n_0\left(\boldsymbol{a}^{(0)\perp}\right)^\perp,$$

and

$$\left\langle \exp\left(h_0^{(0)}\right)p^T\left(\nabla\otimes\nabla\boldsymbol{a}^{(0)}\right)p\right\rangle = n_0\Delta\boldsymbol{a}^{(0)}, \qquad \left\langle 2\alpha\nabla^\perp\left(\nabla a_0^{(0)}\cdot p\right)\right\rangle = 0.$$

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Now we take a look onto the terms where the cross product with $\boldsymbol{h}_1^{(0)}$ appears. The first two upcoming integrals vanish because odd functions with respect to p are integrated and the third follows from Proposition 3.6.4:

$$\begin{aligned}\left\langle \exp\left(h_0^{(0)}\right)\left(\left(\nabla \boldsymbol{a}^{(0)}\right)p\right)\times \boldsymbol{a}^{(0)}\right\rangle =&0,\\ \left\langle \alpha^2 \exp\left(h_0^{(0)}\right)\left(\nabla a_0^{(0)}\right)^{\perp}\times p^{\perp}\right\rangle =&0,\\ \alpha\left\langle \exp\left(h_0^{(0)}\right)\left(\nabla a_0^{(0)}\right)^{\perp}\times \boldsymbol{a}^{(0)}\right\rangle =&\alpha n_0\left(\nabla a_0^{(0)}\right)^{\perp}\times \boldsymbol{a}^{(0)}.\end{aligned}$$

The very last integral gets a bit more attention (notice that in the second equality the odd terms disappear after integration):

$$\begin{aligned}\left\langle \exp\left(h_0^{(0)}\right)\left(\left(\nabla \boldsymbol{a}^{(0)}\right)p\right)\times p^{\perp}\right\rangle =&\left\langle \exp\left(h_0^{(0)}\right)\begin{pmatrix}\partial_{x_1}a_1^{(0)}p_1+\partial_{x_2}a_1^{(0)}p_2\\ \partial_{x_1}a_2^{(0)}p_1+\partial_{x_2}a_2^{(0)}p_2\\ \partial_{x_1}a_3^{(0)}p_1+\partial_{x_2}a_3^{(0)}p_2\end{pmatrix}\times\begin{pmatrix}p_2\\-p_1\\0\end{pmatrix}\right\rangle\\ =&\left\langle \exp\left(h_0^{(0)}\right)\begin{pmatrix}\partial_{x_1}a_3^{(0)}p_1^2\\ \partial_{x_2}a_3^{(0)}p_2^2\\ -\partial_{x_1}a_1^{(0)}p_1^2-\partial_{x_2}a_2^{(0)}p_2^2\end{pmatrix}\right\rangle\\ =&-n_0(\nabla\times e_3)\times \boldsymbol{a}^{(0)}.\end{aligned}$$

Hence we obtain for the integration of $g^{(3)}(1)$ at $\varepsilon=0$ the following

$$\begin{aligned}\left\langle \boldsymbol{g}^{(3)}(1)\Big|_{\varepsilon=0}\right\rangle =&\frac{n_0}{24}\left(\left(3\Delta a_0^{(0)}+\left|\nabla a_0^{(0)}\right|^2\right)\boldsymbol{a}^{(0)}+2\nabla\boldsymbol{a}^{(0)}\cdot\nabla a_0^{(0)}+3\Delta\boldsymbol{a}^{(0)}-12\alpha\nabla^{\perp}\times\boldsymbol{a}^{(0)}\right)\\ &+\frac{n_0}{24}\left[4\left(\left|\boldsymbol{a}^{(0)}\right|^2+2\alpha^2\right)\boldsymbol{a}^{(0)}-8\alpha^2\left(\boldsymbol{a}^{(0)\perp}\right)^{\perp}-\left(\Delta a_0^{(0)}\right)\boldsymbol{a}^{(0)}-\Delta\boldsymbol{a}^{(0)}\right.\\ &\left.-4\left(\alpha\left(\nabla^{\perp}\right)\times\boldsymbol{a}^{(0)}+\alpha\left(\nabla a_0^{(0)}\right)^{\perp}\times\boldsymbol{a}^{(0)}\right)\right]\\ =&\frac{n_0}{24}\left[\left(2\Delta a_0^{(0)}+\left|\nabla a_0^{(0)}\right|^2+4\left(\left|\boldsymbol{a}^{(0)}\right|^2+2\alpha^2\right)\right)\boldsymbol{a}^{(0)}-8\alpha^2\left(\boldsymbol{a}^{(0)\perp}\right)^{\perp}\right.\\ &\left.+2\nabla\boldsymbol{a}^{(0)}\cdot\nabla a_0^{(0)}+2\Delta\boldsymbol{a}^{(0)}-16\alpha\nabla^{\perp}\times\boldsymbol{a}^{(0)}-4\alpha\left(\nabla a_0^{(0)}\right)^{\perp}\times\boldsymbol{a}^{(0)}\right]\\ =&\frac{n_0}{12}\left(\left[\Delta a_0^{(0)}+\frac{1}{2}\left|\nabla a_0^{(0)}\right|^2+2\left(\left|\boldsymbol{a}^{(0)}\right|^2+2\alpha^2\right)\right]\boldsymbol{a}^{(0)}-4\alpha^2\left(\boldsymbol{a}^{(0)\perp}\right)^{\perp}\right)\\ &+\frac{n_0}{12}\left(\Delta\boldsymbol{a}^{(0)}+\nabla\boldsymbol{a}^{(0)}\cdot\nabla a_0^{(0)}-\alpha\left(8\nabla+2\nabla a_0^{(0)}\right)^{\perp}\times\boldsymbol{a}^{(0)}\right).\end{aligned}$$

Before we substitute into equation (B.8) we want to calculate the needed derivatives of $\boldsymbol{a}^{(0)}=\boldsymbol{n}/n_0$:

$$\begin{aligned}\partial_{x_i}\boldsymbol{a}^{(0)} =&\frac{1}{n_0}\partial_{x_i}\boldsymbol{n}-\frac{1}{{n_0}^2}(\partial_{x_i}n_0)\boldsymbol{n}\\ \partial_{x_i}^2\boldsymbol{a}^{(0)} =&\partial_{x_i}\left(\frac{1}{n_0}\partial_{x_i}\boldsymbol{n}-\frac{1}{{n_0}^2}(\partial_{x_i}n_0)\boldsymbol{n}\right)\\ =&\frac{1}{{n_0}^2}\left((\partial_{x_i}^2\boldsymbol{n})n_0-\partial_{x_i}\boldsymbol{n}\,\partial_{x_i}n_0\right)-\frac{1}{{n_0}^4}\left(((\partial_{x_i}^2n_0)\boldsymbol{n}+\partial_{x_i}n_0\,\partial_{x_i}\boldsymbol{n}){n_0}^2-2n_0(\partial_{x_i}n_0)^2\boldsymbol{n}\right)\\ =&\frac{1}{n_0}\partial_{x_i}^2\boldsymbol{n}-2\frac{1}{{n_0}^2}(\partial_{x_i}n_0)\partial_{x_i}\boldsymbol{n}-\frac{1}{{n_0}^2}(\partial_{x_i}^2n_0)\boldsymbol{n}+2\frac{1}{{n_0}^3}(\partial_{x_i}n_0)^2\boldsymbol{n}.\end{aligned}$$

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With the above we can calculate easy the gradient and the Laplacian of $\boldsymbol{a}^{(2)}$:

$$\nabla \boldsymbol{a}^{(0)} = \frac{1}{n_0}\left(\nabla \boldsymbol{n} - \frac{1}{n_0}\boldsymbol{n}\nabla n_0\right),$$
$$\Delta \boldsymbol{a}^{(0)} = \frac{1}{n_0}\left(\Delta \boldsymbol{n} - \frac{2}{n_0}\nabla \boldsymbol{n}\cdot\nabla n_0 - \frac{1}{n_0}(\Delta n_0)\boldsymbol{n} + 2\left|\frac{\nabla n_0}{n_0}\right|^2 \boldsymbol{n}\right).$$

Finally substituting everything together into (B.8) we obtain

$$\begin{aligned}
\boldsymbol{a}^{(2)} =& -\frac{1}{n_0}\left\langle \boldsymbol{g}^{(3)}(1)\Big|_{\varepsilon=0}\right\rangle - \frac{1}{n_0}a_0^{(2)}\boldsymbol{n}\\
=& -\frac{1}{12}\left(\left[\Delta a_0^{(0)} + \frac{1}{2}\left|\nabla a_0^{(0)}\right|^2 + 2\left(\left|\boldsymbol{a}^{(0)}\right|^2 + 2\alpha^2\right)\right]\boldsymbol{a}^{(0)} - 4\alpha^2\left(\boldsymbol{a}^{(0)\perp}\right)^\perp\right)\\
&- \frac{1}{12}\left(\Delta \boldsymbol{a}^{(0)} + \nabla \boldsymbol{a}^{(0)}\cdot\nabla a_0^{(0)} - \alpha\left(8\nabla + 2\nabla a_0^{(0)}\right)^\perp \times \boldsymbol{a}^{(0)}\right)\\
&- \frac{1}{n_0}\left(-\frac{1}{12}\left(\frac{\Delta n_0}{n_0} - \frac{|\nabla n_0|^2}{{n_0}^2}\right) - \frac{1}{24}\left|\frac{\nabla n_0}{n_0}\right|^2 - \frac{1}{2}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 - \alpha^2\right)\boldsymbol{n}\\
=& \frac{1}{12n_0}\left(\left(\frac{\Delta n_0}{n_0} - 2\left|\frac{\nabla n_0}{n_0}\right|^2 + 4\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + 8\alpha^2\right)\boldsymbol{n} + 4\alpha^2\left(\boldsymbol{n}^\perp\right)^\perp - \Delta\boldsymbol{n} + 2\nabla\boldsymbol{n}\cdot\frac{\nabla n_0}{n_0}\right)\\
&- \frac{1}{12n_0}\left(\left(\nabla\boldsymbol{n} - \frac{1}{n_0}\boldsymbol{n}\nabla n_0\right)\cdot\frac{\nabla n_0}{n_0} - \alpha\left(8\nabla + 2\frac{\nabla n_0}{n_0}\right)^\perp \times \boldsymbol{n}\right)\\
=& \frac{1}{12n_0}\left(\left(\frac{\Delta n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2 + 4\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + 8\alpha^2\right)\boldsymbol{n} + 4\alpha^2\left(\boldsymbol{n}^\perp\right)^\perp\right)\\
&- \frac{1}{12}\left(\frac{\Delta\boldsymbol{n}}{n_0} - \frac{\nabla\boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0}\right) + \frac{\alpha}{6n_0}\left(4\nabla + \frac{\nabla n_0}{n_0}\right)^\perp \times \boldsymbol{n}.
\end{aligned}$$

B.4.4. Gradients of the Second Order Lagrange Multiplier

We give here the calculations for $\nabla\boldsymbol{a}^{(2)}$ and we will see that then the explicit form of $\nabla a_0^{(2)}$ follows directly. For the second order we start with applying the product rule

$$\begin{aligned}
\nabla\boldsymbol{a}^{(2)} =& \nabla\left(\left(\frac{1}{3}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \frac{1}{12}\frac{\Delta n_0}{n_0} - \frac{1}{12}\left|\frac{\nabla n_0}{n_0}\right|^2\right)\frac{\boldsymbol{n}}{n_0} - \frac{1}{12}\frac{\Delta\boldsymbol{n}}{n_0} + \frac{1}{12}\frac{\nabla\boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0}\right)\\
=& \frac{\boldsymbol{n}}{n_0}\nabla\left(\frac{1}{3}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \frac{1}{12}\frac{\Delta n_0}{n_0} - \frac{1}{12}\left|\frac{\nabla n_0}{n_0}\right|^2\right) + \left(\frac{1}{3}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \frac{1}{12}\frac{\Delta n_0}{n_0} - \frac{1}{12}\left|\frac{\nabla n_0}{n_0}\right|^2\right)\nabla\left(\frac{\boldsymbol{n}}{n_0}\right)\\
&- \frac{1}{12}\nabla\left(\frac{\Delta\boldsymbol{n}}{n_0}\right) + \frac{1}{12}\nabla\left(\frac{\nabla\boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0}\right).
\end{aligned}$$

Looking at the expressions separately gives us

$$\begin{aligned}
\partial_{x_k}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 =& \partial_{x_k}\left(\frac{1}{{n_0}^2}\sum_{j=1}^3 n_j^2\right) = \frac{1}{{n_0}^4}\left(2\sum_{j=1}^3 n_j(\partial_{x_k}n_j){n_0}^2 - 2n_0(\partial_{x_k}n_0)\sum_{j=1}^3 n_j^2\right)\\
=& 2\left(\frac{1}{{n_0}^2}\boldsymbol{n}\cdot\partial_{x_k}\boldsymbol{n} - \frac{1}{{n_0}^3}|\boldsymbol{n}|^2\partial_{x_k}n_0\right),\\
\nabla\left|\frac{\boldsymbol{n}}{n_0}\right|^2 =& 2\left(\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0} - \left|\frac{\boldsymbol{n}}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right).
\end{aligned} \tag{B.9}$$

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Here the $j-$th row of the matrix $\nabla\left|\frac{\boldsymbol{n}}{n_0}\right|^2\boldsymbol{n}$ reads as follows

$$\left(\nabla\left|\frac{\boldsymbol{n}}{n_0}\right|^2\boldsymbol{n}\right)_{j.} = 2\left(\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0} - \left|\frac{\boldsymbol{n}}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right)n_j.$$

Next term on the list is $\nabla|(\nabla n_0)/n_0|^2$. The calculations are similar to the previous ones where we only need to replace $\boldsymbol{n}$ with ∇n_0. The gradient of the gradient equals the tensor product of the derivatives (or just the hessian) and will be denoted with $\nabla\otimes\nabla$.

$$\begin{aligned}\partial_{x_k}\left|\frac{\nabla n_0}{n_0}\right|^2 &= 2\left(\frac{1}{{n_0}^2}\nabla n_0\cdot\partial_{x_k}\nabla n_0 - \frac{1}{{n_0}^3}|\nabla n_0|^2\partial_{x_k}n_0\right),\\ \nabla\left|\frac{\nabla n_0}{n_0}\right|^2 &= 2\left(\frac{\nabla n_0}{n_0}\frac{(\nabla\otimes\nabla)n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right).\end{aligned}\tag{B.10}$$

Next term is quite straight forward where we only apply the quotient rule.

$$\nabla\left(\frac{\Delta n_0}{n_0}\right) = \frac{\nabla(\Delta n_0)}{n_0} - \frac{\nabla n_0}{n_0}\frac{\Delta n_0}{n_0}, \qquad \nabla\left(\frac{\Delta\boldsymbol{n}}{n_0}\right) = \frac{\nabla(\Delta\boldsymbol{n})}{n_0} - \frac{\Delta\boldsymbol{n}}{n_0}\frac{\nabla n_0}{n_0}.\tag{B.11}$$

The last derivative that will be calculated, needs do be done more in detail, to avoid confusion. Let for $j\in\{1,2,3\}$ and for $k\in\{1,2\}$

$$\begin{aligned}\partial_{x_k}\left(\left(\frac{\nabla\boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0}\right)_j\right) &= \partial_{x_k}\left(\frac{1}{{n_0}^2}\sum_{i=1}^{2}(\partial_{x_i}n_j)\partial_{x_i}n_0\right) =\\ &= \frac{1}{{n_0}^2}\left(\sum_{i=1}^{2}(\partial_{x_k}\partial_{x_i}n_j)\partial_{x_i}n_0 + (\partial_{x_i}n_j)\partial_{x_k}\partial_{x_i}n_0\right) - \frac{2}{{n_0}^3}\left(\sum_{i=1}^{2}(\partial_{x_i}n_j)(\partial_{x_i}n_0)\partial_{x_k}n_0\right),\end{aligned}$$

which means for the gradient of the $j-$component

$$\nabla\left(\left(\frac{\nabla\boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0}\right)_j\right) = \frac{\nabla n_0}{n_0}\left(\frac{(\nabla\otimes\nabla)n_j}{n_0}\right) + \frac{\nabla n_j}{n_0}\left(\frac{(\nabla\otimes\nabla)n_0}{n_0}\right) - 2\left(\frac{\nabla n_j}{n_0}\cdot\frac{\nabla n_0}{n_0}\right)\frac{\nabla n_0}{n_0}.$$

In general we have

$$\nabla\left(\frac{\nabla\boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0}\right) = \frac{\nabla n_0}{n_0}\left(\frac{(\nabla\otimes\nabla)\boldsymbol{n}}{n_0}\right) + \frac{\nabla\boldsymbol{n}}{n_0}\left(\frac{(\nabla\otimes\nabla)n_0}{n_0}\right) - 2\left(\frac{\nabla\boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0}\right)\frac{\nabla n_0}{n_0}.$$

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Therefore we obtain for the gradient of the second order of $\boldsymbol{a}$ the following result

$$
\begin{aligned}
\nabla \boldsymbol{a}^{(2)} &= \frac{\boldsymbol{n}}{n_0}\nabla\left(\frac{1}{3}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \frac{1}{12}\frac{\Delta n_0}{n_0} - \frac{1}{12}\left|\frac{\nabla n_0}{n_0}\right|^2\right) \\
&\quad + \left(\frac{1}{3}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \frac{1}{12}\frac{\Delta n_0}{n_0} - \frac{1}{12}\left|\frac{\nabla n_0}{n_0}\right|^2\right)\nabla\left(\frac{\boldsymbol{n}}{n_0}\right) - \frac{1}{12}\nabla\left(\frac{\Delta \boldsymbol{n}}{n_0}\right) + \frac{1}{12}\nabla\left(\frac{\nabla \boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0}\right) \\
&= \frac{\boldsymbol{n}}{n_0}\left(\frac{2}{3}\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla \boldsymbol{n}}{n_0} - \frac{2}{3}\left|\frac{\boldsymbol{n}}{n_0}\right|^2\frac{\nabla n_0}{n_0} + \frac{1}{12}\frac{\nabla(\Delta n_0)}{n_0} - \frac{1}{12}\frac{\nabla n_0}{n_0}\frac{\Delta n_0}{n_0}\right) \\
&\quad - \frac{1}{6}\frac{\boldsymbol{n}}{n_0}\left(\frac{\nabla n_0}{n_0}\frac{(\nabla\otimes\nabla)n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right) \\
&\quad + \left(\frac{1}{3}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \frac{1}{12}\frac{\Delta n_0}{n_0} - \frac{1}{12}\left|\frac{\nabla n_0}{n_0}\right|^2\right)\left(\frac{\nabla \boldsymbol{n}}{n_0} - \frac{\boldsymbol{n}}{n_0}\frac{\nabla n_0}{n_0}\right) - \frac{1}{12}\frac{\nabla(\Delta \boldsymbol{n})}{n_0} + \frac{1}{12}\frac{\Delta \boldsymbol{n}}{n_0}\frac{\nabla n_0}{n_0} \\
&\quad + \frac{1}{12}\frac{\nabla n_0}{n_0}\left(\frac{(\nabla\otimes\nabla)\boldsymbol{n}}{n_0}\right) + \frac{1}{12}\frac{\nabla \boldsymbol{n}}{n_0}\left(\frac{(\nabla\otimes\nabla)n_0}{n_0}\right) - \frac{1}{6}\left(\frac{\nabla \boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0}\right)\frac{\nabla n_0}{n_0} \\
&= \frac{\boldsymbol{n}}{n_0}\left(\frac{2}{3}\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla \boldsymbol{n}}{n_0} - \left|\frac{\boldsymbol{n}}{n_0}\right|^2\frac{\nabla n_0}{n_0} + \frac{1}{12}\frac{\nabla(\Delta n_0)}{n_0} - \frac{1}{6}\frac{\nabla n_0}{n_0}\frac{\Delta n_0}{n_0} - \frac{1}{6}\frac{\nabla n_0}{n_0}\frac{(\nabla\otimes\nabla)n_0}{n_0}\right) \\
&\quad + \frac{\boldsymbol{n}}{n_0}\left(\frac{1}{4}\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right) + \frac{1}{12}\frac{\nabla \boldsymbol{n}}{n_0}\left(\frac{(\nabla\otimes\nabla)n_0}{n_0} + \left(4\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + \frac{\Delta n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2\right)\sigma_0\right) \\
&\quad + \frac{1}{12}\left(\frac{\Delta \boldsymbol{n}}{n_0} - 2\left(\frac{\nabla \boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0}\right)\right)\frac{\nabla n_0}{n_0} + \frac{1}{12}\frac{\nabla n_0}{n_0}\frac{(\nabla\otimes\nabla)\boldsymbol{n}}{n_0} - \frac{1}{12}\frac{\nabla(\Delta \boldsymbol{n})}{n_0}
\end{aligned}
$$

where $((\nabla n_0(\nabla\otimes\nabla))\boldsymbol{n})_j = \nabla n_0(\nabla\otimes\nabla)n_j$, and we point out that $\nabla\boldsymbol{a}^{(2)}$ is a 3×3 matrix, where the last column equals zero. For the gradient of $a_0^{(2)}$ we need only (B.9), (B.10) and (B.11), which gives us

$$
\begin{aligned}
\nabla {a_0}^{(2)} &= -\frac{1}{12}\nabla\left(\frac{\Delta n_0}{n_0} - \frac{1}{2}\frac{|\nabla n_0|^2}{{n_0}^2}\right) - \nabla\frac{1}{2}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 \\
&= -\frac{1}{12}\left(\frac{\nabla(\Delta n_0)}{n_0} - \frac{\nabla n_0}{n_0}\frac{\Delta n_0}{n_0} - \frac{\nabla n_0}{n_0}\frac{(\nabla\otimes\nabla)n_0}{n_0} + \left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right) \\
&\quad - \left(\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla \boldsymbol{n}}{n_0} - \left|\frac{\boldsymbol{n}}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right)
\end{aligned}
$$

B.5. Another Depiction of the Semiclassical Model (3.106)

For a better overview we give here again the semiclassical model for the spin components:

$$
\begin{aligned}
\partial_t \boldsymbol{n} =& \tau\,\mathrm{div}\,(\nabla\boldsymbol{n} + \boldsymbol{n}\nabla V) - 2\tau\alpha(2\nabla^\perp + \nabla V^\perp)\times\boldsymbol{n} - 4\tau\alpha^2(2\boldsymbol{n} + (\boldsymbol{n}^\perp)^\perp) \\
&+ \frac{\varepsilon^2}{6}\frac{\boldsymbol{n}}{n_0}\times\mathcal{B}(N) + \tau\frac{\varepsilon^2}{12}\,\mathrm{div}\,\Big(\boldsymbol{n}\mathcal{A}(N) - \nabla(\Delta\boldsymbol{n}) + (\nabla\boldsymbol{n})\mathcal{C}(N) + \mathcal{B}(N)\nabla n_0 + \mathcal{D}(N)\Big) \\
&+ \tau\frac{\varepsilon^2}{3}\boldsymbol{n}\times\left(\frac{\boldsymbol{n}}{n_0}\times\mathcal{B}(N) - \mathcal{B}(N)\right),
\end{aligned}
$$

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where

$$\mathcal{A}(N) := 2\left|\frac{\nabla n_0}{n_0}\right|^2 \frac{\nabla n_0}{n_0} - 4\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla \boldsymbol{n}}{n_0} - \frac{\nabla n_0}{n_0}\frac{\Delta n_0}{n_0} - \frac{\nabla n_0}{n_0}\frac{(\nabla\otimes\nabla)n_0}{n_0},$$

$$\mathcal{B}(N) := \frac{\Delta \boldsymbol{n}}{n_0} - \frac{\nabla \boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0},$$

$$\mathcal{C}(N) := \left(\frac{\Delta n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2 + 4\left|\frac{\boldsymbol{n}}{n_0}\right|^2\right)\sigma_0 + \frac{\nabla\otimes\nabla n_0}{n_0},$$

$$\mathcal{D}(N) := \frac{(\nabla n_0(\nabla\otimes\nabla))}{n_0}\boldsymbol{n} - \left(\nabla\boldsymbol{n}\cdot\frac{\nabla n_0}{n_0}\right)\frac{\nabla n_0}{n_0}.$$

We are interested in the divergence that appears in the second line and we want to resolve it. Recalling that the gradient is a row vector, $\nabla = (\partial_{x_1}, \partial_{x_2}, 0)$ and that for a matrix valued function $B(x)$ the divergence is defined as $\operatorname{div} B(x) := \sum_{k=1}^{2} \partial_{x_k} B_{.\,k}(x)$, where $B_{.\,k}(x)$ represents the k-th column of B. For better understanding we recall some done calculations:

$$\partial_{x_k}\left|\frac{\boldsymbol{n}}{n_0}\right|^2 = 2\left(\frac{\boldsymbol{n}\cdot\partial_{x_k}\boldsymbol{n}}{n_0^2} - \frac{|\boldsymbol{n}|^2\partial_{x_k}n_0}{n_0^3}\right), \tag{B.12}$$

$$\partial_{x_k}\left|\frac{\nabla n_0}{n_0}\right|^2 = 2\left(\frac{\nabla n_0\cdot\partial_{x_k}\nabla n_0}{n_0^2} - \frac{|\nabla n_0|^2\partial_{x_k}n_0}{n_0^3}\right). \tag{B.13}$$

The plan is to calculate each term separately so that it is easier to follow.
First term:

$$\operatorname{div}\left(\boldsymbol{n}\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right) = \sum_{k=1}^{2}\partial_{x_k}\left(\boldsymbol{n}\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\partial_{x_k}n_0}{n_0}\right) =$$

$$= \sum_{k=1}^{2}\boldsymbol{n}\partial_{x_k}\left(\left|\frac{\nabla n_0}{n_0}\right|^2\right)\frac{\partial_{x_k}n_0}{n_0} + \left|\frac{\nabla n_0}{n_0}\right|^2\partial_{x_k}\left(\boldsymbol{n}\frac{\partial_{x_k}n_0}{n_0}\right)$$

$$= \sum_{k=1}^{2}2\boldsymbol{n}\left(\frac{\nabla n_0\cdot\partial_{x_k}\nabla n_0}{n_0^2} - \frac{|\nabla n_0|^2\partial_{x_k}n_0}{n_0^3}\right)\frac{\partial_{x_k}n_0}{n_0} + \left|\frac{\nabla n_0}{n_0}\right|^2\left(\boldsymbol{n}\frac{\partial^2_{x_k}n_0}{n_0} - \boldsymbol{n}\frac{(\partial_{x_k}n_0)^2}{n_0^2} + (\partial_{x_k}\boldsymbol{n})\frac{\partial_{x_k}n_0}{n_0}\right)$$

$$= 2\left(\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0}\cdot\frac{\nabla n_0}{n_0}\right)\boldsymbol{n} - 2\left|\frac{\nabla n_0}{n_0}\right|^4\boldsymbol{n} + \left|\frac{\nabla n_0}{n_0}\right|\frac{\Delta n_0}{n_0}\boldsymbol{n} - \left|\frac{\nabla n_0}{n_0}\right|^4\boldsymbol{n} + \left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0}\cdot\nabla\boldsymbol{n}$$

$$= \left(2\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0}\cdot\frac{\nabla n_0}{n_0} - 3\left|\frac{\nabla n_0}{n_0}\right|^4 + \left|\frac{\nabla n_0}{n_0}\right|^2\frac{\Delta n_0}{n_0}\right)\boldsymbol{n} + \left(\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right)\cdot\nabla\boldsymbol{n}.$$

Second term:

$$\operatorname{div}\left(\boldsymbol{n}\left(\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0}\right)\right) = \sum_{k=1}^{2}\boldsymbol{n}\partial_{x_k}\left(\sum_{j=1}^{3}\frac{n_j}{n_0}\frac{\partial_{x_k}n_j}{n_0}\right) + \partial_{x_k}\boldsymbol{n}\left(\frac{\boldsymbol{n}}{n_0}\cdot\frac{\partial_{x_k}\boldsymbol{n}}{n_0}\right)$$

$$= \sum_{k=1}^{2}\sum_{j=1}^{3}\boldsymbol{n}\left(\frac{(\partial_{x_k}n_j)^2 + n_j\partial^2_{x_k}n_j}{n_0^2} - 2\frac{n_j(\partial_{x_k}n_j)\partial_{x_k}n_0}{n_0^3}\right) + \partial_{x_k}\boldsymbol{n}\left(\frac{n_j}{n_0}\frac{\partial_{x_k}n_j}{n_0}\right)$$

$$= \sum_{j=1}^{3}\left|\frac{\nabla n_j}{n_0}\right|^2\boldsymbol{n} + \frac{n_j\Delta n_j}{n_0^2}\boldsymbol{n} - 2\frac{n_j\nabla n_j\cdot\nabla n_0}{n_0^3}\boldsymbol{n} + \frac{n_j\nabla n_j}{n_0^2}\cdot\nabla\boldsymbol{n}$$

$$= \left[\left|\frac{\nabla\boldsymbol{n}}{n_0}\right|^2 + \frac{\boldsymbol{n}}{n_0}\cdot\frac{\Delta\boldsymbol{n}}{n_0} - 2\left(\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0}\right)\cdot\frac{\nabla n_0}{n_0}\right]\boldsymbol{n} + \left(\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0}\right)\cdot\nabla\boldsymbol{n}.$$

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Third term:

$$\operatorname{div}\left(\boldsymbol{n}\frac{\nabla n_0}{n_0}\frac{\Delta n_0}{n_0}\right) = \sum_{k=1}^{2}\partial_{x_k}\left(\boldsymbol{n}\frac{\partial_{x_k} n_0}{n_0}\frac{\Delta n_0}{n_0}\right) =$$
$$= \sum_{k=1}^{2}\frac{\partial_{x_k}^2 n_0\Delta n_0 + \partial_{x_k} n_0\partial_{x_k}\Delta n_0}{{n_0}^2}\boldsymbol{n} - 2\frac{(\partial_{x_k} n_0)^2\Delta n_0}{{n_0}^3}\boldsymbol{n} + \frac{\partial_{x_k} n_0\Delta n_0}{{n_0}^2}\partial_{x_k}\boldsymbol{n}$$
$$= \left[\left(\frac{\Delta n_0}{n_0}\right)^2 + \frac{\nabla n_0}{n_0}\cdot\frac{\nabla\Delta n_0}{n_0} - 2\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\Delta n_0}{n_0}\right]\boldsymbol{n} + \left(\frac{\Delta n_0}{n_0}\frac{\nabla n_0}{n_0}\right)\cdot\nabla\boldsymbol{n}.$$

Fourth term:

$$\operatorname{div}\left(\boldsymbol{n}\left(\frac{\nabla n_0}{n_0}\frac{(\nabla\otimes\nabla)n_0}{n_0}\right)\right) = \sum_{k=1}^{2}\partial_{x_k}\left(\boldsymbol{n}\left(\frac{\nabla n_0}{n_0}\cdot\frac{\nabla\partial_{x_k} n_0}{n_0}\right)\right)$$
$$= \sum_{k=1}^{2}\sum_{l=1}^{2}\boldsymbol{n}\frac{(\partial_{x_k}\partial_{x_l} n_0)^2 + \partial_{x_l} n_0\partial_{x_l}\partial_{x_l}^2 n_0}{{n_0}^2} - 2\frac{\partial_{x_k} n_0\partial_{x_k}\partial_{x_l} n_0\partial_{x_l} n_0}{{n_0}^3}\boldsymbol{n} + \frac{\partial_{x_l} n_0\partial_{x_l}\partial_{x_k} n_0}{{n_0}^2}\partial_{x_k}\boldsymbol{n}$$
$$= \left[\left\|\frac{\nabla\otimes\nabla n_0}{n_0}\right|^2 + \frac{\nabla n_0}{n_0}\cdot\frac{\nabla\Delta n_0}{n_0} - 2\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0}\cdot\frac{\nabla n_0}{n_0}\right]\boldsymbol{n} + \left(\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0}\right)\cdot\nabla\boldsymbol{n}.$$

Fifth term:

$$\operatorname{div}(\nabla\Delta\boldsymbol{n}) = \Delta(\Delta\boldsymbol{n}).$$

For the upcoming calculations we use formulas (B.12) - (B.13) and the product rule of the divergence of a scalar function f times vector field $\overrightarrow{F}$, which would be $\operatorname{div}\left(f\overrightarrow{F}\right) = \nabla f\cdot\overrightarrow{F} + f\operatorname{div}\overrightarrow{F}$.

Sixth term:

$$\operatorname{div}\left(\frac{\Delta n_0}{n_0}\nabla\boldsymbol{n}\right) = \left[\frac{\nabla\Delta n_0}{n_0} - \frac{\Delta n_0}{n_0}\frac{\nabla n_0}{n_0}\right]\cdot\nabla\boldsymbol{n} + \frac{\Delta n_0}{n_0}\Delta\boldsymbol{n}.$$

Seventh term:

$$\operatorname{div}\left(\left|\frac{\nabla n_0}{n_0}\right|^2\nabla\boldsymbol{n}\right) = \nabla\left|\frac{\nabla n_0}{n_0}\right|^2\cdot\nabla\boldsymbol{n} + \left|\frac{\nabla n_0}{n_0}\right|^2\Delta\boldsymbol{n}$$
$$= 2\left[\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right]\cdot\nabla\boldsymbol{n} + \left|\frac{\nabla n_0}{n_0}\right|^2\Delta\boldsymbol{n}.$$

Eighth term:

$$\operatorname{div}\left(\left|\frac{\boldsymbol{n}}{n_0}\right|^2\nabla\boldsymbol{n}\right) = \nabla\left|\frac{\boldsymbol{n}}{n_0}\right|^2\cdot\nabla\boldsymbol{n} + \left|\frac{\boldsymbol{n}}{n_0}\right|^2\Delta\boldsymbol{n}$$
$$= 2\left[\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0} - \left|\frac{\boldsymbol{n}}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right]\cdot\nabla\boldsymbol{n} + \left|\frac{\boldsymbol{n}}{n_0}\right|^2\Delta\boldsymbol{n}.$$

Ninth term:

$$\operatorname{div}\left(\nabla\boldsymbol{n}\left(\frac{(\nabla\otimes\nabla)n_0}{n_0}\right)\right) = \sum_{k=1}^{2}\partial_{x_k}\left(\nabla\boldsymbol{n}\cdot\frac{\nabla\partial_{x_k} n_0}{n_0}\right)$$
$$= \sum_{k=1}^{2}\nabla\partial_{x_k}\boldsymbol{n}\cdot\frac{\nabla\partial_{x_k} n_0}{n_0} + \nabla\boldsymbol{n}\cdot\left(\frac{\nabla\partial_{x_k}^2 n_0}{n_0} - \frac{\nabla\partial_{x_k} n_0\partial_{x_k} n_0}{{n_0}^2}\right)$$
$$= \nabla\otimes\nabla\boldsymbol{n}\cdot\frac{\nabla\otimes\nabla n_0}{n_0} + \left[\frac{\nabla\Delta n_0}{n_0} - \frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0}\right]\cdot\nabla\boldsymbol{n}.$$

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Tenth term:

$$\operatorname{div}\left((\Delta \boldsymbol{n})\frac{\nabla n_0}{n_0}\right) = \left[\frac{\Delta n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2\right]\Delta \boldsymbol{n} + \frac{\nabla n_0}{n_0}\cdot\nabla\Delta\boldsymbol{n}.$$

Eleventh and thirteenth term:

$$\begin{aligned}
\operatorname{div}\left(\left(\nabla\boldsymbol{n}\cdot\frac{\nabla n_0}{n_0}\right)\frac{\nabla n_0}{n_0}\right) &= \sum_{k=1}^{2}\partial_{x_k}\left(\left(\nabla\boldsymbol{n}\cdot\frac{\nabla n_0}{n_0}\right)\frac{\partial_{x_k} n_0}{n_0}\right) = \\
&= \sum_{k=1}^{2}\sum_{l=1}^{2}\partial_{x_k}\partial_{x_l}\boldsymbol{n}\frac{\partial_{x_l} n_0}{n_0}\frac{\partial_{x_k} n_0}{n_0} + \partial_{x_l}\boldsymbol{n}\left(\frac{\partial_{x_k}\partial_{x_l} n_0}{n_0}\frac{\partial_{x_k} n_0}{n_0} - \frac{\partial_{x_l} n_0(\partial_{x_k} n_0)^2}{{n_0}^3}\right) \\
&\quad + \partial_{x_l}\boldsymbol{n}\frac{\partial_{x_l} n_0}{n_0}\left(\frac{\partial^2_{x_k} n_0}{n_0} - \frac{(\partial_{x_k} n_0)^2}{{n_0}^2}\right) \\
&= \left(\frac{\nabla n_0}{n_0}(\nabla\otimes\nabla\boldsymbol{n})\right)\cdot\frac{\nabla n_0}{n_0} + \left[\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0} - 2\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0} + \frac{\Delta n_0}{n_0}\frac{\nabla n_0}{n_0}\right]\cdot\nabla\boldsymbol{n}.
\end{aligned}$$

Twelfth term:

$$\begin{aligned}
\operatorname{div}\left(\frac{\nabla n_0}{n_0}(\nabla\otimes\nabla)\boldsymbol{n}\right) &= \sum_{k=1}^{2}\partial_{x_k}\left(\frac{\nabla n_0}{n_0}\cdot\nabla\partial_{x_k}\boldsymbol{n}\right) \\
&= \sum_{k=1}^{2}\sum_{l=1}^{2}\left(\frac{\partial_{x_l}\partial_{x_k} n_0}{n_0}\partial_{x_l}\partial_{x_k}\boldsymbol{n} - \frac{\partial_{x_l} n_0\partial_{x_k} n_0}{{n_0}^2}\partial_{x_l}\partial_{x_k}\boldsymbol{n}\right) + \frac{\partial_{x_l} n_0}{n_0}\partial_{x_l}\partial^2_{x_k}\boldsymbol{n} \\
&= \frac{\nabla\otimes\nabla n_0}{n_0}\cdot(\nabla\otimes\nabla)\boldsymbol{n} - \left(\frac{\nabla n_0}{n_0}(\nabla\otimes\nabla\boldsymbol{n})\right)\cdot\frac{\nabla n_0}{n_0} + \frac{\nabla n_0}{n_0}\cdot\nabla\Delta\boldsymbol{n}.
\end{aligned}$$

Now every term was calculated and now everything can be put together. For a better overview

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we colorize $\boldsymbol{n}, \nabla\boldsymbol{n}$ and $\Delta\boldsymbol{n}$, leading us to

$$
\begin{aligned}
&\operatorname{div}\Big(\boldsymbol{n}\mathcal{A}(N) - \nabla(\Delta\boldsymbol{n}) + (\nabla\boldsymbol{n})\mathcal{C}(N) + \mathcal{B}(N)\nabla n_0 + \mathcal{D}(N)\Big) = \\
&=2\left(\left[2\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0}\cdot\frac{\nabla n_0}{n_0} - 3\left|\frac{\nabla n_0}{n_0}\right|^4 + \left|\frac{\nabla n_0}{n_0}\right|^2\frac{\Delta n_0}{n_0}\right]\boldsymbol{n} + \left[\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right]\cdot\nabla\boldsymbol{n}\right) \\
&\quad -4\left(\left[\left|\frac{\nabla\boldsymbol{n}}{n_0}\right|^2 + \frac{\boldsymbol{n}}{n_0}\cdot\frac{\Delta\boldsymbol{n}}{n_0} - 2\left(\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0}\right)\cdot\frac{\nabla n_0}{n_0}\right]\boldsymbol{n} + \left(\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0}\right)\cdot\nabla\boldsymbol{n}\right) \\
&\quad -\left(\left[\left(\frac{\Delta n_0}{n_0}\right)^2 + \frac{\nabla n_0}{n_0}\cdot\frac{\nabla\Delta n_0}{n_0} - 2\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\Delta n_0}{n_0}\right]\boldsymbol{n} + \left(\frac{\Delta n_0}{n_0}\frac{\nabla n_0}{n_0}\right)\cdot\nabla\boldsymbol{n}\right) \\
&\quad -\left(\left[\left|\frac{\nabla\otimes\nabla n_0}{n_0}\right|^2 + \frac{\nabla n_0}{n_0}\cdot\frac{\nabla\Delta n_0}{n_0} - 2\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0}\cdot\frac{\nabla n_0}{n_0}\right]\boldsymbol{n} + \left(\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0}\right)\cdot\nabla\boldsymbol{n}\right) \\
&\quad +\Delta(\Delta\boldsymbol{n}) - \left(2\left[\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right]\cdot\nabla\boldsymbol{n} + \left|\frac{\nabla n_0}{n_0}\right|^2\Delta\boldsymbol{n}\right) \\
&\quad +4\left(2\left[\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0} - \left|\frac{\boldsymbol{n}}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right]\cdot\nabla\boldsymbol{n} + \left|\frac{\boldsymbol{n}}{n_0}\right|^2\Delta\boldsymbol{n}\right) + \nabla\otimes\nabla\boldsymbol{n}\cdot\frac{\nabla\otimes\nabla n_0}{n_0} \\
&\quad +\left[\frac{\nabla\Delta n_0}{n_0} - \frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0}\right]\cdot\nabla\boldsymbol{n} + \left(\left[\frac{\nabla\Delta n_0}{n_0} - \frac{\Delta n_0}{n_0}\frac{\nabla n_0}{n_0}\right]\cdot\nabla\boldsymbol{n} + \frac{\Delta n_0}{n_0}\Delta\boldsymbol{n}\right) \\
&\quad +\left(\left[\frac{\Delta n_0}{n_0} - \left|\frac{\nabla n_0}{n_0}\right|^2\right]\Delta\boldsymbol{n} + \frac{\nabla n_0}{n_0}\cdot\nabla\Delta\boldsymbol{n}\right) \\
&\quad +\left(\frac{\nabla\otimes\nabla n_0}{n_0}\cdot(\nabla\otimes\nabla)\boldsymbol{n} - \left(\frac{\nabla n_0}{n_0}(\nabla\otimes\nabla\boldsymbol{n})\right)\cdot\frac{\nabla n_0}{n_0} + \frac{\nabla n_0}{n_0}\cdot\nabla\Delta\boldsymbol{n}\right) \\
&\quad -2\left(\left(\frac{\nabla n_0}{n_0}(\nabla\otimes\nabla\boldsymbol{n})\right)\cdot\frac{\nabla n_0}{n_0} + \left[\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0} - 2\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0} + \frac{\Delta n_0}{n_0}\frac{\nabla n_0}{n_0}\right]\cdot\nabla\boldsymbol{n}\right)
\end{aligned}
$$

Putting everything together provides

$$
\begin{aligned}
&\operatorname{div}\Big(\boldsymbol{n}\mathcal{A}(N) - \nabla(\Delta\boldsymbol{n}) + (\nabla\boldsymbol{n})\mathcal{C}(N) + \mathcal{B}(N)\nabla n_0 + \mathcal{D}(N)\Big) = \\
&=\Bigg[6\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0}\cdot\frac{\nabla n_0}{n_0} - 6\left|\frac{\nabla n_0}{n_0}\right|^4 + 4\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\Delta n_0}{n_0} - 4\left|\frac{\nabla\boldsymbol{n}}{n_0}\right|^2 - 4\frac{\boldsymbol{n}}{n_0}\cdot\frac{\Delta\boldsymbol{n}}{n_0} \\
&\quad +8\left(\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0}\right)\cdot\frac{\nabla n_0}{n_0} - \left(\frac{\Delta n_0}{n_0}\right)^2 - 2\frac{\nabla n_0}{n_0}\cdot\frac{\nabla\Delta n_0}{n_0} - \left|\frac{\nabla\otimes\nabla n_0}{n_0}\right|^2\Bigg]\boldsymbol{n} \\
&\quad +\left[8\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0} - 4\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0} - 4\frac{\Delta n_0}{n_0}\frac{\nabla n_0}{n_0} - 6\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0} + 2\frac{\nabla\Delta n_0}{n_0} - 8\left|\frac{\boldsymbol{n}}{n_0}\right|^2\frac{\nabla n_0}{n_0}\right]\cdot\nabla\boldsymbol{n} \\
&\quad +\left[4\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + 2\frac{\Delta n_0}{n_0} - 2\left|\frac{\nabla n_0}{n_0}\right|^2\right]\Delta\boldsymbol{n} + 2\frac{\nabla n_0}{n_0}\cdot\nabla\Delta\boldsymbol{n} + 2\frac{\nabla\otimes\nabla n_0}{n_0}\cdot(\nabla\otimes\nabla)\boldsymbol{n} \\
&\quad -3\left(\frac{\nabla n_0}{n_0}(\nabla\otimes\nabla\boldsymbol{n})\right)\cdot\frac{\nabla n_0}{n_0} + \Delta(\Delta\boldsymbol{n}).
\end{aligned}
$$

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Hence we can rewrite the equations for the spin components and obtain:

$$
\begin{aligned}
\partial_t \boldsymbol{n} =& \tau \operatorname{div}(\nabla \boldsymbol{n} + \boldsymbol{n}\nabla V) - 2\tau\alpha(2\nabla^\perp + \nabla V^\perp)\times \boldsymbol{n} - 4\tau\alpha^2(2\boldsymbol{n} + (\boldsymbol{n}^\perp)^\perp) \\
&+ \frac{\varepsilon^2}{6}\frac{\boldsymbol{n}}{n_0}\times \mathcal{B}(N) + \tau\frac{\varepsilon^2}{12}\left[\widetilde{\mathfrak{A}}(N)\boldsymbol{n} + \widetilde{\mathfrak{B}}(N)\cdot\nabla\boldsymbol{n} + \widetilde{\mathfrak{C}}(N)\Delta\boldsymbol{n}\right] \\
&+ \tau\frac{\varepsilon^2}{12}\left[\Delta(\Delta\boldsymbol{n}) + 2\frac{\nabla n_0}{n_0}\cdot\nabla\Delta\boldsymbol{n} + 2\frac{\nabla\otimes\nabla n_0}{n_0}\cdot(\nabla\otimes\nabla)\boldsymbol{n} - 3\left(\frac{\nabla n_0}{n_0}(\nabla\otimes\nabla\boldsymbol{n})\right)\cdot\frac{\nabla n_0}{n_0}\right] \\
&+ \tau\frac{\varepsilon^2}{3}\boldsymbol{n}\times\left(\frac{\boldsymbol{n}}{n_0}\times\mathcal{B}(N) - \mathcal{B}(N)\right) + \mathcal{O}(\varepsilon^3),
\end{aligned}
$$

where

$$
\begin{aligned}
\widetilde{\mathfrak{A}}(N) :=& 6\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0}\cdot\frac{\nabla n_0}{n_0} - 6\left|\frac{\nabla n_0}{n_0}\right|^4 + 4\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\Delta n_0}{n_0} - 4\left|\frac{\nabla\boldsymbol{n}}{n_0}\right|^2 - 4\frac{\boldsymbol{n}}{n_0}\cdot\frac{\Delta\boldsymbol{n}}{n_0} \\
&+ 8\left(\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0}\right)\cdot\frac{\nabla n_0}{n_0} - \left(\frac{\Delta n_0}{n_0}\right)^2 - 2\frac{\nabla n_0}{n_0}\cdot\frac{\nabla\Delta n_0}{n_0} - \left|\frac{\nabla\otimes\nabla n_0}{n_0}\right|^2 \\
\widetilde{\mathfrak{B}}(N) :=& 8\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0} - 4\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0} - 4\frac{\Delta n_0}{n_0}\frac{\nabla n_0}{n_0} - 6\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0} + 2\frac{\nabla\Delta n_0}{n_0} - 8\left|\frac{\boldsymbol{n}}{n_0}\right|^2\frac{\nabla n_0}{n_0} \\
\widetilde{\mathfrak{C}}(N) :=& 4\left|\frac{\boldsymbol{n}}{n_0}\right|^2 + 2\frac{\Delta n_0}{n_0} - 2\left|\frac{\nabla n_0}{n_0}\right|^2.
\end{aligned}
$$

For the double cross product we use the formula $(\vec{b}\times\vec{c})\times\vec{d} = (\vec{b}\cdot\vec{d})\,\vec{c} - (\vec{c}\cdot\vec{d})\,\vec{b}$ for $\vec{b},\ \vec{c},\ \vec{d}$ in $\mathbb{R}^3$, where in our case we have that $\vec{b} = \mathcal{B}(N),\ \vec{c} = \boldsymbol{n}/n_0,\ \vec{d} = \boldsymbol{n}$. Therefore

$$
\left(\mathcal{B}(N)\times\frac{\boldsymbol{n}}{n_0}\right)\times\boldsymbol{n} = \left(\mathcal{B}(N)\cdot\frac{\boldsymbol{n}}{n_0}\right)\boldsymbol{n} - \frac{|\boldsymbol{n}|^2}{n_0}\mathcal{B}(N)
$$

We see, that these terms above also appear in either $\widetilde{\mathfrak{A}}$, $\widetilde{\mathfrak{B}}$ and $\widetilde{\mathfrak{C}}$, which leads us to a simpler version for our model:

Equation for the spin components:

$$
\begin{aligned}
\partial_t \boldsymbol{n} =& \tau \operatorname{div}(\nabla \boldsymbol{n} + \boldsymbol{n}\nabla V) - 2\tau\alpha(2\nabla^\perp + \nabla V^\perp)\times \boldsymbol{n} - 4\tau\alpha^2(2\boldsymbol{n} + (\boldsymbol{n}^\perp)^\perp) \\
&+ \frac{\varepsilon^2}{6}\frac{\boldsymbol{n}}{n_0}\times \mathcal{B}(N) + \tau\frac{\varepsilon^2}{12}\left[\mathfrak{A}(N)\boldsymbol{n} + \mathfrak{B}(N)\cdot\nabla\boldsymbol{n} + \mathfrak{C}(n_0)\Delta\boldsymbol{n} + 4\mathcal{B}(N)\times\boldsymbol{n}\right] \\
&+ \tau\frac{\varepsilon^2}{12}\left[\Delta(\Delta\boldsymbol{n}) + 2\frac{\nabla n_0}{n_0}\cdot\nabla\Delta\boldsymbol{n} + 2\frac{\nabla\otimes\nabla n_0}{n_0}\cdot(\nabla\otimes\nabla)\boldsymbol{n} - 3\left(\frac{\nabla n_0}{n_0}(\nabla\otimes\nabla\boldsymbol{n})\right)\cdot\frac{\nabla n_0}{n_0}\right]
\end{aligned}
$$

where

$$
\begin{aligned}
\mathfrak{A}(N) :=& 6\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0}\cdot\frac{\nabla n_0}{n_0} - 6\left|\frac{\nabla n_0}{n_0}\right|^4 + 4\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\Delta n_0}{n_0} - 4\left|\frac{\nabla\boldsymbol{n}}{n_0}\right|^2 + 4\left(\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0}\right)\cdot\frac{\nabla n_0}{n_0} \\
&- \left(\frac{\Delta n_0}{n_0}\right)^2 - 2\frac{\nabla n_0}{n_0}\cdot\frac{\nabla\Delta n_0}{n_0} - \left|\frac{\nabla\otimes\nabla n_0}{n_0}\right|^2 \\
\mathfrak{B}(N) :=& 8\left|\frac{\nabla n_0}{n_0}\right|^2\frac{\nabla n_0}{n_0} - 4\frac{\boldsymbol{n}}{n_0}\cdot\frac{\nabla\boldsymbol{n}}{n_0} - 4\frac{\Delta n_0}{n_0}\frac{\nabla n_0}{n_0} - 6\frac{\nabla n_0}{n_0}\frac{\nabla\otimes\nabla n_0}{n_0} + 2\frac{\nabla\Delta n_0}{n_0} - 4\left|\frac{\boldsymbol{n}}{n_0}\right|^2\frac{\nabla n_0}{n_0} \\
\mathfrak{C}(n_0) :=& 2\frac{\Delta n_0}{n_0} - 2\left|\frac{\nabla n_0}{n_0}\right|^2, \qquad \mathcal{B}(N) = \frac{\Delta\boldsymbol{n}}{n_0} - \frac{\nabla\boldsymbol{n}}{n_0}\cdot\frac{\nabla n_0}{n_0}
\end{aligned}
$$

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B.6. Separate Equations for the Spin Components

The advantage we obtain from the second depiction of the semiclassical model for the spin components, derived in Appendix B.5, is that it is then much easier to separate them into the single equations for n_1, n_2 and n_3, which are still connected. For the single component equations we have some twisted cross products, which we unravel here:

$$\Delta \boldsymbol{n} \times \boldsymbol{n} = \begin{pmatrix} (\Delta n_2)n_3 - (\Delta n_3)n_2 \\ -(\Delta n_1)n_3 + (\Delta n_3)n_1 \\ (\Delta n_1)n_2 - (\Delta n_2)n_1 \end{pmatrix}, \quad (\nabla \boldsymbol{n} \cdot \nabla n_0) \times \boldsymbol{n} = \begin{pmatrix} (\nabla n_2 \cdot \nabla n_0)n_3 - (\nabla n_3 \cdot \nabla n_0)n_2 \\ -(\nabla n_1 \cdot \nabla n_0)n_3 + (\nabla n_3 \cdot \nabla n_0)n_1 \\ (\nabla n_1 \cdot \nabla n_0)n_2 - (\nabla n_2 \cdot \nabla n_0)n_1 \end{pmatrix},$$

$$\nabla^\perp \times \boldsymbol{n} = \begin{pmatrix} -\partial_{x_1} n_3 \\ -\partial_{x_2} n_3 \\ \partial_{x_1} n_1 + \partial_{x_2} n_2 \end{pmatrix}, \qquad \nabla^\perp V \times \boldsymbol{n} = \begin{pmatrix} -\partial_{x_1} V n_3 \\ -\partial_{x_2} V n_3 \\ \partial_{x_1} V n_1 + \partial_{x_2} V n_2 \end{pmatrix}.$$

Using $\mathfrak{A}(N), \mathfrak{B}(N)$ and $\mathfrak{C}(n_0)$ from the previous section (Appendix B.5), we obtain for the single components :

$$\begin{aligned}
\partial_t n_1 &= \tau \left(\operatorname{div}\left(\nabla n_1 + \nabla V n_1\right)\right) + 4\tau\alpha\partial_{x_1} n_3 + 2\tau\alpha\partial_{x_1} V n_3 - 4\tau\alpha^2 n_1 + \\
&+ \frac{\varepsilon^2}{6{n_0}^3}\left((\nabla n_2 \cdot \nabla n_0 - (n_0\Delta n_2))n_3 - (\nabla n_3 \cdot \nabla n_0 + (n_0\Delta n_3))n_2\right) \\
&+ \tau\frac{\varepsilon^2}{12}\left[\mathfrak{A}(N)n_1 + \mathfrak{B}(N)\cdot\nabla n_1 + \mathfrak{C}(n_0)\Delta n_1 - \frac{4}{{n_0}^2}\Big((\nabla n_2 \cdot \nabla n_0 - (n_0\Delta n_2))n_3 - (\nabla n_3 \cdot \nabla n_0 + (n_0\Delta n_3))n_2\Big)\right] \\
&+ \tau\frac{\varepsilon^2}{12}\left[\Delta(\Delta n_1) + 2\frac{\nabla n_0}{n_0}\cdot\nabla\Delta n_1 + 2\frac{\nabla\otimes\nabla n_0}{n_0}\cdot(\nabla\otimes\nabla n_1) - 3\left(\frac{\nabla n_0}{n_0}(\nabla\otimes\nabla n_1)\right)\cdot\frac{\nabla n_0}{n_0}\right],
\end{aligned}$$

$$\begin{aligned}
\partial_t n_2 &= \tau \left(\operatorname{div}\left(\nabla n_2 + \nabla V n_2\right)\right) + 4\tau\alpha\partial_{x_2} n_3 + 2\tau\alpha\partial_{x_2} V n_3 - 4\tau\alpha^2 n_2 \\
&+ \frac{\varepsilon^2}{6{n_0}^3}\left((\nabla n_3 \cdot \nabla n_0 - (n_0\Delta n_3))n_1 - (\nabla n_1 \cdot \nabla n_0 - (n_0\Delta n_1))n_3\right) + \\
&+ \tau\frac{\varepsilon^2}{12}\left[\mathfrak{A}(N)n_2 + \mathfrak{B}(N)\cdot\nabla n_2 + \mathfrak{C}(n_0)\Delta n_2 - \frac{4}{{n_0}^2}\Big((\nabla n_3 \cdot \nabla n_0 - (n_0\Delta n_3))n_1 - (\nabla n_1 \cdot \nabla n_0 - (n_0\Delta n_1))n_3\Big)\right] \\
&+ \tau\frac{\varepsilon^2}{12}\left[\Delta(\Delta n_2) + 2\frac{\nabla n_0}{n_0}\cdot\nabla\Delta n_2 + 2\frac{\nabla\otimes\nabla n_0}{n_0}\cdot(\nabla\otimes\nabla n_2) - 3\left(\frac{\nabla n_0}{n_0}(\nabla\otimes\nabla n_2)\right)\cdot\frac{\nabla n_0}{n_0}\right],
\end{aligned}$$

$$\begin{aligned}
\partial_t n_3 &= \tau \left(\operatorname{div}\left(\nabla n_3 + \nabla V n_3\right)\right) - 4\tau\alpha(\partial_{x_1} n_1 + \partial_{x_2} n_2) - 2\tau\alpha(\partial_{x_1} V n_1 + \partial_{x_2} V n_2) - 8\tau\alpha^2 n_3 \\
&+ \frac{\varepsilon^2}{6{n_0}^3}\left((\nabla n_1 \cdot \nabla n_0 - (n_0\Delta n_1))n_2 - (\nabla n_2 \cdot \nabla n_0 - (n_0\Delta n_2))n_1\right) + \\
&+ \tau\frac{\varepsilon^2}{12}\left[\mathfrak{A}(N)n_3 + \mathfrak{B}(N)\cdot\nabla n_3 + \mathfrak{C}(n_0)\Delta n_3 - \frac{4}{{n_0}^2}\Big((\nabla n_1 \cdot \nabla n_0 - (n_0\Delta n_1))n_2 - (\nabla n_2 \cdot \nabla n_0 - (n_0\Delta n_2))n_1\Big)\right] \\
&+ \tau\frac{\varepsilon^2}{12}\left[\Delta(\Delta n_3) + 2\frac{\nabla n_0}{n_0}\cdot\nabla\Delta n_3 + 2\frac{\nabla\otimes\nabla n_0}{n_0}\cdot(\nabla\otimes\nabla n_3) - 3\left(\frac{\nabla n_0}{n_0}(\nabla\otimes\nabla n_3)\right)\cdot\frac{\nabla n_0}{n_0}\right].
\end{aligned}$$

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C. Addendum Large Time Asymptotics

C.1. A boundedness result

The following lemma is an extension of a result due to Kowalczyk [Kow05], based on an iteration technique [Ali79]. It slightly generalizes [JNS15, Lemma A.1]. Although the result should be known to experts, we present a proof for completeness.

Lemma C.1.1 (Boundedness from iteration)**.** *Let $\Omega \subset \mathbb{R}^d$ ($d \geq 1$) be a bounded domain and let $w_i^{q/2} \in L^2(0,T;H^1(\Omega)) \cap C^0([0,T];L^2(\Omega))$ for all $q \in \mathbb{N}$ with $q \geq 2$ with $w_i \geq 0$, $w_i = 0$ on $\partial\Omega$, and $w_i(0) = 0$ in Ω for $i = 1,\dots,n$. Assume that there are constants K_0, K_1, $K_2 > 0$ and α, $\beta \geq 0$ such that for all $q \geq 2$, $t > 0$,*

$$\int_\Omega e^t \sum_{i=1}^n w_i(t)^q dx + K_0 \int_0^t \int_\Omega e^s \sum_{i=1}^n |\nabla w_i^{q/2}|^2 dxds \\ \leq K_1 q^\alpha \int_0^t \int_\Omega e^s \sum_{i=1}^n w_i^q dxds + K_2 q^\beta e^t. \tag{C.1}$$

Then

$$w_i(t) \leq K = K_3 \Big(\sum_{i=1}^n \|w_i\|_{L^\infty(0,\infty;L^1(\Omega))} + 1 \Big) \quad \text{in } \Omega,\ t > 0,$$

where K_3 depends only on α, β, d, Ω, K_0, K_1, and K_2.

Proof. We apply the Gagliardo–Nirenberg inequality [Zei90b, p. 1034] with $\theta = d/(d+2) < 1$ and the Poincaré inequality to deal with the integral over w_i^q on the right-hand side of (C.1):

$$\int_\Omega w_i^q dx = \|w_i^{q/2}\|_{L^2(\Omega)}^2 \leq C_1 \|\nabla w_i^{q/2}\|_{L^2(\Omega)}^{2\theta} \|w_i^{q/2}\|_{L^1(\Omega)}^{2(1-\theta)} \\ \leq \varepsilon \|\nabla w_i^{q/2}\|_{L^2(\Omega)}^2 + C_1^{1+d/2} \varepsilon^{-d/2} \|w_i^{q/2}\|_{L^1(\Omega)}^2$$

for any $\varepsilon > 0$. Choosing $\varepsilon = K_0/(2q^\alpha K_1)$, which is equivalent to $K_1 q^\alpha \varepsilon = K_0/2$, (C.1) becomes

$$\int_\Omega e^t \sum_{i=1}^n w_i(t)^q dx + \frac{K_0}{2} \int_0^t \int_\Omega e^s \sum_{i=1}^n |\nabla w_i^{q/2}|^2 dxds \\ \leq C_2 q^{\alpha(1+d/2)} \int_0^t e^s \sum_{i=1}^n \|w_i\|_{L^{q/2}(\Omega)}^q ds + K_2 q^\beta e^t,$$

where C_2 depends on d, K_0, and K_1. We obtain

$$\sum_{i=1}^n \|w_i(t)\|_{L^q(\Omega)}^q \leq C_2 q^{\alpha(1+d/2)} \int_0^t e^{-(t-s)} \sum_{i=1}^n \|w_i(s)\|_{L^{q/2}(\Omega)}^q ds + K_2 q^\beta$$

and, taking the supremum over time,

$$\sup_{0<s<t} \sum_{i=1}^n \|w_i(s)\|_{L^q(\Omega)}^q \leq C_2 q^{\alpha(1+d/2)} (1 - e^{-t}) \sup_{0<s<t} \sum_{i=1}^n \|w_i(s)\|_{L^{q/2}(\Omega)}^q + K_2 q^\beta \\ \leq C_2 q^{\alpha(1+d/2)} \sup_{0<s<t} \sum_{i=1}^n \|w_i(s)\|_{L^{q/2}(\Omega)}^q + K_2 q^\beta.$$

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We choose $q = 2^k$ for $k \geq 0$ and set $b_k = \sum_{i=1}^n \|w_i\|_{L^\infty(0,T;L^{2^k}(\Omega))}^{2^k} + 1$. Then

$$\begin{aligned} b_k &\leq C_2 2^{\alpha(1+d/2)k} \sum_{i=1}^n \|w_i\|_{L^\infty(0,T;L^{2^{k-1}}(\Omega))}^{2^k} + (K_2+1)2^{\beta k} \\ &\leq \max\left\{C_2 2^{\alpha(1+d/2)}, (K_2+1)^{1/k} 2^\beta\right\}^k \left(\sum_{i=1}^n \|w_i\|_{L^\infty(0,T;L^{2^{k-1}}(\Omega))}^{2^k} + 1\right) \\ &\leq \max\left\{C_2 2^{\alpha(1+d/2)}, (K_2+1) 2^\beta\right\}^k \left(\sum_{i=1}^n \|w_i\|_{L^\infty(0,T;L^{2^{k-1}}(\Omega))}^{2^{k-1}} + 1\right)^2 \\ &= \gamma^k b_{k-1}^2, \end{aligned}$$

where

$$\gamma = \max\left\{C_2 2^{\alpha(1+d/2)}, (K_2+1)2^\beta\right\}.$$

To solve this recursion, we set $c_k = \gamma^{k+2} b_k$. Then

$$c_k \leq \gamma^{2(k+1)} b_{k-1}^2 = (\gamma^{k+1} b_{k-1})^2 = c_{k-1}^2,$$

which gives $c_k \leq c_0^{2^k} \leq \gamma^{2^{k+1}} b_0^{2^k}$. Consequently, $b_k = \gamma^{-k-2} c_k \leq \gamma^{2^{k+1}-k-2} b_0^{2^k}$ and, after taking the 2^kth root,

$$\|w_i\|_{L^\infty(0,T;L^{2^k}(\Omega))} \leq b_k^{2^{-k}} \leq \gamma^{2-2^{-k}(k+2)} \left(\sum_{i=1}^n \|w_i\|_{L^\infty(0,T;L^1(\Omega))} + 1\right).$$

The limit $k \to \infty$ concludes the proof. $\square$

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