

Entanglement in Bragg Scattering

Ao. Univ. Prof. Peter Schattschneider¹, Assoc.-prof. Stefan Löffler¹

¹TU Wien, Wien, Austria

Whenever two quantum systems interact and their state changes (in a non-separable way), they become entangled. In essence, they can no longer be seen as two separate systems, but rather as a single, large system (until they decohere). Since electron microscopy deals with elementary particles as well as structures and processes on the atomic scale – i.e., quantum objects – entanglement is fundamental. In inelastic scattering (EELS), this has been embraced fully for quite some time by the use of the mixed dynamic form factor (MDFF) [1,2]. To our knowledge, the same cannot be said for the much more widespread (and theoretically simpler) case of elastic scattering.

The strange effects of entanglement occur also in Bragg diffraction, as we are dealing with the two interacting quantum systems of the probe beam and the crystal. Take the two-beam case as an example: Measuring in the diffraction plane and detecting the probe electron in the 0 or in the g diffracted beam results in a momentum transfer of either 0 or $-g \hbar$ to the scatterer. On the other hand, measuring in the image plane leaves the scatterer in a quantum superposition of two states with different momenta like Schrödinger's cat. This shows that a measurement on one part of an entangled system can have an effect on the other [3]. Therefore, it is critical to include entanglement in the theoretical description of the process to get complete and accurate predictions.

In this work, the joint quantum state of the probe beam and crystal system is described by its density matrix [4] which captures all aspects of the state. It allows to predict the evolution of the state and the outcome of measurements on parts of the system (the beam electron in the present context) by virtue of the reduced density matrix. In the 1-dimensional case, the N degrees of freedom of the scatterer (the positions of the N atoms) can be rewritten as $N-1$ relative coordinates of a rigid lattice and the position of the center of mass (CM). It is shown that the diagonal elements of the density matrix in a momentum basis correspond to the well-known scattering distribution from conventional kinematic scattering theory. The relative coordinates define the amplitude whereas the CM position imprints a lattice periodic phase factor. Apart from the diagonal terms, the reduced density matrix features off-diagonal elements, which give insight into correlation and interference effects. Among other things, these can be used for determining the decoherence properties of the electron beam.

A rigorous treatment of the entangled system “probe electron/crystal” leads to the standard (reciprocal space) description of Bragg diffraction as scattering on a static periodic Coulomb potential. But on top of that, it also

contains additional information on the quantum system, that is accessible in other bases (such as in position space). This work sheds light onto the quantum mechanical measuring process in the context of electron microscopy and therefore contributes to a better understanding on a fundamental level.

[5]

Keywords:

scattering, entanglement, interaction, quantum mechanics

Reference:

- [1] H. Kohl, H. Rose: *Adv. El. El. Phys.* 65 (1985) 173
- [2] P. Schattschneider et al.: *Micron* 31 (2000) 333
- [3] P. Schattschneider, S. Löffler: *Ultramicroscopy* 190 (2018) 39
- [4] K. Blum: *Density Matrix Theory and Applications*. Springer 1996
- [5] SL acknowledges financial support by the Austrian Science Fund (FWF) under grant nr. I4309-N36. PS thanks Helmut Kohl for valuable comments