Type of presentation: Oral

IM6-O-1 Entanglement in Bragg Scattering

Stefan Löffler[a], Stefan Nimmrichter[b], Dennis Rätzel[c], Philipp Haslinger[a], Peter Schattschneider[a]

[a]*TU Wien, Austria*

[b]*Universität Siegen, Germany*

[c]*Universität Bremen, Germany*

Contact email: stefan.loeffler@tuwien.ac.at

The transmission electron microscope (TEM) is a ubiquitous tool for material characterization. One of its core features is its supreme spatial resolution down to the sub-Angstrom range, owing to the electron beam's short wavelength. The dominant method of interaction between the electron beam and the sample is the long-ranged Coulomb interaction, which gives rise (among other things) to the well-known Bragg scattering in crystalline samples. Therefore, at its core, Bragg scattering is a quantum-mechanical process, which we can describe by a unitary transformation acting on the joint quantum state of electron and sample. Given that such a unitary transformation can entangle the two systems [1,2], the question naturally arises in what way this affects the Bragg scattering signal.

In this work, we present a full quantum-mechanical treatment of Bragg scattering based on a density matrix that describes the joint quantum state of the electron and of the atoms in the sample. Unlike the traditional description as scattering of the probe electron's wavefunction in a fixed external potential that is treated as a perturbation in a one-electron model, the density matrix allows us to describe changes in the combined electron-scatterer wavefunction, e.g., upon Bragg scattering.

We show that the electron beam and the sample do become entangled and that the purity of the electron beam state after tracing out the sample states decreases as a function of the overlap between different sample states. This can have measurable consequences, e.g., reducing the contrast of the lattice fringes in high-resolution images [3]. However, in the limit of an increasingly heavy rigid lattice, our model approaches the standard treatment of a single probe electron in a fixed external potential.

Another interesting aspect that can be studied in the density-matrix formulation of Bragg scattering is time dependence. When the sample can be considered to be in a single, freely evolving quantum state, this state naturally broadens over time. This, in turn, affects the interaction with the electron beam, leading to a change in purity depending on the evolution time after the preparation of the sample state. With latest-generation ultra-fast TEMs, it should be possible to detect and exploit these changes, giving rise to a new way for studying quantum decoherence with a TEM. In fact, it was recently proposed to exploit the entanglement between an electron and a levitated nanocrystal sample as a means to bring the sample's centre of mass into a quantum superposition state [4].

The full quantum description of Bragg scattering not only broadens our horizon and allows deeper insights into the quantum mechanical scattering occurring inside a TEM, it also paves the way for novel quantum metrology. At the same time, it confirms inherited convictions that in the limit of heavy rigid lattices, "classical TEM" works as we have come to expect.

References:
1. P. Schattschneider, S. Löffler, *Ultramicroscopy*, **2018**, 190, 39-44.
2. P. Schattschneider, S. Löffler, H. Gollisch, R. Feder, *Ultramicroscopy*, **2020**, 241, 146810
3. S. Löffler et al., in preparation
4. S. Nimmrichter, D. Rätzel, I. Bicket, M. Seifner, P. Haslinger, arXiv:2502.13821, **2025**