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Simulation of electron-material interactions in electron microscopy using quantum trajectories SAMANTHA RUDINSKY, McGill University, ANGEL S. SANZ, Complutense University of Madrid, RAYNALD GAUVIN, McGill University — Experimental data obtained from transmission imaging in scanning electron microscopy (SEM) is complex and must be coupled with simulations in order to be properly interpreted. Current methods rely on fast electron assumptions which restrict their applicability to high energy systems. This work utilizes the Bohmian formulation of the quantum theory in order to simulate electron-specimen interactions such as diffraction and particle scattering using parameters specific to SEM, such as low energies and high tilt angles, in order to improve current methods. With this computational technique, trajectories whose equation of motion is dependent upon the wave function can provide a physical representation of the system and indicate the quantum flow. Trajectories representing a beam of electrons incident on a thin specimen show how electron-material interactions affect resulting diffraction data under a variety of initial SEM conditions. Comparisons are made to current dynamical diffraction theories in order to explain their underlying mechanisms. Use of a spectral method to compute the wave function emulates a time-dependent system and can display phenomena such as electron backscattering, currently not possible with existing diffraction image simulation algorithms.

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