Conceptual issues, practicalities and applications of Bohmian Trajectories in Nanoelectronics

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Abstract

For many years quantum transport in nanostructures has benefited from the interpretive power of Bohmian trajectories by the *post-processing* of direct quantum calculations for either wave-functions or non-equilibrium Green's Functions. The resulting trajectories are deterministic with interesting topological properties. Non-deterministic trajectories have also been advocated in an extension of Bohmian mechanics to a stochastic form but have had limited application. The possibilities for using *ab initio* Bohmian mechanics as a direct self-contained simulation tool is discussed in the light of modern semiconductor device simulation where the quantum potential is widely deployed as a calibratable function for incorporating effects of quantum confinement, quantum transport and tunnelling within drift-diffusion modelling. Similar quantum corrections have been made to Ensemble Monte Carlo methodology. However, there are severe limitations to using the quantum potential alone, particularly if vortex motion is present in the current flow. It is then not possible to derive the velocity field from the carrier density alone. Generalisations, based on gauge invariance, to include a quantum vector potential have been suggested and explicit examples constructed. These simple pictures have been corroborated by full self-consistent Non-Equilibrium Green's function computations on nano-structured devices where the quantum hydrodynamic velocity field is obtained directly. A heuristic topologically-based method to derive *ab initio* velocity fields (trajectory families) is outlined and a quasi-string formalism is used to show that coherent quantum states are reconstructible from a variational principle for quantum trajectories. Finally, the impact of dissipation and decoherence is briefly discussed in the context of atomistically variable semiconductor devices.