Quantum Wavepacket Dynamics using the de Broglie-Bohm Formulation of Quantum Mechanics

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Abstract

A time-dependent quantum wavepacket propagation method based on the de Broglie-Bohm formulation of quantum mechanics is discussed. The quantum hydrodynamical equations are solved in the Lagrangian viewpoint using a meshless method based on a Moving Least Squares (MLS) approach. A grid adaptation scheme is described which adds computational particles in regions where the particle density becomes too small or the gradient of the wavefunction becomes too large. Similarly, particles are removed in regions where the particle density becomes too large or the magnitude of the wavefunction becomes too small. Numerical errors in the calculated transmission and reflection probabilities for 1D and 2D tunneling problems are shown to be related to the grid spacing and the order of the local polynomial expansion in the MLS approach. As the reflected wavepacket develops nodes, the quantum potential and force become singular and numerical instabilities occur. By using a grid adaptation scheme and a 4th order MLS, the wavepacket can be propagated for long enough times to give converged probabilities before the instabilities become problematic. However, state-to-state quantum reactive scattering calculations will require even longer propagation times and possible schemes for overcoming the instabilities are discussed.