An Iterative Finite Difference Method for Solving the Quantum Hydrodynamic Equations of Motion

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Abstract

The direct numerical solution of the quantum hydrodynamic equations of motion associated with the de Broglie-Bohm formulation of quantum mechanics is non-trivial. Even for the simplest problems, the quantum "probability fluid" exhibits characteristics that are numerically very challenging to deal with, such as: unsteady compressible flow with zero viscosity. In addition to these properties, the quantum potential ("pressure") is a non-linear function of the probability density itself. Furthermore, the quantum potential is non-local and can become singular during the course of a calculation. In recent years, much progress has been made in developing numerical methods for overcoming these difficulties. A promising new approach called the Iterative Finite Difference Method (IFDM) will be discussed. The methodology is based on an iterative solution of the coupled non-linear hydrodynamic equations using a finite difference approximation for evaluating the numerical derivatives. The method is second order accurate in both space and time and exhibits exponential convergence with respect to the iteration count. It is stable, computationally efficient, and straightforward to implement on a computer. Several example scattering calculations using this method will be presented.