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A novel approach to Bohmian mechanics using an uncompressed particle method

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ABSTRACT

We propose extending Bohmian mechanics (BM) with the moving particle semi-implicit method, a particle method for uncompressed fluids. The application of this method prevents the node of the Bohm quantum potential from breaking numerical calculations while maintaining a low calculation cost. We validated our extended method by comparing our results with those from the conventional method for a one-dimensional harmonic oscillator, Gaussian barrier and rectangular barrier. The proposed method was found to simulate the temporal changes in the probability density for a rectangular barrier. In addition, the relational equation obtained by this method reveals an interesting correspondence between the pressure of a classical fluid and the Bohm quantum potential.

1. Introduction

Quantum wave packet dynamics methods have been used to understand dynamical phenomena with quantum effects across a wide range of fields in chemistry and physics. Quantum wave packet dynamics simulations rely on solving the time-dependent Schrödinger equation (TDSE) using numerical methods, namely, the Euler method, the Fourier method, and the perturbation method. In 1999, the quantum trajectory method (QTM) was proposed by Wyatt [1,2] as a quantum wave packet dynamics method. The QTM is a numerical method based on a hydrodynamic formulation of quantum mechanics, which was first proposed by Madelung [3] and de Broglie [4] and subsequently developed as Bohmian mechanics (BM) by Bohm [5,6]. In contrast to the conventional methods, the QTM can be simulated in Lagrange coordinates. As the use of Lagrange coordinates allows the coordinate grids to be moved, rather than being fixed, the QTM affords the following advantages: (1) the calculation cost can be reduced because the frame of interest can be extracted, (2) it is not necessary to consider boundary conditions because the grids move during the calculations, and (3) hydrodynamic algorithms can easily be adapted.

BM is derived by assuming that the wave function is described by a polar form and substituting it into the TDSE. The equations derived are identical in form to the classical Hamilton–Jacobi equation, but also incorporate the Bohm quantum potential. The Bohm quantum potential is known to be the source of the quantum force, and as such, it is a useful term for understanding quantum mechanics.

Since the QTM is interesting from the standpoints of both theory and numerical calculations, many researchers have attempted to develop BM. For example, Tannor and co-workers [7,8] proposed a BM framework referred to as “Bohmian mechanics with complex action” (BOMCA) by reformulating BM in complex space. Many approaches based on BOMCA have subsequently been reported, such as the development and improvement of the QTM [8–16], its expansion to adiabatic and diabatic forms [17,18], and its application to electronic quantum motions [19], slit experiments [20], quantum dot [21], and the photodissociation dynamics [22]. Furthermore, approaches to solving the Schrödinger–Langevin equation using the QTM [23–25] and adapting the QTM to general physical problems [26–30] have also attracted attention over the last few years.

However, it is known that the node of the Bohm quantum potential breaks the numerical calculation of the QTM. This problem has been resolved in a number of different ways, including incorporating artificial viscosity into the QTM [31–36], the covering function method [37,38], the bipolar decomposition approach [39–44], the phase space method [45], and the selection of transmitted trajectories for the scattering problem [46,47]. However, the optimal treatment of the Bohm quantum potential remains an open question.

In this study, to prevent the node of the Bohm quantum potential

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from breaking the numerical calculations of the QTM, we focus on the so-called "moving particle semi-implicit" (MPS) method [48–50] for uncompressed fluids, a type of particle method used in hydrodynamics that was recently proposed by Koshizuka and co-workers. By using the MPS method, we can adapt the gradient and Laplacian models to the QTM and directly calculate the gradient of the Bohm quantum potential without differentiation of the probability density. Thus, we derive the "Bohmian mechanics on particle formulation" (BOMPF) method by adapting MPS to BM. In addition, we find an interesting correspondence: the Bohm quantum potential behaves very similarly to classical pressure.

In Section 2, we describe the proposed new method for adapting MPS to BM. In Section 3, we determine the initial conditions necessary for the numerical calculation and validate this method using one-dimension harmonic oscillator, Gaussian barrier, and rectangular barrier systems. Section 4 presents our conclusions.

2. Theory

2.1. Hydrodynamic formulation of quantum mechanics

Conventional BM is formulated using the polar form of the wave function:

$$\psi(x,\,t) = \sqrt{\rho(x,\,t)}\exp\left(\frac{i}{\hbar}S(x,\,t)\right), \tag{1}$$

where $\rho(x,\,t)$ is the probability density, $S(x,\,t)$ is the action function of a real number, $i = \sqrt{-1}$, and $\hbar$ is the reduced Planck constant. By inserting the ansatz into the TDSE and separating the result into real and imaginary parts, we obtain two equations:

$$\frac{\partial\rho}{\partial t} + \nabla\left(\frac{\rho}{m}\nabla S\right) = 0, \tag{2}$$

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + Q_B + V = 0. \tag{3}$$

In these equations, m is the mass, V is the classical potential, and Q_B is the Bohm quantum potential:

$$Q_B = -\frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}. \tag{4}$$

Eq. (2) is a continuity equation. Eq. (3) is a quantum Hamilton–Jacobi equation (QHJE), which is identical in form to the classical Hamilton–Jacobi equation but also includes the Bohm quantum potential. We transform from the Euler frame to the Lagrange frame by using the following equation:

$$\frac{d}{dt} = \frac{\partial}{\partial t} + v\frac{d}{dq}, \tag{5}$$

where $v = \nabla S/m$ is the flow velocity. Substituting Eqs. (2) and (3) into Eq. (5) yields the following Lagrange equations:

$$\frac{\partial\rho}{\partial t} = -\rho\nabla v, \tag{6}$$

$$m\frac{\partial v}{\partial t} = -\nabla(Q_B + V) = \boldsymbol{f_q} + \boldsymbol{f_c}\ , \tag{7}$$

where $\boldsymbol{f_q} = -\nabla Q_B$ and $\boldsymbol{f_c} = -\nabla V$ represent the quantum and classical forces, respectively. Since Eqs. (6) and (7) resemble the formulations used in classical hydrodynamics, the quantum trajectories can be calculated by selecting and adapting the appropriate techniques from computational fluid dynamics (CFD). This method is the QTM, and it can be applied to various systems in combination with the derivative propagation method [51] and the arbitrary Lagrangian-Eulerian method [52].

2.2. Bohmian mechanics on particle formulation

In this study, we focus on the MPS method for uncompressed fluids, which is a particle method used in CFD, and adapt it to BM. The most fundamental definition for uncompressed fluids in the particle method is

$$\frac{d\rho_i}{dt} = -\rho_i\nabla\cdot v = 0. \tag{8}$$

This equation implies that the probability density ρ_i of each particle i is always constant. Instead, we introduce the particle number density $n_i(x)$ for each particle i, which enables the calculation of the probability density as a function of the coordinate:

$$n_i(x) = \sum_{j\neq i} w_{\rho(x)}(r_{ij}), \tag{9}$$

where the subscripts i and j denote each particle, $r_{ij} = |r_j - r_i|$ is the interparticle distance between i and j, and w is the weight function with respect to r_{ij}. The subscript of each weight function denotes the physical quantity expressed by that weight function. In this study, to describe the probability density $\rho(x)$ as a function of the coordinate, the Bohm quantum potential Q_B, and the gradient of the Bohm quantum potential, we use the following weight functions:

$$w_{\rho(x)}(r_{ij}) = a_1\exp(-a_2 r_{ij}^2), \tag{10}$$

$$w_{Q_B}(r_{ij}) = a_3\exp(-a_4 r_{ij})\exp(-a_5 r_{ij}^2)\exp(-a_6 r_{ij}^3), \tag{11}$$

$$w_g(r_{ij}) = a_7\exp(-a_8 r_{ij}^2), \tag{12}$$

where a_1 to a_8 are arbitrary constants. The use of a weight function allows the introduction of an influence area r_e to eliminate the influence of particles that are separated from each other. Thus, unnecessary calculations can be avoided, which reduces the calculation cost as well as preventing the node of the Bohm quantum potential from breaking the numerical calculations. The values of a and r_e will be determined in Section 3.

It is known that the probability density $\rho^k(x)$ and the particle number density $n^k(x)$ are related via the following equation [53]:

$$\frac{\rho^k(x) - \rho^0}{\rho^0} \cong \frac{n^k(x) - n^0}{n^0}\ , \tag{13}$$

where the superscript k represents the time step, n^0 is the standard particle number density, and ρ^0 is the standard fluid density.

We can then rewrite the QHJE on Lagrange coordinate in Eq. (7). Since $\hbar$ is the source of quantum effects, all of the quantum effects of a system are concentrated in the Bohm quantum potential Q_B. Thus, we can separate Eq. (7) into a classical mechanics component and a quantum mechanics component:

$$\text{classical mechanics component: } m\frac{v(t+\alpha) - v(t)}{\partial t} = -\nabla V \tag{14}$$

$$\text{quantum mechanics component: } m\frac{v(t+dt) - v(t+\alpha)}{\partial t} = -\nabla Q_B\ , \tag{15}$$

where α is the time affected by ∇V. Naturally, if we take the limit as $\hbar \to 0$, Q_B and α become zero. Thus, the wave packet behaves like a classical fluid. Differentiation of both sides of Eq. (15) affords the following equation:

$$m\frac{\nabla v(t+\alpha)}{dt} = \nabla^2 Q_B\,, \tag{16}$$

where we used $\nabla v(t) = \nabla v(t+dt) = 0$ derived from Eq. (8). For time $t+\alpha$, the probability density is not constant because ∇v changes only with the classical potential. Therefore, Eq. (16) has the effect of making the probability density constant again. Then, taking the time difference of Eq. (6) gives