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Computation of transmission probabilities for thin potential barriers with transmitted quantum trajectories

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ABSTRACT

A computational method is presented for the evaluation of transmission probabilities for thin potential barriers by evolving an ensemble of transmitted quantum trajectories. A single row of second-order trajectories computed using the derivative propagation method is propagated to determine the initial conditions for transmitted quantum trajectories. As time evolves, trajectories reflected from the potential barrier are deleted from the ensemble. This method is applied to a two-dimensional system involving either a thin Eckart or Gaussian barrier along the reaction coordinate coupled to a harmonic oscillator. Transmission probabilities are in good agreement with the exact results.

1. Introduction

As an alternative interpretation to nonrelativistic quantum mechanics, Bohmian mechanics provides an insightful trajectory description of quantum phenomena from a hydrodynamic point of view [1–3]. For example, it has been shown that the Bohmian paths of the electrons for Rydberg atoms are ellipses to a high degree of approximation even for arbitrary widths of the wave packets [4]. Bohm's interpretation has been applied to the quantized spherically-symmetric blackhole coupled to a massless scalar field [5]. Quantum recurrences for the excited hydrogen atom in a magnetic field have been analyzed using Bohmian trajectories [6]. The geometric phase has been studied within the complex quantum Hamilton–Jacobi formalism [7]. The uncertainty principle in one-dimensional systems has been analyzed using complex Bohmian trajectories [8]. Moreover, the trajectory formulation of quantum mechanics has been utilized to analyze a broad range of physical processes [9,10], such as atom-surface diffraction and the dissociation of molecules at metallic surfaces [11,12], quantum nonlocality [13], and quantum interference [14,15].

Quantum wave packet dynamics can provide considerable insight into problems of interest in chemical physics. Wave packet methods can achieve solutions for far more complicated systems than the time independent methods [16,17], and these methods have been applied to quantum reactive scattering [18–22]. Various synthetic quantum trajectory approaches have been developed to study quantum barrier scattering problems. The quantum trajectory method (QTM) has been introduced as a computational tool to solve the time-dependent Schrödinger equation (TDSE) by evolving ensembles of quantum trajectories through the integration of the hydrodynamic equations *on the fly* [23–25]. Since then, more robust QTMs have been developed and applied to a diverse range of quantum systems with increasing complexity and dimensionality [26].

An important feature of the QTM is that quantum trajectories follow along with the evolving probability density. Because of this property, the quantum trajectory formalism significantly reduces the computational effort relative to conventional computational (fixed grid or basis set) techniques for solving the TDSE. However, singularities in the quantum hydrodynamic equations of motion may occur in regions of wave interferences, and this results in numerical breakdown of the trajectory propagation. Thus, much effort has been spent on developing methods to deal with the node problem. For example, artificial viscosity can be introduced into the equations of motion to moderate the strong quantum force in nodal regions by preventing nodes from fully forming [27–33]. Based on the propagation of node-free functions, the covering function method [34,35] and the bipolar decomposition approach [36–44] have been utilized to avoid the node formation during the trajectory evolution.

In our previous study [45], a straightforward computational method was proposed to compute time-dependent reaction probabilities by evolving *transmitted* quantum trajectories. An ensemble

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of trajectories is initially launched from the reactant region toward the potential barrier. As time progresses, trajectories with negative translational velocities are deleted, and this process gradually removes the reflected trajectories from the trajectory ensemble. After the wave packet splits into reflected and transmitted parts, the reflected trajectories are completely deleted from the ensemble. All the remaining trajectories are definitely headed for the transmitted region, and they describe the transmitted subensemble of the wave packet. The removal process of reflected trajectories avoids numerical instabilities resulting from singularities in the quantum potential near nodal regions. This method is specifically suitable for *thick* barrier scattering problems. However, as discussed in the previous studies [46–48], solutions depend strongly on the quantum potential for *thin* barrier scattering problems. Thus, the removal of the reflected trajectories from the ensemble cannot yield accurate solutions for thin barriers.

The purpose of this study is to extend our previous computational method for thick barriers to thin barriers. For two-dimensional barrier scattering problems, a single row of second-order trajectories computed using the derivative propagation method (DPM) [49–52] along the translational coordinate is propagated to determine the appropriate initial conditions for transmitted quantum trajectories. The complex quantum Hamilton–Jacobi equation (CQHJE) is solved for the complex action by evolving an ensemble of *transmitted* quantum trajectories. As time evolves, trajectories reflected from the potential barrier are deleted from the ensemble. Because the initial trajectory ensemble is sampled from the appropriate initial positions, most trajectories correspond to the transmitted component of the wave packet. Then, the computational methodology is applied to a two-dimensional system involving either a thin Eckart or Gaussian barrier along the reaction coordinate coupled to a harmonic oscillator. In addition, computational results are presented for time-dependent transmission probabilities evaluated by the time integration of the probability flux using transmitted quantum trajectories.

The organization of the remainder of this study is as follows. In Section 2, the potential energy surfaces involving both thin Eckart and Gaussian barriers are described and the initial wave packet is presented. In Section 3, we employ the arbitrary Lagrangian–Eulerian (ALE) method to derive the CQHJE along Bohmian trajectories. The moving least squares (MLS) algorithm employed in quantum trajectory calculations is described for the calculation of the spatial derivatives of the complex action. We propose a method to determine the appropriate initial positions for transmitted trajectories. In Section 4, computational results and analysis are presented for the transmitted wave packet and transmission probabilities. In Section 5, we make some comments and present suggestions for further study.

2. Model two-dimensional scattering problem

We consider a Gaussian wave packet scattering from a two-dimensional potential barrier given by

$$V(x, y) = V_{\text{trans}}(x) + \frac{1}{2}k(x)y^2, \tag{1}$$

where x and y denote the translational and vibrational coordinates, respectively. The potential energy surface is either an Eckart or a Gaussian barrier of height V_0 centered at $x = 0$, which is coupled to a vibrational mode with a variable force constant along x. The translational component of the potential is either an Eckart barrier, $V_{\text{trans}}(x) = V_0\,\text{sech}^2(\alpha x)$, or a Gaussian barrier, $V_{\text{trans}}(x) = V_0\,\exp(-\gamma x^2)$. The variable force constant $k(x) = k_0[1 - \sigma\exp(-\lambda x^2)]$ reaches its minimum value, $k_0(1-\sigma)$, at the barrier maximum ($x = 0$). The values of the parameters are given as $V_0 = 0.035$, $k_0 = 0.09$, $\sigma = 0.1$, and $\lambda = 1$. All quantities are given in atomic units throughout this study ($\hbar = 1$). Two width parameters were used: $\alpha = 3$ for the Eckart barrier and $\gamma = 7$ for the Gaussian barrier [47,48].

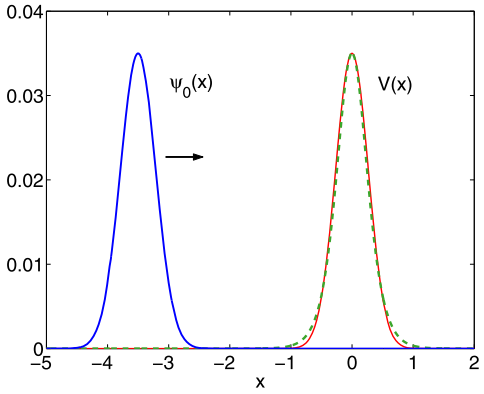

Fig. 1. (Color online.) Absolute value of the initial wave function (blue solid curve) and the thin Eckart (green dashed curve) and Gaussian (red solid curve) barriers plotted along the x axis. The wave function has been scaled to have the same height as the potential barrier.

The initial Gaussian wave packet is given by

$$\psi_0(x, y) = \left(\frac{4\beta_x\beta_y}{\pi^2}\right)^{1/4} e^{[-\beta_x(x-x_c)^2-\beta_y y^2+ik_x x]}, \tag{2}$$

where the center of wave packet is located at $x_c = -3.5$ and $y = 0$. The initial wave packet has a momentum $\hbar k_x$ toward the product region, where $k_x = \sqrt{2mE}/\hbar$, $m = 2000$, and E is the mean translational energy. The width parameters for the translational and vibrational motion are given by $\beta_x = 6$ and $\beta_y = \sqrt{mk_0}/(2\hbar)$. As shown in Fig. 1, the Eckart or Gaussian potential energy surface described in this study has slightly smaller half-width than the initial wave packet. Hence, these two barriers are considered to be "thin" barriers.

3. Computational method

3.1. Complex quantum Hamilton–Jacobi equation with Bohmian trajectories

The CQHJE-BT method has been proposed to solve the CQHJE by evolving an ensemble of Bohmian trajectories (BT) [53,54]. Substituting the exponential form of the wave function, $\psi(\vec{r}, t) = \exp[iA(\vec{r}, t)/\hbar]$, into the TDSE yields the CQHJE

$$-\frac{\partial A}{\partial t} = \frac{1}{2m}(\vec{\nabla}A)^2 + V(\vec{r}) + \frac{\hbar}{2mi}\nabla^2 A, \tag{3}$$

where $A(\vec{r}, t)$ is the complex action. In order to derive the equations of motion for the complex action along Bohmian trajectories, we consider a transformation from the Eulerian partial time derivative to the total time derivative

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \left(\frac{d\vec{r}}{dt}\right)\cdot\vec{\nabla}. \tag{4}$$

In the real-valued quantum trajectory method [26], the grid velocities are specified according to the guidance equation for Bohmian trajectories

$$\frac{d\vec{r}}{dt} = \frac{1}{m}\text{Re}\left[\vec{\nabla}A\right], \tag{5}$$

where Re represents the real part. These grids behave as fluid elements which follow the evolving probability density. In the ALE representation, the CQHJE in Eq. (3) can be written as

$$\frac{dA}{dt} = -\frac{1}{2m}(\vec{\nabla}A)^2 - V(\vec{r}) - \frac{\hbar}{2mi}\nabla^2 A + \frac{1}{m}\text{Re}\left[\vec{\nabla}A\right]\cdot\vec{\nabla}A. \tag{6}$$