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Quantum-trajectory calculations of proton–hydrogen model collisions

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ABSTRACT

We investigate a proton–hydrogen model collision using a method based on the de Broglie–Bohm formulation of quantum dynamics. By studying the quantum-trajectories of the particles we obtain approximate ionization and capture cross sections that are in good agreement with the exact values. In particular, the implementation of this high-order approximation method allows us to solve each *trajectory* independently. The method has a relatively low computational cost and can be straightforwardly parallelized for many bodies systems.

1. Introduction

The theoretical investigation on atomic transition processes has recently seen dramatic improvements through the growth of computing power and development of new computational techniques that allows the implementation of fully-numerical solutions to the Schrödinger equation [1,2]. Despite the bright future of numerical-extensive full solutions, they are currently available only for the simpler three- and four-body systems [3]. A complementary approach is given by methods based on perturbative approximations, providing good results with relatively low-computer requirements [4,5]. However, there is an increasing interest on pursuing the development of fully-numerical methods that could be generalized to more complex systems. In fact, nowadays one of the main requirements of computer-intensive methods is their scalability for increasing degrees of freedom of the system.

The hydrodynamical formulation of quantum mechanics, based on the de Broglie–Bohm interpretation, allows the exact resolution of a system's time evolution in an alternative approach to those employing spatial grids or basis expansions [6–8]. The method was proposed initially as an interpretative tool to quantum mechanics [8,9] except for a few early efforts [10–12]. However, recently there has been a renewed interest in employing this formulation as a computing method. Several authors implemented resolutions of quantum mechanical problems in this framework by means of the so-called "quantum-trajectories method" (QTM) [13–17]. This approach, based on Bohm's formulation of quantum mechanics [6,7], describes the quantum dynamics in terms of pseudo-particles that evolve obeying equations similar to those of classical-mechanics. While this treatment in terms of trajectories represents a full solution of the time-dependent Schrödinger equation (TDSE), its main drawbacks are due to the strong coupling among trajectories and the instability of some of the resulting equations [17]. Nonetheless, its scalability characteristics, through parallel implementations and Monte Carlo methods, make the quantum-trajectory approach a promising field for the investigation of many-particle collision processes.

In this communication, we present benchmark model calculations of ion–atom collisions employing approximations to the quantum-trajectory method. In particular, we implement and investigate a method suggested a few years ago in order to circumvent the problems arising from the strong coupling among the trajectories [18]. The resulting equations, obtained from rewriting the de Broglie–Bohm equations, uncouple the quantum-trajectories, allowing us to solve each of them individually. Each trajectory becomes the solution of a system of infinite coupled differential equations that can be solved at different levels of approximation.

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2. General approach

The hydrodynamical formulation of quantum mechanics may be obtained by writing the wavefunction in polar form $\psi(\vec{r},\vec{t}) = \sqrt{\rho(\vec{r},\vec{t})}\exp^{iS(\vec{r},\vec{t})/\hbar}$ [17]. Thus, the time-dependent Schrödinger equation (TDSE),

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)\right)\psi(\vec{r},t)$$

may be transformed to a system of coupled differential equations, similar to those obtained in classical-mechanics,

$$\frac{\partial\rho(\vec{r},t)}{\partial t} = -\vec{\nabla}\vec{j}(\vec{r},t), \tag{1}$$

$$-\frac{\partial S(\vec{r},t)}{\partial t} = \frac{(\vec{\nabla}S(\vec{r},t))^2}{2m} + V(\vec{r}) + Q(\vec{r},t), \tag{2}$$

where m is the mass particle and the current is defined by $\vec{j}(\vec{r},t) = \frac{\rho}{m}\vec{\nabla}S$.

Eqs. (1) and (2) describe the evolution of an ensemble of correlated nodes or *particles* with well-defined trajectories. The first of the above equations expresses conservation of the density of probability. The second is a modified quantum Hamilton–Jacobi (QHJ) equation with an extra term, depending on the curvature of the amplitude, given by the so-called *quantum potential*,

$$Q(\vec{r},t) = -\frac{\hbar^2}{8m}\left[2\frac{\nabla^2\rho(\vec{r},t)}{\rho(\vec{r},t)} - \left(\frac{\nabla\rho(\vec{r},t)}{\rho(\vec{r},t)}\right)^2\right], \tag{3}$$

which comprises the quantum nature of the problem. Observe that by defining the velocity of the node as $\vec{v} = \vec{\nabla}S/m$, the QHJ may be rewritten in a reference system that moves with the node, taking the form of a Newton-like equation. We obtain for the evolution of the nodes,

$$m\frac{d\vec{v}}{dt} = -\vec{\nabla}(V+Q) = F_{\mathrm{Ext}}(\vec{r},t) + F_{\mathrm{QM}}(\vec{r},t), \tag{4}$$

$$\frac{d\rho}{dt}(\vec{r},t) = -\rho\vec{\nabla}\cdot\vec{v}(\vec{r},t). \tag{5}$$

A modern, full implementation of this method would be superior to traditional numerical methods based on griding of the space or expansion of the wavefunction in a basis. The main advantage would be that the computation is carried out only in those regions of space where the probability density is appreciable, leading to better scaling with the dimensionality of the problem. However, the calculation of the quantum potential (3) involves numerical second-order derivatives of the probability density, which are computationally expensive and prone to introducing numerical instability. There is abundant literature on implementations of the quantum-trajectory method from the above equations [13–16,19,20]. These methods include moving least square (MLS) fitting to the densities, re-sampling of the nodes and the inclusion of artificial viscosity terms that allow to stabilize the equations. Besides the success of these methods, mainly on low-dimensionality problems, their use on three-dimensional collisions involving several fragments is still uncertain.

Alternative methods, based on approximate treatment of the hydrodynamical equations have recently been developed [15,18]. These formulations provide computationally feasible solutions that may be applied to multidimensional systems.

3. Uncoupling of the quantum-trajectories

As commented above, the main obstacle for the implementation of methods based on QTM arises from the lack of reliable computations of the quantum potential. Moreover, due to the strong coupling of the trajectories they must all be solved simultaneously, requiring great computing power.

A few years ago, Liu and Makri proposed a method that allows the uncoupling of the quantum-trajectories by using their stability properties and study the evolution of wavepackets at the second-order of approximation [18]. We now discuss the proposed method and investigate some higher-order approximations in one-dimensional collision problems.

The dynamical Bohm equations from the Lagrangian point of view ((4) and (5)) may be rewritten in terms of the Jacobian $J(x(t),t) = \partial x(t)/\partial x(0)$. Thus, evolution of the probability density along a quantum-trajectory $x(t)$ is given by its initial value and the evolution of the Jacobian,

$$\rho(x_t,t) = \frac{\rho(x_0,0)}{J(x(t),t)}.$$

The evolution of the Jacobian is obtained by deriving (4) respect to the initial position x_0,

$$m\frac{d^2J(x_0,t)}{dt^2} = F^{(1)}(x,t)J(x_0,t). \tag{6}$$

In order to evaluate the quantum force, the first three derivatives of the Jacobian are needed. At the same time the evolution of the Jacobian involves the computation of high-order derivatives of the quantum force. This entanglement creates an infinite hierarchy of coupled equations that can be truncated at different orders.

The quantum force, derived from the quantum potential (3), depends on the third-order derivatives to the probability density. However, the derivatives of the Jacobian vanish at the second-order of approximation and the quantum force for a pseudo particle depends only on its initial value and the Jacobian,

$$F_q(t) = \frac{F_q(0)}{J^3(t)}. \tag{7}$$

The derivative of the quantum force needed to solve the evolution is obtained from this equation.

This simple approximation has been shown to provide good results for wavepacket evolution and some smooth barrier transmission problems [18]. However, the approximation may fail because the approximated quantum force expression (7) introduces instabilities in the evolution when the Jacobian becomes very small.

In order to obtain higher-order approximations, we start writing the general form of the quantum potential in terms of the Jacobian along the trajectories,

$$Q(t) = \frac{Q_0}{J^2(t)} + \frac{\hbar^2}{2m}\frac{J^{(1)}(t)}{J^3(t)}\frac{\rho_0^{(1)}}{\rho_0} - \frac{5\hbar^2}{8m}\left(\frac{J^{(1)}(t)}{J^2(t)}\right)^2 + \frac{\hbar^2}{4m}\frac{J^{(2)}(t)}{J^3(t)}. \tag{8}$$

Thus, the quantum force may be obtained by taking the derivatives of (8). The resulting expressions no longer have the simple form of the second-order approximation (7) and depend on high-order derivatives of the Jacobian.

4. Model of proton–hydrogen collision

In this communication, we show results from a one-dimensional proton–hydrogen collision model. We investigate the electron distribution evolution, initially bounded to the target proton at the ground hydrogen state. In this approximation model, the projectile is moving at a constant velocity against the target. Both protons are described by an Eckart potential,

$$V(x) = \frac{-1}{\cosh^2[(x-x_c)]}, \tag{9}$$

where x_c represents the position for each proton. In this approximation the target nucleus is fixed at the origin, while the electron moves at constant velocity v_p. Initially the centers are separated at a distance of 10 a.u.