Quantum dynamics simulations using quantum trajectories

Lidice Cruz Rodriguez[a]

Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK

In this work we give a short overview of the hydrodynamic formulation of quantum mechanics, together with some examples of its application to quantum dynamics simulations using the Quantum Trajectory Method.

Investigating the real-time dynamics of many-body correlated systems is one of the major challenges in contemporary theoretical physics and chemistry. The full quantum-mechanical description requires the solution of the time-dependent Schrödinger equation (TDSE). The standard methods for exact numerical computations are based on spatial grids, basis sets of functions, or discrete variable representation. These methods have the disadvantage that while retrieving the full quantum mechanical solution, they scale exponentially with the system's dimensions, making them not applicable beyond ten degrees of freedom. In contrast, if we can treat them classically, the classical molecular dynamics methods (MD) allow modeling systems of thousands of particles by propagating ensembles of trajectories.

Therefore, looking for trajectory-based methods to perform quantum dynamics simulations is a very active field of research. A natural way of addressing this problem is to use quantum trajectories. An extended explanation of the fundamental principles and equations of this theory can be found in Ref. [1]. The starting point is expressing the wave function in terms of a real phase $S(x,t)$, and density $\rho(x,t)$,

$$\Psi(x,t) = \sqrt{\rho(x,t)}e^{iS(x,t))}. \tag{1}$$

The quantum trajectories are defined such that their velocity is,

$$\dot{x} := \left.\frac{\nabla S(x,t)}{m}\right|_x = x(t). \tag{2}$$

After substituting in the TDSE, this leads to a set of hydrodynamic equations,

$$\frac{dS}{dt} = \frac{1}{2}mv^2 - (V+Q)\ , \tag{3}$$

$$\frac{d\rho}{dt} = -\rho\frac{\partial v}{\partial x}\ , \tag{4}$$

$$m\frac{dv}{dt} = -\frac{\partial(V+Q)}{\partial x}\ . \tag{5}$$

The first two equations determine the time evolution of the hydrodynamic fields, and the last one is the equation of motion of the quantum trajectories. To solve them, we need the initial positions of the trajectories x_0 and the wave function Ψ_0 at $t=0$. The ensemble is initially distributed according to $|\Psi_0|^2 = \rho_0$, and their initial velocity is defined from Eq. (2). Under these conditions, the time evolution of the quantum trajectories renders the wave function $\Psi(x,t)$ at every time t. It is important to remember that this ensemble doesn't represent the actual material particle; each trajectory is a possible realization of a single particle. Eq. (3) is a Hamilton-Jacobi-like equation, but it has an additional term known as the quantum potential,

$$Q = -\frac{\hbar^2}{4m}\left(\frac{\nabla^2\rho}{\rho} - \frac{1}{2}\left(\frac{\nabla\rho}{\rho}\right)^2\right)\ , \tag{6}$$

which is the one bringing all the non-local effects to the dynamics. The gradient of this quantum potential is identified as the quantum force, and it enters the Newton-like equation (5) together with the classical force acting on the particles. Details about this theory and how the hydrodynamic equations are derived are given in Refs. [1] and [2].

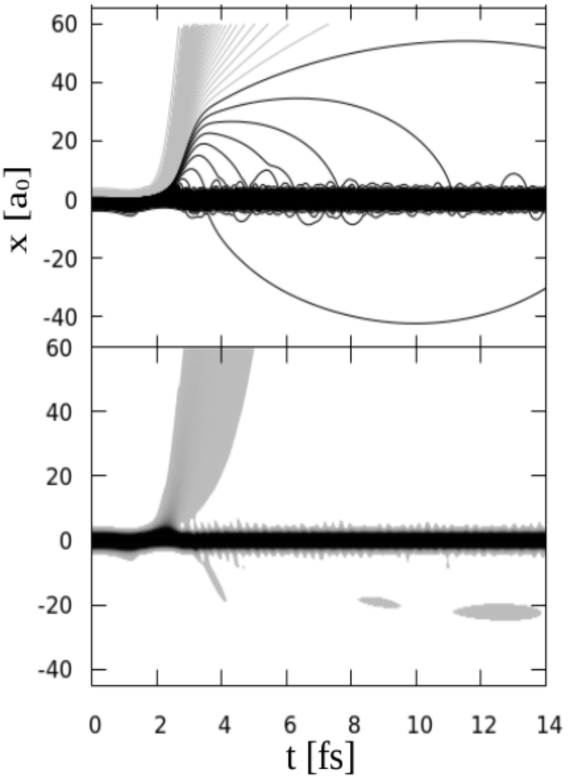

Figure 1: In the top panel we show the time evolution of an ensemble of $N = 501$ trajectories. In the bottom panel the time-dependent probability density evaluated via wave packet propagation is plotted. The figure was adapted from [5].

From the computational point of view, there are two ways of determining the time evolution of quantum trajectories. The first approach consists of solving the TDSE and, hence computing the trajectories. This leaves us with the problem we described initially, as we need to apply the standard and very computationally expensive methods to solve the TDSE.

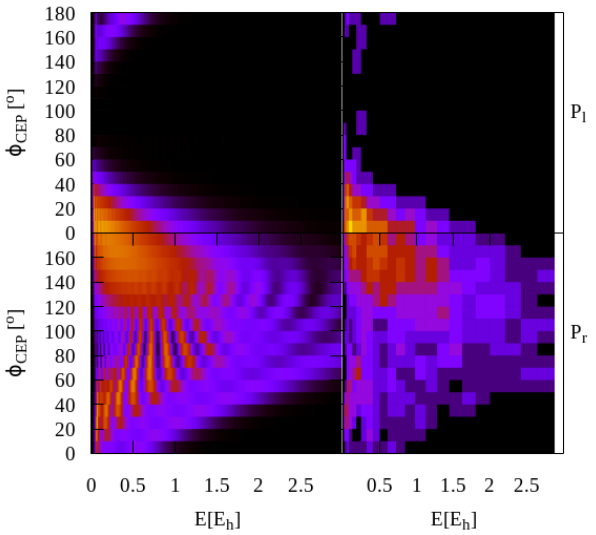

Figure 2: Density map of the left/right photo-electron spectra P_l (upper panel) and P_r (lower panel) as a function of energy and CEP parameter. The figure was taken from [5]

A different approach is based on using the trajectories as a tool to solve the Schrödinger equation. Using Eqs. (3)-(5), we can propagate the ensemble of trajectories together with the density and phase and build the wave function and any observable at every time step. A particular implementation of this approach was proposed in [3], and it is known as the Quantum Trajectory Method (QTM).

The QTM possesses many challenges from the computational point of view. One of the more important ones is evaluating the quantum potential and force at the trajectories as they form a very unstructured grid. An extended discussion about the QTM and its practical difficulties can be found in Ref [2].

In our work [4], we proposed an analytical approximation to the quantum potential and force valid for one-dimensional model systems. We applied the method to model the zero-point energy of harmonic and an-harmonic potentials and the real-time dynamics of bound and scattering problems. Furthermore, we study the laser-driven electron dynamics by strong and ultrashort laser pulses [5]. Here we will show some of the results of the latest application. More results and details about the implementation of the model and the pulse shape are given in our original publication [5].

In Fig. 1, the top panel shows the time evolution of an ensemble of $N = 501$ trajectories driven by the influence of a strong laser pulse. The bottom panel shows the results of a standard wave packet simulation used as a benchmark. The figure illustrates how the trajectories are a powerful tool to visualize the dynamics.

An interesting phenomenon to study with very short laser pulses is the impact of the Carrier Envelope Phase on the electron dynamics. In very short laser pulses, we can evaluate the asymmetry in the photo-electron spectra. The top panel of Fig. 2 shows the ionization probability (P_l) to the left, and the bottom panel the ionization probability (P_r) to the right. Within our trajectory-based approach, this is calculated by adding up how many trajectories end up in each direction. The results from our method are shown in the left column, while in the right column, we show the benchmark calculations.

Notes

a. Email: lidicecruzr@gmail.com

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