The shortest simulation-box for time-dependent computation of (Bohmian) wave packets

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INTRODUCTION

Most of our understanding of quantum electron transport is based on single-particle time-independent conditions. Studying quantum transport beyond DC requires manageable approximations for the many-body problem and the non-unitary evolution due to decoherence/measurements [1] .

We have recently shown that the Bohmian conditional wave function is a very powerful tool to deal with both quantum many-body problems and non-unitary evolutions [2], [3]. By constructions, such (Bohmian conditional) wave functions require a time-dependent evolution. In this work, we discus the numerical viability of such time-dependent (Bohmian conditional) wave-packets.

As seen in Fig. 1(a), the simulation box for time-dependent wave-packets has to include the initial state and avoid spurious reflections at $t \rightarrow \infty$. These considerations can imply simulation boxes 10 times larger than the ones used for quantum time-independent algorithms.

SHORTENING THE SIMULATION BOX

In this conference we present an algorithm that allows the time-evolution of wave packets with the shortest "time-dependent" simulation box. It has two steps:

A. Absorbing boundary conditions

The first step is using a function $g(x)$ which is 1 during the physical length L_p and goes to zero at the end of the absorbing boundary (see red lines in Fig. 1). Then, at each time step, the original wave packet $\psi(x,t)$ solution of the time-dependent Schrödinger equation (TDSE) can be substituted by $\psi'(x,t) = \psi(x,t)g(x)$, if $g(x)$ is smooth enough to commute with the Hamiltonian H [4]. The new function ψ' evolving in the simulation box in Fig. 1 (b) avoids possible spurious reflections with the absorbing boundary. The error between ψ and ψ' is:

$$Error = \frac{1}{L_p}\int_{L_p} |\psi(x,t) - \psi'(x,t)|^2 dx \qquad (1)$$

which remains very small for reasonable boundary length L_B, as seen in Fig. 3.

B. Analytical injection

The second step is an analytical injection of the wave packet outside L_P, as seen in Fig. 1(c). We decompose $\psi = \psi_0 + \psi''$ where ψ_0 is given by an analytical Gaussian wave packet in free space [4]. Using the linearity of TDSE, it can be found that ψ'' is the solution of TDSE with an explicit time-dependent potential U:

$$i\hbar\frac{\partial\psi''(x,t)}{\partial t} = H\psi''(x,t) + U(x,t)\psi_0(x,t), \quad (2)$$

Where H is the Hamiltonian operator. See the initial time in Fig. 2, $\psi''(x,0) = 0$ (blue). Then, at each time step, the original wave packet $\psi(x,t)$ is substituted by $\psi'(x,t) = \psi_0 + \psi''g(x)$. The error when using ψ'' solution of Eq. (2) with the simulation box (c) is very small for all practical situations studied in Figs. 4 and 5.

CONCLUSION

We have shown that time-dependent wave-packets are accurately computed from Eq. (2) with the simulation box of Fig. 1(c), which is 10 times smaller (faster) than typical ones of Fig. 1(a). The new algorithm presented in this conference can be applied to any type of time-dependent quantum algorithm. In particular, it certifies the computational viability of the quantum Monte Carlo BITLLES algorithm developed in Ref. [2], [3] where each electron has its own (Bohmian conditional) time-dependent wave packet.

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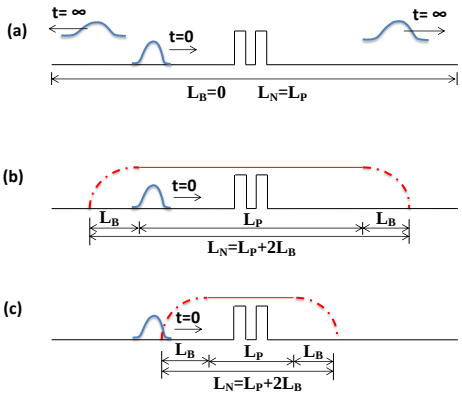

Fig. 1. Different simulation boxes. (a) the largest numerical length L_N to avoid spurious reflection. (b) With absorbing boundary length L_B. (c) The shortest L_N when absorbing boundary conditions and analytical injection are considered. We use $g(x) = 1 - tan^n(\pi x/(4L_B))$

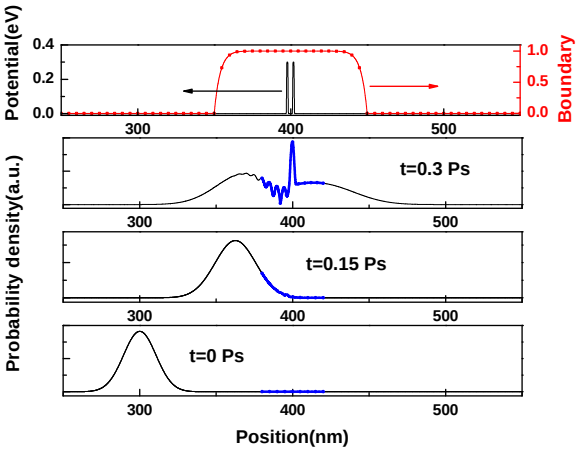

Fig. 2. Time-evolution of the wave function ψ (black) with simulation box (a) and ψ' (blue) with simulation box (c) for an electron with $E = 0.1eV$ in a double barrier $0.8/3.2/0.8$ nm with a height of 0.3 eV and an effective mass of 0.2 times the free electron mass. The time step $\Delta t = 0.03fs$ and spatial step $\Delta x = 0.2nm$. Simulation box (a) with $L_P = 800\ nm$ while simulation box (c) with $L_B = 30\ nm$ and $L_P = 40\ nm$.

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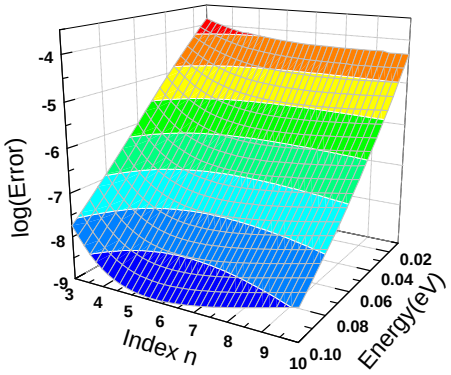

Fig. 3. Error from Eq. (1) (for different electron energies and indexes n) when ψ in simulation box (a) with $L_P = 800\ nm$ is compared with ψ' in simulation box (b) with $L_B = 50\ nm$ and $L_P = 150\ nm$. The condition $[H, g] \approx 0$ is better satisfied at high energies.

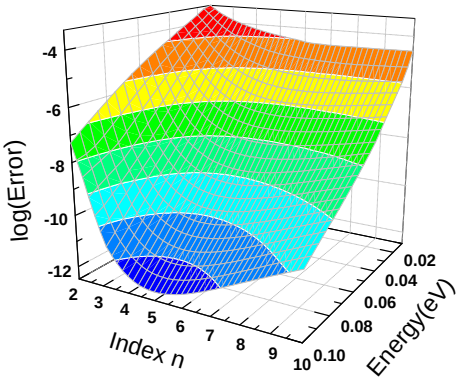

Fig. 4. The same error as in Fig. 3 when ψ in simulation box (a) is compared with ψ' in simulation box (c) with $L_B = 80\ nm$ and $L_P = 40\ nm$.

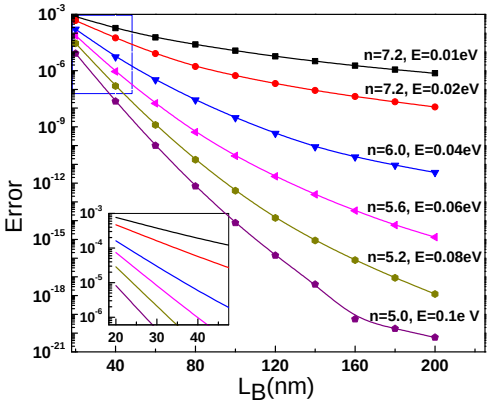

Fig. 5. The same error as in Fig. 4 as a function of L_B for different energies E and optimum index n.