Explicit computation of Coulomb and exchange interactions for N-electrons in open quantum systems using Bohm trajectories

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From a computational point of view, the direct solution of the many-particle Schrödinger equation is inaccessible for more than very few electrons. This issue is at the heart of almost all the unsolved problems in quantum transport. Recently, a novel many-particle quantum transport formalism using Bohm trajectories has been presented for dealing with Coulomb and exchange interaction among electrons [1]. We discuss the computational burden associated with the explicit consideration of the electron spin in the previous formalism [1]. In particular, we provide a numerical justification that shows the viability of the previous formalism for a system with a large ($N \approx 100$) number of electrons. We consider a system of N electrons described by a many-particle wave-function $\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3..\uparrow_1,\downarrow_2,\downarrow_3..;t)$ with $\vec{r}_i$ the electron position and $\uparrow_i / \downarrow_i$ its (up/down) spin. We use an uncoupled spin-base which is adequate for (non-conservative spin) open systems. In the previous formalism [1], the Bohm velocity of each electron has to be computed directly from the many-particle wave-function. Since this formalism is intrinsically time-dependent [1], the standard simplifications in the computation of the many-particle wave-function, obtained from Hamiltonian (orthogonal) eigenstates, cannot be used. In addition, the explicit evaluation of $N!\cdot N!$ products of permutations for the computation of the many-particle system is intractable for more than very few electrons because of computational limitations (note that $8!^2 = 40320^2$). The previous computational limitation is overcome by computing the many-particle velocity with the assumption that the many-particle wave-function can be separated into a product of spin-up $(\uparrow)$ and spin-down $(\downarrow)$ many-particle wave functions:

$$\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3..\uparrow_1,\downarrow_2,\downarrow_3..,t) \approx \Psi(\vec{r}_1,\vec{r}_4..\uparrow_1,\uparrow_4..,t)\cdot\Psi(\vec{r}_2,\vec{r}_3,..\downarrow_2,\downarrow_3..,t). \qquad (1)$$

Then, the numerical difficulties in the computation of the many-particle Bohm velocity disappear because it can be computed from a complex matrix (Slater) determinant. In order to numerically verify the correctness of our assumption, we compute the Bohm velocity associated to electron 1 in four different (exchange-interacting) situations. We have defined the parameter *d* as a normalized (i.e. without units) phase-space distance [2] between electron 1 and the others (see insets in all Figures). We have chosen arbitrary initial Gausssian wave-packets. In Fig. 1, we show the Bohm velocity (with an approximate value of $6\text{x}10^4$ m/s) for one independent (spin-up) electron. In Fig. 2, we plot the same Bohm velocity for the same electron when other 4 exchange-interacting electrons are present. As we decrease the distance *d* among electrons, the Bohm velocity becomes very different from Fig. 1 as a consequence of the Pauli (Exclusion) Principle. In Fig. 3, we show one spin-up electron and two spin-down electrons. Surprisingly, when Fig. 3 is compared with Fig. 1, an exchange interaction between spin-up and spin-down electrons is present due to the non-orthogonal spatial behavior of our "arbitrary" wave-functions. However, the effect of such spin-up-spin-down interaction in the Bohm velocity is quite small when compared to its effect with the spin configuration of Fig. 4, where the 3 spin-up electrons of Fig. 2 are considered. The strong resemblance between the Bohm velocities of Figs. 2 and 4 for the different values of *d* provides a numerical justification

of expression (1) for the computation of many-particle Bohm velocities. The same result is obtained for many other spin schemes.

In conclusion, we present a powerful proposal to study quantum transport with the explicit consideration of Coulomb and exchange interaction among electrons. We show the practical numerical viability of our proposal for large, $N \approx 100$, number of electrons. Since the algorithm deals with time-dependent Schrödinger equations in terms of quantum trajectories, it can be applied for the computation of the average current or its fluctuations [3] in zero or high frequency [4] quantum scenarios.

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References:

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[3] G. Albareda, J.Suñe, X. Oriols, Phys. Rev. B 79, 075315 (2009).
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Figures:

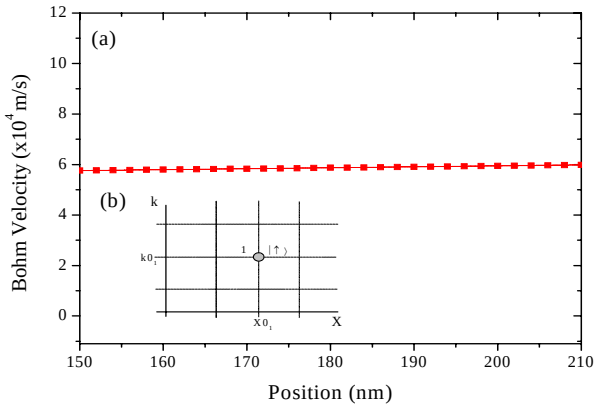

Fig. 1. (a) Bohm velocity for an independent electron. (b) Schematic representation of the system for an electron where we indicate the central value of the X0 and wave-vector K0.

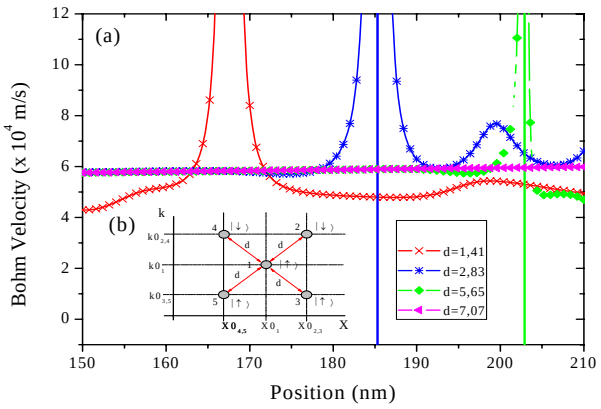

Fig. 2. (a) Bohm velocities for 1-electron using different values of *d* for a system of 5 electrons (3 spin-up and 2 spin-down). (b) In this scheme we indicate the central value of the X0 and wave-vector K0 of these electrons.

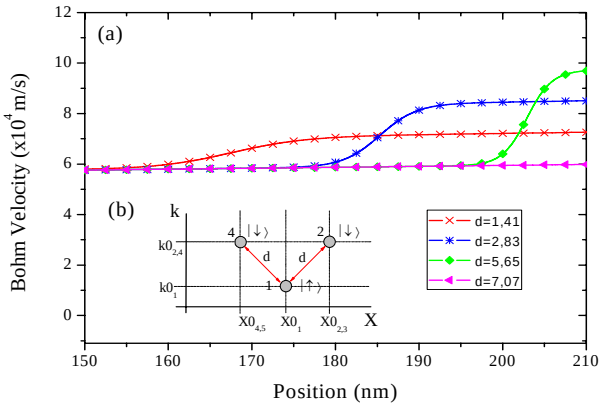

Fig. 3. (a) Bohm velocities for 1-electron using different values of *d* for a system of 3 electrons (1 spin-up and 2 spin-down). (b) In this scheme we indicate the central value of the X0 and wave-vector K0 of these electrons.

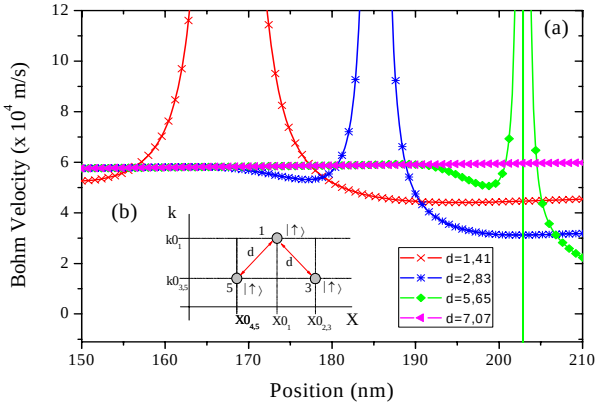

Fig. 4. Bohm velocities for 1-electron using different values of *d* for a system of 3 electrons (spin-up). (b) In this scheme we indicate the central value of the X0 and wave-vector K0 of these electrons.