# Explicit computation of Bohm velocity for N-electrons in open quantum systems

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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 have provided a numerical justification that shows the viability of previous formalism for studying systems with a large (N~100) number of electrons. We consider a system of $N$ electrons described by a many-particle wave-function $\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3..\uparrow_1,\downarrow_2,\downarrow_3..)$ 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. 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 Bohm 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:

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

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. 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). Also, we have chosen arbitrary initial Gaussians wave-packets. In order to numerically verify the correctness of our assumption, we compute the Bohm velocity associated to electron 1 in three different (exchange-interacting) situations: independent electron, exact computation and computational approximation showed in the schemes of Fig. 1, Fig. 2, and Fig. 3 respectively. In detail, 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 exact computation of Bohm velocity for a system of 5 electrons studying the electron 1 when other 4 exchange-interacting electrons are present. In this case, when 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 consider a computational approximation for the system with 5 electrons studying only the 3 spin-up electrons of Fig. 2. The strong resemblance between the Bohm velocities of Figs. 2 and 3 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. The differences between the two schemes presented in Figs. 2 and 3 are explained in Fig. 4. For a particular position (X=150nm) of Figs. 2 and 3 we plot the Bohm velocity in function distance *d* among electrons for these two different electron scenarios. We observe in Fig. 4 two different zones: zone with for *small d* and zone for *large d* (circle dashed lines). For justify the differences between the exact computation and the computational approximation that we observe for *small d* inside Fig.4 is necessary to treat with detail the total norm that we use for compute the Bohm velocity of particle 1. In detail, the total norm is divided in two parts: principal contribution and spurious contribution. In the particular scenario for *small d* we find a significant spurious contribution. Or contrary, in the particular scenario for *large d* the spurious contribution is almost zero.

In conclusion, we present an approximation expression (1) to study the many-particle Schrödinger equation in spin-dependent systems. In order to overcome the computational limitations associates to these systems, we propose that a many particle wave functions can be separated in a product of spin up and spin down many-particle wave functions. To verify our assumption we present a numerical justification computing the Bohm velocity in three different (exchange–interacting) schemes. The practical viability of our proposal can be used for study systems of large (N~100) number of electrons using Slater determinants. Also, this study has significant implications in electron quantum transport with Coulomb and exchange interactions among electrons. In next future we will treat with time-dependent Schrödinger equations in terms of Bohm trajectories. This approach will apply 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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**Figures:**

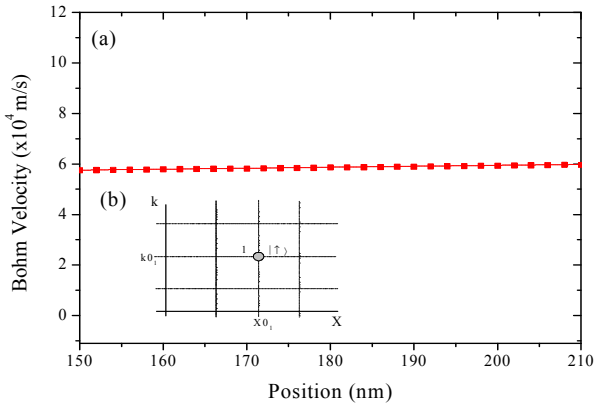


Fig. 1. (a) Bohm velocity for an independent electron. (b) Schematic representation of the system for an electron where we indicate the central value of the X0 and wave-vector K0.

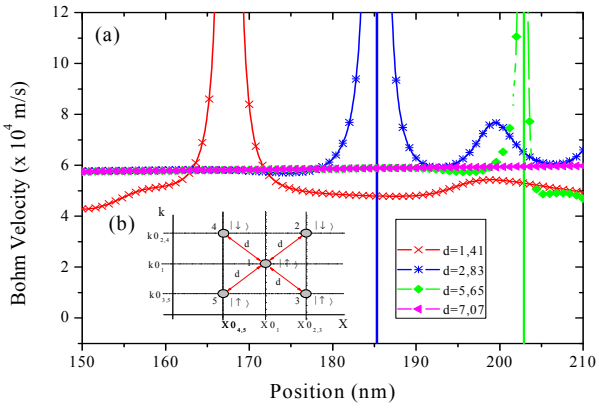


Fig. 2. (a) Bohm velocities for 1-electron using different values of *d* for a system of 5 electrons (3 spin-up and 2 spin-down). (b) In this scheme we indicate the central value of the X0 and wave-vector K0 of these electrons.

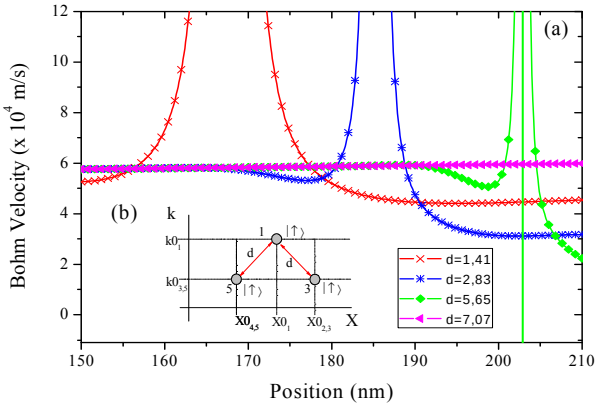


Fig. 3. Bohm velocities for 1-electron using different values of *d* for a system of 3 electrons (spin-up). (b) In this scheme we indicate the central value of the X0 and wave-vector K0 of these electrons.

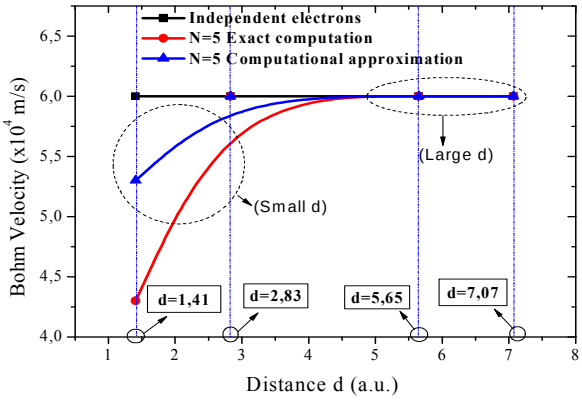


Fig.4. For a particular position (X=150nm) of Bohm velocity of Fig. 2 and Fig. 3. We plot the Bohm velocity in function distance *d* among electrons for two different electron scenarios.