A procedure for calculating the many-particle Bohm quantum potential.

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Abstract

In a recent work, M. Kohout (M. Kohout, Int. J. Quant. Chem. 87, 12 2002) raised the important question of how to make a correct use of Bohm’s approach for defining a quantum potential. In this work, by taking into account Kohout’s results, we propose a general self-consistent iterative procedure for solving this problem.

Key-words:
Bohm’s quantum potential, many-electron systems, partial differential equations, self-consistent procedure.

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I. INTRODUCTION

Bohm’s formulation of quantum mechanics in terms of single-particle trajectories ([1, 2, 3, 4, 5, 6]) has been, and still is, a continuous matter of dispute, often in rather philosophical terms above all ([5, 6, 7, 8, 9, 10, 11, 12, 13, 14]) concerning the fundamental meaning of quantum mechanics. At a concrete level such a theory has been used as a theoretical tool for understanding and interpreting several processes in different fields, from molecular physics to plasma physics, from scattering theory to simulation of quantum wires [15, 16, 17, 18, 19, 20, 21], to name a few. Recently M.Kohout [22] raised the important question of how to treat the more rigorous and realistic $3N$-dimensional formulation of the quantum potential generated by $N$ electrons. Rigorously speaking, in an $N$-particle system Bohm’s potential is a $3N$-dimensional function and the one-particle Bohm’s potential, usually considered in literature, is the simplest 3-dimensional reduced form which systematically does not take into account the effects due to the presence of other particles. He proposed a formal interpretation of the wavefunction as a product of a one-particle marginal function and a conditional many-particle function where somehow the effects due to the other particles are taken into account, then a formal expression of the quantum potential is obtained. However, as the author underlines, for the conditional many-particle function an explicit expression is required and this is a rather difficult problem. In this work, by taking into account Kohout results we build a reasonable initial guess for the many-particle potential and, following this choice, we develop an iterative self-consistent procedure for obtaining a general (numerical) expression of the potential. We restrict our analysis to a spinless system, in any case there exists the possibility to extend the procedure to wavefunctions which explicitly consider the spin variables. To conclude, we must underline that the intention of this work is simply to show that the widely used Bohm potential (used in the approximation of one particle) can actually be reasonably treated in its true form of many-particle and we propose a method to do so. It is not our intention to prove that such a procedure is preferable to other quantum approaches, such as Hartree-Fock or Density Functional Theory, for determining general many-body effects in electronic systems.
II. A BRIEF ACCOUNT OF BOHM’S THEORY

Bohm’s formulation of quantum mechanics in terms of single-particle trajectory is based on the assumption that the wavefunction determines the dynamics of more fundamental variables (hidden variables). The essence of the theory can be summarized by quoting Bohm’s original work ”The first step in developing this interpretation in a more explicit way is to associate with each electron a particle having precisely definable and continuously varying values of position and momentum” [1]. Within this assumption, the system is described by its wavefunction $\psi(x_1, ..., x_N, t)$ and the positions of its particles $x_i$; these two fundamental quantities are governed respectively by Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi$$

(1)

where $H$, as usual, is the Hamiltonian of the system, and by the dynamical equation:

$$\frac{d}{dt}x_i = v_i$$

(2)

where $v_i = \frac{\hbar}{m}Im \frac{\psi^* \nabla x_i \psi}{\psi^* \psi}$. This procedure leads to a non-Newtonian equation of motion which becomes Newtonian in the classical limit of $\hbar \to 0$; the connection of such an approach with quantum mechanics is provided by the fact that the quantum formalism automatically emerges from Bohm mechanics. In simple terms this approach ”...implies however the particle moves under the action of a force which is not entirely derivable from the classical potential, $V(x)$, but which also obtains contributions from the quantum mechanical potential...” [1]. Given the $N$-particle electronic wavefunction whose general form can be written as $\psi(R, t) = \chi(R, t)e^{i\hbar S(R, t)}$; $R \in \mathbb{R}^{3N}$, substituting it into the time-dependent Schrödinger equation and then separating real and imaginary part, once the velocity is defined as $v = \frac{i\hbar}{2m} \frac{\psi^* \nabla \psi - \psi^* \nabla \psi}{R^2} = \frac{1}{m} \nabla S$, and $\rho = |\psi|^2 = \chi^2$ one obtains the equations:

$$\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho v) = 0$$

(3)

and

$$\frac{\partial S}{\partial t} + \frac{[\nabla S(R, t)]^2}{2m} = -[V(R, t) + Q(R, t)].$$  

(4)

where $m$ is the mass of the particle, $V(R, t)$ is the potential characterizing the system (e.g. electrostatic for interacting fermions), $Q(R, t) = -\frac{\hbar^2}{2m} \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}}$ is the Bohm potential and
\[ \nabla = \sum_{i=1}^{N} \nabla_i \] the sum of the gradients of the \( N \)-particles. We restrict our analysis to the stationary case, thus we can write in terms of the wavefunction phase factor:

\[ \frac{[\nabla S(R)]^2}{2m} = -[V(R) + Q(R)]. \] (5)

### III. KOHOUT'S FORMULATION OF THE MULTI-PARTICLE POTENTIAL PROBLEM

Bohm’s potential in three dimensions is used in many applications, within this framework \( \rho(r) \), a one-particle electron density, is defined as:

\[ \rho(r) = N \int_{\Omega(N-1)} |\psi(r, r_2, r_3, \ldots, r_N)|^2 dr_2 dr_3 \ldots dr_N \] (6)

(\( \Omega \) domain of definition of the system in real space) and the single-particle wavefunction writes:

\[ \psi(r) = \frac{\sqrt{\rho(r)}}{N} e^{i\hbar s(r)}; r \in \mathbb{R}^3. \] (7)

The wavefunction’s form of Eq.7 corresponds to the procedure of separating Bohm’s dynamical equations into independent and indistinguishable single-particle equations and describe a set of identical particles moving in an average potential where specific mutual interactions are neglected. In simple terms it is sufficient to describe only one particle, embedded in an average potential generated by the other particles, in order to automatically describe the whole system. In this case \( S(r_1, \ldots, r_N) = s(r_1) + \ldots + s(r_M) \). It must be noticed that, within the approximation done, what we called the one-particle Bohm potential, does not correspond to the Bohm potential for a system composed by only one particle. In fact, if this was the case, Bohm equations could not be defined at the nodes of the electron wavefunction, instead the definition of \( \psi(r) \) given in Eq.7 with \( \rho(r) \) defined by Eq.6 suggests that it is unlikely to have a \( \psi \) which contains zeros at least for dense systems.

The one-particle potential is the simplest approximation that can be used for describing an electronic system. Recently M.Kohout proposed another approach, by redefining the wavefunction \( \psi(r, r') \) (\( r' \) indicates the remaining \( N-1 \) particles of an \( N \)-particle system when one focuses the attention on particle \( r \)):

\[ \psi(r, r') = \chi(r, r') e^{i\hbar S(r, r')} = \phi(r) \cdot \beta(r'|r) e^{i\hbar S(r, r')}. \] (8)
φ(r) is the marginal function while β(r′|r) is the conditional function, conditionally dependent on the coordinate r. These two functions satisfy the following normalization conditions:

\[ \int_\Omega |\phi(r)|^2 dr = 1 \quad (9) \]

and

\[ \int_\Omega |\beta(r′|r)|^2 dr′ = 1; \forall r. \quad (10) \]

By using this factorization, he obtains a formal expression of the potential \( Q(r, r′) \) as a sum of the one-particle Bohm potential and a conditional multi-particle potential \( Q_{\text{cond}}(r|r′) = -\frac{\hbar}{2m\beta(r′|r)} \sum_{i=1,N} \nabla^2_i \beta(r′|r) \). This expression bares a rather difficult problem: to find a reasonable expression for \( \beta(r′|r) \). In this work we will circumvent this problem by using a suitable expression for \( \chi(r, r′) \) which recovers the properties of the factorized wavefunction introduced by Kohout, and leads to an iterative procedure for \( Q(r, r′) \); this is reported in the next sections.

IV. MANY-PARTICLE DENSITY AND BOHM’S WAVEFUNCTION.

As anticipated in previous sections our final aim is to develop a procedure for obtaining a Bohm’s potential where many-particle effects are somehow incorporated. For this purpose, we redefine the wavefunction of the system by extending the form \( \psi(r) = \phi(r)e^{i\hbar S(r)} \) for one-particle to \( \psi(r_1, r_2...r_M) = \phi(r_1, r_2...r_M)e^{i\hbar S(r_1, r_2...r_M)} \), an \( M \)-particle wavefunction in an \( N \)-particle system, with \( M \leq N \). We should also require \( \phi \) to be antisymmetric and \( S \) to be symmetric with respect to the \( M! \) possible pair permutations of the \( M \) particles; this requirement will preserve the antisymmetry of \( \psi \). Later we will show that the symmetry of \( S \) corresponds to the fundamental physical property of indistinguishable particles. In the next sections, to remind the analogy with the one-particle case we will identify \( r \) with \( r_1 \), thus \( \phi(r_1, r_2...r_M) = \phi(r, r_2...r_M) \). This basically means that given \( N \) particles, our system is characterized by (or alternatively, we are interested in considering) \( M \)-particle interactions which produce observable effects on the average behavior of the system, thus \( M \) particles must be treated explicitly; we can describe those effects by considering the \( M \)-th approximation, where \( M = 1, ... N \), the case \( M = 1 \) is the trivial one-particle case, \( M = 2 \) counts two-particle effects etc.etc.. For the moment we are not interested in \( S(r_1, r_2...r_M) \) whose role will be clear later on. Let us focus on \( \phi(r, r_2...r_M) \). In the one-particle case
\[ N \cdot |\phi(r)|^2 = \rho(r) = N \int_{\Omega(N-1)} |\psi(r, r_2, r_3, \ldots, r_N)|^2 dr_2 dr_3 \ldots dr_N = \rho(r), \] i.e. the average electron density of \( N \) indistinguishable particles projected on the real (3-dimensional) space. In analogy we can define an \( M \)-particle electron density as:

\[ N|\phi(r_\ldots, r_M)|^2 = \rho(r_\ldots, r_M) = N \int_{\Omega(M-1)} |\psi(r, r_2, \ldots, r_M, r_{M+1}, \ldots, r_N)|^2 dr_{M+1} \ldots dr_N \quad (11) \]

where, in analogy to the one-particle case, one has:

\[ \int_{\Omega_M} |\phi(r_\ldots, r_M)|^2 dr_\ldots dr_M = 1. \quad (12) \]

This form of \( \phi(r, r_2, \ldots, r_M) \) satisfies the requirements of the factorization in marginal and conditional part as defined by Kohout:

\[ \psi(r, r_2, \ldots, r_M) = \phi(r) \cdot \frac{\phi(r, r_2, \ldots, r_M)}{\phi(r)} e^{i\hbar S(r_1, \ldots, r_M)}. \quad (13) \]

In fact the conditional function of Eq. 11, \( \beta(r' | r) \), can be written as: \( \beta(r' | r) = \frac{\phi(r, r_2, \ldots, r_M)}{\phi(r)} \) and (as can be easily verified) one obtains \( \int_{\Omega_M} |\beta(r' | r)|^2 d^M r' = 1; \forall r' \in \Omega, \) where \( r' = r_2, r_3, \ldots, r_M \). This kind of factorization was already considered by Hunter [23] who, once more, underlines that the nature of \( \phi(r) \), as a marginal probability density function, makes unlikely the existence of zeros. In terms of probability \( \frac{\phi(r, r_2, \ldots, r_M)}{\phi(r)} \) is interpreted as the square root of the classical expression for the conditional probability density. The conditional probability density, i.e. the probability density for \( M - 1 \) particles given the position of the particle \( r \), is written as the probability density of the particles \( r, r_2, \ldots, r_M \), \(|\phi(r, r_2, \ldots, r_M)|^2\), divided by the probability density of particle \( r \), \(|\phi(r)|^2\). In general the mathematical structure of quantum mechanics leads to a non-commutative probability theory which coincides with the classical one only in case we treat commuting spaces [24]. Here for a commuting space we intend a set of variables representing physical quantities, such as positions, which do commute. In the language of quantum mechanics this means for example that position operators of the \( M \)-particles commute, i.e. a measurement of the position of particle 1 does not influence the measurement of the position of particle 2. The same example does not hold in the space of spins, however since we have restricted our analysis to spinless systems, we can apply the rules of classical probability. In Ref. [24] is reported a study about the possibility of defining a quantum correction which takes into account a non-commutative probability for the conditional function. Once we have formally defined the many-electron
wavefunction via Eq.13, we can determine a reasonable initial guess for Bohm’s potential, by defining a reasonable \( \phi(r, r_2, \ldots, r_M) \):

\[
Q(r, r_2, \ldots, r_M) = -\frac{\hbar}{2m\phi} \sum_{i=1,M} \nabla_i^2 \phi. \tag{14}
\]

V. BOHM’S DYNAMICAL SYSTEM FOR \( M \) NON-INDEPENDENT PARTICLES

In the previous section we defined, in analogy to the one-particle case, an \( M \)-particle wavefunction for an \( N \)-particle system. Clearly the larger the value of \( M \) the more difficult the determination of the wavefunction, although in many cases two or three-particle effects may be enough for a basic understanding of some physical properties. So far by defining the many-particle wavefunction we simply gave a first approximation for the potential \( Q \), within, for example, Slater orbitals or similar appropriate approximations (e.g. plane-waves expansion). The idea for an effective coupling of \( M \) electrons is to insert an approximation of \( Q \), as an initial guess, in a system of equations which do couple the \( M \) electrons. This set of equations is obtained by inserting the \( M \)-particle wavefunction in Schrödinger equation and repeating the procedure followed for the one-particle case within Bohm’s framework as it is shown next. In fact, by inserting \( \psi(r, r_2, \ldots, r_M) \) in Schrödinger equation for the stationary case, similarly to Eq.5, one obtains:

\[
\sum_{i=r, r_M} \frac{[\nabla_i S(r, \ldots, r_M)]^2}{2m} = -V(r, \ldots, r_M) - Q(r, \ldots, r_M) \tag{15}
\]

where \(-V(r, \ldots, r_M)\) is the electrostatic potential experienced by each single particle. In this form, Eq.15 is not very useful thus we should find a way for a simplification which can be based on physical well founded hypothesis. The first thing to notice is that \( \nabla_i S(r, \ldots, r_M) = v_{r_i}(r, \ldots, r_M) \) represents, within Bohm’s framework, the velocity field of particle \( r_i \) which depends upon (or alternatively, is influenced by) the positions of the other \( M - 1 \) particles as well. We can also notice that \(-V(r, \ldots, r_M)\) can be represented as the electrostatic potential per particle and can be expressed in good approximation as:

\[
V(r, \ldots, r_M) = \sum_{i=1,M} \frac{1}{N} \left[ \frac{1}{2} \int_{\Omega} \frac{\rho(w)}{r_i - w} dw \right]. \tag{16}
\]

In Eq.16 \( \rho(w) \) is the one-particle electron density, obtained by integrating the \( M \)-particle density over \( M - 1 \) variables. The meaning of Eq.16 is that in a system of indistinguishable
particles the average electrostatic potential experienced by one-particle is the same as that experienced by another particle. The "average" character is obtained by considering the one-particle electron density instead of the $M$-particle one. The use of a simpler rather than a more complicated expression for $V$ can be justified by the fact that we know how to express electrostatic properties and we know that Eq.16 is reasonable. What is unknown are the quantum effects represented by $Q$, for this reason we can take known quantities in their simplest approximation as far as they are known to be reasonable. In any case the important fact is that following Eq.16 one can write:

$$V(r,\ldots r_M) = V(r) + V(r_2) + \ldots + V(r_M).$$

(17)

The expression for $V(r,\ldots r_M)$ given in Eq.17 is particularly useful for simplifying Eq.15. In fact Eq.15 can be written as:

$$\sum_{i=r,r_M} \left[ \frac{\nabla_i S(r,\ldots r_M)^2}{2m} \right] = - \sum_{i=1,M} \left[ V(r_i) + \frac{1}{M} Q(r, r_2, \ldots, r_M) \right]$$

(18)

where $\frac{1}{M} Q(r, r_2, \ldots, r_M)$ is the quantum potential per interacting particle. At this point we can proceed having in mind the following points:

Eq.18 is a $3M$-dimensional non-linear partial differential equation and we would like to have a solution which somehow recovers the dynamical physics contained in Bohm’s approach. The natural simplification of Eq.18 is to decompose it in a system of $M$ one-particle equations coupled through $S(r, r_2, \ldots, r_M)$ and $Q(r, r_2, \ldots, r_M)$, where each equation describes the squared modulus of the velocity field of a particular electron $\nabla_i S(r, \ldots r_M)$ subject to a potential per particle $[V(r_i) + \frac{1}{M} Q(r, r_2, \ldots, r_M)]$. Clearly the sum of solutions of single equations is also a solution for the initial one. In mathematical terms this kind of solution represents only one possible way (a particular solution), while in physical terms this represents the direct extension of Bohm’s one-particle dynamical description to a system of $M$-particle non-independent electrons. In this way we obtain a set of equations coupling the $M$ interacting electrons as we postulated at the beginning of this section. The $M$-equation system takes the
form:

\[(1) [v_r(r, ... r_M)]^2 = \frac{[\nabla_r S(r, ... r_M)]^2}{2m} = - [V(r) + \frac{1}{M} Q(r, r_2, ..., r_M)]\]

\[(2) [v_{r_2}(r, ... r_M)]^2 = \frac{[\nabla_{r_2} S(r, ... r_M)]^2}{2m} = - [V(r_2) + \frac{1}{M} Q(r, r_2, ..., r_M)]\]

\[(3)............................................................\]

\[(4)............................................................\]

\[(5)............................................................\]

\[(6)............................................................\]

\[(M) [v_{r_M}(r, ... r_M)]^2 = \frac{[\nabla_{r_M} S(r, ... r_M)]^2}{2m} = - [V(r_M) + \frac{1}{M} Q(r, r_2, ..., r_M)]\]

In the next section we show that, by using Eq. 19, a self-consistent procedure for \(Q(r, ... r_M)\) can be determined.

VI. SELF-CONSISTENT ITERATIVE PROCEDURE FOR \(Q(r, ... r_M)\)

The basic idea is to start from the approximative form of \(Q = Q_0(r, ... r_M)\) obtained via the \(M\)-particle density within a Slater orbitals or similar approach and then introduce it in equation (1) of system 19. Next by solving the first order non linear partial differential equation for \(S(r, ... r_M)\) with respect to \(r\) one find an "initial" value for \(S(r, ... r_M) = S_1(r, ... r_M)\). At this point \(S_1(r, ... r_M)\) is substituted in equation (2) and leads to a new value of \(Q\), \(Q_1(r, ... r_M) = \frac{[\nabla_{r_2} S_1(r, ... r_M)]^2}{2m} + [V(r_2)]\). The next step consists in substituting \(Q_1\) in equation (3) and solve it (as for equation (1) ) with respect to \(r_3\) to find a new \(S(r, ... r_M) = S_2(r, ... r_M)\), the procedure is repeated until the convergence of \(Q\) meets a given criterion of acceptance. It must be noticed that the procedure is iterative in the sense that one should go through all the \(M\)-equations of the system and then take the final \(Q\) or \(S\) for repeating the process by going through the \(M\) equations again as is illustrated for the case \(M = 3\) and \(M = 4\) in Fig.11. Finally \(Q(r, r_1, ..., r_M)\) can be integrated with respect to \(M - 1\) variable and so be reduced to a one particle potential where the many-particles effects are integrated out (averaged). However, in practical terms this procedure is not straightforward since a first order non linear partial differential equations must be solved, for example with
with respect to \( \mathbf{r} = (x, y, z) \) at the very first step:

\[
\frac{1}{2m} \left[ \left( \frac{\partial S(\mathbf{r}, \ldots \mathbf{r}_M)}{\partial x} \right)^2 + \left( \frac{\partial S(\mathbf{r}, \ldots \mathbf{r}_M)}{\partial y} \right)^2 + \left( \frac{\partial S(\mathbf{r}, \ldots \mathbf{r}_M)}{\partial z} \right)^2 \right] = -\left[ V(\mathbf{r}) + \frac{1}{M} Q_0(\mathbf{r}, \ldots \mathbf{r}_M) \right]
\]

and formally a solution of the following form should be obtained:

\[
S(\mathbf{r}, \ldots \mathbf{r}_M) = f(\mathbf{r}, \mathbf{r}_2, \ldots \mathbf{r}_M) + G(\mathbf{r}_2, \ldots \mathbf{r}_M) + \text{const.}
\]

\[ (20) \]

\( G(\mathbf{r}_2, \ldots \mathbf{r}_M) \) is a function constant with respect to \( \mathbf{r} \) and \( \text{const} \) is a constant which can be neglected since we are interested in gradients of \( S \). \( G(\mathbf{r}_2, \ldots \mathbf{r}_M) \) cannot be obtained by solving a single equation since in principle one should solve the whole system of equations and find the global solution (basically \( G(\mathbf{r}_2, \ldots \mathbf{r}_M) \) would be an artifact of the procedure). On the other hand to find a global solution would represent a formidable, if not impossible, task.

We need a well founded approximation which allow us to remove the artifact represented by the function \( G(\mathbf{r}_2, \ldots \mathbf{r}_M) \). At this point we notice that there exists a fundamental physical property of the system which can reasonably solve this problem. In fact \( S(\mathbf{r}, \mathbf{r}_1, \ldots, \mathbf{r}_M) \) must be symmetric under any permutation of the \( N \) particles. This fundamental property is a direct consequence of the fact that the particles are indistinguishable and implies that the velocity field of one particle can be obtained from that of another via particle permutation (see Appendix).

The symmetry of the total wavefunction can be preserved by taking \( \phi(\mathbf{r}, \mathbf{r}_1, \ldots, \mathbf{r}_M) \) antisymmetric with respect to any pair exchange of the \( M \) particles. The property of symmetry for \( S \) allows us to make the iterative procedure possible and physically reasonable. In fact we solve Eq.\[20\] with respect to \( \mathbf{r} \) and obtain \( S(\mathbf{r}) \) as:

\[
S_1(\mathbf{r}, \ldots \mathbf{r}_M) = f(\mathbf{r}, \mathbf{r}_2, \ldots \mathbf{r}_M)
\]

\[ (22) \]

formally neglecting, for the moment, the part \( G(\mathbf{r}_2, \ldots \mathbf{r}_M) \) of Eq.\[21\].

Then in order to obtain a global solution which satisfies the permutation (symmetry) criterion we write the solution for \( S \) at the first iterative step as:

\[
S_{1\text{tot}}(\mathbf{r}, \mathbf{r}_2, \ldots \mathbf{r}_M) = \frac{1}{M!} \sum_i P_i S_1(\mathbf{r}, \ldots \mathbf{r}_M)
\]

\[ (23) \]

where \( \sum_i P_i \) is the sum over all the possible \( M \)-coordinate pair permutations and \( P_i \) is the permutation operator for the \( i \)-th permutation. This procedure, by making a fully symmetric
solution $S$, does not require to consider the term $G(r_2,...,r_M)$ which would formally come from a direct mathematical approach. This point can be considered from an alternative point of view; we extract a solution of a multi-variable function problem by considering only one equation instead of considering all the equations. Such a solution is valid for the variable $r$ (integration variable) as long as the other variables are considered as constants (fixed at a particular parametric value). Next, by using the physical condition of indistinguishable particles, we can extend, reasonably well, this solution to the whole set of variable by making the global solution a fully symmetric function of the whole set of coordinates. We can then go to the next equation to find $Q$, make it fully symmetric with the same procedure we used before for $S$ and go to the next equation, again solve for $S$, make it symmetric and proceed on in the same way. A formal argument for the symmetry of $S$ is given in Appendix. Technically the major problem is the fact that in general to solve a non linear partial differential equation in three dimensions is not an easy task, however Eq.20 is the well known equation of the eikonal in an anisotropic media. In this case the boundary condition for $S$ must be assigned when the Schrödinger equation is formulated and should depend on the particular nature of the system under consideration. The problem of the solution of this equation goes beyond the purposes of this work, however there exists a massive list of references dealing with this problem for both mathematical properties and numerical techniques (see for example [25, 26, 27, 28, 29, 30, 31, 32, 33] and references therein). In particular the fast sweeping algorithms of Ref.[30], and the robust algorithms for multidimensional Hamilton-Jacobi equations of Refs.[31, 32, 33] represent an extremely useful approach to a computer implementation of this procedure. In particular these latter algorithms, although dealing with the more general non stationary problem, in principle can be adapted to the stationary case and in general would make it possible also to extend the procedure to non stationary cases.

VII. CONCLUSIONS

We propose a general method to treat Bohm’s potential in its $3N$-dimensional rigorous form. Inevitably, there are several physical approximations that one should accept; we use a spinless system, thus we can apply the concept of classical probability to a quantum system in a stationary state. This choice offers technical advantages but is not physically obvi-
ous; in case the spin variables are explicitly considered, the basis of our procedure remains valid, but we should find an opportune way to define a more general wavefunction where the conditional function is determined by non-commutative probability principles as suggested in Ref. [24]. The separation of the many-electron equation in single but mutually dependent one-particle equations is not unique from a rigorous mathematical point of view but it is based on a reasonable physical approximation. From a technical-mathematical point of view the major problem is the solution of the non-linear partial differential equations for $S$ (eikonal equation). As it is commented in several textbooks of quantum mechanics (see for example [34]), to solve this equation is not an easy task, however the literature relative to the solution of the eikonal equation is sufficiently large and several methods are available. For small $M$ (e.g. 2, 3) it should be possible to apply the procedure with a reasonable effort; moreover there exists systems which can be described with simplified unidimensional models such as electrons in a one dimensional wire or an isolated atom considered spherically symmetric. Other simple examples are those where it is possible to proceed to a separation of variables (i.e. $f(x_i, x_j, y_i, y_j, z_i, z_j) = X(x_i, x_j) + Y(y_i, y_j) + Z(z_i, z_j)$ or $f(x_i, x_j, y_i, y_j, z_i, z_j) = X(x_i, x_j)Y(y_i, y_j)Z(z_i, z_j)$) in this case the eikonal equation is reduced to independent ordinary first order differential equations which can be easily solved. The simple cases listed above can be used as a first approximation of more complicated systems. As stated before, it is important to underline that the intention of this work is that of proposing a procedure to properly treat and use Bohm potential in fields where it is currently (and extensively) employed for practical applications. We do not claim that this procedure is computationally or methodologically more convenient than others in solving general many-electron problems, however, this method may also represent a complementary theoretical approach to the standard ones used in current research; due to the deterministic interpretation of Quantum Mechanics, on which the method is based, effects which cannot be describe by standard Hartree-Fock or DFT may be revealed. This issue, anyway, involves a much deeper analysis which goes beyond the purpose of this work and will be possibly treated elsewhere.
VIII. ACKNOWLEDGMENTS

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IX. APPENDIX

For simplicity let us consider a two-particle system \((r, r')\). Let us suppose that from Eq 20 for \((r, r')\), integrated with respect to \(r\), the following solution is found:

\[ f(r, r') = g(r, r') + h(r) + l(r') \]  

(24)

where \(g(r, r') = g(r', r)\) and \(l(r')\) is unknown since it represents the constant (with respect to \(r\)) obtained by solving the equation with respect to \(r\). From Eq 24 it follows that the formal expression for the velocity field for the particle \(r\) is

\[ v_r(r, r') = \nabla_r [g(r, r') + h(r)] \]  

(25)

this means

\[ v_r(r, r') = v_1(r, r') + v_2(r) \]  

(26)

while for particle \(r'\) we have:

\[ v_{r'}(r, r') = \nabla_{r'} [g(r, r') + l(r)] = v_1(r', r) + v_3(r'). \]  

(27)

Because the particles are indistinguishable one must obtain \(v_{r'}(r', r)\) from \(v_r(r, r')\) by permutation of \((r, r')\) thus the unknown function \(l(r')\) must coincide with \(h(r')\). As one can easily see, by taking \(f(r, r') = g(r, r') + h(r)\) and making it symmetric with respect to the permutation \((r, r') \rightarrow (r', r)\), we reach the same result for \(l(r')\). In the most general case \(g(r, r')\) is not necessarily equal to \(g(r', r)\), however the same procedure (and principles) can be applied with the only difference that \(g\) must be also made symmetric, i.e. \(g_{fin}(r, r') = \frac{g(r, r') + g(r', r)}{2}\) and \(h_{fin}(r, r') = \frac{h(r) + h(r')}{2}\). In case of more than 2 particles the same argument can be used by taking into account all possible particle permutations.

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FIG. 1: The figure represents the pictorial illustration of the self-consistent iterative procedure shown in this work. For STEP we intent the process of going through all the 3 (4) equations. Next by using the final Q or S, obtained at the first STEP, it is possible to start a second STEP. $S_{ij}$ ($Q_{ij}$) is the function S calculated at different stages of the procedure. i corresponds to the number of equations solved within the system, $i = 0$ corresponds to the starting (initial guess) expression for $Q$, j indicates the number of global iterations (STEP).