Density-functional theory, finite-temperature classical maps, and their implications for foundational studies of quantum systems

M W C Dharma-wardana

National Research Council of Canada, Ottawa, Canada, K1A 0R6

E-mail: `chandre.dharma-wardan@nrc-cnrc.gc.ca`

Abstract. The advent of the Hohenberg-Kohn theorem in 1964, its extension to finite-T, Kohn-Sham theory, and relativistic extensions provide the well-established formalism of density-functional theory (DFT). This theory enables the calculation of all static properties of quantum systems *without* the need for an n-body wavefunction ψ. DFT uses the one-body density distribution instead of ψ. The more recent time-dependent formulations of DFT attempt to describe the time evolution of quantum systems without using the time-dependent wavefunction. Although DFT has become the standard tool of condensed-matter computational quantum mechanics, its foundational implications have remained largely unexplored. While all systems require quantum mechanics (QM) at $T=0$, the pair-distribution functions (PDFs) of such quantum systems have been accurately mapped into classical models at effective finite-T, and using suitable non-local quantum potentials (e.g., to mimic Pauli exclusion effects). These approaches shed light on the quantum → hybrid → classical models, and provide a new way of looking at the existence of non- local correlations without appealing to Bell's theorem. They also provide insights regarding Bohmian mechanics. Furthermore, macroscopic systems even at 1 Kelvin have de Broglie wavelengths in the micro-femtometer range, thereby eliminating macroscopic cat states, and avoiding the need for *ad hoc* decoherence models.

1. Introduction.

In 1964, Hohenberg and Kohn [1] proved a theorem asserting that the ground- state properties of a stationary, non-relativistic system can be calculated from a variational principle involving only the one-body density $n(\vec{r})$ of the system, without recourse to the Schrödinger equation and its wavefunction. The theorem was soon generalized to finite-T [2], and to relativistic systems [3]. Thus it became clear that all thermodynamic properties of n-particle quantum systems, entangled, interacting, or not, could be calculated without recourse to the n-body wavefunction. The method, re-written in the form of the Kohn-Sham theory has now become the preferred method in computational quantum mechanics (QM). Furthermore, since linear transport properties depend only on equilibrium correlation functions (c.f., the Kubo relations), a large class of quantum phenomena depends only on the density $n(r)$, a measurable quantity having a familiar 'ontology' in quantum as well as classical mechanics. Unlike the many-electron wavefunction of conventional QM, the one-body density is an observable. For instance, the X-ray scattering from a specimen of matter gives direct information regarding $n(r)$. The development of 'time-dependent' density functional theory [4], if substantiated, implies that

density functional theory may enable a very different discussion of quantum phenomena than has been the custom in foundational studies. In this article, for the sake of brevity and simplicity, we limit ourselves mainly to non-relativistic equilibrium systems. In the following presentation we look at DFT and compare it with relevant aspects of Bohmian mechanics, treatment of hybrid systems within DFT, as well as classical representations inspired by DFT ideas. Furthermore, finite-T physics leads us to conclude that there is no need for *ad hoc* decoherence theories to eliminate macroscopic cat states from QM.

2. Density functionals and Bohmian mechanics

To be specific, we consider a system of electrons subject to an external potential $v_{ext}(\vec{r})$, and interacting with one another via the Coulomb potential. In many cases this external potential is produced by a fixed set of nuclei, as in molecular physics or quantum chemistry calculations at $T = 0$. However, the ions cannot be treated as fixed in dealing with liquid metals and hot plasmas. Hence, in discussing true hybrid systems, we allow the nuclei (or ions) to be a second interacting subsystem, interacting with the electron subsystem, and the finite-T discussion becomes not only appropriate, but also necessary. However, in simplified models, e.g., the jellium model, the ions provide a fixed uniform positive distribution of charge that exactly neutralizes the negative charge of the electron distribution. The $q \to 0$ singularities in the Coulomb potential $4\pi/q^2$ for electron-electron or ion-ion interactions are exactly canceled by the corresponding term in the ion-electron interactions.

However, while keeping such specific models in mind, we can simply work with an unspecified external potential v_{ext} and a corresponding one-body electron distribution $n(r)$. Then according to Hohenberg and Kohn [1], the exact ground state density $n(r)$ and the ground-state energy $E_v[n]$ corresponding to that external potential v_{ext} are obtained by the minimization of the following energy functional.

$$E_v[n] = T[n] + U_{cou}[n] + \int d\vec{r}\, v_{ext}(\vec{r})n(\vec{r}) \tag{1}$$

The kinetic energy contribution, viz., $T[n]$, and the Coulomb electrostatic energy $U_{coul}[n]$ are said to be 'universal functionals' of $n(r)$, in the sense that they do not depend on the external potential $v_{ext}(\vec{r})$ specific to the system. The original Hohenberg-Kohn theorem was established for non-degenerate ground states at $T = 0$. This has since been restated within the language of functional analysis [5], while degenerate ground states, spin-polarized systems, finite-T systems, relativistic systems, multi-component hybrid systems, superconductors, liquids and plasmas etc., have been studied within the first three decades of DFT [7].

It is clear that a direct minimization of $E_v[n]$ via $\delta E_v/\delta n(\vec{(r)})$ would require a knowledge of the kinetic energy functional $T[n]$, and the electrostatic potential $U_{cou}[n]$. The latter is a known functional of $n(r)$, but $T[n]$ is unknown. Although this is a universal functional of $n(\vec{r})$, it turns out to be highly non-local. Hence gradient expansions merely lead to Thomas-Fermi like theories. These, sometimes known as 'orbital-free DFT' [6], presently lack the full accuracy of methods that use a wavefunction. Since DFT is presented via a one-body density, the Kohn-Sham formulation of DFT uses a one-body 'Kohn-Sham wavefunction' to construct a non-local kinetic energy, where a single Kohn-Sham electron moves in the electrostatic potential of the other electrons and an additional exchange-correlation potential $V_{xc}[n]$ which is a functional of the one-body density. Thus, the many-electron problem is replaced by an effective one electron problem in Kohn-Sham theory. Here the Kohn-Sham electron moves in a non-local Kohn-Sham potential that is made up of the electrostatic potential $U_{cou}[n]$, and the non-local $V_{xc}[n]$. However, unlike $T[n]$, approximate models of $V_{xc}[n]$ have proved to be quite successful, when used in the Kohn-Sham equation where $T[n]$ is constructed for each case, instead of relying on a knowledge of the universal functional $T[n]$.

It is of interest at this stage to examine Bohmian mechanics, where the Schrödinger many-particle wavefunction $\psi(\vec{x}_1, \cdots \vec{x}_n)$ is used to construct a non-linear equation of motion containing the external potential as well as a quantum potential $Q(\vec{x}_1, \cdots \vec{x}_n)$. Let us limit ourselves to a single particle problem in 1-D for the sake of brevity. Bohm [8] writes the wavefunction in the form:

$$\phi(x,t) = R(x,t)\exp\{iS(x,t)/\hbar\} \tag{2}$$
$$R(x,t) = \sqrt{n(x,t)}; \ n(x,t) = |\phi(x,t)|^2 \tag{3}$$

so that R (positive), and S are real functions. Substituting this form of the wavefunction into the Schrödinger equation, one obtains Bohm's form of the equations as:

$$\frac{\partial n}{\partial t} + \nabla \cdot \left[n \frac{\nabla S}{m} \right] = 0 \tag{4}$$

$$\frac{\partial S}{\partial t} + v_{ext} + \frac{(\nabla S)^2}{2m} + Q(x,t) = 0 \tag{5}$$

$$Q(x,t) = \frac{-\hbar^2}{2m} \frac{\nabla^2 R}{R} \tag{6}$$

Eq. 4 is simply the equation of continuity. The term $(\nabla S)^2/2m$ in Eq. 5 is interpreted as the kinetic energy of a point-like particles with momentum $p = \nabla S$. In effect, Eq. 5 has the form:

$$\partial S/\partial t + H(p,x) + Q(x,t) = 0 \tag{7}$$

This is exactly like a classical Hamilton-Jacobi equation with the extra potential $Q(x,t)$, called the quantum potential, or the Bohm potential. Since we are interested in the simplest form of DFT (systems in equilibrium) in this presentation, let us consider an electron confined within an infinite potential well of width a. The eigenfunctions are of the form $\psi_n(x) = \sqrt{(2/a)} \sin(k_n x); \quad n = 1, 2, \cdots$. It is easily shown that the particle current $j(x,t)$ is zero, and the Bohmian particle is *at rest* in some unknown location x in the well, with the probability $|\psi_n(x)|^2$ of *being* there. Einstein felt that the particle being at rest in the well was not the correct physical picture. A more detailed discussion of the Bohmian particle in a well, and a possible resolution to Einstein's objections [9] are given in Chapter 6 of Ref. [10].

Does the Bohmian particle in the well have no kinetic energy? It is easy to show that the kinetic energy is completely resident in Bohm's quantum potential while the particle current is zero. In fact, the kinetic energy functional $T[n(x)]$ per electron confined in the quantum well, given by Hohenberg-Kohn theory (or conventional QM) is essentially the quantum potential of Bohm. Although some advocates of Bohmian mechanics have moved away from the quantum potential (mainly due to philosophical reasons), we find it to be of a sort similar to the effective potentials based on density-functionals used in condensed-matter many-body physics.

For instance, one of the objections adduced against the quantum potential is that it has the 'unusual effect' of making the particle density n influence the dynamics of individual particles. However, that is precisely the message of DFT. It is typical of many-particle physics that the individual dynamics is influence by the over-all particle distribution. For instance, a low-order (mean-field) many-body theory like the Hartree theory of many electrons requires that an electron moves in the many-body field of the other electrons produced by the density distribution $n(x)$. Hartree-Fock theory involves a highly non-local Hartree-Fock potential dependent on the density $n(r)$.

Interestingly, Dürr, Goldstein and Zhangi [11] summarize their attitude to the quantum potential with the statement, 'We believe that the most serious flaw in the quantum-potential formulation of Bohmian mechanics is that it gives a completely wrong impression of the lengths

to which we must go in order to convert orthodox quantum theory into something more rational. The quantum potential suggests ... we must incorporate into the theory a quantum potential of a *grossly* non-local character'. We emphasized the word 'grossly' in the above to high-light where the attitudinal squeamishness resides. In contrast, most physicists who use the highly non-local Hartree-Fock potential as a basic first step in their calculations have given up any such squeamishness. Regarding 'the lengths' needed to reach the classical Hamilton-Jacobi form, as seen from above, we need only a few lines.

The insights from DFT enable us to consider the Bohm potential as a functional of the density, without invoking a wavefunction. Furthermore, Eq. 6 may be used as a differential equation for the direct determination of Q given in terms of $R = \sqrt{n}$, subject to satisfying the equation of continuity, and minimizing the energy. Once R is determined by iteratively solving Eq. 6, S can be obtained from the continuity equation. In effect, a time-dependent system is described by the four vector consisting of the current $j(x,t)$ and the density $n(x,t)$. These are precisely the quantities treated in DFT, and in Bohmian mechanics.

The above considerations suggest that Bohmian mechanics can be formulated entirely in a language free of the wavefunction, using only density functionals, exactly as in DFT.

3. Pair-distributions and classical maps

The Hohenberg-Kohn theorem reduces the n-electron problem to that of a functional of an effective one-body problem and an exchange-correlation potential $V_{xc}[n]$. Given that the basic electron-electron interactions (that lead to quantum correlations including those of the Bell type) are pair-interactions and Pauli exclusion effects, the reduction to a one-body problem achieved in DFT appears a bit mysterious, and one would expect that fundamental two-particle correlations are embedded in the V_{xc}. In fact, the latter is most transparently evaluated as a coupling constant integration over the pair-distribution function (PDF), i.e., $g(\vec{r}_1, \vec{r}_2)$ of the system. This is the probability of finding an electron at r_2, given an electron at r_1.

The PDF is well-defined both classically and quantum mechanically. In QM, the PDF is calculated from the many-particle wavefunction by integrating over all except two space variables $\vec{r}_1, \vec{r}_2$ of two electrons. In a classical system, we can consider a uniform electron fluid (as in jellium), with a mean density n and Wigner-Seitz radius $r_s = \{3/(4\pi n)\}^{1/3}$. We position the origin on the first electron, so that $\vec{r}_1 = 0$. Then, invoking radial symmetry and uniformity, we can use $g(r)$ rather than $g(\vec{r})$ for the PDF, where r is the radial distance of the (second) electron from the origin. When classical mechanics holds (i.e., for $T > 0$ and for very small de Broglie wavelengths), this $g(r)$ for an interacting Coulomb fluid can be calculated using the modified-hyper-netted-chain (MHNC) equation [21], or via molecular dynamics (MD).

In QM, even the non-interacting electron system is of interest if all the particles have the same spin. Then the Pauli exclusion principle controls the entanglement of the n-electron system. This non-interacting set of n-entangled electrons is described by a Slater determinantal wavefunction. The fully spin-polarized system (parallel spins σ), and the fully unpolarized system (anti-parallel spins $\sigma_1 \neq \sigma_2$) are of interest. They can be analytically treated at $T = 0$ as in Ref. [12], and extended to finite-T as in Ref. [13]. Furthermore, the Pauli exchange effect (which leads to entanglement since the wavefunction is a Slater determinant) can be re-written as a non-local quantum potential which is a universal function of r/r_s. This 'Pauli-exclusion' potential $P(r/r_s)$ can be constructed such that it reproduces the quantum $g(r)$ when used in the classical MHNC equation. This provides an interesting and useful classical map of the quantum problem that has been very fruitful in applications to interacting quantum problems ranging from 2-D electron layers [14], hydrogen plasmas, electrons in graphene, and quantum dots [15]. That is, correlated, interacting quantum problems can be replaced by equivalent classical problems where pair-potentials involve additional potentials containing quantum effects which are usually non-local. Bohmian mechanics achieves this directly from the $R = \sqrt{(n)}$ part of the wavefunction. DFT
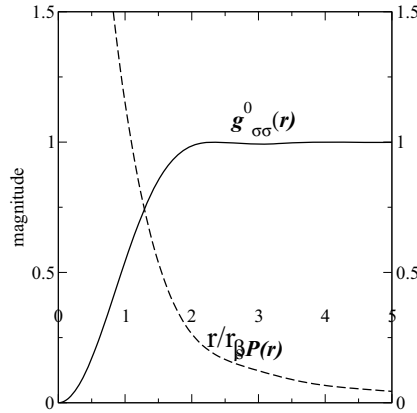
Figure 1. The pair-distribution function $g^0_{\sigma\sigma}(r)$ gives the probability of finding a σ-spin electron at r if there is already a σ-spin electron at the origin (Coulomb repulsion neglected). We plot r/r_s on the x axis, and the result is valid for any density, r_s being the sphere-radius containing an average of one electron. Thus the 'entanglement' due to Pauli exclusion holds even if r_s is a lunar distance. The Pauli exclusion is exactly mimicked by a scale-independent repulsive potential $\beta P(r)$ when used in a classical MHNC equation.

achieves this via functionals of the one-body density $n(r)$. Naturally, non-local contributions are usually quite important in both DFT and Bohmian mechanics.

The PDF of non-interacting fully spin-polarized entangled electrons, denoted by $g^0_{\sigma,\sigma}(r)$ is shown in Fig. 1. It has the form:

$$g^0_{\sigma\sigma'}(r) = 1; \quad \sigma \neq \sigma' \tag{8}$$
$$g^0_{\sigma\sigma}(r) = 1 - \{3j_1(rk_F)/(rk_F)\}^2 \tag{9}$$

(The large-r behavior is normalized to unity, whereas if $\zeta = 0$, it is natural to normalize the spin-resolved functions to 1/2). Here $j_1(x)$ is the spherical Bessel function, while its argument x contains $k_F = 1/(\alpha r_s), \alpha = 0.52106$, where k_F is the Fermi momentum. The probability of finding an electron at r, given that there is an electron at the origin of coordinates is affected by their mutual Coulomb interaction. This is not included in the above calculation, and hence the superfix 'zero' in g^0. A treatment including the Coulomb potential is given in Ref. [13], where it is shown that remarkably good agreement with Monte-Carlo quantum simulations is obtained for these classical maps.

Since the PDF scales as r/r_s, the correlations remain undiminished, whatever be the mean-separation $R = 2r_s$ that is imposed on any two electrons in the entangled system. That is, *local realism* as required by the Einstein-Podolsky-Rosen gedanken experiment does not hold. Thus the correlations unearthed by the Bell inequalities are very transparently and simply revealed by an examination of the PDF of correlated electron systems. This topic is discussed in greater detail in Chapters 7 and 8 of Ref. [10].

4. Finite temperatures, hybrid systems and decoherence

Formal discussions of hybrid systems (i.e., systems containing quantum particles as well as classical particles) [16, 17] rarely bother to discuss the role of temperature, partly because some of these discussions deal with model problems dealing with just one or two particles. In reality, all particles in any system obey quantum mechanics. However, if some particles have de Broglie

wavelengths λ smaller than some assigned length scales associated with the system, then such particles among themselves can be treated within classical mechanics. The interactions between the particle deemed to be classical, and those deemed to be quantum occur via a Hamiltonian H_{int} whose characteristic length scales and energy scales have to be investigated separately. In the following we look at systems at finite temperature T.

If a system is coupled to a heat bath and held at some finite temperature T, the average kinetic energy of the particles is a function of T. In the classical limit the average kinetic energy of an atom is $3T/2$, using energy units for T where the Boltzmann constant becomes unity. At $T = 0$, for our model system of fermions (jellium), the kinetic energy becomes $3E_F/5$, where E_F is the Fermi energy. The latter can be thought of as a temperature $T = 2E_f/5$. Hence we see that we can ascribe a de Broglie wavelength λ and a thermal momentum mv to any particle in a system at an effective temperature T, with v and λ given by:

$$v = \sqrt{3T/m}, \quad \lambda = h/p = h/\sqrt{3mT} \tag{10}$$

It is clear that λ is infinite for systems at $T = 0$, or for sufficiently dilute quantum systems ($E_F \to 0$ as $n \to 0$). Thus all systems become quantum systems as $T \to 0$ since their de Broglie wavelengths become infinite. However, if at some finite (even if low) temperature, e.g., 1 Kelvin, if the mass of a particle is sufficiently large, then if $\lambda \ll 1$ atomic unit, we may assume that superposition and entanglement become unimportant. Such heavy particles are classical particles. Hence, since all systems are quantum systems at $T = 0$, and heavy particles become classical at some finite-T, any quantum theory of hybrid systems [16] has to ultimately incorporate a quantum treatment of thermal fields.

The conventional quantum approach to finite-T problems is difficult, and involves a typical doubling of the Hilbert space as in Umezawa's thermofield dynamics [18], or in the Martin-Schwinger-Kedysh contour technique [19]. These methods are useful for tackling a class of non-equilibrium physics. However, even static finite-T quantum calculations (e.g., via the Matsubara method [12]) are restricted to perturbation theory.

On the other hand, finite-T density functional theory [2] presents a computationally and conceptually much simpler approach to finite-T problems, as well as two-temperature quasi-equilibria. Here the finite T one-body density functionals $n(\vec{x}, T)$ determine all the thermodynamics and linear transport properties of the system *without* the need for a wavefunction.

The explicit construction of a DFT and the calculation of such finite-T hybrid systems for a system of protons (classical) and electrons (quantum) at finite-T has been given in Ref. [20]. The method is applicable to any electron-ion system, where the ions are treated classically. The usual Born-Oppenheimer approximation is not needed. If the ion distribution is denoted by $\rho(\vec{r})$, and the electron distribution is $n(\vec{r})$, the total free energy $F([\rho], [n])$ is a functional of both distributions. Hence we have two coupled Hohenberg-Kohn-Mermin type equations to determine the finite-T distributions of the hybrid system. That is, the functional derivatives with respect to variations $\delta n, \delta \rho$ lead to two coupled Euler-Lagrange equations.

$$\frac{\delta F[\rho, n]}{\delta n} = 0, \quad \frac{\delta F[\rho, n]}{\delta \rho} = 0. \tag{11}$$

The first of these equation can be reduced to a Kohn-Sham equation for electrons at finite-T, or simply retained as a Hohenberg-Kohn variational form. The second equation leads to a classical Hohenberg-Kohn equation for the ion distribution that is identified as a form of the MHNC equation. In effect, it is a Boltzmann distribution for the density ρ in terms of the 'potential of mean force' (PMF) used in the statistical mechanics of liquids [21]. The PMF is the appropriate Kohn-Sham potential for this classical system. The full practical implementation

of this approach to a typical hybrid system (an interacting gas of electrons and protons at finite T inclusive of the formation of hydrogenic bound states) is given in Ref. [20].

4.1. Decoherence and macroscopic cat states

The equation 10 is of great importance in showing us that there is no need for *ad hoc* theories of decoherence to eliminate macroscopic cat states from QM. Let us consider a 1 kg cat at room temperature (300 K, i.e., 9.500×10^{-4} Hartees). The atoms in the cat have internal energies with approximately $3T/2$ arising from translational motion. The center of mass will also make random oscillatory motions about an equilibrium position consistent with its temperature and any motion of the cat. The corresponding center-of-mass de Broglie wavelength λ_c turns out to be

$$\lambda_c \simeq 9.45 \times 10^{-23} \text{ meters} \tag{12}$$

The 'radius' of a proton is about 0.88 femtometers (1 fm=10^{-15} meters). The de Borglie wavelength of the cat is about one hundred-millionth of the size of a proton! Even when cooled to one Kelvin, the de Broglie wavelength remains totally negligible. Even a free electron close to a cat's body would not get entangled with the cat's quantum energy states. Matter has to be squashed to densities where nuclear reactions begin before superpositions are possible at such small values of λ_c. Clearly, Schrödinger's cat states of macroscopic bodies (entanglements or superpositions) do not exist in nature except at T=0, or possibly in white dwarfs.

One may argue that the mass M of the center of mass is not the proper quantity to use. One may claim that QM should be applied to some molecules of the cat that are specific to it being dead or alive in Schrödinger's cat paradox. In that case we are no longer applying QM to a macroscopic system and then there is no difficulty in having superpositions or entangled states. Chemical reactions (e.g., cyanide reacting with the cat) are simply processes where reactive atomic groups enter into entanglements. Such processes pose no difficulty and are not 'paradoxical'.

One may also question the use of a momentum calculated from $3T/2$. This is the classical kinetic energy of an ideal gas. We know from Dulong and Petit's law (or from the more modern Einstein-Debye theory of solids) that classically, a system held together by chemical bonds, e.g., a cat, has three degrees of vibration per atom, and three degrees of translation, each having an energy $T/2$. For solids in the low-temperature limit, we need the Fermi energy of the system. Such detailed treatments merely introduce numerical factors of little consequence. The basic conclusion that λ_c is very very small remains firm.

These considerations imply that explicit decoherence theories like those of Penrose ('objective reduction' due to quantum gravity) [22], or the 'spontaneous localization' model of Ghirardi, Rimini and Weber [23] are unnecessary additions to quantum mechanics, if we grant that the relevant de Broglie lengths are much smaller than even nuclear radii.

5. Conclusion

The tradition of studying just one or two quantum particles, usually in a two-state model has a long history in foundational studies. However, if the many-body problem is examined, QM can be approached using one-body density functionals, without recourse to wavefunctions, both at $T = 0$ and at finite-T. An examination of Bohmian mechanics within the perspective of DFT is conceptually rewarding and clarifies the nature of the Bohmian quantum potential. Finite-T quantum mechanics leads us to consider the thermal de Broglie wavelength which, being negligible for macroscopic systems, ensures that there are no macroscopic Schrödinger cat states.

References
[1] Hohenberg P and Kohn W 1964 *Phys. Rev.* B **136** 864

[2] Mermin N D 1965 *Phys. Rev.* A **137** 1441
[3] Rajagopal A K and Callaway J 1973 B *Phys. Rev .* **7** 1912;
    MacDonald A H and Vosko S H 1979 *J. Phys.* C **12** 2977
[4] Runge E and Gross E K U 1984 *Phys. Rev. Lett.* **52** 997
[5] Lieb E 1985 *Density functional methods in Physics* NATO Series **B123** ed R M Dreizler and J Providencia
    (New York: Plenum)
[6] Karasiev V V and Trickey S B 2012 *Preprint* arXiv:1109.6602
[7] Gross E K U and Dreizler R M 1993 *Density Functional Theory* NATO ASI Series **337** (New York: Plenum)
[8] Bohm D 1952 *Phys. Rev.* **85** 166; *do.* 1953 *Phys. Rev.* **89** 1040
[9] Einstein A 1953 *Scientific papers presented to Max Born* (*Festschrift*) (New York: Hafner) p 33 and Bohm
    D in the same volume, p 13-19
[10] Dharma-wardana M W C 2013 *A physicist's view of Matter and Mind* (World Scientific Singapore)
[11] Dürr D Goldstein S and Zhangi N 1995 *Bohmian Mechanics and Quantum Theory: An Appraisal* ed J T
    Cushing, A Fine and S Goldstein (New York: Kluwer Academic Press) (*Preprint* quant-ph/9511016)
[12] Mahan G D 1981 *Many-Particle Physics* (New York: Plenum)
[13] Dharma-wardana M W C and Perrot F 2000 *Phys. Rev. Lett.* **84** 959
[14] Perrot F and Dharma-wardana M W C 2001 *Phys. Rev. Lett.* **87** 206404
[15] Dharma-wardana M W C 2012 *Int. J. Quant. Chem.* **112** 53
[16] Heslot A 1985 *Phys. Rev.* D **31** 1341
[17] Elze H-T 2012 *Phys. Rev.* A **85** 052109
[18] Umezawa H 1993 *Advanced field theory: Micro, Macro and Thermal Physics* (New York: AIP)
[19] Rammer J and Smith H 1986 *Rev. Mod. Phys.* **58** 323
[20] Dharma-wardana M W C and Perrot F 1982 *Phys. Rev.* A **26** 2096
[21] Hansen J-P and MacDonald I R 2006 *Theory of Simple Liquids* (London: Academic)
[22] Penrose R 1996 *Gen. Relativ. Grav.* **28** 581
[23] Ghirardi C, Rimini A and Weber T 1986 *Phys. Rev.* D **34** 470