Can decoherence make quantum theories unfalsifiable? Understanding the quantum-to-classical transition without it

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Abstract. Exact predictions for most quantum systems are computationally inaccessible. This is the so-called many body problem, which is present in most common interpretations of quantum mechanics. Therefore, predictions of natural quantum phenomena have to rely on some approximations (assumptions or simplifications). In the literature, there are different types of approximations, ranging from those whose justification is basically based on theoretical developments to those whose justification lies on the agreement with experiments. This last type of approximations can convert a quantum theory into an “unfalsifiable” quantum theory, true by construction. On the practical side, converting some part of a quantum theory into an “unfalsifiable” one ensures a successful modeling (i.e. compatible with experiments) for quantum engineering applications. An example of including irreversibility and dissipation in the Bohmian modeling of open systems is presented. On the ontological level, however, the present-day foundational problems related to controversial quantum phenomena have to avoid (if possible) being contaminated by the unfalsifiability originated from the many body problem. An original attempt to show how the Bohmian theory itself (minimizing the role of many body approximations) explains the transitions from a microscopic quantum system towards a macroscopic classical one is presented.

1. Introduction: the many body problem
The role of all physical theories (and the quantum theory among them) is to employ mathematical models implementing physical laws to predict natural phenomena. The correctness of a theory is judged by the extent to which its predictions agree with empirical observations. In this sense, it seems to me that the deep consequences of the many body problem [1, 2, 3] on ontological issues of quantum mechanics have not been properly recognized.

The many body problem is present in almost all interpretations of quantum mechanics (Copenhagen [4, 5], many-worlds [6, 7], Bohmian mechanics [8, 9, 10, 11, 12, 13], etc). This problem is due to the fact that the Schrödinger equation (or any other equation of motion) is analytically unsolvable most of the times, and its numerical integration is out of today’s present computer capabilities, even for quantum systems with very few degrees of freedom. This computational difficulty is the reason why our predicting capability of quantum phenomena is, indeed, very limited. In 1929, Dirac wrote the following [1]:

The general theory of quantum mechanics is now almost complete. The underlying physical laws necessary for the mathematical theory of a large part of physics and the
entire chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.

Three decades later, Born rephrased the issue [2]:

It would indeed be remarkable if Nature fortified herself against further advances in knowledge behind the analytical difficulties of the many body problem.

I really believe that, as indicated by Born, many advances in our ability to understand the quantum world are limited by this computational difficulty [3]. We can successfully solve the Schrödinger equation for a single-particle quantum system in an isolated environment (for example, an hydrogen atom whose electronic wave function is solved with an external potential generated by fixed nuclei). However, isolated quantum systems that appear in all textbooks of quantum mechanics are so simple that they have to be understood as a kind of toy-model of the quantum systems of interest. No real quantum system is completely isolated from its surroundings [14, 15, 16].

One of the most common strategies to study quantum systems is to differentiate between the “active” particles (or degrees of freedom) and the rest of particles, which are considered as “external” or “passive”. The set of active particles are collected under the name open quantum system\(^1\) and all the rest, the passive part, are named the environment or the bath [17]. For the type of discussion in the paper, the measuring apparatus can also be considered as part of the environment. In general, a quantum system has few degrees of freedom, while the environment typically has a large number. As emphasized above, the many body problem makes the exact solution of the system plus environment impossible. The environment is not explicitly simulated, but its effect is introduced through some type of external operator (or potential energy) acting on the degrees of freedom of the quantum system. How do we specify the external operators or potentials to get concrete predictions of a natural phenomenon?

This paper revolves around the implications of the different types of answers to the question posed above. There are (approximated) external operators that are basically based on theoretical developments, while others are justified by the agreement with experiments. This last type of (approximated) external operators can convert any formal quantum theory into an “unfalsifiable” theory, true by construction. In section 2, the modeling of open quantum systems is explained. I discuss how easy it is to develop approximations that traverse the subtle line that differentiates falsifiable and unfalsifiable theories. As an example, in section 3, I discuss a Bohmian modeling of open systems where irreversibility and dissipation in electronic devices is introduced [18]. I also emphasize how useful this type of unfalsifiable model can be (not for ontological discussion but) for practical simulations of quantum phenomena and their applications. On the contrary, in section 4 I will show how the conditions for the classicality for the center of mass of a macroscopic system, not for each degree of freedom, at each individual experiment, not for an ensemble of experiments, can be obtained within the Bohmian theory (minimizing the mentioned many body problem) [19]. Finally, I provide some conclusion of the paper in section 5 comparing the intrinsic tendency towards unfalsifiability in different interpretations of quantum mechanics.

2. Can decoherence make quantum theories unfalsifiable?
Over the course of the past decade, decoherence has become an ubiquitous scientific term popular in all kinds of research, from fundamental theories of quantum physics to applications in nanoengineering and quantum computing [15]. While decoherence has been directly observed in various experiments, its meaning, scope and consequences are still diffusely and ambiguously

\(^1\) For commodity, whenever possible, I will omit the word “open”. 
understood by the scientific community. For example, decoherence has been invoked as the solution to long-standing foundational problems dating back to the beginnings of quantum mechanics. Perhaps, the key example of the “magical” explanatory power of decoherence is the attempt to explain the quantum-to-classical transition as something simple due to the loss of coherence of quantum particles (but, why do the particles lose the coherence?). Certainly, this transition remains one of the most intriguing features of the quantum world [15, 20].

The mathematical definition of decoherence is more simple and concrete than its physical consequences: Decoherence is the result of the entanglement between the quantum system and its environment. [15, 20] If the mathematical definition of decoherence is so simple and clear, why are its physical implications so ambiguous? Because of the many body problem. We cannot know which is the exact physical effect of this quantum entanglement by directly solving the many body Schrödinger equation, and we have to relay on (more or less imprecise and vague) approximations.

2.1. Modeling an open quantum system in terms of the reduced density matrix

In order to explain better how the many body problem forces us to explain decoherence with approximations, let us consider a simple example for a non-relativistic quantum world with spinless particles “living” in a 1D physical space. The generalization to a 3D physical space with particles with spin does not change any of the conclusions presented here, but only makes the many body problem more dramatic. We consider $N$ particles of mass $m$ governed by the wave function $\Psi(\vec{x}, t)$ solution of the many-particle Schrödinger equation,

$$i\hbar \frac{\partial \Psi(\vec{x}, t)}{\partial t} = \hat{H}\Psi(\vec{x}, t) = \left(-\frac{\hbar^2}{2m} \sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} + U(\vec{x}, t)\right)\Psi(\vec{x}, t), \quad (1)$$

where $\vec{x} = \{x_1, x_2, ..., x_N\}$ are the positions of all the particles and the Hamiltonian operator $\hat{H}$ contains the dynamical laws of the particles of the system, of the environment and the interaction among particles. The potential $U(\vec{x}, t)$ is responsible for the non-separability of Eq. (1). I emphasize that Eq. (1) can only be solved for $N = 1$, $N = 2$, or perhaps with powerful computational abilities, for $N = 3$ degrees of freedom. This is the many body problem [3, 17].

Alternatively to the (universal) wave function $\Psi(\vec{x}, t)$ in Eq. (1), the whole quantum system of $N$ particles can be tackled with the (universal) density matrix $\hat{\rho}_{\text{tot}}(t) = |\Psi\rangle\langle\Psi|$. Its (unitary) time evolution is determined by the Liouville–von Neumann equation [4]:

$$i\hbar \frac{d\hat{\rho}_{\text{tot}}(t)}{dt} = [\hat{H}, \hat{\rho}_{\text{tot}}(t)], \quad (2)$$

Because of the many body problem, obviously, the exact solution of Eq. (2) is inaccessible too. A quite common strategy $^2$ for treating Eq. (2) is based on defining the density matrix of the open system $\hat{\rho}_{\text{sys}}(t)$ by integrating or tracing out the degrees of freedom of the environment of the full (universal) density matrix $\hat{\rho}_{\text{tot}}(t) = Tr_{\text{env}}\{\hat{\rho}_{\text{tot}}(t)\}$. A standard approximation (under the consideration that the environment “lose” memory of their internal correlations [25, 26, 27]) is that the density matrix of the system is governed by the following master equation:

$$\frac{d\hat{\rho}_{\text{sys}}(t)}{dt} = -\frac{i}{\hbar} [\hat{H}_{\text{sys}}, \hat{\rho}_{\text{sys}}(t)] + \hat{D}[\hat{\rho}_{\text{sys}}(t)], \quad (3)$$

$^2$ There are other approximations for overcoming the many body problem of time-independent (closed system) Hamiltonian eigenstates with several degrees of freedom. For example, the Hartree - Fock approximation [21, 22], Density Functional Theory [23, 24], etc.
where $\hat{H}_{\text{sys}}$ is the part of the Hamiltonian that acts on the degrees of freedom of the system and the superoperator $\hat{D}$ converts the values of the density matrix operator at one time into new values at another time. This superoperator $\hat{D}$ is usually defined as the dissipation operator. Perhaps, the name decoherence operator would also be adequate. According to the work of Lindblad, Gorini, Kossakoneski and Sudarshan [25, 26, 27], such operator $\hat{D}$ can be defined by,

$$\hat{D}[\rho_{\text{sys}}(t)] = -\frac{1}{2} \hat{A}^{\dagger} \hat{A} \rho_{\text{sys}}(t) - \frac{1}{2} \rho_{\text{sys}}(t) \hat{A}^{\dagger} \hat{A} + \hat{A} \rho_{\text{sys}}(t) \hat{A}^{\dagger}$$  \hspace{1cm} (4)$$

where $\hat{A}$ is an unknown operator (not necessarily hermitian). The ultimate reason why $\hat{A}$ is unknown (which means that $\hat{D}$ is also unknown) is the many body problem [3]. To exactly identify $\hat{D}$ from Eq. (3) we require the knowledge of $\hat{\rho}(t)_{\text{tot}}$, that implies the full knowledge of $\Psi(\vec{x}, t)$, which is numerically inaccessible [28].

To further elaborate $\hat{D}$ some approximation is mandatory. The second term of the right hand side of Eq. (3), if needed, can include dissipative (inelastic) scattering not achievable from a unitary operator. For example, the electron-phonon interaction. The typical semi-classical Boltzmann-like scattering term (based on the Fermi Golden rule) deals with scattering mechanics in the phase space. In order to be able to use the same tools to tackle electron-phonon interaction we need a type of density matrix in the phase-space. This can be obtained through a Wigner–Weyl transformation of $\hat{\rho}_{\text{tot}}$ that is named Wigner distribution function [29]. This Wigner distribution function is a really powerful tool for the simulation of quantum systems of interest, because it mixes the pure quantum unitary dynamic present in the first term of the right hand side of Eq. (3) together with dissipative and decoherence dynamics introduced by the second term. However, What is the justification for this type of external (approximated) operators that includes electron-phonon interactions? Part of the justification comes from the theory, but another part from the experimental evidences.

2.2. Modeling an open quantum system in terms of the (Bohmian) conditional wave function

In order to enlarge the previous discussion about different models and approximations for open systems, in this subsection I explain an original algorithm to deal with open systems within Bohmian mechanics. The wave function of an open quantum (sub) system does not exist. This is the reason why the (reduced) density matrix is invoked in section 2.1. Fortunately, the concept of wave function of an open system can be rigorously formulated within the Bohmian explanation of quantum phenomena, by means of the conditional wave function [10, 11, 12]. In Bohmian mechanics, a system of $N$ particles is composed by the (universal) wave function $\Psi(\vec{x}, t)$ described by Eq. (1) plus the position of all the particles that I denote here by capital letters $\vec{Y}[t] = \{X_1[t],...,X_0[t],...,x_N[t]\}$. The time evolution of the wave function $\Psi(\vec{x}, t)$ is described by Eq. (1). Clearly, the many body problem in Bohmian mechanics is hidden here. The time evolution of the particles position is determined by the following guiding equation:

$$v_k(\vec{x}, t) = \frac{dX_k[t]}{dt} = \frac{J_k(\vec{x}, t)}{|\Psi(\vec{x}, t)|^2},$$  \hspace{1cm} (5)$$

where $J_k(\vec{x}, t)$ is the standard quantum current density. The formal presentation of the theory requires a discussion on the selection of the initial positions according to the quantum equilibrium hypothesis, plus an explanation of the symmetry of the wave function of identical particles. See many reviews, for example [8, 9, 10, 11, 12, 13].

What I have explained about Bohmian mechanics is enough to define the conditional wave function. Let us consider the mentioned many-particle wave function $\Psi(\vec{x}, t)$ solution of the unitary Schrödinger equation (1). If we focus only on the trajectory $X_0[t]$ of one specific particle
Bohmian mechanics defines the so-called conditional wave function \[\Psi_{a}(x,t) = \Psi(x_{a}, \vec{Y}[t], t),\] where \(\Psi_{a}(x, t)\) constitutes a slice of the whole multi-dimensional wave function \(\Psi(\vec{x}, t)\) solution of Eq. (1). \(^\text{3}\) I have defined \(\vec{Y}[t] = \{x_{1}[t], \ldots, x_{a-1}[t], x_{a+1}[t], \ldots, x_{N}[t]\}\) as the Bohmian trajectories of all particles except \(a\). It has been demonstrated by the author [30] that \(\Psi_{a}(x_{a}, t)\) obeys the following wave equation:

\[
i\hbar \frac{\partial \Psi_{a}(x_{a}, t)}{\partial t} = \left\{ -\frac{\hbar^{2}}{2m} \frac{\partial}{\partial x_{a}^{2}} + U(x_{a}, \vec{Y}[t], t) + G_{a}(x_{a}, \vec{Y}[t], t) + iJ_{a}(x_{a}, \vec{Y}[t], t) \right\}\Psi_{a}(x_{a}, t),
\]

where \(U(x_{a}, \vec{Y}[t], t)\) is the potential that appears in Eq. (1) evaluated at \(\vec{x} = \{x_{a}, \vec{Y}[t], t\}\). The additional potentials \(G_{a}(x_{a}, \vec{Y}[t], t)\) and \(J_{a}(x_{a}, \vec{Y}[t], t)\) are defined through the (universal) wave function [30, 31]. By using Eq. (7) for each particle, \(x_{a}[t]\) for \(a = 1, \ldots, N\), we obtain a system of \(N\) coupled single-particle pseudo-Schrödinger equations. In principle, such system of equations is able to compute many-particle Bohmian trajectories without knowing the many-particle wave function [11]. The great merit of Eq. (7) is to demonstrate that such a single-particle solution of a many-particle problem exists, although we do not know exactly the values of the terms \(G_{a}(x_{a}, \vec{Y}[t], t)\) and \(J_{a}(x_{a}, \vec{Y}[t], t)\). The ultimate reason why it is not possible to know such terms is because they depend on the knowledge of the (universal) wave function \(\Psi(\vec{x}, t)\) that remains inaccessible because of the many body problem [31]. In summary, the situation is quite similar to that found in Eq. (3). We have a quantum equation of motion to tackle a many body system, but there are some operators in Eq. (3) or external potentials in Eq. (7) that require approximations to arrive to some specific predictions.

The formalism of the conditional (single-particle) wave function just described is the base of the simulator BITLLES [32], which already includes electron-electron interaction beyond mean field [33], open system boundaries [34], exchange (fermion) interactions [35, 36], noise computation [37, 38] and high-frequency displacement currents [39]. After, in section 3, I will use the conditional wave equation (7) to explain an \textit{ad hoc} approximation for including the electron-phonon interactions mentioned in section 2.1. After, in section 4, I will use the same equation (7) to develop a quantum-to-classical transition minimizing the approximations needed to overcome the many body problem.

### 2.3. Falsifiable and unfalsifiable theories

After two examples on how approximations are mandatory in the quantum treatment of open systems, let us discuss the role of such approximations in the falsifiability of quantum theories. In 1963, Karl R. Popper [40] wrote his idea about the importance of developing theories that can be falsified. He argued that irrefutability is not a virtue of a theory (as people often think) but just the contrary. He wrote the following example explaining how theories that predict things too vaguely can imply that the predictions can hardly fail. He compared astronomers and astrologers in the following sentence [40]:

It is a typical soothsayer’s trick to predict things so vaguely that the predictions can hardly fail: that they become irrefutable.

A similar point of view was shared by Einstein [41] when he emphasized that physical theories have to be risky (avoid ambiguities that minimize the possibility of being refuted):

\(^{3}\) The generalization of the conditional wave function for a set of particles, not only for one, can be trivially obtained.
No amount of experimentation can ever prove me right; a single experiment can prove me wrong.

Because of the many body problem, as I repeatedly stressed in this paper, approximations are mandatory to make predictions of most quantum systems. Unfortunately, an approximation introduces some degree of ambiguity into the predictions. There are many types of approximations in the literature. Most of them are basically hanged on the theory. Although the many body problem does not allow us to exhaustively define the external operators or potentials, we can take advantage of some mathematical properties provided by the quantum theory at hand (for example the hermiticity of the observable results or the unitary evolution of the whole system) to get some (partial and) useful information about the shape of such operators.

On the other side, there are approximations to fix the external operators in Eq. (4) (or the potentials in Eq. (7)) whose justification is, in some part, the agreement with experiments. Initially, one can make a hand made proposal for the operators (or potentials). If such operators do not provide good agreement with the experiment, we slightly “tune” them to improve the agreement. In principle, this second route to fix the external potentials seems very satisfactory. However, we have to realize about the ontological implications of this second route. If we select the external operators (or the potentials $J_a(x,t)$ and $G_a(x,t)$ in Eq. (7)) to ensure that we correctly reproduce the experimental results, then, our theory will reproduce experiments by construction.

When dealing with practical applications of quantum mechanics, this route seems less dangerous. However, when dealing with foundational questions much more care is required. Such external operators can explain by themselves the appearance of the arrow of time, why the entropy grows, why quantum systems become classical, etc. All these intriguing quantum phenomena are, somehow, behind the umbrella term of decoherence. One can erroneously conclude that these foundational problems are, already solved, by the “magic” explanatory power of decoherence. Any disagreement between predictions and experiments can always be attributed to the lack of a “proper” modeling of decoherence (a proper computation of the quantum entanglement between the system and the environment), not to a limitation of the theory itself. This flexible understanding of the role of the external operators can convert a quantum theory into a unfalsifiable (true by construction) and universal one (valid for any system by definition).

As far as we cannot avoid the many body problem, all approximations for open quantum systems have a mix of theoretical and experimental justification, with different proportions. Therefore, I am not saying that some approximations are scientific and others non-scientific. I am just saying here that, when discussing foundational questions of quantum mechanics, one has to be worried about the possible contamination of the final conclusions by the unfalsifiability, i.e. because of the unsurmountable many body problem.

3. An example of the practical utility of developing unfalsifiable quantum theories
The quantum theory is today an old theory with more than a century of history. Many researchers work on quantum mechanics applications without worrying at all about foundational issues. I am not criticizing this attitude at all since I sincerely believe that it has provided an unquestionable success in our ability to develop quantum applications. For example, in the next subsection, I explain the recent work of our research group to include irreversibility and dissipation in the Bohmian modeling of open systems [18], and how interesting these capabilities can be in many applied disciplines.

One common approximation to simplify the many body problem in the simulation of electronic devices is the Born-Oppenheimer assumption, which states that the motion of atomic nuclei and
electrons in a (semiconductor) crystal can be separated because of the very different masses of the electrons and atomic nuclei [42]. The (approximated) electronic wave-function can be solved alone. However, since it is well-known from experiments that electrons do effectively interact with the nuclei, we can reintroduce the collision of the electron with a phonon (a collective excitation in a periodic arrangement of atoms) through the external potentials discussed in section 2.2. The electron loses/gains energy during the emission/absorption of a phonon. In order to include the effect of the interaction of an electron with phonons we need an effective Schrödinger type evolution for the conditional wave function like Eq. (7), not a single-particle Schrödinger equation. According to Eq. (7), for a system with $U(x,t) = 0$, we suggest the following equation for the electron [18]:

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - \frac{i\hbar \lambda f(t)}{m \psi(x,t)} \frac{\partial \psi(x,t)}{\partial x} + \frac{1}{2m} \lambda^2 f^2(t) \right] \psi(x,t),$$

(8)

with

$$J_a(x,t) = -\frac{\hbar \lambda f(t)}{m \psi(x,t)} \frac{\partial \psi(x,t)}{\partial x},$$

(9)

and

$$G(x,t) = \frac{1}{2m} \lambda^2 f^2(t),$$

(10)

where $f(t)$ is a time dependent function which mimics the electron-phonon interaction. On the other hand, the parameter $\lambda$ is the momentum of the phonon emitted ($\lambda > 0$) or absorbed ($\lambda < 0$). The motivation for defining Eq. (8) can be understood by rewriting it as :

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \frac{1}{2m} \left( -i\hbar \frac{\partial}{\partial x} + \lambda f(t) \right)^2 \psi(x,t).$$

(11)

It is quite simple to realize that Eq. (11) satisfies the following desired features. First, the conservation of the total momentum between the electron and the phonon. And second, the electron (i.e. the conditional wave functions assigned to the electron) gains/loses an amount of energy proportional to the energy of the phonon absorbed/emitted. I notice that the momentum operator for Eq. (11) is given by $P = p + \lambda f(t) = -i\hbar \partial/\partial x + \lambda f(t)$.

The trajectories of the particle can be straightforwardly obtained inserting the conditional wave function in the polar form, $\psi(x,t) = R(x,t)e^{iS(x,t)/\hbar}$, into Eq. (11). Taking the imaginary part, one obtains a modified continuity equation

$$\frac{\partial R^2}{\partial t} + \frac{\partial}{\partial x} \left( R^2 \left( \frac{\partial S/\partial x}{m} + \frac{\lambda f(t)}{m} \right) \right) = 0,$$

(12)

from which it is easy to realize that the velocity field of the particles is:

$$m \frac{dX[t]}{dt} = m v(x,t) \bigg|_{x=X[t]} = \frac{\partial S(x,t)}{\partial x} + \lambda f(t) = \hbar \text{Im} \left[ \frac{\partial \Psi(x,t)/\partial x}{\Psi(x,t)} \right] + \lambda f(t).$$

(13)

4 In particular, we have tested in [18] two specific examples: an instantaneous interaction $f(t) \equiv \Theta(t) = 0$ for $t < t_1$, $\Theta(t) = 1$ for $t > t_1$ and a gradual interaction $f(t) \equiv \Gamma(t) = 0$ for $t < t_0$, $\Gamma(t) = 1$ for $t > t_1$ and $\Gamma(t) = (t-t_0)/(t_1-t_0)$ for $t_0 < t < t_1$. 
One can see that the velocity field has two terms, the usual one of Bohmian mechanics \((\partial S(x,t))/\partial x\) [11] and an additional term proportional to \(\lambda\), i.e. the momentum of the phonon. Because of the function \(f(t)\) the velocity of the electron changes after the interaction with the phonon. The new velocity of the electron (i.e. the conditional wave function assigned to the electron) is the old one plus a quantity proportional to the momentum of the absorbed/emitted phonon itself. It can increase or decrease depending on whether the phonon is emitted \((\lambda < 0)\) or absorbed \((\lambda > 0)\). I also notice that the present development includes electron-phonon scattering without violating the continuity equation, a problem that could appear in different formalisms [29]. Before the interaction with the phonon the momentum and the energy of the electron are:

\[
\langle P \rangle = \langle p \rangle, \\
\langle E \rangle = \langle p \rangle^2 + \frac{\Delta p^2}{2m},
\]

(14)

(15)
after the interaction with the phonon they are:

\[
\langle P \rangle = \langle p \rangle + \lambda, \\
\langle E \rangle = \frac{(\langle p \rangle + \lambda)^2}{2m} + \frac{\Delta p^2}{2m},
\]

(16)

(17)

where \(\langle p \rangle = -i\hbar \int \psi^*(\partial \psi/\partial x)dx\). Here I underline that the interaction among electrons and phonons briefly introduced here and explained in detail in Ref. [43] is flexible enough to guarantee an agreement with experiments. The scattering rates (i.e. the number of collisions per second) in our time-dependent scenario are defined according to the standard Fermi golden rule. Therefore, a proper selection of the absorption and emission rates (more emission than absorption) provides dissipation of energy (heat) in electronic devices. Obviously, these rates can be tuned to better reproduce experimental scenarios. I emphasize that the hand made scattering rates in our approach are introduced directly into the (conditional) wave function (not into transitions between phase space points as in the Wigner formalism [29]).

4. Understanding the quantum-to-classical transition with Bohmian mechanics

Since the beginning of quantum theory a century ago, the study of the frontier between classical and quantum mechanics has been a constant topic of debate. Let us now briefly explain an attempt developed by the author and co-workers [19] to discuss the quantum-to-classical transition without being (much) contaminated by the approximations needed to overcome the many body problem. Among the attempts from different interpretations of quantum mechanics to reach the classical limits from quantum theories, Bohmian mechanics [8, 9, 11, 13] has some attractive features. Like in classical mechanics, it describes a unique quantum experiment in terms of a trajectory and, remarkably, the quantum measurement is unproblematically treated as another type of interaction [12]. In section 4.1, I discuss how a single-particle quantum system is an ill-defined scenario to reach classical mechanics. Then, in section 4.2, I briefly explain our recent result [19] on how the quantum-to-classical transition can be successfully tackled with the center of mass of a many body system.

4.1. The unsuccessful single-particle scenario

Let us start by discussing the difficulties of studying the quantum-to-classical transition in single particle scenarios. The Newton law that fully determines a classical trajectory \(X[t]\) is:

\[
m \frac{d}{dt} v(X[t], t) = \left[ -\frac{\partial}{\partial x} \left( U(x, t) \right) \right]_{x=X[t]},
\]

(18)
where \(v(X[t], t)\) is the velocity of such particle at the position \(X[t]\) and \(U(x, t)\) is a scalar energy (classical) potential. It is well-known that Newtonian mechanics is compatible with the following Hamilton–Jacobi equation [11]:

\[
H \left( x, \frac{\partial S(x, t)}{\partial x}, t \right) + \frac{\partial S(x, t)}{\partial t} = \frac{1}{2m} \left( \frac{\partial S(x, t)}{\partial x} \right)^2 + U(x, t) + \frac{\partial S(x, t)}{\partial t} = 0, \tag{19}
\]

where \(H\) is the Hamiltonian of the single-particle system that contains a kinetic energy plus a potential energy \(U(x, t)\), and \(S(x, t)\) can be identified with the Hamilton’s principal function. In general, the direct solution of Eq. (19) is more difficult than using the Newton formulation in Eq. (18). In any case, Eq. (19) can be interesting when dealing with an (infinite) ensemble of classical trajectories, i.e. in classical statistics. For example, for a classical (single-particle) experiment with some practical difficulties in specifying the initial position and velocity of the particle, such that different experimental realizations can have slightly different initial conditions. For such an experiment, we can define some distribution of the initial position of the particles of different experiments \(R^2(x, 0) \geq 0\). Such an ensemble of trajectories will evolve in time according to Eq. (18) so that we will obtain a function \(R^2(x, t)\) that describes the particular distribution of particles at any time. All these classical particles will move, in a continuous way, from one unit of volume of the physical space to another. Therefore, we can ensure that the ensemble of trajectories accomplishes the following local conservation law [11]:

\[
\frac{\partial R^2(x, t)}{\partial t} + \frac{\partial}{\partial x} \left( \frac{1}{m} \frac{\partial S(x, t)}{\partial x} R^2(x, t) \right) = 0. \tag{20}
\]

The two previous (real) equations, Eqs. (19) and (20), for \(S(x, t)\) and \(R(x, t)\) are equivalent to the following (complex) classical wave equation [11]:

\[
i\hbar \frac{\partial \psi_{cl}(x, t)}{\partial t} = \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x, t) - Q(x, t) \right) \psi_{cl}(x, t), \tag{21}
\]

where \(\psi_{cl}(x, t) = R(x, t) \exp(iS(x, t)/\hbar)\) is defined as a classical\(^5\) (complex) wave function. The new function \(Q(x, t)\) in Eq. (21) is the so-called quantum potential in the hydrodynamic or Bohmian interpretation of quantum mechanics:

\[
Q(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2 |\psi_{cl}(x, t)|^2/\partial x^2}{|\psi_{cl}(x, t)|^2} = \frac{\hbar^2}{2m} \frac{\partial^2 R(x, t)/\partial x^2}{R(x, t)}. \tag{22}
\]

The reader can be, perhaps, surprised that \(Q(x, t)\) appears in a pure classical context, while it is referred to as a quantum entity. The justification is based on historical arguments [11, 8].

Let us move to the quantum modeling of the same single-particle system. The wave equation that describes the quantum wave function \(\psi(x, t)\) of such experiment is just the typical single-particle Schrödinger equation:

\[
i\hbar \frac{\partial \psi(x, t)}{\partial t} = \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x, t) \right) \psi(x, t). \tag{23}
\]

I notice that the \(Q(x, t)\) term is missing when comparing the quantum wave equation (23) to the classical wave equation (21). Again, when putting \(\psi(x, t) = R(x, t) \exp(iS(x, t)/\hbar)\) into Eq.

\(^5\) For simplicity, I assume that \(R(x, t)\) and \(S(x, t)\) are single valued. This condition is equivalent to assigning a unique velocity to each position of space. If this is not the case, different wave functions (i.e. a mixed state) will be needed to describe the different velocity fields of the classical system.
(23) we arrive at a quantum continuity equation identical to the classical continuity equation, Eq. (20), and at a quantum Hamilton–Jacobi equation quite similar to the classical one, Eq. (19), but now with the presence of a quantum potential [8]:

$$\frac{1}{2m} \left( \frac{\partial S(x,t)}{\partial x} \right)^2 + U(x,t) + Q(x,t) + \frac{\partial S(x,t)}{\partial t} = 0. \quad (24)$$

The last step in this description of similitudes and differences between classical and quantum modelings is getting a quantum Newton-like equation. It can be easily demonstrated using Eq. (20) and Eq. (24) that a Newton-like equation can be developed for the quantum (Bohmian) trajectories [8, 11]:

$$m \frac{d}{dt} v(X[t], t) = \left[ - \frac{\partial}{\partial x} (U(x,t) + Q(x,t)) \right]_{x=X[t]} . \quad (25)$$

In summary, the development performed in this section provides a common language for classical and quantum theories, in terms of either wave functions or trajectories. Here I emphasize that one has to compare either classical and quantum wave functions or classical and quantum ensembles of trajectories (not a single classical trajectory with a quantum wave function).

The presence of $Q(x,t)$ in the quantum Hamilton–Jacobi equation, Eq. (24), and in the Newton-like equation, Eq. (25), implies that Bohmian trajectories depend not only on the classical potential $U(x,t)$ but also on the quantum potential $Q(x,t)$, which is a function of $R(x,t)$. In fact, it is the shape and not the absolute value of $R(x,t)$ that acts on each individual quantum trajectory. On the contrary, each classical trajectory can be computed from Eq. (18) and Eq. (19) independently of the shape of the classical ensemble. In conclusion, the differences between quantum and classical ensembles of trajectories is not a difference between waves and particles, because both waves and particles can be used to study classical or quantum systems. It is a difference on what is the role of $R(x,t)$ on the trajectory of a unique particle. Classically, it has no role. Quantum mechanically, $R(x,t)$ provides the information about how particles are distributed in an ensemble of experiments, and it also affects each individual trajectory, through the quantum potential.

In 1964, Nathan Rosen [44] used these features to develop the conditions needed to reach a classical regime for a one-particle system. I follow here his single-particle arguments. Classical trajectories in Eq. (25) can be obtained by imposing, as a third equation [44, 45, 46], a negligible spatial derivative of a quantum potential:

$$Q(x,t) = \frac{\hbar^2}{2m} \frac{\partial^2 R(x,t)/\partial x^2}{R(x,t)} = \text{cst.} \quad (26)$$

Most of the time, this route to recover classical dynamics from quantum systems is incompatible with a well-defined wave function solution of Eq. (23). The reason is because we have three quantum equations, Eq. (20), Eq. (24) and Eq. (26), imposed on only two unknowns, the amplitude $R(x,t)$ and the phase of the wave function $S(x,t)$.

4.2. The successful many-particle scenario

In this subsection I explain briefly the recent work of the author and co-authors through a generalization of Rosen’s attempt to the center of mass of a many-particle system [19]. I show

6 In the literature, sometimes we see a way of increasing the number of unknowns by assuming the (classical) potential $U(x,t)$ as an additional unknown that has to be fixed by the three equations. So, there are some exotic potentials where quantum and classical solutions can live together [47] (one simple example is a plane wave $R(x,t) = 1$ and $S(x,t) = k x$ with $p = h k$ the momentum in a free space with $U(x,t) = 0$). However, it is a clearly unphysical solution to say that classical scenarios do only appear in quantum systems for very exotic potentials.
that classicality appears as a natural quantum limit for most macroscopic objects, i.e. the effect of the quantum potential becomes negligible while retaining a well-defined wave function. Our work opens the path for a new wave equation for decoherent (sub)systems that are neither purely quantum nor classical (similar to Ref. [48]). The ultimate reason of the unsuccessful attempt to reach classical mechanics from a single-particle quantum system is the fact that we cannot introduce, by hand, any new term on the single particle Schrödinger equation. However, by looking at the (conditional) wave equation for an open quantum system, Eq. (7), we realize that apart from kinetic and (classical) potential energy, there is an additional (complex) term. New possibilities appear that were unaccessible for a single-particle (closed) system.

I consider a quantum system described by Eq. (1) and the center of mass \( x_{cm} \) and a set of relative coordinates \( \vec{y} = \{ y_2, ..., y_N \} \) defined as

\[
x_{cm} = \frac{1}{N} \sum_{i=1}^{N} x_i
\]

\[
y_j = x_j - \frac{\sqrt{N} x_{cm} + x_1}{\sqrt{N} + 1},
\]

which allows rewriting Eq. (1) for \( N \) particles of mass \( m \) in terms of the wave function with the new variables \( \Psi(x_{cm}, \vec{y}, t) \) as [19]

\[
\frac{i\hbar}{\partial_t} \Psi(x_{cm}, \vec{y}, t) = \left( -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x_{cm}^2} - \frac{\hbar^2}{2m} \sum_{j=2}^{N} \frac{\partial^2}{\partial y_j^2} + U(x_{cm}, \vec{y}, t) \right) \Psi(x_{cm}, \vec{y}, t),
\]

with \( M = Nm \). The force acting on the (Bohmian) center of mass trajectory is given by:

\[
M \frac{d^2x_{cm}[t]}{dT^2} = -\left( \frac{\partial}{\partial x_{cm}} (U(x_{cm}, \vec{y}, t) + Q_{cm}(x_{cm}, \vec{y}, t) + \sum_{j=2}^{N} Q_j(x_{cm}, \vec{y}, t)) \right) \bigg|_{x_{cm}=x_{cm}[t]}^{\vec{y}=\vec{y}[t]},
\]

with the quantum potentials

\[
Q_{cm}(x_{cm}, \vec{y}, t) = -\frac{\hbar^2}{2MR(x_{cm}, \vec{y}, t)} \frac{\partial^2 R(x_{cm}, \vec{y}, t)}{\partial x_{cm}^2},
\]

\[
Q_j(x_{cm}, \vec{y}, t) = -\frac{\hbar^2}{2mR(x_{cm}, \vec{y}, t)} \frac{\partial^2 R(x_{cm}, \vec{y}, t)}{\partial y_j^2},
\]

Hereafter, I develop the wave equation that determines the (conditional) wave function for the center of mass \( \psi(x_{cm}, t) = \Psi(x_{cm}, \vec{Y}[t], t) \) computed from Eq. (29). According to section 2.2, the trajectory \( x_{cm}[t] \) can be equivalently computed from \( \psi \) or \( \Psi \). Following Refs. [19, 30], we get:

\[
\frac{i\hbar}{\partial t} \psi = -\frac{\hbar^2}{2M} \frac{\partial^2 \psi}{\partial x_{cm}^2} - \frac{\hbar^2}{2m} \sum_{j=2}^{N} \frac{\partial^2 \psi(x_{cm}, \vec{y}, t)}{\partial y_j^2} \bigg|_{\vec{y}=\vec{y}[t]} - i\hbar \sum_{j=2}^{N} \psi_j^{[t]} \frac{\partial \psi(x_{cm}, \vec{y}, t)}{\partial y_j} \bigg|_{\vec{y}=\vec{y}[t]} + U \psi.
\]

Eq. (33) is just our previous equation Eq. (7) where the terms \( G(x_{cm}, t) \) and \( J(x_{cm}, t) \) can be identified as follow. If we define \( \psi(x_{cm}, t) = r(x_{cm}, t) \exp(i s(x_{cm}, t)/\hbar) \) into Eq. (33), one can then develop a continuity-like equation:

\[
0 = \frac{\partial^2}{\partial t} + \frac{\partial}{\partial x_{cm}} \left( r^2 \frac{1}{M} \frac{\partial s}{\partial x_{cm}} \right) + J,
\]
with

\[
J = \hbar \sum_{j=2}^{N} \left[ \frac{\partial^2 \rho}{\partial y_j} v_j[t] - \frac{\partial}{\partial y_j} \left( \frac{1}{m} \frac{r^2}{\partial y_j} \right) \right],
\]

(35)

where \(v_j[t]\) is the Bohmian velocity of \(y_j\). In addition, we get a quantum Hamilton–Jacobi-like equation:

\[
0 = \frac{\partial s}{\partial t} + \frac{1}{2M} \left( \frac{\partial s}{\partial x_{cm}} \right)^2 + U + G,
\]

(36)

with

\[
G = Q_{cm} + \sum_{j=2}^{N} \left( \frac{1}{2m} \left( \frac{\partial s}{\partial y_j} \right)^2 + Q_j - v_{j}[t] \frac{\partial s}{\partial y_j} \right).
\]

(37)

The relevant point in this many-particle generalization of Rosen’s attempt is that the new equation (33) has the additional environment degrees of freedom, i.e. \(G(x_{cm}, t) + iJ(x_{cm}, t)\), included. Now, contrarily to the single-particle case, we will see that the number of equations and unknowns in the quantum-to-classical transition is well balanced.

To obtain a classical solution for the (quantum) center of mass (not other degrees of freedom) using Eq. (30), the additional requirement is needed:

\[
\frac{\partial U(x_{cm}, \vec{y}, t)}{\partial x_{cm}} \gg \frac{\partial Q_{cm}(x_{cm}, \vec{y}, t)}{\partial x_{cm}} + \sum_{j=2}^{N} \frac{\partial Q_{j}(x_{cm}, \vec{y}, t)}{\partial x_{cm}},
\]

(38)

along the path \(X_{cm}[t]\). Therefore, we have again three real equations (that is Eq. (34), Eq. (36) and Eq. (38)) to get a classical solution and, now, we have three unknowns \(r(x_{cm}, t), s(x_{cm}, t)\) and \(G(x_{cm}, t)\). In summary, a classical solution for the center of mass is possible, while still remaining a quantum solution.

In our recent work [19] we have shown that the natural conditions required for a quantum system of identical particles to ensure that its center of mass has a classical behavior. In particular, we discuss when and why it is reasonable to expect that the spatial derivatives of the classical potential in Eq. (38) are expected to be larger than those of the quantum potentials. We conclude there [19], without invoking ambiguous arguments about the role of decoherence, that a large number of identical particles \((N \rightarrow \infty)\) under an external potential is enough to ensure classical dynamics for its center of mass in a single experiment. This result can also be interpreted as a single-experiment generalization of the well-known multiple-experiment Ehrenfest theorem.

5. Conclusion

In summary, I have discussed the ontological and practical implications in quantum theories of the many body problem that makes exact predictions for most quantum systems computationally inaccessible. This problem is present in most common interpretations of quantum mechanics. Therefore, most predictions of natural quantum phenomena have to rely on some type of approximations. Such approximations are, in some part, justified by theoretical developments.

\[\text{One can argue that } J(x_{cm}, t) \text{ is an additional unknown. It is true. However, although it is not mandatory for a conditional wave function, one can usually fix } J(x_{cm}, t) \text{ using Eq. (34) to ensure a conservation of probability.}\]

In any case, for the many-body system, the number of unknowns is equal or higher than the number of equations to satisfy. In the single-particle case, the balance was opposite.
and, in another part, by the agreement of the outputs (of such approximate model) with experiments.

The progress on many different quantum applications, some of them already present in our society, is due to these approximations that allow us to go far beyond the single-particle understanding of quantum mechanics. An example of including irreversibility and dissipation in the Bohmian modeling of open systems is presented in section 3. On the ontological level, however, the present-day foundational problems related to controversial quantum phenomena (such as the arrow of time, the quantum-to-classical frontier or the increment of the entropy) have to avoid being contaminated by the unfalsifiability originated from the many body problem discussed in this paper. An original attempt to show how the Bohmian theory itself (minimizing the role of many body problem) explains the transitions from a microscopic quantum system towards a macroscopic classical one is shown in section 4. In all cases, I emphasize in this paper that, either for practical or foundational issues, there is no exact solution for quantum systems of interest with most common quantum theories. Therefore, we always have some degree of ambiguity and vagueness in our predictions.

Finally, apart from the many body problem discussed in this paper, I want to make a brief comment about the intrinsic ambiguity (and exposure to refutation) of the different interpretations of quantum mechanics. Paraphrasing Karl R. Popper [40], “every test of a theory is an attempt to falsify it, or to refute it”. However, there are quantum theories that are more testable, more exposed to refutation, than others. They take a greater risk. I want to compare here Copenhagen and Bohmian interpretations. One of the basic postulates of the Copenhagen interpretation is: For every observable in classical mechanics, a linear, Hermitian operator in quantum mechanics exists [5]. But, Which operator do I have to choose? Although the Copenhagen theory does not specify which operator, the answer seems obvious. You have to select that operator that exactly reproduces the experiment. This seems not a very concrete answer and not too risky. Somehow, perhaps, this vagueness in the definition of the operator can explain the success of the Copenhagen (or orthodox) interpretation in front of others. There is a general belief that the Copenhagen interpretation perfectly explains all phenomena of the quantum world, for few or many degrees of freedom. You just need to find the proper operator that ensures the agreements of the predictions with the experiments. I summarize my argument here, by rephrasing the famous sentence “shut-up-and-calculate” by the new one, “shut-up-and-find-the-proper-operator”. These ideas are lined up with the point of view of John Bell. He said that the orthodox theory is “unprofessional” [49] because of this vagueness of operators (either the external ones discussed in this paper or the operator that encapsulates the measurement process). He wrote [50]:

The concept of “measurement” becomes so fuzzy on reflection that it is quite surprising to have it appearing in physical theory at the most fundamental level. Less surprising perhaps is that mathematicians, who need only simple axioms about otherwise undefined objects, have been able to write extensive works on quantum measurement theory—which experimental physicists do not find it necessary to read.

There are other interpretations of quantum phenomena whose postulates are, in my opinion, more concrete, more risky. For example, Bohmian mechanics is a quantum theory without operators [10, 51, 52]. In simple words, operators are not needed in Bohmian mechanics, although they can be a very helpful mathematical trick in practical computational issues by encapsulating the environment in a simple mathematical function. These ideas are emphasized by Goldstein, [8] Here, in this last paragraph, I am talking about the operators associated to the measurement processes. In rest of the paper, I was talking about external operators related to environment. In both cases, the orthodox definition of such operators is ambiguous. In the external operators, the reason is the many body problem, while in the measurement operators it is because of the own theory.
Dürr, Teufel, and coworkers when they refer to the “naive realism about operators” [10, 52, 53]. In Bohmian mechanics, the measurement process is explained as any other type of interaction among particles. There is no measuring postulate. In this sense, the Bohmian theory provides a more definitive answer of how to treat a particular measurement. You just have to include the kinetic energy of the particles of the measuring apparatus and their interaction with the particles of the quantum system into the global Hamiltonian. By knowing the trajectories of the particles of the pointer of the apparatus, you will finally get the observable result without ambiguity.

In summary, in my opinion, the Bohmian explanation of the quantum world (and quantum measurement in particular) is more concrete, more risky, with less ambiguity than the orthodox explanation. However, the many body problem makes the exact solution of the system plus apparatus (or system plus environment) computationally inaccessible in both interpretations. Therefore, at the end of the day, both theories are subject to approximations that imply, more or less, a similar ambiguity in (practical and foundational) predictions. In case of disagreement with the experiments, is the theory incorrect or the approximation too rude? It seems that Nature (through the many body problem) fortified herself against giving a concrete answer to this question. Is it possible to develop other quantum theories free from the many body problem? [54, 55]

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