Aspects of nonlocality from a quantum trajectory perspective: A WKB approach to Bohmian mechanics

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Abstract

Nonlocality is a property of paramount importance both conceptually and computationally exhibited by quantum systems, which has no classical counterpart. Conceptually, it is important because it implies that the evolving system has information on what happens at any space point and time. Computationally, because such a knowledge makes any calculation intractable as the number of degrees of freedom involved increases beyond a few of them. Bohmian mechanics, with its trajectory-based formalism in real configuration space, can help to better understand nonlocality. A detailed analysis of how nonlocal information is transmitted to quantum trajectories in simple systems (free particle and harmonic oscillator) turns out to be very interesting when compared to analogous systems in classical mechanics.

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I. INTRODUCTION

Since the early steps of quantum theory there has always been much interest in establishing a connection between this theory and classical mechanics. A lot of work has been devoted to derive quantization rules based on the correspondence principle [1], to propose and improve semiclassical approximations [2, 3, 4, 5], or to develop quantum-classical studies by using the Liouvillian formulation of quantum mechanics [6, 7, 8, 9] or some sort of approximations where quantum-classical mixed dynamics are involved [10]. However, there is an alternative pathway consisting of exploiting the properties offered by the so-called quantum Hamilton-Jacobi equation, as done by Leacock and Padgett [11] in 1983. This equation can be derived from the time-dependent Schrödinger equation by means of a simple transformation which allows to express the wave function in terms of a complex phase (which also contains all the information that carries the wave function). The formulation based on the quantum Hamilton-Jacobi equation was formerly aimed to obtain bound-state energy levels of quantum systems with no need to solve the equation of motion involved in the calculation of the system wave function.

Leacock and Padgett formulation leads straightforwardly to quantum trajectory approaches, which have also been an alternative to understand the relationship between quantum and classical mechanics. Bohmian mechanics, which was proposed before, is also one of these approaches. Nonetheless, it presents an inconvenient when dealing with (energy) eigenstates. These states are associated with zero velocity fields, and therefore particles remain steady when described by them [12]. To solve this problem, Floyd [13, 14] and Faraggi and Matone [15, 16] developed quantum Hamilton-Jacobi like formulations starting from (real) *bipolar ansatzs*, though they did not claim full equivalence with standard quantum mechanics regarding their predictions. This problem was also treated by John [17] by means of a theory based on *complex quantum trajectories* derived from the ansatz used by Leacock and Padgett, and that was applied to some simple analytical cases, such as the harmonic oscillator and the step barrier. This trajectory-based approach has been used recently [18, 19, 20, 21] to propose different numerical algorithms that allow to obtain transition probabilities and bound-state energies.

When quantum trajectory-based approaches are used, a full *localization* underlies the particle dynamics since we are dealing with well-defined trajectories in (either real or com-

plex) configuration space. Then, one might have the wrong impression that nonlocal effects are somewhat washed out. Remember that nonlocality is present in so remarkable phenomena such as entanglement, which is the cornerstone of quantum information theory and quantum computation, for instance. Hence nonlocality becomes an important issue when working with quantum trajectories (mainly when proposing alternative methods to solve quantum problems by means of them), because not only it does not disappear at all, but plays a key role in the particular topology displayed by such trajectories. Independently of connotations coming from entanglement and quantum information theory, nonlocality is present even when considering the time evolution of a single particle. This can be nicely seen by means of Bohmian mechanics, where quantum trajectories are defined in the (real) configuration space where experiments are carried out. In order to reproduce experimental outcomes, one needs to collect many particles which (we assume) describe certain trajectories within the Bohmian approach. All these particles are independent (i.e., there is no physical interaction among them) and reach the detector (whatever it is) one by one. Despite their independence, all of them are "guided" by identical initial wave functions (or wave fields); the corresponding trajectories are then obtained from the time evolution of the wave field, and the outcomes from the asymptotic limits in space and time of $\rho(x,t) = |\Psi(x,t)|^2$ (we can consider one dimension in this description without loss of generality). The effects of Ψ on the particle motion can be then considered as a manifestation of how nonlocality arises in quantum mechanics.

In this Letter a discussion on nonlocality is carried out in terms of the WKB-like formulation of Bohmian mechanics (WKB-BM), proposed by Sanz *et al.* [5, 22, 23] to understand the quantum-classical correspondence. This correspondence has been recently considered in the study of different problems appearing in realistic atom-surface scattering problems [24, 25, 26].

II. WKB FORMULATION OF BOHMIAN MECHANICS

The starting point of the WKB-BM approach consists of using the general ansatz [11, 17, 22]

$$\Psi(x,t) = e^{i\bar{S}(x,t)/\hbar}, \tag{1}$$

where $\bar{S}$ is a complex (phase) function. This simple relation allows to express the time-dependent Schrödigner equation as a quantum Hamilton-Jacobi equation,

$$\frac{\partial \bar{S}}{\partial t} + \frac{\left(\nabla \bar{S}\right)^2}{2m} + V - \frac{i\hbar}{2m}\nabla^2 \bar{S} = 0. \tag{2}$$

Equivalently, applying the ∇ operator, this equation can be expressed in its hydrodynamical form,

$$\frac{d\bar{v}}{dt} = -\frac{\nabla V}{m} + \frac{i\hbar}{2m}\nabla^2 \bar{v}, \tag{3}$$

where $\bar{v} = \nabla \bar{S}/m$ is a complex velocity field and $d/dt = \partial/\partial t + \bar{v}\nabla$ is the associated Lagrangian operator. This equation is the starting point of different numerical algorithms proposed in the literature [20, 27] to deal with a large variety of quantum problems, particularly high-dimensional ones, where standard quantum mechanics is difficult to apply.

After Eq. (2), the WKB-BM approach considers an expansion of $\bar{S}$ as a power series of $\hbar/i$,

$$\bar{S}(x,t) = \sum_{n=0}^{\infty} \left(\frac{\hbar}{i}\right)^n \bar{S}_n(x,t), \tag{4}$$

where the functions $\bar{S}_n$ are real (as seen below, they satisfy a hierarchy of real coupled equations). We are interested in knowing how and when nonlocality appears, and therefore whether a motion can or cannot be regarded as classical. Therefore, the functions $\bar{S}_n$ have to obey the usual conditions of the standard WKB approximation [28]. Substituting (4) into Eq. (2), the latter can be conveniently decoupled in powers of $\hbar/i$ to yield

$$\frac{\partial \bar{S}_0}{\partial t} + \frac{(\nabla \bar{S}_0)^2}{2m} + V = 0 \tag{5}$$

for the zeroth order (i.e., the classical Hamilton-Jacobi equation, with $\bar{S}_0$ being the classical action), and

$$\frac{\partial \bar{S}_n}{\partial t} + \frac{1}{2m}\sum_{k=0}^{n} \nabla \bar{S}_k \nabla \bar{S}_{n-k} + \frac{1}{2m}\nabla^2 \bar{S}_{n-1} = 0 \tag{6}$$

for higher orders, $n \geq 1$. Eq. (6) together with Eq. (5) provides an iterative scheme to compute higher orders in the expansion of $\bar{S}$. In particular, when the series is truncated at $n = 1$ one gets the well-known WKB approximation. This scheme is not based on the propagation of individual trajectories, but on the propagation of functions displaying the global behavior of ensembles of particles. In this sense, the $\bar{S}_n$ functions can be considered as fields.

Once every $\bar{S}_n$ is known, the series (4) will also be known. One can then compute the real fields R and S that define the Bohmian (polar) ansatz

$$\Psi(x,t) = R(x,t)e^{iS(x,t)/\hbar} \tag{7}$$

in terms of the $\bar{S}_n$ functions by identifying Eqs. (1) and (7) to give

$$R \;=\; \exp\left[\sum_{n=0}^{\infty}(-1)^n\hbar^{2n}\,\bar{S}_{2n+1}\right], \tag{8a}$$

$$S \;=\; \sum_{n=0}^{\infty}(-1)^n\hbar^{2n}\,\bar{S}_{2n}. \tag{8b}$$

We would like to stress that although S is given in terms of even powers of $\hbar$, eventually one could observe constant or time-dependent terms depending linearly on $\hbar$ (see below). Note also that the wave function is always well defined except an overall phase that does not depend on the coordinate space, which is not taken into account in (1). By substituting Eq. (8b) into the Bohmian velocity field,

$$\dot{x} = v = \frac{\nabla S}{m}, \tag{9}$$

we reach

$$\dot{x} = \dot{x}^{(\mathrm{cl})} + \frac{1}{m}\sum_{n=1}^{\infty}(-1)^n\hbar^{2n}\,\nabla\bar{S}_{2n}, \tag{10}$$

where $\dot{x}^{(\mathrm{cl})} = \nabla\bar{S}_0/m$ is the classical law of motion. From Eq. (10) one can therefore interpret quantum trajectories as classical trajectories "dressed" with a series of terms coming from quantum interference. This result makes apparent the important difference between both types of trajectories, classical and Bohmian. Within the WKB-BM approach, nonlocal effects are contained in the second term of the r.h.s. of Eq. (10) and start appearing at very small times.

III. APPLICATIONS OF THE WKB-BM APPROACH

In the light of the WKB-BM approach the effects of the nonlocality are nicely illustrated by means of the following well-known examples. First, we consider the case of the free propagation of a Gaussian wave packet,

$$\Psi(x,t) = \left(\frac{1}{2\pi\tilde{\sigma}_t^2}\right)^{1/4} e^{-(x-v_0t)^2/4\tilde{\sigma}_t\sigma_0 + ip_0(x-v_0t)/\hbar + iEt/\hbar}, \tag{11}$$

where the time complex spreading is given by $\tilde{\sigma}_t = \sigma_0(1 + i\hbar t/2m\sigma_0^2)$, the initial velocity by $v_0 = p_0/m = \langle \hat{p}/m \rangle$, and the initial energy by $E = p_0^2/m = \langle \hat{H} \rangle$. The corresponding (Bohmian) action is then

$$S(x,t) = -\frac{\hbar}{2} \arctan\left(\frac{\hbar t}{2m\sigma_0^2}\right) + Et + p_0 x + \frac{\hbar^2 t}{8m\sigma_0^2\sigma_t^2}(x - v_0 t)^2, \tag{12}$$

with $\sigma_t = \sigma_0[1 + (\hbar t/2m\sigma_0^2)^2]^{1/2}$ being the time-dependent real spreading. For $\hbar$ small (or, in general, $\hbar t/2m\sigma_0^2$ small), note that S can be expressed, effectively, as a series of even powers of $\hbar$ when the arctangent function and the spreading of the wave packet are expanded in a Taylor expansion.

Introducing (12) into Eq. (9), we obtain the exact expression for the quantum trajectories,

$$x(t) = v_0 t + \frac{\sigma_t}{\sigma_0} x_0, \tag{13}$$

where the initial condition is $x(0) = x_0$. If we assume $\hbar t/2m\sigma_0^2 < 1$, (13) can be expressed as

$$x(t) = x_0 + v_0 t + \sum_{n=1}^{\infty} (-1)^{(n-1)} \frac{(2n-3)!!}{2^n \cdot n!} \left(\frac{\hbar t}{2m\sigma_0^2}\right)^{2n} x_0. \tag{14}$$

As expected, the two first terms in the r.h.s. of this expression are exactly the same that one would expect from a classical trajectory; note that the first term arises precisely when there is no spreading. However, the presence of the $\hbar$-dependent (third) term makes that a divergence with respect to the classical motion be observable: it leads to a hyperbolic spreading of the trajectories. This is a very remarkable effect where the nonlocality, as defined above, plays an important role; in order to avoid crossing among trajectories, those with the outmost initial conditions (with respect to $x_0 = 0$) will spread at a faster rate than the innermost ones. This information is contained in the spreading ratio σ_t/σ_0, which provides *global* information (i.e., it transmits the information carried by the wave function) on how the full velocity field has to be at any time. In other words, in this simple example the second term of Eq. (13) is responsible for nonlocal effects. Nevertheless, note that for relatively small $\hbar$ (or, equivalently, very short timescales, wide wave packets, and/or massive particles), the quantum trajectories will basically follow a similar behavior as classical particles, this explaining the good agreement between quantum mechanics and semiclassical approaches in this case.

The general trend described above is illustrated in Fig. 1, where a sample of Bohmian and classical trajectories with equal initial conditions are shown. Observe that after a very

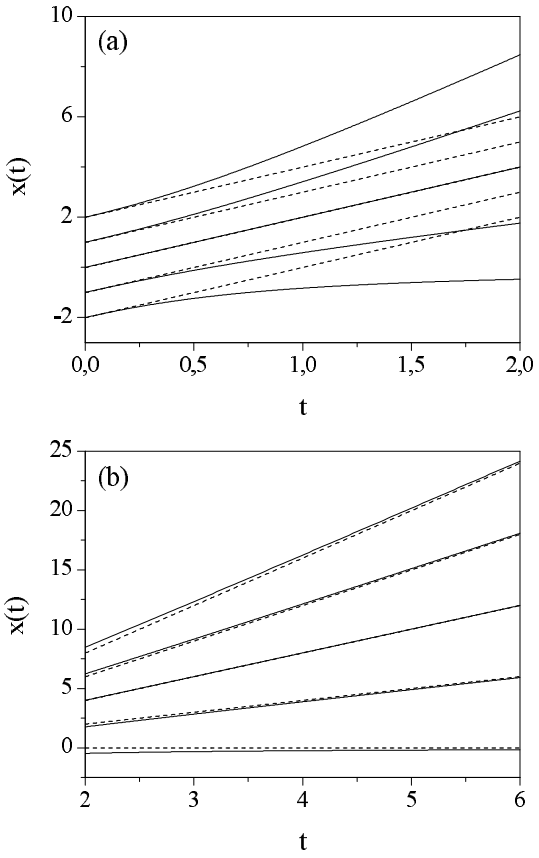

FIG. 1: Bohmian trajectories (solid lines) corresponding to a free Gaussian wave packet and obtained by means of Eq. (13) at: (a) short timescales (region around $\hbar t/2m\sigma_0^2 \lesssim 1$) and (b) asymptotic times ($\hbar t/2m\sigma_0^2 \gg 1$). To compare, the corresponding classical trajectories have also been represented with dashed lines. In part (b), dashed lines indicate the classical-like asymptotes described by Eq. (15).

short time, Bohmian trajectories start displaying a completely different behavior than their classical counterparts. Moreover, note also that at $\hbar t/2m\sigma_0^2 \sim 1$ the series given by Eq. (14) breaks down and can no longer be used to describe the long-time behavior of the Bohmian trajectories. It is then interesting to consider the asymptotic limit of Eq. (13), given by

$$x(t) \approx \left(v_0 + \frac{\hbar x_0}{2m\sigma_0^2} \right) t. \tag{15}$$

This result shows us that asymptotically (within the so-called Fraunhofer regime of motion [22, 23, 29, 30]) quantum trajectories (as classical trajectories) describe a uniform rectilinear motion. However, the corresponding quantum constant velocity given by $v_0' = v_0 + \hbar x_0/2m\sigma_0^2$ contains a residual term coming from the nonlocality (the velocity of each particle depends

on its corresponding initial position). As discussed elsewhere [22, 23, 24, 25, 26, 29, 30], the nonlocal and context-dependence information transmitted to the quantum trajectories is through the quantum potential, which is related to the curvature of the wave function and therefore is responsible for the residual contribution of the constant velocity.

Next example is the harmonic oscillator, which is also worth discussing. In this case, the time-evolution of a Gaussian wave packet centered around $x = a$ is described by

$$\Psi(x,t) = \left(\frac{1}{2\pi\sigma_0^2}\right)^{1/4} e^{-(x-a\cos\omega t)^2/4\sigma_0^2 - i\omega t/2 - im\omega(4xa\sin\omega t - a^2\sin 2\omega t)/4\hbar}, \tag{16}$$

where $\sigma_0^2 = \hbar/2m\omega$. Here, the quantum action is

$$S(x,t) = -\frac{1}{2}\hbar\omega t - \frac{m\omega}{4}(4xa\sin\omega t - a^2\sin 2\omega t), \tag{17}$$

and therefore the quantum trajectory is given by

$$x(t) = (x_0 - a) + a\cos\omega t, \tag{18}$$

which satisfy the motion equation $\ddot{x} + \omega^2 x = \omega^2(x_0 - a)$. As clearly seen from (18), particles will display oscillations parallel to both the classical trajectory (which oscillates around $x = a$ with frequency ω) and other quantum trajectories [i.e., given two particles, labeled as 1 and 2, their respective trajectories will satisfy the property $x^{(2)}(t) - x^{(1)}(t) = x_0^{(2)} - x_0^{(1)}$]. To understand how nonlocality operates here, note that the wave packet does not spread with time but remains the same, with its center following the path tracked by the corresponding classical trajectory. This implies that the quantum motion is constrained. Thus, since trajectories cannot cross, the only possibility for their topology is to be the same as the classical one (different initial positions will give different parallel trajectories). That is, the nonlocality manifests in the distribution of initial conditions, but not in the particular value of $\hbar$, since $\omega t = \hbar t/2m\sigma_0^2$ can acquire any value.

IV. CONCLUSIONS

As shown here, nonlocality is strongly related to the fact that, at any time, the evolution of a (quantum) system strongly depends on the full configuration of the *real* (coordinate) space, rather than the features presented by the particular formulation used to describe it. In other words, the topology of the trajectories is strongly affected by the information carried

in the full wave function (nonlocality could be thus described saying that *at every time any particle has information about the whole system configuration*, unless $\hbar \equiv 0$). Therefore, the nonlocal behavior arises from having a complete information encoded within the wave function, which is transmitted to the (quantum) particles and indicates how they should evolve according to certain rules as illustrated with the above two examples. Due to the fact that the classical limit $\hbar \to 0$ is carried out analytically, one can then observe at each time step the classical and quantum behaviors. Of course, as the system becomes more complex, the classical limit is not carried out analytically and nonlocal effects are not easily detected. When mixed dynamics [10] are proposed to solve problems with high dimensionality, a detail analysis of the nonlocality should also be carried out in order to give a complete interpretation of the results in terms of trajectories because residual contributions, as those seen in Eq. (15), can be masked by a fully classical analysis.

On the other hand, we would like to emphasize the insight that Bohmian mechanics renders when applied to the study of physical systems. In general, trajectory schemes can be of great help to develop efficient computational algorithms to solve quatum problems. However, at some point, one should also balance this efficiency with the insight that they can provide. Here we have seen that a WKB-BM scheme allows a nice comparison between Bohmian and classical trajectories and, at the same time, constitutes a method to tackle a quantum problem at different levels of approximation depending on the (relative) value of $\hbar$. In particular, this scheme is useful when trying to compare real Bohmian trajectories with trajectories obtained from the WKB wave function. Generally, when using the WKB approximation, one only calculates the first terms in the expansion [24, 25, 26], $\bar{S}_0$ and $\bar{S}_1$, which already contain nonlocality, as seen above. Nevertheless, sometimes it could be necessary to go to higher orders in semiclassical approximations as happens, for example, for deep tunneling where one needs more terms in order to account for the longer tunneling times involved in the process [31]. Finally, we would like to emphasize that due to the large number of works in WKB and WKB-like formalisms, the Bohmian analysis as proposed here could be of great help to provide a deeper inside in nonlocal effects.

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