Comment on “Bohmian mechanics with complex action: A new trajectory-based formulation of quantum mechanics” [J. Chem. Phys. 125, 231103 (2006)]

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In a recent publication, Goldfarb *et al.*¹ have proposed a new trajectory scheme to solve quantum problems: *Bohmian mechanics with complex action* (BOMCA). According to these authors, their contribution represents “a novel formulation of Bohmian mechanics.” In our opinion, rather than a new formulation of Bohmian mechanics, the proposal of Goldfarb *et al.* consists of a novel quantum computational scheme, which is based on solving the complex trajectory equations resulting from an already known *complex* version of Bohmian dynamics. On the other hand, Goldfarb *et al.* also claimed that their numerical scheme describes “*fully local* complex quantum trajectories,” with the reward of a significantly higher degree of localization than in the conventional Bohmian mechanics by lowering the magnitude of the quantum potential. At least from a theoretical and interpretative point of view, we consider that it is very important to clarify what “fully local quantum trajectories” means. Bohmian mechanics is a nonlocal theory because (standard) quantum mechanics is a nonlocal theory. This nonlocality manifests via the presence of a quantum potential, and therefore the corresponding quantum trajectories will display features that reflect such nonlocality. Something similar should also occur for any trajectory-based approach that intends to be equivalent to standard quantum mechanics. In this Comment we would like to provide a general discussion on these two aspects arising from the work of Goldfarb *et al.*, which can be of much interest to the Chemical Physics community. In particular, we would like to stress the special interest relying on how the term *locality* should be employed.

The approach of Goldfarb *et al.* starts with the time-dependent quantum Hamilton-Jacobi equation. This equation was considered by Leacock and Padgett² in 1983 within the context of the quantum transformation theory^{3,4} as a way to obtain bound-state energy levels of quantum systems with no need to calculate the corresponding eigenfunctions. According to Leacock and Padgett, the quantum Hamilton-Jacobi equation can be either stated as a postulate (as done by these authors) or derived from the Schrödinger equation through a simple connection formula. In the second case, the quantum action corresponds to the complex phase of the wave function when the latter is expressed as a pure complex exponential function. This relationship allows one to pass straightforwardly from the quantum Hamilton-Jacobi formalism to the standard one in terms of the time-dependent Schrödinger

(and vice versa). Although both the *Ansatz* and the formulation used by Leacock and Padgett are similar to those considered in the standard (quantum) WKB semiclassical approximation,^{5,6} as pointed out by these authors, their approach *conceptually* differs from the WKB one.

Within Bohmian mechanics, (energy) eigenstates present an inconvenience: they give rise to zero velocity fields. Hence, when particles are described by this type of states, they will remain steady (motionless). To overcome this problem, Floyd⁷ and Faraggi and Matone⁸ developed (time-independent) quantum Hamilton-Jacobi-like formulations starting from (real) *bipolar Ansätze*, though they did not claim full equivalence with standard quantum mechanics regarding their predictions. Later, John^{9,10} proposed a time-dependent complex quantum trajectory formalism (based on the same connection formula mentioned by Leacock and Padgett) to study the dynamics associated with some simple analytical cases, such as the harmonic oscillator or the step barrier. This “modified de Broglie–Bohm approach to quantum mechanics,” as termed by John, is formally equivalent to the BOMCA formulation of Goldfarb *et al.* Nevertheless, we would like to specify that, due to the fundamental (theoretical) nature of John’s contribution, a separate calculation of the wave function is required in order to obtain the corresponding trajectories (John makes use of the “guiding wave” idea from Bohmian mechanics). Meanwhile, in the version of Goldfarb *et al.* the modified de Broglie–Bohm approach is formulated in terms of a closed set of equations (in the spirit of quantum hydrodynamical formalisms), which avoids the calculation of the wave functions, thus providing a new, practical use to such an approach. Furthermore, within the approach of Goldfarb *et al.*, the expression for the quantum force happens to be typically much smaller than in standard Bohmian mechanics. On the other hand, we would also like to note that a related formulation has also been used by Chou and Wyatt,¹¹ though they developed a different, novel numerical scheme to tackle the problem of bound-energy levels and scattering in one dimension.

When trying to understand the quantum-classical correspondence from the perspective of a WKB-like formulation of Bohmian mechanics (WKB-BM), Sanz and co-workers^{12–16} reached the complex quantum Hamilton-Jacobi equation the same year as John, but independently. The WKB-BM formulation constitutes an excellent, compre-

hensive framework to discuss the nonlocality issue; as seen elsewhere,^{15,17-19} the clear correspondence between classical and quantum (Bohmian) trajectories arising from it is very convenient for the interpretation of realistic atom-surface scattering problems, for instance. The starting point of this approach is the same as in all formulations mentioned above, i.e., the (general) *Ansatz*

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

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

$$\frac{\partial \bar{S}}{\partial t} + \frac{(\nabla \bar{S})^2}{2m} + V - \frac{i\hbar}{2m} \nabla^2 \bar{S} = 0, \quad (2)$$

which was termed by Goldfarb *et al.* as “a single newly defined quantum Hamilton-Jacobi equation.” Equivalently, Eq. (2) can also be recast as a quantum hydrodynamical equation,

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

taking into account that the characteristic curves obtained from Eq. (2) define the complex velocity field $\bar{v} = \nabla \bar{S}/m$ (according to the Hamilton-Jacobi theory), and making use of the Lagrangian operator, $d/dt = \partial/\partial t + \bar{v} \cdot \nabla$. Note that, because of analytic continuation, the x coordinate has to be considered as complex (eventually, the time could also be complex⁹), and then both Ψ and $\bar{S}$ will depend on a complex coordinate. From Eq. (3), proposed and used for the first time for practical purposes by Goldfarb *et al.*,¹ a hierarchy of coupled complex equations for the spatial derivatives of $\bar{S}$ can be obtained.

Because of the relationship between Ψ and $\bar{S}$ [through *Ansatz* (1)], it is clear that all the information provided by the former will also be contained in the latter, even the nonlocality underlying quantum mechanics. In virtue of this, nonlocality will also be present in the complex quantum trajectories of Goldfarb *et al.* because of their dependence on the whole quantum state via $\bar{S}$. It is in this sense that they cannot be regarded as “fully local;” even if Ψ is not calculated explicitly, $\bar{S}$ is obtained (at different orders of approximation) by means of a set of coupled ordinary differential equations, and the trajectories are computed one by one (as also done in the case of real Bohmian trajectories). Note that nonlocality does not disappear with the particular method used to solve a quantum problem unless truncations are taken into account (as it may happen, for instance, in semiclassical approximations). This is in a sharp contrast with classical mechanics, which is *local* because each particle only depends on the action of the potential V , but not on how the full ensemble of particles is distributed. Nevertheless, it must be stressed that even with semiclassical approximations, nonlocal effects may be apparent as soon as *a few terms* are included in the corresponding expansions.¹²⁻¹⁶ This statement can be nicely illustrated by means of the WKB-BM approach as follows.

After reaching Eq. (2), $\bar{S}$ can be expanded in a power series of $\hbar/i$ as

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

where the $\bar{S}_n$ functions are real and satisfy a hierarchy of (real) coupled equations (see below). Once all $\bar{S}_n$ are known, series (4) is also known. Then, the real fields R and S that define the Bohmian *Ansatz*, $\Psi(x, t) = R(x, t)e^{iS(x, t)/\hbar}$, can be easily obtained. In particular, the real phase S is given by

$$S = \sum_{n=0}^{\infty} (-1)^n \hbar^{2n} \bar{S}_{2n}. \quad (5)$$

Substituting Eq. (5) into the expression for the Bohmian velocity field, $\dot{x} = v = \nabla S/m$, we obtain

$$\dot{x} = \dot{x}^{(cl)} + \frac{1}{m} \sum_{n=1}^{\infty} (-1)^n \hbar^{2n} \nabla \bar{S}_{2n}, \quad (6)$$

where $\dot{x}^{(cl)} = \nabla \bar{S}_0/m$ is the classical law of motion ($\bar{S}_0$ being the classical action). From Eq. (6) one can therefore interpret quantum (Bohmian) trajectories as classical trajectories “dressed” with a series of terms coming from quantum interference, which give the nonlocal behavior observed in quantum mechanics. That is, setting aside connotations coming from quantum information theory, nonlocality should be regarded as the fact that *at every time any particle has information about the whole system configuration*, unless $\hbar \equiv 0$. This statement stresses the capital difference between both types of trajectories, classical and Bohmian (either real or complex), the former regarded as “fully local” and the latter as “(fully) nonlocal.” Nonetheless, we would like to add that sometimes the nonlocal topology displayed by the trajectories could be regarded as “local” to some extent.¹⁰ As shown elsewhere,^{16,19} this is particularly true in the case of the Fraunhofer regime (or at very short time scales within the Fresnel regime), where quantum trajectories can be expressed as classical-like trajectories with an effective classical velocity (“effective” in the sense that it does not correspond exactly to a classical velocity, but it includes some quantum parameters, such as $\hbar$).

Finally, it is worth commenting that when one uses real trajectories, the physical insight gained in interpretative as well as comparative work can balance the relatively high computational effort needed to calculate them. However, such an insight is lost when working with complex quantum trajectories, since physical phenomena are measured in “real” coordinate space. Moreover, when dealing with problems with two or higher dimensions, the computational effort of complex trajectories is significantly increased since the dimensionality of the working space is double.

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