Comment on "Quantum Backreaction through the Bohmian Particle"

In a recent Letter [1] Prezhdo and Brooksby forwarded a solution to the long-standing problem of properly dealing with a mixed quantum-classical system, namely, to couple the classical sector, not directly to the quantum one, but to its associated Bohmian particle [2]. The precise proposal is to make replicas of the quantum-classical system, each one with a different position of the Bohmian particle obtained by sampling the "initial" quantum sector density. Each copy of the system is then to be evolved as follows: (i) the quantum sector evolves as usual, i.e., by taking the classical degrees of freedom as time-dependent parameters of the quantum Hamiltonian, (ii) the Bohmian particle evolves *à la* de Broglie–Bohm, its velocity depending solely on the quantum degrees of freedom, and (iii) the classical sector evolves following Hamilton's equations but this time with the Bohmian particle position as a time-dependent parameter in the Hamiltonian. The expectation values of observables are obtained by averaging over the "final" sample of quantum-classical degrees of freedom. In practice this proposal coincides with that in [3] (in its simplest version), although there it was derived as an approximation rather than introduced as a postulate. In this Comment I want to point out some limitations of the proposed prescription if it is pushed too far.

Without loss of generality, it can be assumed that the initial state is given by some probability distribution $n(u, \psi)$ defined on the combined manifold with coordinates $u = (\boldsymbol{x}, \boldsymbol{k})$ (the position momentum of the classical particle) and $|\psi\rangle$ (the normalized wave function of the quantum particle). The full distribution $f(u, \psi, \boldsymbol{y})$ including the Bohmian particle (with coordinates $\boldsymbol{y}$) will then equal $n(u, \psi)|\psi(\boldsymbol{y})|^2$. In this way f is initially fully determined by n. The evolution equations then define a flow for f in the manifold $(u, \psi, \mathbf{y})$. The flow of f has no diffusion (an initial Dirac delta distribution evolves as a delta all the time). Of course, its marginal density $n(u, \psi; t) = \int d\mathbf{y} f(u, \psi, \boldsymbol{y}; t)$ does show diffusion, which is interpreted as branching and backreaction of the quantum-classical system.

The first problem of the proposal is that the initial relation noted between f and n is not preserved by the evolution; that is, at later times the Bohmian particle is no longer distributed as $|\psi(\mathbf{y})|^2$ since a bias is introduced by its coupling to the classical particle coordinates. Some negative consequences of this fact are (i) the proof given in [1] that the total quantum-classical energy is conserved no longer applies. In fact energy is not conserved (no such claim was made in [3]). (ii) Unlike f, the distribution $n(u, \psi; t)$ does not satisfy an evolution equation; that is, the knowledge of this distribution at some intermediate time t is insufficient to predict its future evolution since the distribution of the Bohmian particle is also needed. Unfortunately, physics lies in n not f: If the proposal in the Letter is taken seriously as a prescription to evolve n from an initial time t to a final time t' [let us denote this operation by $U(t', t)$] it will be found that $U(t_2, t_1)U(t_1, t_0)$ differs from $U(t_2, t_0)$ since the proposed prescription requires one to resample the Bohmian particle distribution at the intermediate time t_1.

A second problem is as follows. As is well known in pure quantum mechanics, given an ensemble of pure states, only the combination $\sum_i p_i|\psi_i\rangle\langle\psi_i|$ is relevant to physics, since nothing else can be extracted from the knowledge of the expectation values of all possible observables. For the same reason, in the mixed quantum-classical case, only the quantity $\hat{\boldsymbol{\rho}}(u) = \int D\psi n(u, \psi)|\psi\rangle\langle\psi|$ (the mixed density matrix-density distribution in phase space) characterizes the physical state. Note that there are many different n producing the same $\hat{\boldsymbol{\rho}}$. The trouble is that in the proposed method, two different initial distributions n corresponding to the same $\hat{\boldsymbol{\rho}}$ will in general evolve into different $\hat{\boldsymbol{\rho}}$ at later times (as is readily shown); in other words, identical initial physical states $\hat{\boldsymbol{\rho}}$ will branch into different states $\hat{\boldsymbol{\rho}}(t)$ at later times, depending on which initial distribution n was chosen to represent it. This is a general problem whenever the evolution is not directly based on the quantity $\hat{\boldsymbol{\rho}}(u)$.

This said, we have to distinguish between practical and theoretical points of view. At a practical level the method has been found to be useful and give good results in concrete applications [1,3,4]. Our critique implies, however, that at an exigent theoretical level the method fails to be fully internally consistent (this merely reflecting its intrinsically approximate nature) and cannot be regarded as a final answer to the quantum-classical mixing problem.

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[1] O. V. Prezhdo and C. Brooksby, Phys. Rev. Lett. **86**, 3215 (2001).
[2] P. R. Holland, *The Quantum Theory of Motion* (Cambridge University Press, Cambridge, 1993).
[3] E. Gindensperger, C. Meier, and J. A. Beswick, J. Chem. Phys. **113**, 9369 (2000).
[4] E. Gindensperger, C. Meier, J. A. Beswick, and M.-C. Heitz, J. Chem. Phys. **116**, 10 051 (2002).

