

Hydrodynamic methods for mixed-state dynamics and dissipation

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While the usual perspective on Bohmian mechanics focuses on the description of wavefunctions, or pure quantum states, we have recently explored the connection to a hydrodynamic description for statistical mixtures [4]. The latter has previously been discussed in the context of moment expansions for the density matrix $\rho(x, x')$ or, equivalently, the Wigner function $\rho_W(q, p)$ [1–3]. Here, a local-in-space formulation is derived in terms of moments in the momentum operator $\mathcal{P} = \hbar/2i (\partial/\partial x - \partial/\partial x')$, i.e., $\langle \mathcal{P}^n \rho \rangle_q = \int dp p^n \rho_W(q, p)$, the moments thus being a family of functions in a single spatial variable $q = 1/2(x + x')$. Specifically, the zeroth moment corresponds to the local density $P(q) = \langle \rho \rangle_q$, the first-order moment relates to the current density $j(q) = \langle \mathcal{P} \rho \rangle_q / m$, and the second-order moment corresponds to the kinetic-energy density $T(q) = \langle \mathcal{P}^2 \rho \rangle_q / 2m$. The dynamical equations for these moments represent an infinite hierarchy which, in its entirety, is equivalent to the Liouville-von-Neumann equation for the density operator.

Against this background, the following issues shall be addressed [4]: (i) The derivation, from the above formulation, of pure-state hydrodynamics as familiar from the Bohmian picture. The moment hierarchy now truncates with the two lowest-order members – i.e., the local density and the current density – which fully characterize the wavefunction. Special emphasis will be placed on the interpretation of the fluid-particle momentum, which is subject to a “quantum force”, in the Bohmian theory vs. the hydrodynamic context as outlined above. (ii) The application of the hydrodynamic equations to describe the dynamics of general mixed quantum states. This entails, as a crucial issue, to find a suitable way of truncating the moment hierarchy. Both global and local truncation schemes are discussed. (iii) Inclusion of dissipative effects in the moment equations, in accordance with simple Markovian master equations. We discuss the effect on the hydrodynamic trajectories of a generalized quantum force, augmented by dissipation [5]. (iv) The extension of the hydrodynamic formulation to non-adiabatic dynamics. We propose a general formulation that, by describing the coupling between electronic populations and coherences, properly takes into account coherent effects in the dynamics. For the particular case of pure states, the coupled-state equations by Wyatt et al. [6] are recovered.

As a final consideration, we comment upon the particular nature of hydrodynamic trajectories in the quantum vs. classical pictures [5]. This has some bearing upon mixed quantum-classical schemes emerging from the hydrodynamic description.

- [1] J. E. Moyal, *Proc. Cambridge Philos. Soc.*, **45**, 99 (1949).
- [2] W. R. Frensley, *Rev. Mod. Phys.*, **62**, 745 (1990).
- [3] L. M. Johansen, *Phys. Rev. Lett.*, **80**, 5461 (1998).
- [4] I. Burghardt and L. S. Cederbaum, *J. Chem. Phys.* **115**, 10303 (2001), **115**, 10312 (2001).
- [5] K. B. Møller and I. Burghardt, in preparation.
- [6] R. E. Wyatt, C. L. Lopreore, and G. Parlant, *J. Chem. Phys.*, **114**, 5113 (2001).