Quantum and semiclassical dynamics as fluid theories where gauge matters

Dmitry V. Zhdanov\textsuperscript{1, *} and Denys I. Bondar\textsuperscript{2}

\textsuperscript{1}Institute of Spectroscopy of the Russian Academy of Sciences, Moscow, 142190, Russia
\textsuperscript{2}Tulane University, New Orleans, LA 70118, USA

The family of trajectories-based approximations employed in computational quantum physics and chemistry is very diverse. For instance, Bohmian and Heller’s frozen Gaussian semiclassical trajectories seem to have nothing in common. Based on a hydrodynamic analogy to quantum mechanics, we furnish the unified gauge theory of all such models. In the light of this theory, currently known methods are just a tip of the iceberg, and there exists an infinite family of yet unexplored trajectory-based approaches. Specifically, we show that each definition for a semiclassical trajectory corresponds to a specific hydrodynamic analogy, where a quantum system is mapped to an effective probability fluid in the phase space. We derive the continuity equation for the effective fluid representing dynamics of an arbitrary open bosonic many-body system. We show that unlike in conventional fluid, the flux of the effective fluid is defined up to Skodjes gauge [R. T. Skodje et. al. Phys. Rev. A 40, 2894 (1989)]. We prove that the Wigner, Husimi and Bohmian representations of quantum mechanics are particular cases of our generic hydrodynamic analogy, and all the differences among them reduce to the gauge choice. Infinitely many gauges are possible, each leading to a distinct quantum hydrodynamic analogy and a definition for semiclassical trajectories. We propose a scheme for identifying practically useful gauges and apply it to improve a semiclassical initial value representation employed in quantum many-body simulations.

I. INTRODUCTION

Fluid analogies for complex multidimensional quantum dynamics lay the basis for modern semiclassical computational methods \cite{1–12} \ of many-body physics \cite{13–16}, chemistry \cite{17–21} and optics \cite{22}. In these analogies, the evolution of a quantum state is represented as a flow of an effective compressible probability fluid in the phase space (akin to classical statistical mechanics). Three fluid representations of quantum mechanics used are the Wigner \cite{23–25}, Husimi \cite{26} and Bohmian \cite{27, 28}. Each of them is exact and fully captures the effects of quantum nonlocality and quantum interference. This fact became universally accepted in 1950s after numerous and intriguing debates \cite{1}. Nowadays, the mathematical correspondence between quantum mechanics and classical hydrodynamics can even be demonstrated in actual experiments with fluids \cite{30, 31}. More importantly, this very correspondence enables the description of quantum evolution in terms of phase-space trajectories – the ultimate way to beat the curse of dimensionality in numerical applications. However, none of existing fluid analogies are fully developed. Namely, the exact form of fluid trajectories is unknown, except for one-dimensional systems \cite{32, 33} and a special class of multidimensional closed systems \cite{34}.

In this work, the general exact fluid analogy for an open multidimensional bosonic system is fully developed. The derived continuity equation for effective fluid has an ambiguity (pointed by Skodje \cite{34}) akin to the gauge invariance in electrodynamics. Consequently, the form of fluid trajectories is a matter of Skodje’s flux gauge fixing, which has been overlooked in earlier studies \cite{35, 36}. Our findings unify the fluid analogies to quantum mechanics. They reveal that the “conventional” Wigner, Husimi and Bohmian quantum hydrodynamic representations are just a tip of the iceberg and represent three out of infinitely many possible Skodje’s gauge fixings. In particular, we show that the Bohmian mechanics (Fig. 1d)

\begin{itemize}
  \item[(a)] “Default” gauge $A^H=0 \ (w_p=w_x=1/\sqrt{2})$
  \item[(b)] Regularized Bohmian gauge
  \item[(c)] Gauge $A^H=A^H_2 \ (w_p=w_x=1/\sqrt{2})$
  \item[(d)] Bohmian gauge $w_p/w_x \to \infty$
\end{itemize}

Figure 1. The fluid analogies for the ground state of a quantum harmonic oscillator with the Hamiltonian $H=\frac{1}{2}(p^2+x^2)$ ($\hbar=1$): (a) the standard Husimi representation (Eqs. \textsuperscript{31}); (b) the regularized Bohmian gauge; (c) the gauge $A^H_2=\frac{\pi}{2}\sum_{\delta x, \delta p} \exp[-\frac{1}{2}(x+\delta x)^2+(p+\delta p)^2]$; (d) the Bohmian gauge (Eq. \textsuperscript{40}). The probability fluid density is shown in blue. Black arrows show the vector field of fluid flow.

* dm.zhdanov@gmail.com

\textsuperscript{1} See, e.g., the historic debates between José Moyal and Paul Dirac on possibility to express quantum mechanics in terms of classical-valued phase space variables \cite{29}. A simple illustration of phase space representations of quantum superposition and entangled states is given in Appendix D.
is nothing but a singular limiting case of the Husimi representation (Fig. 1a) in a specific gauge. As exemplified in Fig. 1, different gauges result in strikingly different fluid analogies reflecting incompatible aspects of the wave-particle duality. For instance, the fluxes in the Husimi (Fig. 1a) and Bohmian (Fig. 1d) gauges highlight the non-vanishing zero-point energy and the stationarity of ground states, respectively.

Moreover, we prove by example that yet unexplored Skodje's gauges constitute a powerful resource to improve the accuracy of semiclassical numerical methods. We develop a methodology to screen for useful gauges and employ it to solve the Schr"odinger equation in the basis of time-dependent squeezed coherent states evolving along fluid trajectories. A comparison with benchmark initial value representations, such as the coupled coherent states (CCS) approach [12], confirms a superiority of our numerical method to capture tunneling dynamics.

The paper is organized as follows. The next section II reviews the Wigner-Weyl formalism from dynamical perspective, which, to our knowledge, has not been systematically presented in literature but is critical for understanding our reasoning. Readers not interested in methodological details may skip Sec. II and go directly to Sec. III–V containing our key results. Sec. VI provides a simple numerical example demonstrating the superiority of the developed framework over traditional semiclassical initial value representations used in computational quantum physics and chemistry. A broader impact of our gauge analysis on quantum science and engineering is addressed in concluding remarks. Proofs of all the theorems and important technical details for applying the developed methods to real-world multidimensional problems are moved into the appendices.

Throughout the paper, we use bold symbols to denote vector quantities characterizing multidimensional systems. In particular, $\mathbf{p} = \{p_1, ..., p_N\}$ and $\mathbf{x} = \{x_1, ..., x_N\}$ denote the momentum and position coordinates of an $N$-dimensional system in the $2N$-dimensional phase space, and $|\mathbf{x}\rangle$ denotes a quantum position eigenstate in Dirac notations.

II. INFORMAL INTRODUCTION TO WIGNER-WEYL QUANTIZATION

The detailed expositions of the Wigner-Weyl formalism [24, 25, 37, 38] can be found in a variety of articles, tutorials and textbooks. Wigner’s works [24, 39, 40] can serve as the physically appealing and intuitive introduction. Readers seeking for a more formal and axiomatic presentation might prefer the Stratonovich approach detailed in Refs. [41, 42]. For thorough discussions on the semiclassical limits, classical analogies and applications one can refer to Refs. [23, 43].

This introduction to the Wigner-Weyl formalism is somewhat non-standard and largely informal. It is not intended to be a substitute of above-mentioned works. Rather, its objective is to introduce the ideas of the Wigner quantization from dynamical perspective in the spirit of our earlier works relying on the operational dynamical modelling (ODM) [44, 45], which enables a smooth transition to the hydrodynamic interpretation of quantum mechanics.

It will be convenient for us to treat the general quantum Hamiltonian operators $A=A(\hat{\mathbf{p}}, \hat{\mathbf{x}})$ as symmetrized polynomials of the form

$$A(\hat{\mathbf{p}}, \hat{\mathbf{x}})= \sum_{\mathbf{r}_1, ..., \mathbf{r}_{2N}} a_{\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_{2N}} \{\hat{p}^{r_1}_1, ... \hat{p}^{r_N}_N, \hat{x}^{r_{N+1}}_1, ..., \hat{x}^{r_{2N}}_N\},$$

(1)

where $\{\circ, \circ\}_+$ stands for the anticommutator and $a_{\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_{2N}}$ are some real coefficients. This assumption is not really critical and just helps us to avoid extra complications by dealing with complex expansion coefficients.

A. Key concepts in nutshell

Quantum mechanics prescribes that the momentum and position operators $\hat{\mathbf{p}}$ and $\hat{\mathbf{x}}$ must satisfy identities

$$[\hat{p}_{n_1}, \hat{x}_{n_2}]=-i\hbar \delta_{n_1,n_2}, \quad [\hat{x}_{n_1}, \hat{x}_{n_2}]= [\hat{p}_{n_1}, \hat{p}_{n_2}]=0.$$

(2)

The way to represent these operators is solely up to us. The coordinate representation

$$\hat{x}_n=x_n, \quad \hat{p}_n=-i\hbar \frac{\partial}{\partial x_n},$$

(3a)

and momentum representation

$$\hat{x}_n=i\hbar \frac{\partial}{\partial p_n}, \quad \hat{p}_n=p_n$$

(3b)

are the most typical choices. However, nothing prevents us from choosing something more interesting

$$\hat{x}_n=x_n+i\hbar \frac{\partial}{\partial p_n}, \quad \hat{p}_n=p_n-i\hbar \frac{\partial}{\partial x_n}.$$  

(4)

Here we replaced the common “hat” above the quantum mechanical operator with the right-pointing curved arrow. The reason will become clear shortly. The operators (4) are called the “left” Bopp operators. It is straightforward to verify that they satisfy the identities (2).

At the first glance, the representation (4) looks inconvenient: We doubled the number of variables for no reason. However, one already can notice the remarkable feature that the Bopp operators (4) reduce to the conventional phase space variables $x_n$ and $p_n$ in the classical limit $\hbar \to 0$. This is clearly not the case for the representations (3).

What kind of representation do the Bopp operators lead to? To answer this question, it is instructive first to review the position representation (3a) in more detail. Let $\hat{\rho}$ be a density matrix describing the generic state of a quantum system. Its position representation
In the case of a pure state \( \rho(x',x'')=|x'|\rho|x''\rangle \). The generic term of the form
\[
A(\hat{p},\hat{x})\tilde{B}(\hat{p},\hat{x})
\]
is represented as
\[
\tilde{A}'\tilde{B}''\rho(x',x'')=\tilde{B}''\tilde{A}'\rho(x',x''),
\]
where \( \tilde{A}'=A(-ih\frac{\partial}{\partial x'},x') \) and \( \tilde{B}''=B(ih\frac{\partial}{\partial x''},x'') \). Note the absence of the “-” sign in the momentum argument of \( \tilde{B}'' \). This is the consequence of the fact that \( \rho B=(B\tilde{\rho})' \). For this reason, the left-acting “double-primed” operators satisfy the commutation relations, which are complex conjugate of (2)
\[
[A',\tilde{B}'']=[i\hbar\delta_{n_1,n_2}],
\]
addition, the “primed” and “double-primed” operators act on different variables and hence commute
\[
[A',\tilde{B}'']=0.
\]
What will happen if we switch to the Bopp representation (4)? What will be the analogs of “double-primed” operators? It appears that they can be expressed in terms of the following “right” Bopp operators:
\[
\tilde{x}_n=x_n-i\frac{\hbar}{2}\frac{\partial}{\partial p_n}, \quad \tilde{p}_n=p_n+i\frac{\hbar}{2}\frac{\partial}{\partial x_n},
\]
which will be marked with the left-pointing curved arrows. Indeed,
\[
[A',\tilde{B}'']=[i\hbar\delta_{n_1,n_2}]
\]
and
\[
[A',\tilde{B}'']=[0]
\]
for any \( \tilde{A}=A(\tilde{p},\tilde{x}) \) and \( \tilde{B}=B(\tilde{p},\tilde{x}) \). It is obvious that the relations (9) and (10) are identical to the equalities (6) and (7). Hence, the generic correspondence rule for the Bopp representation should read
\[
A(\hat{p},\hat{x})\tilde{B}(\hat{p},\hat{x})\rightarrow A(\tilde{p},\tilde{x})\tilde{B}(\tilde{p},\tilde{x})P(p,x).
\]
Let us apply the inverse Fourier transform to \( P(p,x) \) with respect to the momentum variables \( p \):
\[
P(\tilde{p},\tilde{x})=\overline{P(\hat{p},\hat{x})} \Rightarrow \tilde{P}(\lambda,\tilde{x})=\overline{P(\hat{p},\hat{x})} \]
\[
\int_\mathbb{R}^n P(p,x)e^{-i\frac{\hbar}{2}\frac{\partial}{\partial p}\frac{\partial}{\partial x}}d^npd^nx.
\]
It can be shown in a similar fashion that
\[
\int_\mathbb{R}^n P(p,x)e^{i\frac{\hbar}{2}\frac{\partial}{\partial p}\frac{\partial}{\partial x}}d^npd^nx=\int_\mathbb{R}^n P(p,x)e^{-i\frac{\hbar}{2}\frac{\partial}{\partial p}\frac{\partial}{\partial x}}d^npd^nx.
\]
References

1. Leonard Cohen, “Progress in the Theory of Quantum Statistics” in Quantum Statistics and the Theory of Classical and Quantum Systems, edited by R. W. P. Dreves, Academic Press, New York, 1969.

2. According to the prominent result of Leon Cohen, one can introduce infinitely many different phase space representations of quantum mechanics [16]. However, the relations (9) and (10) make the Wigner representation special and unique.

3. The function \( P(\lambda,\tilde{x}) \), known as the Blokhintsev function, was first introduced in Ref. [17].

4. The normalization prefactor in Eq. (14) is chosen such that \( \int \int_\mathbb{R}^n P(p,x)e^{-i\frac{\hbar}{2}\frac{\partial}{\partial p}\frac{\partial}{\partial x}}d^npd^nx=1 \).
rewrite the correspondence relation (11) in an appealing form
\[ A(\hat{p}, \hat{x}) \hat{\rho} B(\hat{p}, \hat{x}) \rightarrow \hat{A}(p, x) \ast P(p, x) \ast \hat{B}(p, x). \] (11')

However, there is a complication that generally \( \hat{A}(p, x) \neq A(p, x) \), \( \hat{B}(p, x) \neq B(p, x) \) in the above formula, except for operators of the separable form (16). Here we will not go deeper into the construction and properties of the quantities \( A \) and \( B \), called the Weyl symbols of operators, and instead refer readers to excellent review [48], where an interesting historical remark can be also found.

C. Quantum dynamics in Wigner representation

Using the correspondence relations (11) and (11'), one can write the Liouville–Neumann equation
\[ \frac{\partial}{\partial t} \hat{\rho} = \frac{i}{\hbar} [\hat{H}, \hat{\rho}] \] (19)
in the Wigner representation as
\[ \frac{\partial}{\partial t} P = \{ \hat{H}, P \}, \] (20)
where the right-hand side
\[ \{ \hat{H}, P \} = \frac{1}{i\hbar} (\hat{H} - \hat{\rho} \hat{P} - \hat{P} \hat{\rho}) = \frac{2}{\hbar} \hat{H} \sin \left( \frac{\hbar}{2} (\frac{\partial}{\partial p} - \frac{\partial}{\partial x}) \right) P \] (21)
is called the Moyal bracket of \( \hat{H} \) and \( P \). Eq. (20) is often referred as the quantum Liouville equation. The reason for such a name becomes clear once the Moyal bracket (21) is expanded into the series with respect to \( \hbar \)
\[ \frac{\partial}{\partial t} P = \{ \hat{H}, P \} + O(\hbar^2), \] (22)
where \( \{ \hat{H}, P \} = \frac{\partial\hat{H}}{\partial p} \frac{\partial P}{\partial \phi} - \frac{\partial\hat{H}}{\partial \phi} \frac{\partial P}{\partial p} \) is the usual classical Poisson bracket. Thus, because of relations (4) the quantum Liouville equation (20) directly reduces to its expected classical counterpart in the limit \( \hbar \rightarrow 0 \).

III. FLUID ANALOGY FOR BOSONIC SYSTEMS

Consider a generic \( N \)-dimensional open system with Hamiltonian \( \hat{H} \) obeying the Lindblad-like master equation [49–51]
\[ \frac{\partial}{\partial t} \hat{\rho} = \frac{i}{\hbar} [\hat{\rho}, \hat{H}] + \frac{1}{2} \sum_k \{ (\hat{L}_k(t) \hat{\rho}, \hat{L}_k^\dagger(t)) ] + h.c., \] (23)
where dissipation operators \( \hat{L}_k \) are generally time- and \( \hat{\rho} \)-dependent. We wish to cast Eq. (23) for the density matrix \( \hat{\rho} \) into an evolution equation for effective multi-dimensional probability fluid. Our starting point is the Wigner–Weyl formalism reviewed in the previous section, where the state of the system is described by the Wigner function (15).

**Theorem 1** (see Appendix A for proof). Master equation (23) can be cast into the continuity equation
\[ \frac{\partial}{\partial t} P(p, x) = -\nabla \cdot J^W(p, x) = -\frac{\partial}{\partial p} J^W_x - \frac{\partial}{\partial x} J^W_p, \] (24)
where the components of the 2N-dimensional flow are
\[ J^W_p = -P \otimes \frac{\partial}{\partial p} + \frac{i\hbar}{2} \sum_k ((\hat{L}_k^* P) \otimes \frac{\partial}{\partial x} + c.c.), \] (25a)
\[ J^W_x = P \otimes \frac{\partial}{\partial x} - \frac{i\hbar}{2} \sum_k ((\hat{L}_k^* P) \otimes \frac{\partial}{\partial p} + c.c.). \] (25b)
Here \( \hat{L}_k(p, x) \) and \( \hat{H}(p, x) \) are the Weyl symbols of the operators \( \hat{H} \) and \( \hat{L}_k \). The binary operations \( \ast \) and \( \otimes \) are defined as
\[ \ast = \delta^{\hat{p}} \left( \frac{\partial}{\partial p} - \frac{\partial}{\partial \phi} \right), \quad \otimes = \text{sinc}(\frac{\hbar}{2} (\frac{\partial}{\partial p} - \frac{\partial}{\partial \phi})), \]
where \( \text{sinc}(z) = \sin(z)/z \) and the arrows indicate the directions of differentiation, e.g., \( f(p, x) \frac{\partial}{\partial p} g(p, x) = g(p, x) \frac{\partial}{\partial p} f(p, x) \)

The analogy between classical fluid density and \( P(p, x) \) is incomplete because the latter typically has negative values [52]. To fix this issue, we introduce the **generalized Husimi function** \( Q(p, x) \) as a Gaussian convolution of \( P(p, x) \):
\[ Q(p, x) = \tilde{Q}_{w_p, w_x} P(p, x) = \int \cdots \int P(p', x') \times K^W_{w_p, w_x} (p - p', x - x') \, d^N p' \, d^N x', \] (26)
where \( w_p \) and \( w_x \) are arbitrary width parameters obeying the inequality \( w_p, w_x > \frac{\hbar}{2} \), and the kernel \( K^W_{w_p, w_x} \) is
\[ K^W_{w_p, w_x}(\delta p, \delta x) = \prod_{n=1}^N \frac{1}{2 \pi w_p w_x} e^{-\frac{\delta p^2}{2 w_p^2} - \frac{\delta x^2}{2 w_x^2}}. \] (27)
Function (26) is everywhere strictly positive. It reduces to the standard Husimi function (which can have zeros) in the limit \( w_p, w_x \rightarrow \frac{\hbar}{2} \)
\[ Q(p, x) = \tilde{Q}_{\frac{\hbar}{2}, \frac{\hbar}{2}} P(p, x) = \frac{\langle p, x | \hat{\rho} | p, x \rangle}{(2\pi \hbar)^N} \geq 0, \] (28)

5 The convolution operator can also be written in the differential form \( \tilde{Q}_{w_p, w_x} = \prod_{n=1}^N \exp \left( \frac{1}{2} w_p^2 \frac{\partial^2}{\partial p^2} + \frac{1}{2} w_x^2 \frac{\partial^2}{\partial x^2} \right) \) (see, e.g., Ref. [53]).

6 Note that the Husimi kernels (27) with \( w_p, w_x = \frac{\hbar}{2} \) and \( w_p, w_x > \frac{\hbar}{2} \) can be related to thermal states of a harmonic oscillator with zero and non-zero temperatures, respectively [38, 54]. It worth stressing that, unlike physical thermal averaging, the “thermal” Husimi transform remains invertible and does not lead to any loss of information contained in the original Wigner function.
where \(| \hat{p}, \hat{x} \rangle \) is the multidimensional squeezed coherent state localized at \(\{ \hat{p}, \hat{x} \rangle \):

\[
\langle \hat{x} | \hat{p}, \hat{x} \rangle = \prod_{n=1}^{N} \left( \omega_n^{-\frac{1}{2}} \right) e^{-\frac{1}{2} \hat{p}^2_{\hat{n}} - \frac{1}{2} \delta p_n(x_n - \bar{x}_n)^2} \phi_p(x_n - \bar{x}_n).
\]

Theorem 2 (see Appendix B for proof). Master equation (23) can be cast into the continuity equation

\[
\frac{\partial}{\partial t} Q(p, x) = -\nabla \cdot J^H(p, x) = -\frac{\partial}{\partial p} \cdot J^H - \frac{\partial}{\partial x} J^H_x,
\]

for the generalized Husimi function \(Q(p, x)\), where the components of the Husimi flow vector field \(J^H\) are expressed via the Wigner flows (25) as

\[
J^H_p = \hat{\mathcal{G}}_{p_w, w_x} J^W_p, \quad J^H_x = \hat{\mathcal{G}}_{w_p, w_x} J^W_x.
\]

Theorem 2 and strict positivity of \(Q(p, x)\) allow to introduce the trajectories of elementary parcels of the effective Husimi fluid in the Lagrangian picture:

\[
\frac{D}{Dt} x = v^H_x(p, x), \quad \frac{D}{Dt} p = v^H_p(p, x),
\]

where the components of the velocity field are \(v^H_x(p, x) = J^H(p, x)/Q(p, x)\), and \(v^H_p(p, x) = J^H_x(p, x)/Q(p, x)\).

IV. GAUGE TRANSFORMATIONS

In classical fluid dynamics, equations governing mass density redistribution follow from underlying velocity fields. The situation is reverse in quantum hydrodynamics: The flow fields (25) and (31) were recovered from the master equation (23). Such a recovery is not unique [34]: The substitutions

\[
J^W \to J^W + \delta J^W, \quad J^H \to J^H + \delta J^H
\]

leave the quantum dynamics (i.e., Eqs. (24) and (30)) intact if the auxiliary gauge fields \(\delta J^W\) and \(\delta J^H\) have zero divergences: \(\nabla \cdot \delta J^W = \nabla \cdot \delta J^H = 0\). For instance, \(\delta J^H_p\) may represent invariable swirls in the phase space:

\[
\delta J^H_p = -\frac{\partial}{\partial x} A^H_p(p, x), \quad \delta J^H_x = -\frac{\partial}{\partial p} A^H(p, x),
\]

where the gauge potentials \(A^H_p(p, x)\) are arbitrary bounded twice continuously differentiable functions.

This gauge freedom has been highlighted in, e.g., Refs. [10, 11, 32, 34], although has been utilized only once [55]. However, it has been overlooked that the price for the gauge freedom is the constraint

\[
J^W, J^H |_{x,p,p\to\pm\infty} \to 0
\]

ensuring that there is no probability sources and drains at \(|p, \hat{x}| = \pm\infty\). For instance, the constraint (35) rules out uniform gauge flows \(\delta J^H = \text{const}\) allowed by Eqs. (34).

It is noteworthy that the analytical expressions (25) linearly depend on \(P\) and hence satisfy Eq. (35) for all localized quasiprobability densities. This feature opens opportunities to design dynamical models obeying desired constraints \(f_r(J^H) = 0\) \((r = 1, \ldots R)\) without explicitly solving the complicated boundary value problem (35). Namely, one can start from Eqs. (25), (31) defining the “default” gauge \(A^H = 0\) and then seek new gauge potentials \(A^H(p, x)\) obeying the following constraints:

\[
A^H, \nabla A^H |_{x,p,p\to\pm\infty} \to 0, \quad f_r(J^H + \delta J^H (A^H, \ldots, A^H)) = 0.
\]

Let us demonstrate this generic scheme on an example.

V. BOHMIAN MECHANICS

Consider a closed \(N\)-dimensional quantum system with the Hamiltonian

\[
\hat{H} = \sum_{n=1}^{N} \frac{1}{2m_n} \hat{p}_n^2 + V(\hat{x}),
\]

whose Weyl symbol is \(\hat{H}(p, x) = \sum_{k=1}^{N} \frac{\hat{p}_n^2}{2m_n} + V(x)\). We assume that the system is in a pure state described by the wavefunction \(\psi(x, t) = |x(\psi(t))\).

Our aim is to construct the hydrodynamic analogy (marked by double primes “) to the dynamics of this system, where every \(n\)-th component \(v^H_n\) of the fluid velocity field (32) is independent of the corresponding conjugate momentum \(p_n\).

The constraint (36b) of \(J^H_x\) becomes

\[
J^H_x(p, x) = \frac{\partial}{\partial p} Q^R(p_n, p_n, \ldots, p_n, p_n, \ldots, p_n, x|x) \langle n \rangle(p, x).
\]

Here the velocities \(v^H_n\) are expressed in terms of yet-unknown \(p_n\)-independent functions \(w^R_m\), which we will call the regularized Bohmian momenta for the reasons below. Following our scheme, one first deduces the \(x\)-components of the gauge field from Eq. (38) using the definition (33) and Eqs. (31),

\[
\delta J^H_x = \frac{1}{m_n} \left( p^R_n Q^R(p, x) - \hat{G}_{w^R_n, w^R_n} (p_n P(P(p, x))) \right).
\]

This allows to find the gauge potential \(A^H(p, x)\) from the second of Eqs. (34),

\[
A^H(p, x) = \int_{0}^{\infty} \delta J^H_x dp = \frac{1}{m_n} (p^R_n P_{\infty} Q^R(p, x) \langle p_n P(p, x) \rangle dp).
\]

The boundary constraints (36a) in the limit \(p_n \to +\infty\) specialize the regularized Bohmian momenta \(p^R_n\),

\[
p^R_n = \frac{\int_{-\infty}^{\infty} dp \hat{G}_{w^R_n, w^R_n} (p_n P(P(p, x)))}{\int_{-\infty}^{\infty} Q^R(p, x) \langle p_n P(p, x) \rangle dp}.
\]

Now the gauge (40) is fully specified, and we can compute all the components of the gauge flow field using Eqs. (34).

Of special interest is the limiting case (marked by single primes “) of the just-constructed hydrodynamic analogy, where

\[
w^H_n = w^R_n \to 0, \quad w^H_n \to -\infty.
\]
Theorem 3 (see Appendix C for proof). The evolution of the generalized Husimi fluid \( Q(p,x) = \hat{S}_{w_p, w_x} P(p,x) \) in the gauge (40) in the one-dimensional case \( N=1 \) and in the limit (42) is represented by the flow

\[
J'_x = \frac{\dot{p}(x)}{m} Q(p,x), \quad J'_p = -\frac{\partial (V(x) + \mathcal{G}(x))}{\partial x} Q(p,x),
\]

(43)

where \( p(x) = p^\text{reg} |_{w'_p \to 0, w'_x \to \infty} = \mathcal{R} \hat{S}_{w_p, w_x} \psi(x) \) is the Bohmian momentum and \( \mathcal{G}(x) = -\frac{\hbar^2}{2m|\psi(x)|^2} |\psi(x)|^2 \) is the quantum potential introduced in the Bohmian theory.

Theorem 3 indicates that the phase space velocities \( \nu' = J'/Q' = \{ -\frac{\partial}{\partial x} (V(x) + \mathcal{G}(x)); \frac{\dot{p}(x)}{m} \} \) are independent of \( p \). Hence, it follows from Eqs. (32) and (41) that

\[
\frac{\partial}{\partial t} p = -\frac{\partial}{\partial x} (V(x) + \mathcal{G}(x)), \quad \frac{\partial}{\partial t} x = \frac{\dot{p}(x)}{m}.
\]

(44)

Furthermore, one can verify by direct substitution that

\[
\psi(x) = |\psi(x)| \exp \left( \int_{-\infty}^{x} \frac{\dot{p}(x')}{m} \, dx' \right).
\]

(45)

Equations (44) and (45) fully specify the evolution of pure state \( |\psi\rangle \) in terms of \( |\psi(x)| \exp(\int_{-\infty}^{x} \frac{\dot{p}(x')}{m} \, dx') \) and \( p \). They reproduce the familiar equations of the Bohmian mechanics, the oldest quantum hydrodynamic formalism introduced by Madelung and de Broglie in 1927 [27, 28].

The physical meaning of the Bohmian gauge specialized by theorem 3 can be clarified on the example of the quantum harmonic oscillator in Fig. 1. Panels a and d of Fig. 1 compare two fluid representations of the oscillator’s ground state \( |\psi_0\rangle \). In the “default” gauge (panel a), the quantum advection, shown by black arrows, reproduces classical dynamics. In contrast, the flow fields vanish in the Bohmian gauge (panel d) in line with the notion of the stationary state.

The classical-like drift of the Husimi fluid (Fig. 1a) is an obstacle for simulating quantum tunneling effects as in the case of the double-well potential shown in Fig. 2. Due to quantum advection in the “default” gauge of Fig. 2a, a dense sampling of the entire phase space is needed to capture a small fraction of trajectories crossing the barrier. In contrast, tunneling trajectories in the Bohmian gauge, Fig. 2b, originate from a localized region near the barrier permitting a local dense sampling. This very property of the Bohmian mechanics has caught the eye of applied physicists and chemists [56, 57], leading to a recent remarkable progress in modelling complex many-body systems [2].

The Bohmian formalism found a variety of applications [58–61] including studies of molecular processes (e.g., reactive scattering and nonadiabatic vibronic dynamics [62–64]), elastic collisions [65], and quantum measurements [66]. Parallels between the Bohmian mechanics and the classical dynamical effects in silicone oil have also been drawn [67].

However, the transition to the Bohmian gauge is not invertible for a generic mixed quantum state: The singular convolution \( \hat{S}_{w'_p, w'_x} \to \mathcal{R} \hat{S}_{w_p, w_x} \) in Eq. (26) irrecoverably destroys the momentum information in the original Wigner function. Also, the Bohmian fluid spreads over an infinite phase space area (see Fig. 2b). The associated natural coherent states (29), following from the relation (28), collapse to a set of \( \delta \)-functions with undefined parameters \( \hat{p}_k \). Such a singular basis is not suitable for numerical simulations.

In order to circumvent all these issues, we propose the regularized Bohmian transformation, where the gauge (40) is applied to the localized Husimi function \( Q'' = \hat{S}_{w'_p, w'_x} P \) constructed using finite width parameters \( w'' \neq 0, \infty \). This gauge inherits the aforementioned advantages of the Bohmian mechanics – vanishing flows for steady states (Fig. 1b) and the localized origins of tunneling trajectories in the phase space (Fig. 2c). Moreover, compared to Fig. 2b, the resulting effective fluid trajectories in Fig. 2c are smooth and completely free of the \( \delta \)-like singularities.

Figure 2. The three fluid representations of the quantum dynamics in the double-well potential \( V^{\text{dw}} = \frac{1}{2} (x-5)^2 x^2 \): (a) the “default” Husimi gauge (Eqs. (25) and (31)); (b) the Bohmian gauge; (c) the regularized Bohmian gauge. The Husimi function \( Q \) of the initial state \( \langle x|\psi_0\rangle |_{x=0} = \frac{\sqrt{\pi}}{2\sqrt{2}} e^{-x^2/2} \) is in blue. Colored curves depict the trajectories of effective fluid parcels.

VI. NUMERICAL EXAMPLE

During last two decades, notable progress has been achieved in simulating quantum dynamics directly in the Wigner [68, 69] or Husimi representations, especially thanks to the Martens group [10, 11, 55, 70]. However, such simulations are inherently challenging. A particular issue is vanished quantum interference (and hence, the phase information) in the Husimi picture (see Appendix D for details and an example). We argue that this issue can be turned into a numerical advantage when combined with the CCS- and FMS-type quantum chemistry methods [9] to solve the Schrödinger equation.
that the trajectory accompanied by multiple scattering. The quantum dynamical systems theory \[ t \text{ tum processes via recently proposed inventive use of the Husimi fluid} \]

The results, summarized in Fig. 3, show that the accuracy of simulating weak tunneling effects improves significantly if the “default” Husimi gauge $A^H=0$ (green curves) is replaced by the regularized Bohmian gauge (blue curves). Moreover, the latter gauge also delivers substantially better long-term estimates for both the shape of the quantum state and the tunneling probabilities than the standard CCS method [12] (black curves).

**VII. OUTLOOK**

The demonstrated utility of our theory calls for revisiting other applications of phase space methods in quantum mechanics and beyond. For instance, an open question is the optimal Skodje’s gauge for examining quantum processes via recently proposed inventive use of the dynamical systems theory [73, 74]. Exploring the fluid analogies to other initial value representations, such as G-MCTDH [75, 76], could help to improve their numerical stability. The close ties between the phase space approaches to signal processing and quantum mechanics (see, e.g., Refs. [46, 48, 77]) make the developed methodology transferable to the time-frequency analysis of propagating signals in engineering applications. Connections with the gauge-dependent trajectory-based methods relying on the Voronoi tessellation [78, 79] also deserve a detailed exploration. Finally, we believe that our results blur the boundary between classical and quantum worlds by shedding new light on the controversial interpretation of trajectories in quantum mechanics [80, 81] and offer new ways to construct quantum-classical hybrid models [82, 83].

**ACKNOWLEDGMENTS**

D. Zh. thanks Francisco González Montoya for fruitful discussions and relevant advises. D.I.B. was supported by AFOSR (grant FA9550-16-1-0254), ARO (grant W911NF-19-1-0377), and DARPA (grant D19AP00043). The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of AFOSR, ARO, DARPA, or the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for Government purposes notwithstanding any copyright notation herein.

**Appendix A: Proof of theorem 1**

Our starting point is the Liouville-von Neumann equation (20). Unlike the classical Liouville equation, Eq. (20) does not preserve the phase space volume. However, it preserves the normalization

\[
\int_{-\infty}^{+\infty} d^N p \, d^N x \, F(p, x) = \text{Tr} [\hat{\rho}] = 1. \tag{A1}
\]
Using the correspondence rule (11) and the definition (21) of the Moyal bracket, one can convert a master equation
\[ \frac{\partial}{\partial t} P = -\nabla \cdot J^W, \] (A2)
where \( \nabla = \left( \frac{\partial}{\partial \phi}, \frac{\partial}{\partial \chi} \right) \) and \( J^W = (J^W_p, J^W_x) \) are the Wigner flows. In order to find \( J^W_p \) and \( J^W_x \), we will need the following lemma:

**Lemma 1.** The Moyal bracket (21) of two Weyl symbols \( \hat{A} \) and \( \hat{B} \) can be written as
\[ \{ \hat{A}, \hat{B} \} = \frac{\partial}{\partial \phi} (\hat{A} \circ \hat{B}) - \frac{\partial}{\partial \chi} (\hat{A} \circ \hat{B}), \] (A3)
where \( \circ \) denotes the binary operation
\[ \circ = \text{sinc}(\frac{\phi}{2}, \frac{\chi}{2}). \] (A4)

**Proof.**
\[ \frac{\partial}{\partial \phi} (\hat{A} \circ \hat{B}) - \frac{\partial}{\partial \chi} (\hat{A} \circ \hat{B}) = (\hat{A} (\frac{\partial}{\partial \phi} + \frac{\partial}{\partial \chi}) \circ \hat{B} + \hat{B} \circ \hat{A} (\frac{\partial}{\partial \phi} + \frac{\partial}{\partial \chi})) = \hat{A} \left( \frac{\partial}{\partial \phi} \circ \frac{\partial}{\partial \chi} \right) \circ \hat{B} = \{ \hat{A}, \hat{B} \}. \]

**Proof of theorem 1.** Using the correspondence rule (11) and the definition (21) of the Moyal bracket, one can convert a master equation
\[ \frac{\partial}{\partial t} \hat{\rho} = i \left[ \hat{H}, \hat{\rho} \right] + \frac{i}{2} \sum_k \left( \{ \hat{\mathcal{L}}_k(t) \hat{\rho}, \hat{\mathcal{L}}^\dagger_k(t) \} + \text{h.c.} \right) \]
into the Wigner representation as
\[ \frac{\partial}{\partial t} P = \{ \hat{H}, P \} - \frac{i}{2} \sum_k \left( \{ \{ \hat{\mathcal{L}}_k(t) \ast P, \hat{\mathcal{L}}^\dagger_k(t) \} \right) \] (A5)

Using Lemma 1, Eq. (A5) can be further rewritten as
\[ \frac{\partial}{\partial t} P = -\frac{\partial}{\partial \phi} (P \circ \hat{\mathcal{L}}^\dagger_k(t)) + \frac{\partial}{\partial \chi} (P \circ \hat{\mathcal{L}}^\dagger_k(t)) + \frac{i}{2} \sum_k \left( \frac{\partial}{\partial \phi} (\{ \hat{\mathcal{L}}_k(t) \ast P \}) + \frac{\partial}{\partial \chi} (\{ \hat{\mathcal{L}}^\dagger_k(t) \ast P \}) + \right) \]
\[ \text{h.c.} \]
\[ = \frac{\partial}{\partial \phi} J^W_p - \frac{\partial}{\partial \chi} J^W_x, \] (A6)

where finally
\[ J^W_p = -P \circ \hat{\mathcal{L}}^\dagger_k(t) + \frac{i}{2} \sum_k \left( \{ \hat{\mathcal{L}}_k(t) \ast P \} \right) \]
\[ \text{h.c.} \]
\[ (\frac{\partial}{\partial \phi} \circ (P \circ \hat{\mathcal{L}}^\dagger_k(t))) \], (A7a)

\[ J^W_x = P \circ \hat{\mathcal{L}}^\dagger_k(t) + \frac{i}{2} \sum_k \left( \{ \hat{\mathcal{L}}^\dagger_k(t) \ast P \} \right) \]
\[ \text{h.c.} \]
\[ (\frac{\partial}{\partial \phi} \circ (P \circ \hat{\mathcal{L}}^\dagger_k(t))) \]. (A7b)

Let us make a remark about the important special case of a closed system with the Hamiltonian
\[ \hat{H} = H(\hat{p}, \hat{x}) = \sum_n \frac{\hat{p}^2}{2m_n} + V(\hat{x}). \] (A8)

This Hamiltonian (A8) has the separable form (16), so that \( \hat{H} = H_p(x) \). By substituting this Weyl symbol into Eqs. (A7) and integrating by parts an appropriate number of times, one can show that the state-averaged Wigner flows \( J^W = \int_{-\infty}^{+\infty} J^W(p, x) d^N p d^N x \) coincide with the respective classical expressions:
\[ \langle J^W_p(P) \rangle = \int \cdots \int_{-\infty}^{+\infty} \frac{\partial V(x)}{\partial x} P(p, x) d^N p d^N x \] (A9a)
\[ \langle J^W_x(P) \rangle = \int \cdots \int_{-\infty}^{+\infty} \frac{\partial V(x)}{\partial x} P(p, x) d^N p d^N x. \] (A9b)

**Appendix B: Proof of theorem 2**

The normalization condition (A1) holds for the generalized Husimi function as well. Indeed, one can check that the kernel \( K_{w_p, w_x} \) defined by Eq. (27) satisfies the property
\[ \int \cdots \int_{-\infty}^{+\infty} K_{w_p, w_x}(p-p', x-x') d^N p d^N x = 1. \] (B1)

Using this identity, one finds that
\[ \int \cdots \int_{-\infty}^{+\infty} Q(p, x) d^N p d^N x = \int \cdots \int_{-\infty}^{+\infty} \hat{\mathcal{G}}_{w_p, w_x}(P(p, x)) d^N p d^N x = \int \cdots \int_{-\infty}^{+\infty} P(p, x) d^N p d^N x'. \] (B2)

Identity (B2) implies that the generalized Husimi function should satisfy a continuity-like equation similar to Eq. (A2).

**Proof of theorem 2.** The explicit form of the continuity equation for the generalized Husimi function can be deduced by applying the convolution operator \( \hat{\mathcal{G}}_{w_p, w_x} \) to the both sides of Eq. (A2):
\[ \hat{\mathcal{G}}_{w_p, w_x} \left( \frac{\partial}{\partial t} P \left( \frac{\partial}{\partial \phi} \ast Q \right) \right) = \frac{\partial}{\partial \phi} \ast Q \] (B3a)
\[ \hat{\mathcal{G}}_{w_p, w_x} \left( -\nabla \cdot J^W \right) = -\nabla \cdot \left( \hat{\mathcal{G}}_{w_p, w_x} J^W \right), \] (B3b)

where the Wigner currents are defined by Eqs. (A7). In the last equality we used the fact that the convolution operator \( \hat{\mathcal{G}}_{w_p, w_x} \) can be equivalently represented a in differential form as
\[ \hat{\mathcal{G}}_{w_p, w_x} = \prod_{n=1}^{N} \exp \left( \frac{1}{2} w_p^2 \frac{\partial^2}{\partial \phi^2} + \frac{1}{2} w_x^2 \frac{\partial^2}{\partial x^2} \right), \] (B4)
from which the identity \( \hat{\mathcal{G}}_{wp, w_p} \nabla = \nabla \hat{\mathcal{G}}_{wp, w_p} \) follows. By equating the right hand side of Eqs. (B3), one finds that

\[
J_p^H = \hat{\mathcal{G}}_{wp, w_p} J_p^W, \quad J_x = \hat{\mathcal{G}}_{wp, w_p} J_x^W. \tag{B5}
\]

For completeness, let us also re-express the right hand side of Eqs. (B5) for the Husimi currents solely in terms of the Husimi function \( Q(p, x) \) using the identity

\[
\hat{\mathcal{G}}_{wp, w_p}^{-1} = \hat{\mathcal{G}}_{-iw_p, iw_p}, \tag{B6}
\]

which directly follows from Eq. (B4) and allows to formally write

\[
P(p, x) = \hat{\mathcal{G}}_{-iw_p, iw_p} Q(p, x). \tag{B7}
\]

Substitution of Eq. (B7) into Eqs. (B5) gives

\[
J_p^H = \left( e^{ad_{\Sigma_{n=1}^N 1/2 \frac{\partial}{\partial p}} + \frac{\partial}{\partial x} \frac{\hat{H}(p, x)}{\partial x}} \right) Q(p, x) = Q(p, x) \odot^H \frac{\partial}{\partial x} \left( \hat{\mathcal{G}}_{wp, w_p} \hat{H}(p, x) \right). \tag{B8a}
\]

As a preliminary step, let us specialize the definition of the gauge potential (40) for the case of a pure quantum state \( |\psi\rangle \). For this, we will need the following property of the convolution operator \( \hat{\mathcal{G}}_{wp, w_p} \):

\[
\int_{\pi}^{p_n} \hat{\mathcal{G}}_{wp, w_p} Z(p, x) \, dp_n = \hat{\mathcal{G}}_{wp, w_p} \left( \int_{\pi}^{p_n} Z(p, x) \, dp_n \right), \tag{C1}
\]

which is valid for any function \( Z(p, x) \) exponentially small at \( |p| \to \infty \) and/or \( |x| \to \infty \). With the help of Eqs. (C1), (15) and the equality \( p_n e^{-i \frac{\hat{p} x}{\hbar}} = i \hbar \frac{\partial}{\partial x} e^{-i \frac{\hat{p} x}{\hbar}} \) we obtain

\[
A_n''(p, x) = \int_{\pi}^{p_n} \delta J_x'' \, dp_n = \frac{1}{m_n} (p_n \int_{\pi}^{p_n} Q''(p, x) \, dp_n - \int_{\pi}^{p_n} \hat{\mathcal{G}}_{wp', w_p''} (p_n P(p, x)) \, dp_n) = \frac{1}{m_n} \left( p_n \int_{\pi}^{p_n} \hat{\mathcal{G}}_{wp', w_p''} \int_{\pi}^{p_n} P(p, x) \, dp_n - \int_{\pi}^{p_n} \hat{\mathcal{G}}_{wp', w_p''} \int_{\pi}^{p_n} (p_n P(p, x)) \, dp_n \right) = \frac{1}{m_n} \left( p_n \int_{\pi}^{p_n} \hat{\mathcal{G}}_{wp', w_p''} \int_{\pi}^{p_n} \frac{1}{(2\pi \hbar)^{2N}} \int_{-\infty}^{+\infty} \psi^*(x - \frac{x'}{2}) \psi(x + \frac{x'}{2}) e^{-i \frac{\hat{p} x'}{\hbar}} \, d^N x' \, dp_n - \int_{\pi}^{p_n} \hat{\mathcal{G}}_{wp', w_p''} \int_{\pi}^{p_n} \frac{1}{(2\pi \hbar)^{2N}} \int_{-\infty}^{+\infty} \psi^*(x - \frac{x'}{2}) \psi(x + \frac{x'}{2}) e^{-i \frac{\hat{p} x'}{\hbar}} \, d^N x' \, dp_n \right) = \frac{1}{m_n} \left( p_n \int_{\pi}^{p_n} \frac{1}{(2\pi \hbar)^{2N}} d^N x' \int_{-\infty}^{+\infty} \psi^*(x - \frac{x'}{2}) \psi(x + \frac{x'}{2}) \frac{\partial}{\partial x} e^{-i \frac{\hat{p} x'}{\hbar}} \, d^N x' \right) + \hat{\mathcal{G}}_{wp', w_p''} \left( P.V. \int_{-\pi}^{+\pi} i \hbar \frac{\partial}{\partial x} \frac{\partial}{\partial x} \left( \psi^*(x - \frac{x'}{2}) \psi(x + \frac{x'}{2}) \frac{\partial}{\partial x} e^{-i \frac{\hat{p} x'}{\hbar}} \, d^N x' \right) \right). \tag{C2}
\]

The last equality in (C2) was obtained via the integration by parts with respect to \( x_n \).

**Proof of theorem 3.** We are now interested in the one-dimensional case \( N=1 \) when the Husimi transform is performed in the singular limit \( w''_p \to \infty, \ w''_p \to 0 \). Note that the kernel \( K_{wp', w_p'}^{W} \) defined by Eq. (27) in this

\[\text{limit reduces to} \]

\[K_{wp', w_p'}^{W} (p-p', x-x') \simeq \frac{\delta(x-x')}{\sqrt{\pi \hbar}} \delta(x-x') Q'[p;x]. \tag{C3}\]

After substituting Eq. (C3) into Eq. (41) one finds that

\[ \frac{p^{\text{reg}}}{p^{\text{reg}}} \mid_{w''_p \to \infty, w''_p \to 0} = \frac{P(p, x) \, dp}{\int_{\pi}^{p_n} P(p, x) \, dp} = p(x), \tag{C4} \]

where \( p(x) = \frac{\psi(x)^* \frac{\partial}{\partial x} \psi(x)}{|\psi(x)|^2} \) is the conventional Bohmian momentum, here \( \frac{p}{\pi} \).
Eqs. (C3) and (C4) allow to cast the gauge potential (C2) into the form

\[ A'(p, x) = \frac{Q'(p, x)}{|\psi(x)|^2} \text{P.V.} \int_{-\infty}^{+\infty} \frac{i \hbar \partial y}{m} (\mathbf{p}(x) + i \hbar \frac{\partial}{\partial y} \psi^*(x - \frac{y}{2}) \psi(x + \frac{y}{2})) dy. \quad (C5) \]

Further simplifications can be made by expanding \( \psi^*(x - \frac{y}{2}) \) and \( \psi(x + \frac{y}{2}) \) into the series of \( y \):

\[ A'(p, x) = \frac{Q'(p, x)}{|\psi(x)|^2} \text{P.V.} \int_{-\infty}^{+\infty} \frac{i \hbar \partial y}{m} \left( \mathbf{p}(x) + i \hbar \frac{\partial}{\partial y} \psi(x) + \frac{1}{2 \hbar} \psi^*(x) \frac{\partial^2 \psi(x)}{\partial x^2} - 2 \frac{\partial \psi^*(x)}{\partial x} \frac{\partial \psi(x)}{\partial x} + \frac{\partial^2 \psi^*(x)}{\partial x^2} \psi(x) + o(y^2) \right) dy. \quad (C6) \]

The terms in the curly brackets proportional to \( y^r \) with \( r > 2 \) do not contribute to the integral over \( y \). The rest of Eq. (C6) can be split into even and odd terms with respect to \( y \); the odd terms also do not contribute to the integral. By collecting the even terms and performing the integration, one obtains

\[ A'(p, x) = \frac{\hbar^2}{m} Q'(p, x) \left( \frac{\psi(x)^* \psi(x)}{|\psi(x)|^2} - p(x)^2 \right). \quad (C8) \]

Now we are ready to compute the fluid flow vector field corresponding to the Bohmian gauge. Its momentum component reads

\[ J'_p = -\frac{\partial}{\partial x} A'(p, x) + \frac{\hbar}{2\sigma^2} J^W_p(p, x) \bigg|_{w \to 0}, \quad (C9) \]

where \( J^W_p(p, x) \) is given by Eq. (A7a). Evaluation of the second term in Eq. (C9) using the specific form (C3) of the convolution kernel \( K^W_{w', w''} \) gives

\[ \frac{\hbar}{2\sigma^2} J^W_p(p, x) \bigg|_{w \to 0} = \frac{Q'(p, x)}{|\psi(x)|^2} \times \]

\[ \int_{-\infty}^{+\infty} P(p, x) \left[ \frac{\partial}{\partial x} \left( \frac{\partial}{\partial p} \frac{\partial \psi(x)}{\partial p} \right) - \frac{\partial}{\partial x} \frac{\partial \psi(x)}{\partial p} \right] \frac{\partial \psi(x)}{\partial x} \, dp =
\]

\[ - \frac{Q'(p, x)}{|\psi(x)|^2} \int_{-\infty}^{+\infty} P(p, x) \left[ \frac{\partial}{\partial x} \frac{\partial \psi(x)}{\partial x} - \frac{\partial}{\partial x} \frac{\partial \psi(x)}{\partial p} \right] \, dp =
\]

\[ - \frac{Q'(p, x)}{|\psi(x)|^2} \int_{-\infty}^{+\infty} P(p, x) \left[ \frac{\partial}{\partial x} \frac{\partial \psi(x)}{\partial x} \right] \, dp + \frac{Q'(p, x)}{|\psi(x)|^2} \times \]

\[ \int_{-\infty}^{+\infty} \frac{\partial}{\partial p} \left( P(p, x) \sum_{k=1}^{\infty} \left( \frac{\partial^2 \psi(x)}{\partial x^2} \right)^{2k-1} \right) \, dp =
\]

\[ - \frac{Q'(p, x)}{|\psi(x)|^2} \left[ \frac{\partial \psi(x)}{\partial x} \right]. \quad (C10) \]

The first term in Eq. (C9) can be transformed as

\[ \frac{\partial}{\partial x} A'(p, x) = \frac{\hbar^2}{m} Q'(p, x) \frac{\partial}{\partial x} \left( \psi(x)^2 \left( \frac{\psi(x)}{|\psi(x)|^2} - p(x)^2 \right) \right) = \frac{\partial}{\partial x} Q'(p, x), \quad (C11) \]

where \( \mathfrak{V}(x) \) is the quantum potential defined in theorem 3.

Thus, Eq. (C9) can be rewritten as

\[ J'_p = -Q'(p, x) \frac{\partial}{\partial x} (V(x) + \mathfrak{V}(x)). \quad (C12a) \]

The positional component of the flow can be obtained in a similar fashion using the definition of \( J'_x \) (see Eq. (38)):

\[ J'_x = \frac{\hbar}{m} Q'(p, x). \quad (C12b) \]

Equalities (C12) prove the theorem.

\[ \square \]

Appendix D: Quantum superposition and entangled states in Wigner and Husimi pictures

The possibility of the Wigner function \( P(p, x, t) \) to take negative values compromises its interpretation as a conventional probability distribution (this is why it is often referred as the quasiprobability distribution). The emergence of negative values is more the rule than the exception. For instance, Fig. 4a illustrates the Wigner function \( P_\psi \) of a superposition

\[ |\psi\rangle \propto |\bar{p}_a, \bar{x}_a\rangle + |\bar{p}_b, \bar{x}_b\rangle. \quad (D1) \]

of two squeezed coherent states defined in Eq. (46). One can see that \( P_\psi \) consists of three components

\[ P_\psi(p, x) = P_{aa}(p, x) + P_{bb}(p, x) + 2\Re[P_{ab}(p, x)], \quad (D2) \]

where

\[ P_{ab}(p, x) \propto \frac{1}{2\pi \hbar} \int_{-\infty}^{+\infty} (\bar{p}_a + \frac{\bar{p}_b}{2}) (x - \frac{\bar{p}_b}{2}) (x - \frac{\bar{p}_b}{2}) e^{-i\frac{\bar{p}_b}{2}x} \, dx'. \quad (D3) \]

The first two terms in Eq. (D2) manifest themselves in Fig. 4a by two Gaussian blobs around the points \( \{p_a, x_a\} \) and \( \{p_b, x_b\} \). These blobs are identical to the classical probability distribution for a particle having equal likelihoods of being localized either near \( \{p_a, x_a\} \) or near \( \{p_b, x_b\} \). However, the last term in Eq. (D2) adds non-classical sign-changing interference fringes between these blobs. It is because of this term the phase space velocity field \( J^W(p, x) / P(p, x) \) is both physically and mathematically ill-defined and singular. Consequently, one cannot unambiguously define the trajectories of the elementary parcels of quantum fluid represented by the time-dependent Wigner function [52]. Furthermore, in a general case, the overlapping fringes form a complicated landscape, which is difficult to approximate numerically.
Panels (a) and (b) of Fig. 4 help to compare the Wigner and Husimi representations for the same quantum superposition state. As expected, the Husimi function $Q(p, x)$ is everywhere non-negative. At the same time, one can see that the interference fringes are nearly entirely smeared out in the Husimi representation by the Gaussian convolution (they are nearly two orders of magnitude smaller than the dominant peaks). Consequently, the quantum superpositions with the opposite phases shown in panels (b) and (c) look nearly identical.

Similar conclusions apply to an entangled state of two quantum particles, such as

$$|\text{ent}\rangle \propto |\vec{p}_{1, a}, \vec{x}_{1, a}\rangle |\vec{p}_{2, a}, \vec{x}_{2, a}\rangle + |\vec{p}_{1, b}, \vec{x}_{2, b}\rangle |\vec{p}_{1, b}, \vec{x}_{2, b}\rangle,$$  
where indices 1 and 2 enumerate the particles. The corresponding Wigner function $P_{\text{ent}}$ again consists of three terms

$$P_{\text{ent}}(p, x) = P_{aa}(p_1, x_1)P_{aa}(p_2, x_2) + P_{bb}(p_1, x_1)P_{bb}(p_2, x_2) + 2\Re[P_{ab}(p_1, x_1)P_{ab}(p_2, x_2)].$$

The first two terms describe classical correlations between particles’ positions and momenta. The last term in Eq. (D5) is composed of the product of terms $P_{ab}$, which, as we have learned from Fig. 4a, are non-positive and oscillatory. This additional, markedly non-classical correlation term is the phase space signature of quantum nonlocality. We refer interested readers to Ref. [84] for a thorough analysis of the quantum nonlocality (expressed as a violation of the Bell inequality) in terms of the parameters of the Wigner function.

These illustrations show that simulating quantum dynamics directly in the Wigner and Husimi representations is challenging. Nevertheless, it is worth noting the innovative methods developed in the Martens group, which made such simulations possible for low-dimensional systems [10, 11, 55, 70].

Appendix E: Hydrodynamic interpretation of coupled coherent states (CCS) method

In the CCS method, the trajectories $\{\vec{p}_k(t), \vec{x}_k(t)\}$ of centers of basis states in the time-dependent anzatz (46) are defined as the optimal trajectories minimizing the residual

$$\langle \hat{r}_k | \hat{r}_k \rangle \rightarrow \min |\vec{p}_k(t), \vec{x}_k(t)\rangle,$$

where $|\hat{r}_k\rangle = \left(\frac{\hbar}{2} - \frac{1}{\hbar} \hat{H}\right) |\vec{p}_k(t), \vec{x}_k(t)\rangle$. In other words, the functions $\vec{p}_k(t)$ and $\vec{x}_k(t)$ provide the best fit to the solution of the Schrödinger equation $i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle$ when using the single-Gaussian approximation $|\psi\rangle \propto |\vec{p}_k(t), \vec{x}_k(t)\rangle$. The solution to the problem (E1) is

$$\frac{\partial}{\partial t} \vec{p}_k(t) = -\langle \vec{p}_k(t), \vec{x}_k(t) | \frac{\partial V(\vec{x})}{\partial \vec{x}} | \vec{p}_k(t), \vec{x}_k(t)\rangle,$$
$$\frac{\partial}{\partial t} \vec{x}_k(t) = \langle \vec{p}_k(t), \vec{x}_k(t) | \frac{\hbar}{m} \frac{\partial}{\partial \vec{p}} | \vec{p}_k(t), \vec{x}_k(t)\rangle,$$

where the Hamiltonian of form (A8) is assumed. Straightforward computation shows that Eqs. (E2) can be reduced to

$$\frac{\partial}{\partial t} \vec{p}_k(t) = \langle J^W_p (P_k) \rangle,$$
$$\frac{\partial}{\partial t} \vec{x}_k(t) = \langle J^W_{\vec{p}} (P_k) \rangle,$$

where $P_k(p, x)$ is the Wigner representation of the basis function $|\vec{p}_k, \vec{x}_k\rangle$ (i.e., it is obtained by substituting $|\psi\rangle = |\vec{p}_k, \vec{x}_k\rangle$ into Eq. (15)). The Wigner flows $J^W$ and their averaged values are defined by Eqs. (A7) and (A9). Thus, the CCS solutions for $\vec{p}_k(t)$ and $\vec{x}_k(t)$ allow for a simple interpretation as the trajectories guided by the averaged Wigner phase space velocities for a single basis state.

Appendix F: Regularized Bohmian representation: Closed-form expressions for fluid velocities and fluxes

1. Preliminaries

Assume that a quantum state $|\psi\rangle$ is approximated using the anzatz of squeezed coherent states (46). The respective Wigner and Husimi functions can be represented as

$$P(p, x) = \sum_{k_1=1}^{K} \sum_{k_2=1}^{K} \tilde{a}_{k_1}^\dagger(t) \tilde{a}_{k_2}(t) P_{k_1, k_2}(p, x),$$
$$Q''(p, x) = \sum_{k_1=1}^{K} \sum_{k_2=1}^{K} \tilde{a}_{k_1}^\dagger(t) \tilde{a}_{k_2}(t) Q''_{k_1, k_2}(p, x),$$

where
and correspond to $Q\rightarrow 0$ in the above expressions we used the notations

\[ \langle \bar{\psi}_n \rangle = \frac{1}{\sqrt{\pi \hbar}} \exp \left( -\frac{\bar{\psi}^2}{2\hbar} \right) \]

\[ \langle \bar{\psi}_n \rangle^2 = \frac{1}{\hbar} \sum_{n=1}^{\infty} \frac{1}{n} \exp \left( -\frac{\bar{\psi}^2}{2\hbar} \right) \]

The following relations for $P_{k_1, k_2}(p, x)$ and $Q_{k_1, k_2}(p, x)$ will be needed in the subsequent derivations:

\[ P_{k_1, k_2}(p, x) = \frac{1}{\sqrt{\pi \hbar}} \exp \left( -\frac{\bar{\psi}^2}{2\hbar} \right) \]

\[ Q_{k_1, k_2}(p, x) = \frac{1}{\sqrt{\pi \hbar}} \exp \left( -\frac{\bar{\psi}^2}{2\hbar} \right) \]

where the function $f_n(z)$ is defined as

\[ f_n(z) = \frac{\sqrt{\pi}}{2\hbar} e^{-z^2} \text{erf}(z s_n) + 1 \]

with $s_n = \sqrt{\frac{\bar{\psi}^2}{2\hbar \sum_{n=1}^{\infty} \frac{1}{n} \exp \left( -\frac{\bar{\psi}^2}{2\hbar} \right) \}}$ (erf stands for error function).

2. Regularized Bohmian momentum $p_{\text{reg}}(p, \{p_n\}, x)$

Before turning to a general multidimensional case, let us demonstrate that Eq. (41) takes a particularly simple form for a pure state $|\psi\rangle$ in the one-dimensional case $N=1$.
The above derivation can be straightforwardly generalized to a multidimensional case

\[
p^{\text{reg}}_{n}(p_i \{ p_n \}, x) = \sum_{k_1, k_2 = 1}^{K} \sum_{k_1, k_2 = 1}^{K} a_{k_1}^* (t) a_{k_2} (t) \langle \hat{p}_{k_1, n}, \hat{x}_{k_1, n} | \{ \hat{p}_n, e^{-i \frac{x_n - x_{n'}}{2m}} \} + \langle \hat{p}_{k_2, n}, \hat{x}_{k_2, n} | \{ \hat{p}_n, e^{-i \frac{x_n - x_{n'}}{2m}} \} \rangle_{n \neq n'} Q'_{k_1, k_2, n'} (p_n', x_n') \]  

(F12)

3. Husimi fluxes

The position flux components \( J^p_{x_n} (p, x) \) can be readily evaluated by substituting Eqs. (F1), (F4) and (F5) into Eq. (F13).

The computation of the momentum flux components

\[
J^p_{n}(p, x) = \mathcal{J}^{p}_{n}(p, x) + \delta J^p_{n}(p, x),
\]

(F13)

is more involving. (Recall that the “default” component \( J^p_{n}(p, x) \) of the momentum Husimi flow is defined by Eqs. (B5) and (A7)). We are going to show how one can evaluate both the terms in Eq. (F13).

The gauge term \( \delta J^p_{n}(p, x) \) is given by the first of Eqs. (34). In order to evaluate the right hand side of Eqs. (34), one needs to know the gauge potential defined in Eq. (40). One can proceed by expanding \( A^p_{n}(p, x) \) analogously to Eqs. (F1)

\[
A^p_{n}(p, x) = \sum_{k_1 = 1}^{K} \sum_{k_2 = 1}^{K} a_{k_1}^* a_{k_2} A^p_{n,k_1,k_2}(p, x),
\]

(F14)

where

\[
A^p_{n,k_1,k_2}(p, x) = \frac{1}{m} \left( \frac{\partial}{\partial x} \int_{-\infty}^{p_n} Q'_{p_n, k_2} (p, x) \, dp - \int_{-\infty}^{p_n} \sum_{k_1} a_{k_1}^* a_{k_2} P_{k_1, k_2} (p, x) \, dp \right) \]

(F15)

The terms \( A^p_{n,k_1,k_2}(p, x) \) can be evaluated via Eqs. (F8) and (F9)

\[
A^p_{n,k_1,k_2}(p, x) = \frac{1}{m} \left( (p_{\text{reg}} - \overline{p}_{n,k_1,k_2}) f_n (p_n - \overline{p}_{n,k_1,k_2}) + \frac{k^2 w_n}{2} Q'_{p_n, k_2} (p, x) \right).
\]

(F16)

Substitution of Eq. (F16) into the first of Eqs. (34) gives

\[
\delta J^p_{n}(p, x) = \sum_{k_1 = 1}^{K} \sum_{k_2 = 1}^{K} a_{k_1}^* a_{k_2} \delta J^p_{n,k_1,k_2}(p, x),
\]

(F17)

where

\[
\delta J^p_{n,k_1,k_2}(p, x) = \frac{1}{m} \left( \frac{\partial}{\partial x} \int_{-\infty}^{p_n} Q''_{p_n, k_1,k_2} (p, x) \right) + \left( (p_{\text{reg}} - \overline{p}_{n,k_1,k_2}) f_n (p_n - \overline{p}_{n,k_1,k_2}) + \frac{k^2 w_n}{2} Q''_{p_n, k_2} (p, x) \right).
\]

(F18)

Let us now turn to computing the first term \( J^H_{n}(p, x) \) in Eq. (F13). We will restrict ourselves to the case of the Hamiltonians specified in Eq. (37) with the separable potential

\[
V(x) = \sum_{n} V_n (x_n),
\]

as this case allows for the exact analytical treatment.

We again start by expanding the momentum flow \( J^H_{p} \) defined in Eqs. (B5) and (A7) similarly to Eq. (F17)

\[
J^H_{p}(p, x) = \sum_{k_1 = 1}^{K} \sum_{k_2 = 1}^{K} a_{k_1}^* a_{k_2} J^H_{n,k_1,k_2}(p, x),
\]

(F20)

where

\[
J^H_{n,k_1,k_2}(p, x) = \sum_{n_1 \neq n} Q'_1 \sum_{n_1 \neq n} Q''_{n_1, k_1, k_2} (p_n', x_n'),
\]

(F21)

and

\[
J^H_{n,k_1,k_2}(p, x) = - \sum_{n_1 \neq n} Q'_1 \sum_{n_1 \neq n} Q''_{n_1, k_1, k_2} (p_n', x_n').
\]

(F22)

To simplify notations, hereafter we will use the composite index \( \xi = \{ k_1, k_2, n \} \), i.e., \( J^H_{n,k_1,k_2,n} \), etc. Following the discussion in Sec. II.A, we can reexpress Eq. (F23) in terms of the Blokhintsev function \( \tilde{P}_{\xi}(\lambda, x_n) = \mathcal{F}^{-1}_{p_n - \lambda} [ \mathcal{P}_{\xi}(p_n, x_n) ] \) by applying the Fourier transform (12)

\[
J^W_{n,k_1,k_2,n}(p_n, x_n) = - \mathcal{F}_{p_n - \lambda} \left( \frac{1}{\lambda} \tilde{P}_{\xi}(\lambda, x_n) \sinh \left( \frac{\lambda}{2} \frac{\partial}{\partial x_n} \right) \frac{\partial V_n(x_n)}{\partial x_n} \right) = \frac{2\pi i}{\lambda} \tilde{P}_{\xi}(\lambda, x_n) \sin \left( \frac{\lambda}{2} \frac{\partial}{\partial x_n} \right) V_n(x_n) = \mathcal{F}_{p_n - \lambda} \left( \frac{1}{\lambda} \tilde{P}_{\xi}(\lambda, x_n) \sinh \left( \frac{\lambda}{2} \frac{\partial}{\partial x_n} \right) \right) V_n(x_n).
\]

(F24)

The respective expression (F22) for \( J^H_{n,k_1,k_2,n}(p_n, x_n) \) can be simplified with the help of convolution theorem

\[
J^H_{n,k_1,k_2,n}(p_n, x_n) = \int_{-\infty}^{+\infty} \mathcal{F}_{p_n - \lambda} \left( \frac{1}{\lambda} \tilde{P}_{\xi}(\lambda, x_n - x') \right) \left( \mathcal{F}_{p_n - \lambda} \left( \frac{1}{\lambda} \tilde{P}_{\xi}(\lambda, x_n - x') \right) \right) dx',
\]

(F25)
where
\[
\tilde{K}^W_{w_m',w_n'}(\lambda, \delta x)=\mathcal{F}^{-1} p' \rightarrow \lambda [K^W_{w_m',w_n'} (p_n-p', \delta x)]=
\frac{1}{2\pi \sqrt{\hbar w_{m'}}} \exp \left(-\frac{\delta x^2}{2w_{m'}} - \lambda \left(\frac{w_{m'}^2}{\hbar} + \frac{2ip_n \hbar}{\lambda} \right) \right)
\] (F26)

is the partially Fourier-transformed kernel \( K^W_{w_m',w_n'} \) (see Eq. (27)).

Recall that the squeezed coherent states have the form
\[
\langle x| p_k, x_k \rangle = \prod_{n=1}^{N} \chi_{k,n}(x_n),
\]
\[
\chi_{k,n}(x_n) = \prod_{n=1}^{N} \frac{1}{\sqrt{\pi w_n}} e^{-\left(\frac{x_n - \bar{x}_{k,n}}{2w_n}\right)^2} \hat{p}_{k,n}(x_n - \bar{x}_{k,n}).
\] (F27)

Using this definition and with the help of the substitutions \( y = x - \frac{\lambda}{2}, z = x + \frac{\lambda}{2} \), Eq. (F25) can be reshaped as
\[
I^H_{p_n, \xi}(p_n, x_n) = \int_{-\infty}^{\infty} \chi_{k,1}(y)V_n(y) I^{(1)}_{k,2,n}(y, p_n, x_n) \, dy,
\] (F29)

and
\[
I^{(1)}_{k,2,n}(y, p_n, x_n) = \int_{-\infty}^{\infty} \tilde{K}^W_{w_m',w_n'}(z-y, \frac{\xi}{\sqrt{\hbar}}) \, dz.
\] (F30)

The last integral is of a general form
\[
C_0 \int_{-\infty}^{\infty} e^{-A_0 z^2 + B_0 z} \, d\lambda = \pi C_0 \text{erf} \left( \frac{B_0}{\sqrt{2A_0}} \right),
\]
where, in our case,
\[
C_0 = \frac{C_1}{\sqrt{\pi}} e^{-A_1 y^2 + B_1 y}, \quad A_1 = \frac{1}{2} \left( \frac{1}{w_n} + \frac{1}{w_{m'}} \right),
\]
\[
B_1 = \frac{ip_n}{\hbar} + \frac{2k_{2,n}}{w_n} + \frac{2ip_{2,n}}{\lambda w_n},
\]
\[
C_1 = \frac{\exp \left(-\frac{x^2}{2w_n^2} + \frac{4}{\lambda} \frac{2k_{2,n}}{w_n} + \frac{2i}{\hbar} \frac{ip_{2,n}}{\lambda} \right)}{2\pi \sqrt{\hbar w_n}},
\]
\[
A_0 = \frac{1}{\sqrt{2}} \left( \frac{4}{w_n} + \frac{4w_{m'}^2}{w_n} + \frac{\lambda}{\hbar} \right), \quad B_0 = B_{0,1} y + B_{0,2},
\]
\[
B_{0,1} = -\frac{1}{2w_n} - \frac{1}{2w_{m'}^2}, \quad B_{0,2} = \frac{i}{\hbar} \frac{p_n - p_{2,n}}{w_n} + \frac{x_{2,n}}{2w_{m'}^2}.
\]

Thus,
\[
I^{(1)}_{k,2,n}(y, p_n, x_n) = C_1 e^{-A_1 y^2 + B_1 y} \text{erfi}(B_2 y + C_2),
\]
(F32)

where \( B_2 = \frac{B_{0,1}}{2w_n}, C_2 = \frac{B_{0,2}}{2w_n}, \) and \( \text{erfi}(z) = \frac{\exp(i x)}{i} \).

Assume that the potential \( V_n(y) \) can be cast as a sum
\[
V_n(y) = \sum_k v_{n,k},
\]
(F33)

where each term \( v_{n,k} \) has the following generic form
\[
v_{n,k}(y) = c_{r(k)}(y) v^r_1(y) y^2 + v_2(y)
\]
(F34)

with non-negative integers \( r \) and some constants \( c_r, v_1 \) and \( v_2 \). In this case, the integral (F29) is expandable as
\[
I_{\xi}^{(0)}(p_n, x_n) = \sum_k c_{r(k)} I_{\xi, k}^{(0)}(p_n, x_n),
\]
(F35)

where each \( I_{\xi, k}^{(0)}(p_n, x_n) \) is of the form
\[
I_{\xi, k}^{(0)}(p_n, x_n) = \int_{-\infty}^{\infty} \chi_{k,1}(y) y^r e^{a y^2 + b y} \chi_{k,2,n}(y, p_n, x_n) \, dy =
\]
\[
C_I \int_{-\infty}^{\infty} y^r e^{-\alpha y^2 + \beta y} \text{erfi}(B_2 y + C_2) \, dy =
\]
\[
-ic_I \sqrt{2\pi} e^{-\frac{\pi}{\beta^2}} I^{(2)}(\beta, \sqrt{2\pi} - iC_2, \beta, \sqrt{2\pi}),
\]
(F36)

Here
\[
\alpha = \frac{1}{\lambda} A_1 + A_2, \quad \beta = \frac{ip_n}{\hbar} + \frac{w_{m'}}{w_n} + B_1 + v_1,
\]
\[
C_4 = C_1 e^{\frac{i k_{1,n}}{\sqrt{\hbar}} (\frac{4}{w_n} + \frac{4w_{m'}^2}{w_n} + \frac{\lambda}{\hbar})},
\]
and
\[
I^{(2)}(a, b, \mu) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} x^r e^{-\frac{x^2}{2} + \mu x} \text{erf}(ax+b) \, dx =
\]
\[
P_r(\mu) e^{\frac{\mu^2}{2a}} \text{erf} \left( \frac{\mu + b}{\sqrt{2\pi a}} \right) + Q_r(\mu) e^{\frac{\mu^2}{2a}} \frac{e^{-\frac{\lambda^2}{2\hbar^2}}}{\lambda},
\]
(F37)

where the polynomials \( P_r(\mu) \) and \( Q_r(\mu) \) are defined recursively as
\[
P_0(\mu) = 1, \quad Q_0(\mu) = 0,
\]
\[
P_{r+1}(\mu) = \frac{\partial P_r(\mu)}{\partial \mu} + \mu P_r(\mu),
\]
\[
Q_{r+1}(\mu) = \frac{\partial Q_r(\mu)}{\partial \mu} + \frac{2a P_r(\mu)}{\sqrt{\pi(2a^2 + 1)}}.
\]

4. **Remark on multidimensional computations**

The outlined procedures for computing the components of \( \mathbf{p}_{\text{reg}}^{H^p}, \mathbf{J}_{\mathbf{x}}^{H^p} \) and \( \delta \mathbf{J}_{H^p}^{H^p} \) are applicable to both one- and multidimensional systems. The numerical complexities scale linearly with the number of dimensions. However, the described algorithm for computing the “default” Husimi momentum flow (given by the first of Eqs. (B5)), where \( J^W_p \) is defined by Eq. (A7) is effective only for one-dimensional systems, and its direct extension to multidimensional systems (apart from the special cases of harmonic and separable potentials (F19)) is prohibitively computationally expensive. Here we demonstrate the feasibility of the approximation
\[
\mathbf{J}_{\mathbf{p}}^{H^p}(\mathbf{p}, \mathbf{x}) \approx - \Re \left[ \hat{G}_{w_{m'},w_n'} \left( \frac{1}{2\pi \hbar^2} \right) \int f_{-\infty}^{\infty} d\lambda N \times \right.
\]
\[
\langle \psi | \mathbf{x} - \frac{\lambda}{2} \rangle \langle \psi | x + \frac{\lambda}{2} | \partial H \partial \mathbf{p} | \psi \rangle e^{-i \frac{\mathbf{p}^2}{2\hbar}} \left] \right.,
\]
(F38)

applicable to the case of a pure quantum state $|\psi\rangle$. Note that Eq. (F38) reduces to

$$J^H_p(p, x) \simeq \mathcal{R}[\langle p, x | \hat{\rho}_{\delta} \hat{H} | \psi \rangle | \langle p, x \rangle]$$

(F39)

in the case of the conventional “non-thermal” Husimi representation defined in Eq. (28). The procedures for computing right hand side of Eq. (F39) in a multidimensional case are well-developed [12]. Similarly, Eq. (F38) can be analytically evaluated for generic operators $\hat{O} = -\frac{\partial}{\partial x}$ of the form

$$\hat{O} = \sum_{k,s,r} \alpha_{k,s,r} \prod_{n=1}^{N} \hat{p}_{n}^{k} \hat{x}_{n}^{s} e^{C_{2,k,n} \hat{x}_{n}^{2} + C_{1,k,n} \hat{x}_{n}},$$

(F40)

where $\alpha_{k,s,r}, C_{1,k,n} \in \mathbb{C}$ and $C_{2,k,n} \in \mathbb{R}$ are some coefficients. Using the expansion similar to (F20), the only non-trivial part of evaluating Eq. (F38) is the calculation of an one-dimensional integrals of the form

$$\hat{O} \hat{w}_{\rho, \omega} \left( \frac{1}{2\pi F} \int_{-\infty}^{\infty} \hat{\lambda} e^{-i \hat{\lambda}} \times \langle \hat{p}_{1}, \hat{x}_{1} \mid x_{1} - \frac{\lambda}{2} \rangle \langle x_{1} + \frac{\lambda}{2} \rangle \hat{p}_{2}^{i} \hat{x}_{2}^{i} e^{C_{2,k,n} \hat{x}_{n}^{2} + C_{1,k,n} \hat{x}_{n}} \mid \hat{p}_{2}, \hat{x}_{2} \rangle \right).$$

(F41)

In the following, it will be helpful to explicitly introduce the width parameter into the notation (F27) for the squeezed coherent states

$$|\hat{p}, \hat{x} \rangle \equiv |\hat{p}, \hat{x}, \omega \rangle$$

(F42)

One can check that the following relation holds:

$$e^{C_{2,k,n} \hat{x}_{n}^{2} + C_{1,k,n} \hat{x}_{n}} |\hat{p}, \hat{x}, \omega \rangle \equiv e^{\epsilon} |\hat{p}', \hat{x}', \omega' \rangle,$$

(F43)

where

$$\epsilon = \exp \left( -\frac{\omega^{2} \left(2p \hat{p}_{2} + N_{c} \hat{n} \right) + \omega \left( \hat{n} + 3 \hat{c}_{1} \hat{c}_{1} \right)}{2 \left(2\omega^{2} + 2\omega \right)} \right),$$

$$\hat{p}' = \hat{p} + \alpha \hat{c}_{1}, \quad \hat{x}' = \frac{\hat{x} e^{\omega^{2} \hat{p} \hat{p}_{2} + N_{c} \hat{n}}}{1 - 2\omega^{2} \hat{p} \hat{p}_{2} + N_{c} \hat{n}}, \quad \omega' = \frac{\omega}{\sqrt{1 - 2\omega^{2} \hat{p} \hat{p}_{2} + N_{c} \hat{n}}}.$$

Using the relation (F42), we can reduce the integrals in Eq. (F41) to the evaluation of the following generic term:

$$\hat{O} \hat{w}_{\rho, \omega} \left( \frac{1}{2\pi F} \int_{-\infty}^{\infty} \hat{\lambda} e^{-i \hat{\lambda}} \times \langle \hat{p}_{1}, \hat{x}_{1}, \hat{w}_{1} \mid x_{1} - \frac{\lambda}{2} \rangle \langle x_{1} + \frac{\lambda}{2} \rangle \hat{p}_{2} \hat{x}_{2} \rangle \right).$$

(F44)

Further simplifications can be done by using the equality

$$\hat{p} |\hat{p}, \hat{x}, \omega \rangle = (i \frac{\omega}{\alpha} (x-\hat{\omega}) + \hat{p}) |\hat{p}, \hat{x}, \omega \rangle$$

(F45)

and the canonical commutation relations between position and momentum operators, which allow to rewrite Eq. (F44) as the sum of terms like

$$I^{(4)} = \hat{O} \hat{w}_{\rho, \omega} \left( \frac{1}{2\pi F} \int_{-\infty}^{\infty} \hat{\lambda} e^{-i \hat{\lambda}} \times \langle \hat{p}_{1}, \hat{x}_{1}, \hat{w}_{1} \mid x_{1} - \frac{\lambda}{2} \rangle \langle x_{1} + \frac{\lambda}{2} \rangle \hat{p}_{2} \hat{x}_{2} \rangle \right).$$

(F46)

The latter allow for analytical integration

$$I^{(4)} = \frac{1}{2\pi F} \sqrt{\frac{1}{w_{1} w_{2} w_{\rho} w_{\omega}}} C \bar{H}_{r} \left[ \frac{Z(p, x)}{2C} \right] \times e^{A(x-x)^{2} + B(p-p)^{2} + D(C(p-p))^{2} + (x-x)^{2}},$$

(G47)

where $H_{r}$ denote Hermite polynomials,

$$Z(p, x) = \left( \frac{w_{1}^{2}(2A(x-x)+C(p-p)) + iA(2B(p-p)+C(x-x)))}{w_{1}^{2} w_{2}^{2} + 1} + X \right)$$

(F48)

and the coefficients are

$$E = \frac{1}{2} \left( \frac{1}{w_{1}^{2} + 1 / w_{2}^{2} + 1 / w_{\rho}^{2}} \right), \quad F = \frac{\omega^{2} \left(2p \hat{p}_{2} + N_{c} \hat{n} \right) + \omega \left( \hat{n} + 3 \hat{c}_{1} \hat{c}_{1} \right)}{2 \left(2\omega^{2} + 2\omega \right)} + E,$$

$$A = -\left( \frac{\omega^{2} \left(2p \hat{p}_{2} + N_{c} \hat{n} \right) + \omega \left( \hat{n} + 3 \hat{c}_{1} \hat{c}_{1} \right)}{2 \left(2\omega^{2} + 2\omega \right)} \right), \quad B = -\frac{E}{2F w_{1}},$$

$$C = -\frac{iA}{2F w_{1} w_{2} w_{\rho} w_{\omega}}, \quad X = \frac{\hat{p}_{1} \hat{w}_{1} \hat{w}_{2} + \hat{w}_{1} \hat{w}_{2} \hat{p}_{2} + iA(\hat{x}_{1} - \hat{x}_{2})}{w_{1}^{2} w_{2}^{2}},$$

$$P = \frac{\omega^{2} \left(2p \hat{p}_{2} + N_{c} \hat{n} \right) + \omega \left( \hat{n} + 3 \hat{c}_{1} \hat{c}_{1} \right)}{2 \left(2\omega^{2} + 2\omega \right)} + \frac{E}{2F w_{1}},$$

$$D = \frac{1}{2} \left( \frac{\hat{p}_{1} \hat{x}_{1} - \hat{p}_{2} \hat{x}_{2} + P(\hat{x}_{1} - \hat{x}_{2}) - X(\hat{p}_{1} - \hat{p}_{2})}{2} \right).$$

Note that Eq. (F39) is exact for the case of a harmonic system. In the case of non-harmonic potentials, it can be regarded as a local harmonic approximation of the potential energy surface near the phase space point $(p, x)$. However, Fig. 5 demonstrates that this approximation remains viable even for manifestly anharmonic, rapidly varying potentials. We consider again the model from Fig. 3. We reproduce the solution computed using the exact regularized Bohmian gauge (blue curves) and repeat the same calculation using the approximate expression (F39) (red curves). One can see that the accuracies of both the methods are nearly identical up to $t \approx 7.5$; after that the exact and approximate solutions rapidly diverge due to an insufficient basis size.

**Appendix G: Numerical example: Computational details**

Here we detail the procedure for solving the time-dependent Schrödinger equation

$$\frac{d}{dt} |\psi\rangle = \frac{i}{\hbar} \hat{H} |\psi\rangle = 0,$$

(G1)

within the anzatz of time-dependent squeezed coherent states (46), which is used to obtain the results presented in Fig. 3 and Fig. 5. The problem of propagating $|\psi(t)\rangle$ reduces to determining the $L$ time-dependent parameters in the anzatz (46), such as amplitudes $\hat{a}_{k}(t)$, for which we do not provide analytical expressions. Let us collectively denote these parameters as $\hat{a}$. Then, the time derivative $\frac{d}{dt} |\psi\rangle$ in (G1) can be written as

$$\frac{d}{dt} |\psi\rangle = \sum_{k=1}^{L} \hat{a}_{k} \langle \psi_{k} \rangle + |\psi_{k}\rangle \langle \psi_{k} | \psi \rangle,$$

(G2)
where the shorthand notations $\dot{z}_k = \frac{d^2 z_k}{dt^2}$, $|\psi_{z_k}\rangle = \frac{\partial}{\partial z_k} |\psi\rangle$ are used, and $|\psi_t\rangle = \frac{\partial}{\partial t} |\psi\rangle$ denotes the partial time derivative over all parameters other than $z(t)$. Similarly to the CCS approach [12], we determine $\dot{z}_k$ as the coefficients minimizing the regularized least-square approximation error

$$\langle r | r \rangle + \epsilon \dot{z}^T D \dot{z} \to \min |\dot{z}|.$$  

(G3)

where $D$ is the real diagonal $L \times L$ regularization matrix (chosen here to be equal to the identity matrix) and $\epsilon > 0$ is an empirically chosen small parameter. Assuming that all of the parameters $z$ are real \(^9\) and using the notations (G2), the solution of extremal problem (G3) can be written as

$$\dot{z} = A^{-1} b,$$  

(G4)

where $A$ and $b$ are the $L \times L$ real matrix and the $L$-dimensional real vector with entries

$$A_{i,j} = \Re \langle \psi_{z_j} | \psi_{z_i} \rangle + \epsilon D_{i,j},$$  

(G5)

$$b_{j} = \Re \langle \tilde{z}_{i} | \tilde{H} | \psi_{z_j} \rangle \langle \psi_{z_j} | \psi_{i} \rangle.$$  

(G6)

The role of the regularization matrix $D$ is twofold. First, it guarantees that $A > 0$ and, hence, is invertible for any $\epsilon > 0$. Second, it introduces a bias for solutions minimizing norms $|\dot{z}_k|$ in degenerate cases. The latter feature is especially useful when $z$ are slow-varying parameters. The empirical constant $\epsilon$ should be chosen large enough to provide an effective regularization, but small enough not to influence the computational accuracy.

The specific definitions of parameters $z$ are identical for both the CCS and phase-space-flows-based computations. Namely, $z = \{b_1, \ldots, b_N, \varphi_1, \ldots, \varphi_N\}$, where real parameters $b_k$ and $\varphi_k$ are the amplitude and “slow” phase of the complex amplitudes $\tilde{z}_k$:

$$\tilde{a}_k(t) = \tilde{b}_k(t)e^{i(\varphi_k(t) + \dot{\varphi}_k(t))}.$$  

(G7)

Here the “fast” phase $\varphi_k(t)$ is defined following the standard practice (see, e.g., Ref. [21]) by initial condition $\varphi_k(0)=0$ and the evolution equation

$$\frac{d}{dt} \varphi_k(t) = \frac{1}{2} \langle \tilde{p}_k \cdot \dot{\tilde{x}}_k - \langle \tilde{p}_k, \tilde{x}_k \rangle \tilde{H} | \tilde{p}_k, \tilde{x}_k \rangle \rangle.$$  

In all the simulations (except for CCS) we utilized the generalized (“thermal”) Husimi transform by modifying Eq. (28) as

$$Q(p,x) = \frac{\hat{G}_0}{\hat{G}_1} \alpha \hat{G}_2 P(p,x)$$  

(G8)

using the scaling factor $\alpha = 1.1$. The initial wavefunction $\psi(t=0)$ was expanded to 21 basis squeezed coherent states with $\tilde{w}_k = 1$. The expansion coefficients at $t=0$ are summarized in Table I.

The source code used to produce all the numerical examples can be found in Ref. [72].

\(^9\) Complex parameters can be included, e.g. by representing them in the polar form and treating the amplitude and phase as two new real parameters.

\begin{table}[h]
\centering
\begin{tabular}{cccc}
$k$ & $\tilde{a}_k$ & arg($\tilde{a}_k$) & $\tilde{x}_k$ \\
0 & 0.421935 & -1.52358 & -2 -2.05 \\
1 & 0.160277 & -0.75583 & -2 -1.69 \\
2 & 0.16441 & -0.23255 & 0 -1.93 \\
3 & 0.326508 & 0.48842 & 0 -1.57 \\
4 & 0.227026 & 2.76771 & 2 -1.81 \\
5 & 0.0897529 & 1.74287 & 2 -1.45 \\
6 & 0.363191 & 2.77319 & -2 -2.35 \\
7 & 0.426131 & -0.36959 & 0 -2.25 \\
8 & 0.268861 & 0.0324824 & 2 -2.15 \\
9 & 0.151384 & -2.35028 & -2 -6.08333 \\
10 & 0.201003 & 2.18152 & -2 -5.08333 \\
11 & 1.09911 & -0.950581 & -2 -4.08333 \\
12 & 0.159998 & 2.25803 & -2 -3.08333 \\
13 & 1.09394 & 0.37624 & 0 -5.75 \\
14 & 3.92821 & -0.214463 & 0 -4.75 \\
15 & 6.64557 & 0.282041 & 0 -3.75 \\
16 & 1.75203 & -0.368937 & 0 -2.75 \\
17 & 0.391672 & -0.246873 & 2 -5.41667 \\
18 & 0.0519809 & 1.89087 & 2 -4.41667 \\
19 & 0.925349 & -1.1339 & 2 -3.41667 \\
20 & 0.593327 & 2.0164 & 2 -2.41667 \\
\end{tabular}
\caption{The initial expansion coefficients for representing the wavefunction $\psi(t=0)$ in the anzats of 21 squeezed coherent states.}
\end{table}
[1] J. Weinbub and D. K. Ferry, Recent advances in wigner function approaches, Appl. Phys. Rev. 5, 041104 (2018).
[2] B. Larder, D. O. Gericke, S. Richardson, P. Maebey, T. G. White, and G. Gregori, Fast nonadiabatic dynamics of many-body quantum systems, Science Advances 5, eaaw1634 (2019).
[3] R. C. Brown and E. J. Heller, Classical trajectory approach to photodissociation: The wigner method, J. Chem. Phys. 75, 186 (1981).
[4] W. H. Miller, The semiclassical initial value representation: a potentially practical way for adding quantum effects to classical molecular dynamics simulations, J. Phys. Chem. A 105, 2942 (2001).
[5] R. Saha and M. Ovchinnikov, Herman-kluk semiclassical dynamics in action-angle representation: New approaches to mapping quantum degrees of freedom, J. Chem. Phys. 124, 204112 (2006).
[6] E. Pollak, The semiclassical initial value series representation of the quantum propagator, in Quantum Dynamics of Complex Molecular Systems, Springer Series in Chemical Physics, edited by D. D. A. Micha and D. I. Burghardt (Springer Berlin Heidelberg, 2007) pp. 259–271.
[7] T. J. H. Hele, M. J. Willatt, A. Muolo, and S. C. Althorpe, Boltzmann-conserving classical dynamics in quantum time-correlation functions: matsuabra dynamics, J. Chem. Phys. 142, 134103 (2015).
[8] B. Berg, L. I. Plimak, A. Polkovnikov, M. K. Olsen, M. Fleischhauer, and W. P. Schleich, Commuting heisenberg operators as the quantum response problem: Time-normal averages in the truncated wigner representation, Phys. Rev. A 80, 033624 (2009).
[9] M. Vacher, M. J. Bearpark, and M. A. Robb, Direct methods for non-adiabatic dynamics: connecting the single-set variational multi-configuration gaussian (vmcg) and ehrenfest perspectives, Theor Chem Acc 135, 187 (2016).
[10] A. Donoso and C. C. Martens, Quantum tunneling using entangled classical trajectories, Phys. Rev. Lett. 87, 223202 (2001).
[11] H. Lpez, C. C. Martens, and A. Donoso, Entangled trajectory dynamics in the husimi representation, J. Chem. Phys. 125, 154111 (2006).
[12] D. V. Shalashilin and I. Burghardt, Gaussian-based techniques for quantum propagation from the time-dependent variational principle: Formulation in terms of trajectories of coupled classical and quantum variables, J. Chem. Phys. 129, 084104 (2008).
[13] M. Foss-Feig, P. Niumfa, J. T. Young, M. Hafezi, A. V. Gorshkov, R. M. Wilson, and M. F. Magrebi, Emergent equilibrium in many-body optical bistability, Phys. Rev. A 95, 043826 (2017).
[14] C. V. Chiana and M. K. Olsen, Quantum phase-space analysis of population equilibration in multiwell ultracold atomic systems, Phys. Rev. A 84, 043636 (2011).
[15] S. P. Cockburn, A. Negretti, N. P. Proukakis, and C. Henkel, Comparison between microscopic methods for finite-temperature boson gases, Phys. Rev. A 83, 043619 (2011).
[16] G. Kordas, D. Wihhaut, P. Buonan, A. Vezzani, R. Burioni, A. I. Kuranikas, and S. Wimberger, The dissipative bose-hubbard model, Eur. Phys. J. Spec. Top. 224, 2127 (2015).
[17] P. Carruthers and F. Zachariasen, Quantum collision theory with phase-space distributions, Rev. Mod. Phys. 55, 245285 (1983).
[18] S. Mai, M. Pollum, L. Martinez-Fernandez, N. Dunn, P. Marquetand, I. Corral, C. E. Crespo-Hernandez, and L. Gonzalez, The origin of efficient triplet state population in sulfur-substituted nucleobases, Nat. Commun. 7, 13077 (2016).
[19] L. Orr, L. Hernández de la Peña, and P.-N. Roy, Formulation of state projected centroid molecular dynamics: Microcanonical ensemble and connection to the wigner distribution, J. Chem. Phys. 146, 214116 (2017).
[20] L. Bonnet, Classical dynamics of chemical reactions in a quantum spirit, Int. Rev. Phys. Chem. 32, 171 (2013).
[21] D. V. Makhov, C. Symonds, S. Fernandez-Alberti, and D. V. Shalashilin, Ab initio quantum direct dynamics simulations of ultrafast photochemistry with multiconfigurational ehrenfest approach, Chem. Phys. 493, 200 (2017).
[22] R. F. O’Connell, Wigner distribution function approach to dissipative problems in quantum mechanics with emphasis on decoherence and measurement theory, J. Opt. B: Quantum Semiclass. Opt. 5, S349 (2003).
[23] C. K. Zachos, D. B. Fairlie, and T. L. Curtright, Quantum Mechanics in Phase Space. An Overview with Selected Papers (World Scientific, 2005).
[24] E. Wigner, On the quantum correction for thermodynamic equilibrium, Phys. Rev. 40, 749 (1932).
[25] R. L. Stratonovich, On distributions in representation space, Sov. Phys.-JETP (J. Exp. Theor. Phys.) 4, 891 (1957).
[26] K. Husimi, Some formal properties of the density matrix, Proc. Phys. Math. Soc. Jpn. 22, 264 (1940).
[27] E. Madelung, Quantentheorie in hydrodynamischer form, Z. Phys. 40, 322 (1927).
[28] G. Bacciagaluppi and A. Valentini, Quantum theory at the crossroads: Reconsidering the 1927 Solvay conference (Cambridge University Press, 2009).
[29] T. L. Curtright, D. B. Fairlie, and C. K. Zachos, A concise treatise on quantum mechanics in phase space (World Scientific Publishing Company, 2013).
[30] G. G. Rozenman, M. Zimmermann, M. A. Efremov, W. P. Schleich, L. Shemer, and A. Arie, Amplitude and phase of wave packets in a linear potential, Phys. Rev. Lett. 122, 124302 (2019).
[31] D. Dragoman and M. Dragoman, Quantum-classical analogies (Springer Science & Business Media, 2013).
[32] M. Veronez and M. A. M. d. Aguilar, Phase space flow in the husimi representation, J. Phys. A: Math. Theor. 46, 485304 (2013).
[33] D. Kakofengitis, M. Oliva, and O. Steuernagel, Wigners representation of quantum mechanics in integral form and its
applications, Phys. Rev. A 95, 022127 (2017).
[34] R. T. Skodje, H. W. Rohrs, and J. VanBuskirk, Flux analysis, the correspondence principle, and the structure of quantum phase space, Phys. Rev. A 40, 2894 (1989).
[35] E. Colomés, Z. Zhan, and X. Oriols, Comparing wigner, husimi and bohmian distributions: which one is a true probability distribution in phase space?, J. Comput. Electron. 14, 894 (2015).
[36] B. J. Hiley, On the relationship between the wigner-moyal and bohm approaches to quantum mechanics: A step to a more general theory?, Found. Phys. 40, 356 (2010).
[37] H. J. Groenewold, On the principles of elementary quantum mechanics, Physica 12, 405 (1946).
[38] M. S. Bartlett and J. E. Moyal, The exact transition probabilities of quantum-mechanical oscillators calculated by the phase-space method, Math. Proc. Camb. Philos. Soc. 45, 545 (1949).
[39] R. F. O'Connell and E. P. Wigner, Quantum-mechanical distribution functions: conditions for uniqueness, Phys. Lett. A 83, 145 (1981).
[40] M. Hillery, R. F. O'Connell, M. O. Scully, and E. P. Wigner, Distribution functions in physics: fundamentals, Phys. Rep. 106, 121167 (1984).
[41] C. Brif and A. Mann, A general theory of phase-space quasiprobability distributions, J. Phys. A: Math. Gen. 31, L9 (1998).
[42] B. Calden, Stratonovich-Weyl correspondence for discrete series representations, Arch. Math.(Brno) 47, 51 (2011).
[43] A. Polkovnikov, Phase space representation of quantum dynamics, Ann. Phys. (New York) 325, 1790 (2010).
[44] D. I. Bondar, R. Cabrera, R. R. Lombay, M. Y. Ivanov, and H. A. Rabitz, Operational dynamic modeling transcending quantum and classical mechanics, Phys. Rev. Lett. 109, 190403 (2012).
[45] D. V. Zhidanov and T. Seideman, Wigner representation of the rotational dynamics of rigid tops, Phys. Rev. A 92, 012129 (2015).
[46] L. Cohen, Generalized phase-space distribution functions, J. Math. Phys. 7, 781 (1966).
[47] D. I. Blokhintzev, The gibbs quantum ensemble and its connection with the classical ensemble, J. Phys. (USSR) 2, 71 (1940).
[48] L. Cohen, Time-frequency distributions – A review, Proc. IEEE 77, 941 (1989).
[49] A. Kossakowski, On quantum statistical mechanics of non-hamiltonian systems, Reports on Mathematical Physics 3, 247 (1972).
[50] G. Lindblad, On the generators of quantum dynamical semigroups, Comm. Math. Phys. 48, 119 (1976).
[51] T. F. Havel, Robust procedures for converting among lindblad, kraus and matrix representations of quantum dynamical semigroups, Journal of Mathematical Physics 44, 534 (2003).
[52] M. Oliva, D. Kakofengitis, and O. Steuernagel, Anharmonic quantum mechanical systems do not feature phase space trajectories, Physica A 502, 201 (2018).
[53] W. Ulmer and W. Kaisl, The inverse problem of a gaussian convolution and its application to the finite size of the measurement chambers/detectors in photon and proton dosimetry, Phys. Med. Biol. 48, 707 (2003).
[54] V. V. Dodonov and V. I. Manko, Phase space eigenfunctions of multidimensional quadratic hamiltonians, Physica A 137, 306 (1986).
[55] L. Wang, C. C. Martens, and Y. Zheng, Entangled trajectory molecular dynamics in multidimensional systems: Two-dimensional quantum tunneling through the eckart barrier, J. Chem. Phys. 137, 034113 (2012).
[56] B. Gu and S. Garashchuk, Quantum dynamics with gaussian bases defined by the quantum trajectories, J. Phys. Chem. A 120, 3023 (2016).
[57] S. Garashchuk and V. Rassolov, Quantum trajectory dynamics based on local approximations to the quantum potential and force, J. Chem. Theory Comput. 15, 3906 (2019).
[58] P. R. Holland, The Quantum Theory of Motion: An Account of the de Broglie-Bohm Causal Interpretation of Quantum Mechanics (Cambridge University Press, 1993).
[59] X. Oriols and M. J., eds., Applied Bohmian Mechanics: From Nanoscale Systems to Cosmology (PAN Stanford Publishing PTE LTD, 2012).
[60] A. Benseny, G. Albareda, n. S. Sanz, J. Mompart, and X. Oriols, Applied bohmian mechanics, Eur. Phys. J. D 68, 286 (2014).
[61] A. S. Sanz and S. Miret-Artés, A Trajectory Description of Quantum Processes. II. Applications: A Bohmian Perspective, Lecture Notes in Physics, Vol. 831 (Springer, 2013).
[62] R. E. Wyatt, C. L. Lopreore, and G. Parlant, Electronic transitions with quantum trajectories, J. Chem. Phys. 114, 5113 (2001).
[63] B. F. E. Curchod, U. Rothlisberger, and I. Tavernelli, Trajectory-based nonadiabatic dynamics with time-dependent density functional theory, ChemPhysChem 14, 1314 (2013).
[64] S. K. Min, F. Agostini, I. Tavernelli, and E. K. U. Gross, Ab initio nonadiabatic dynamics with coupled trajectories: A rigorous approach to quantum (de)coherence, J. Phys. Chem. Lett. 8, 3048 (2017).
[65] C. Efthymiopoulos, N. Delis, and G. Contopoulos, Wavepacket approach to particle diffraction by thin targets: Quantum trajectories and arrival times, Ann. Phys. (N. Y.) 327, 438 (2012).
[66] D. Dürr, S. Goldstein, and N. Zangh, Quantum equilibrium and the role of operators as observables in quantum theory, J. Stat. Phys. 116, 959 (2004).
[67] P. A. Milewski, C. A. Galano-Rios, A. Nachbin, and J. W. M. Bush, Faraday pilot-wave dynamics: modelling and computation, Journal of Fluid Mechanics 778, 361 (2015).
[68] R. Cabrera, D. I. Bondar, K. Jacobs, and H. A. Rabitz, Efficient method to generate time evolution of the wigner function
for open quantum systems, Phys. Rev. A 92, 042122 (2015).

[69] D. I. Bondar, A. G. Campos, R. Cabrera, and H. A. Rabitz, Efficient computations of quantum canonical gibbs state in phase space, Phys. Rev. E 93, 063304 (2016).

[70] A. Wang, Y. Zheng, C. C. Martens, and W. Ren, Quantum tunneling dynamics using entangled trajectories: general potentials, Phys. Chem. Chem. Phys. 11, 1588 (2009).

[71] R. Kosloff and D. Kosloff, A Fourier method solution for the time dependent Schrödinger equation: A study of the reaction \( H^+ + H_2, D^+ + HD, \) and \( D^+ + H_2 \), J. Chem. Phys. 79, 1823 (1983).

[72] The source code for the numerical example can be found at https://bitbucket.org/dmzhdanov/objectmce.

[73] O. Steuernagel, D. Kakofengitis, and G. Ritter, Wigner flow reveals topological order in quantum phase space dynamics, Physical Review Letters 110, 030401 (2013).

[74] D. J. Mason, M. F. Borunda, and E. J. Heller, Quantum flux and reverse engineering of quantum wave functions, EPL 102, 60005 (2013).

[75] I. Burghardt, H.-D. Meyer, and L. S. Cederbaum, Approaches to the approximate treatment of complex molecular systems by the multiconfiguration time-dependent hartree method, J. Chem. Phys. 111, 2927 (1999).

[76] H.-D. Meyer, F. Gatti, and G. A. Worth, Multidimensional quantum dynamics: MCTDH theory and applications (John Wiley & Sons, 2009).

[77] P. Rojas, R. Blaser, Y. M. Sua, and K. F. Lee, Optical phase-space-time-frequency tomography, Opt. Express 19, 7480 (2011).

[78] T. M. Coffey, R. E. Wyatt, and W. C. Schieve, Quantum trajectories from kinematic considerations, J. Phys. A: Math. Theor. 43, 335301 (2010).

[79] T. M. Coffey, R. E. Wyatt, and W. C. Schieve, Reconstruction of the time-dependent wave function exclusively from position data, Phys. Rev. Lett. 107, 230403 (2011).

[80] R. Penrose, The road to reality: A complete guide to the laws of the universe (Vintage, London, 2005).

[81] A. J. Leggett, The quantum measurement problem, Science 307, 871 (2005).

[82] D. I. Bondar, F. Gay-Balmaz, and C. Tronci, Koopman wavefunctions and classical-quantum correlation dynamics, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 475, 20180879 (2019).

[83] F. Gay-Balmaz and C. Tronci, Madelung transform and probability densities in hybrid classical-quantum dynamics, arXiv:1907.06624 [math-ph, physics:quant-ph] (2019).

[84] A. Venugopalan and R. Ghosh, Wigner-function description of quantum-mechanical nonlocality, Phys. Rev. A 44, 6109 (1991).