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Anharmonic quantum mechanical systems do not feature phase space trajectories

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Abstract

Phase space dynamics in classical mechanics is described by transport along trajectories. Anharmonic quantum mechanical systems do not allow for a trajectory-based description of their phase space dynamics. This invalidates some approaches to quantum phase space studies. We first demonstrate the absence of trajectories in general terms. We then give an explicit proof for all quantum phase space distributions with negative values: we show that the generation of coherences in anharmonic quantum mechanical systems is responsible for the occurrence of singularities in their phase space velocity fields, and vice versa. This explains numerical problems repeatedly reported in the literature, and provides deeper insight into the nature of quantum phase space dynamics.

1. Introduction and Motivation

The phase space dynamics of classical conservative mechanical systems is described by the transport equations of Hamiltonian flow, along trajectories. For quantum mechanical systems this is only true for harmonic potentials, anharmonic quantum mechanical systems do not transport quantum phase space distributions along trajectories.

This important fact is not appreciated by all: a number of incorrect schemes to model quantum dynamics using phase space trajectories have been devised [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16], leading to confusion [17, 18, 19, 20, 21, 22, 23, 24]. The schemes' failures have, in some quarters, given phase space

representations of quantum mechanics an undeservedly poor standing [25].

Here we revisit the basic features of quantum dynamics in phase space [26, 27, 28] in order to identify concepts of classical dynamics that cannot be applied to quantum systems (recent reviews on quantum-classical methods can be found in [29, 30, 31]). Our analysis deepens our understanding of the behaviour of quantum dynamics in phase space. We show how the generation of quantum coherences renders quantum dynamics in phase space very different from classical dynamics.

In Section 2 we explain how phase space trajectories arise from solutions of first order differential equations as integral curves describing the transport of a density distribution.

In Section 3, we emphasize that quantum phase space-based studies [see 26, 28, 27] of quantum dynamics are no more involved than methods using von Neumann's equation to propagate the density matrix.

Section 4 emphasizes that a priori it is not clear whether quantum dynamics can be described using trajectories.

In Section 5 we show that anharmonic systems are described by evolution equations which are higher order differential equations, these generally do not permit a trajectory description but create quantum coherences; we additionally emphasize that harmonic systems cannot generate quantum coherences.

We explicitly prove in Section 6 that quantum phase space distributions with negative values (such as Wigner's distribution) cannot feature trajectories because the quantum analog of Hamilton's phase space velocity field becomes singular. We show why such singularities are *needed* to create quantum coherences.

The singularities affect numerical performance badly, see references [32], in Section 7 we explain why, using a simple toy system.

Several misconceptions and incorrect conclusions drawn from ill-fated applications of the trajectory concept are reported in the literature. Some are examined in Section 8 in order to explain how they fail and to further illuminate differences between classical and quantum dynamics; before we conclude.

2. Continuity equation, trajectories, classical phase space flow and Liouville's theorem

The transport of a density $\rho(\boldsymbol{r},t)$, where the initial density $\rho(\boldsymbol{r},0)$ and its current $\boldsymbol{j}$ encode the boundary conditions, is governed by a continuity equation

$$\partial_t \rho(\boldsymbol{r},t) + \boldsymbol{\nabla}\cdot\boldsymbol{j}(\boldsymbol{r},t) = 0\ . \tag{1}$$

Here we write $\frac{\partial}{\partial t} = \partial_t$, $\boldsymbol{r} = \binom{\boldsymbol{x}}{\boldsymbol{p}}$ parametrizes locations in phase space and $\boldsymbol{\nabla} = \binom{\partial_{\boldsymbol{x}}}{\partial_{\boldsymbol{p}}}$; we denote vectors in bold face, and '$\cdot$' stands for scalar product.

A time-dependent solution for ρ of the Eulerian type (integrated over a time-differential dt while keeping the position $\boldsymbol{r}$ fixed), is of the form

$$\rho(\boldsymbol{r},t+dt) = \ \rho(\boldsymbol{r},t) - dt\ \boldsymbol{\nabla}\cdot\boldsymbol{j}. \tag{2}$$

From a fluid dynamics perspective, the Eulerian approach tends to be in *conservation form* and its solutions therefore well behaved numerically.

2.1. Trajectories through Lagrangian decomposition

If the current factorizes as

$$\boldsymbol{j}(\boldsymbol{r},t) = \rho(\boldsymbol{r},t)\boldsymbol{v}(\boldsymbol{r},t), \tag{3}$$

where $\boldsymbol{v}$ is the velocity field, the continuity equation (1) can be rewritten in Lagrangian decomposition [33, 13, 12]

$$\frac{d}{dt}\rho = \partial_t\rho + \boldsymbol{v}\cdot\boldsymbol{\nabla}\rho = -\rho\boldsymbol{\nabla}\cdot\boldsymbol{v}\ . \tag{4}$$

If equation (4) is of first order in the derivatives, linear in ρ, and all quantities are mathematically well behaved, its solution allows for a trajectory-based description, in Lagrangian (or co-moving) transport form [12, 13]

$$\rho(\boldsymbol{r}_t,t) = e^{-\int_0^t d\tau \boldsymbol{\nabla}\cdot\boldsymbol{v}(\boldsymbol{r}_\tau,\tau)}\ \rho(\boldsymbol{r}_0,0)\ , \tag{5}$$

where *trajectories* are functions $\boldsymbol{r}_t$, parameterized by time t, arising through integration of $\boldsymbol{v}$ starting from $\boldsymbol{r}_0$

$$\boldsymbol{r}_t(\boldsymbol{r}_0) = \boldsymbol{r}_0 + \int_0^t d\tau\ \boldsymbol{v}(\boldsymbol{r}_\tau,\tau). \tag{6}$$

Trajectories are integral curves describing the transport of a density distribution.

From a fluid dynamics perspective, the Lagrangian approach tends not to be in conservation form and its solutions therefore poorly behaved numerically.

From a mathematical perspective, solution (5) is found using the method of characteristics (also known as Lagrange-Charpit method) which requires the governing equation (4) to be of first order in its derivatives of ρ. For example, diffusion equations are of second order and do not admit trajectory-based solutions.

2.2. Liouvillian flow in conservative classical mechanical systems

The natural setting for the dynamics of a mechanical particle is its phase space [34]. In this work we discuss a particle with mass M moving in one dimension x only. The associated two-dimensional phase space is parameterised by vectors $\boldsymbol{r} = \binom{x}{p}$, subject to a conservative hamiltonian $H = p^2/(2M) + V(x)$. In this case, the particle's phase space velocity

$$\boldsymbol{v}(\boldsymbol{r}) = \frac{d}{dt}\boldsymbol{r}_t = \begin{pmatrix} p/M \\ -\partial_x V(x) \end{pmatrix}, \tag{7}$$

encapsulates Newton's laws, and features volume preserving or 'Liouvillian' dynamics: $\boldsymbol{\nabla} \cdot \boldsymbol{v} = 0$. As a function of $\boldsymbol{r}$ only, $\boldsymbol{v}$ is independent of time t and state $\rho(\boldsymbol{r}, t)$.

The Liouvillian nature of classical Hamiltonian current implies with $\boldsymbol{\nabla} \cdot \boldsymbol{j} = \boldsymbol{v} \cdot \boldsymbol{\nabla}\rho$, that the total derivative (4) is zero: the value of ρ, while the dynamics sweeps it along its trajectories, stays constant $\rho(\boldsymbol{r}_t(\boldsymbol{r}_0), t) = \rho(\boldsymbol{r}_0, 0)$. In this case, solution (5), viewed as the function $\rho(\boldsymbol{r}, t)$, through relabelling $\boldsymbol{r} = \boldsymbol{r}_t$, simplifies to the pull-back form

$$\rho(\boldsymbol{r}, t) = \rho\left(\boldsymbol{r} - \int_0^t d\tau\ \boldsymbol{v}(\boldsymbol{r}_\tau), 0\right). \tag{8}$$

2.3. A simple system with non-Liouvillian flow that features trajectories

A free particle slowed down by friction $\dot{p} = -\gamma p$ is a classical system violating Liouville's theorem. With $p_t = p_0\ e^{-\gamma t}$ and $x_t = x_0 + (1 - e^{-\gamma t})p_0/(m\gamma)$, Kramer's evolution equation $\partial_t \rho = [-p/m\partial_x + \gamma p \partial_p + \gamma]\rho$, where the diffusive

Brownian motion term has been neglected, yields the trajectories-based solution of transport form (5)

$$\rho(x,p,t) = \exp[\gamma t]\ \rho_0(x - \frac{p}{\gamma m}(e^{\gamma t} - 1), p\, e^{\gamma t})\ . \tag{9}$$

The coefficient function $\exp[\gamma t]$ keeps this distribution normalized while the dynamics shrinks volumes uniformly across phase space: $\boldsymbol{\nabla}\cdot\boldsymbol{v} = \boldsymbol{\nabla}\cdot(p/m, -\gamma p) = -\gamma$.

3. Wigner's quantum phase space distribution

Attempts to understand and numerically approximate quantum dynamics of anharmonic systems has frequently relied on the concept of phase space trajectories in a way unsuitable for this task [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]. This seems to be the reason for the fatigue expressed by fellow researchers who perceive the 'Wigner method' (and other phase space methods) as unsuitable for finding ways of reducing computational complexities [25].

We have not found a rigorous explanation for the supposed unsuitability of Wigner's representation of quantum mechanics. In the general case it is not justifiable since *"All calculation methods scale in proportion to the volume of phase space that the molecular encounter occupies. Therefore, phase space is a common denominator by which different methods of calculation can be compared and the feasibility of the calculation estimated."* [35]

Recent work shows that the propagation of the Wigner distribution is suitable for the study of quantum dynamics of anharmonic systems [36] and that its study provides new valuable insight [31].

A quantum state's density matrix $\varrho(x,x',t) = \langle x|\hat{\varrho}(t)|x'\rangle$, can equivalently be described by Wigner's phase space-based quantum distribution $W(x,p,t)$ [37, 38, 27, 39], both are based in spaces of equal dimension:

$$W_\varrho(x,p,t) \equiv \frac{1}{\pi\hbar}\int_{-\infty}^{\infty} dy\, e^{-\frac{2i}{\hbar}py}\langle x+y|\hat{\varrho}(t)|x-y\rangle\ . \tag{10}$$

W can numerically be generated quickly through fast Fourier transforms of ϱ.

W is real-valued (unlike ϱ), non-local (through y), and normalized $\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx\ dp\ W(x,p,t) = 1$.

Generally, the Wigner distribution has negative patches [40], like many other quantum phase space distributions [38], this will be important for part of our discussion, in Section 6.

Specifically, Wigner's distribution is set apart from other quantum phase space distributions [38] by the fact that only Wigner's simultaneously yields the correct projections in Schrödinger's position $\varrho(x,x,t) = \int_{-\infty}^{\infty} dp\ W(x,p,t)$ and momentum representation $\tilde{\varrho}(p,p,t) = \int_{-\infty}^{\infty} dx\ W(x,p,t)$, while maintaining its form (10) when evolved in time and giving the overlap between states in the simple form $|\langle\psi_a|\psi_b\rangle|^2 = 2\pi\hbar \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dp\ W_a\ W_b$. Finally, the Wigner distribution's averages and uncertainties evolve momentarily classically [41, 42]. W is considered the *"closest quantum analogue of the classical phase-space distribution"* [43].

For specificity we choose Wigner's distribution for our discussions of quantum phase space behaviour. Most of our results apply to other quantum phase space distributions as well; the proof in section 6 explicitly applies only to those [38] that have negative patches in phase space.

4. Trajectories in quantum systems

A priori it is not clear that one must not use trajectories for quantum phase space descriptions of anharmonic systems.

Heisenberg's uncertainty principle is at times interpreted to mean that quantum mechanics does not allow for a trajectory-based description. This interpretation is incorrect:

Phase space trajectories are a fruitful mathematical device for the description of quantum dynamics of a system if the potential is of the quadratic form (14). This statement applies to non-dissipative systems, even driven ones. For such systems the trajectory-description (8) (for W rather than ρ) applies. Using trajectories, which in this case follow the classical law (7), is in fact simpler and,

in this sense, even superior to the use of standard Schrödinger wave function propagators, see Takabayasi in Ref. [44] p. 352.

Bohm's representation of quantum theory uses configuration space trajectories [45, 46] and these have experimental relevance [47].

The concept of paths (unlike trajectories, paths do not have to conform with the equations of motion) has been fruitful in path-integral formalisms applied to configuration or phase space.

Semiclassical methods employ classical trajectories along which quantum objects are carried [48, 49, 50].

When trajectory techniques can be implemented for quantum dynamical phase space studies they permit us to launch large numbers of trajectories while allowing us to efficiently parallelize computer code [32, 13].

In what follows, we will, however, see that in anharmonic quantum systems the divergence of the velocity field in phase space is non-zero. One might still hope to describe the propagation of W in phase space by Eq. (5) [or Eq. (19)]. But it turns out that the divergence of the quantum mechanical velocity field in phase space is singular, see Section 6 and Fig. 2 (c). This cannot be avoided [51], and therefore we can explicitly prove, by contradiction, that trajectories do not exist globally for systems whose phase space distributions can develop areas with negative values, see Section 6.

5. Time evolution of the Wigner distribution

The time evolution of $W(x,p,t) = W(\boldsymbol{r},t)$ is given by the Eulerian continuity equation [37]

$$\partial_t W(\boldsymbol{r},t) = -\boldsymbol{\nabla}\cdot\boldsymbol{J}(\boldsymbol{r},t)\ . \tag{11}$$

Generally, the Wigner current $\boldsymbol{J}$ has an integral representation [37, 38, 52, 51], but for potentials $V(x)$ that can be Taylor-expanded, giving rise to finite forces only, $\boldsymbol{J}$ is of the Moyal-form [37, 53]

$$\boldsymbol{J} = \begin{pmatrix} J_x \\ J_p \end{pmatrix} = \boldsymbol{j} + \begin{pmatrix} 0 \\ -\sum\limits_{l=1}^{\infty} \frac{(i\hbar/2)^{2l}}{(2l+1)!}\partial_p^{2l} W \partial_x^{2l+1} V \end{pmatrix}. \tag{12}$$

Here, with $\boldsymbol{j} = W\boldsymbol{v}$, $\boldsymbol{J} - \boldsymbol{j}$ are the 'quantum-correction' terms.

Fieldlines of Wigner current are well defined and their depiction has helped to reveal the topological charge conservation of $\boldsymbol{J}$'s stagnation points [54, 55].

In analogy to the classical Euler solution (2), the integration of the continuity equation (11) yields

$$W(\boldsymbol{r}, t + dt) = W(\boldsymbol{r}, t) - dt\, \boldsymbol{\nabla} \cdot \boldsymbol{J}, \tag{13}$$

which is in conservation form.

5.1. Formation of coherences and negativities of the Wigner distribution

The primary difference between classical and quantum states is the ability of a quantum particle to form non-local coherences (to be present in both holes of a double slit [56, 48]). Precisely these nonlocal coherences in configuration space are revealed by the Wigner distribution's negative patches [56] in phase space, and vice versa [57, 43, 58]. Coherences or negative patches can only be generated in anharmonic systems. Harmonic systems (and their isomorphic partners [59]) are of the quadratic form

$$\hat{H}_{quadratic}(\hat{x}, \hat{p}) = \frac{\hat{p}^2}{2M} + \frac{K}{2}\hat{x}^2 + a\hat{x} + b \tag{14}$$

(here K, a and b are any real constants). They can feature negative patches of the Wigner distribution only if these are inserted into the initial condition, $W_0(\boldsymbol{r})$, but they cannot *generate* them, see Eq. (19) below.

6. Singularities in the velocity field are needed: trajectories are ill-defined

We now prove that the Lagrangian transport form is ill-defined in the quantum case. Following references [33, 13, 12] we rewrite continuity equation (11) for W in Lagrangian decomposition (4)

$$\frac{dW}{dt} = \partial_t W + \boldsymbol{w} \cdot \boldsymbol{\nabla} W = -W \boldsymbol{\nabla} \cdot \boldsymbol{w}\ . \tag{15}$$

Here, the quantum phase space velocity field $\boldsymbol{w}$ [33, 13, 12], corresponding to the hamiltonian velocity field $\boldsymbol{v}$, is

$$\boldsymbol{w} = \frac{\boldsymbol{J}}{W} = \boldsymbol{v} + \frac{1}{W} \begin{pmatrix} 0 \\ -\sum\limits_{l=1}^{\infty} \frac{(i\hbar/2)^{2l}}{(2l+1)!} \partial_p^{2l} W \partial_x^{2l+1} V \end{pmatrix} . \tag{16}$$

$\boldsymbol{w}$ is singular at zeros of W since, generally, zeros of W do not coincide with zeros of its derivatives [55].

For time-differentials dt, the formal solution of Eq. (15), written in pull-back form, like Eq. (8), has the transport form [12, 13]

$$W(\boldsymbol{r}, t + dt) = e^{-dt \boldsymbol{\nabla} \cdot \boldsymbol{w}} \; W(\boldsymbol{r} - dt \; \boldsymbol{w}, t) \; , \tag{17}$$

where the transport shift can be expressed via a translation using the convective operator $\boldsymbol{w} \cdot \boldsymbol{\nabla}$

$$W(\boldsymbol{r} - dt \; \boldsymbol{w}, t) = e^{-dt \; \boldsymbol{w} \cdot \boldsymbol{\nabla}} \left[W(\boldsymbol{r}, t) \right] \; . \tag{18}$$

We emphasize that the Lagrangian decomposition, although technically correct, splits up the well behaved expressions in the continuity equation (11) and in this way creates singularities in the evolution equation (15) and the exponents of its solution (17) and (18).

Following references [12, 13] we formally extend the integration in time for the transport form (17). To this end we temporarily assume that globally $W > 0$ in order to remove singularities in $\boldsymbol{w}$ in Eq. (16) and that, additionally, W and V are of such a form that $|\boldsymbol{\nabla} \cdot \boldsymbol{w}| < \infty$. We formally arrive at the integrated transport form [12, 13]

$$W(\boldsymbol{r}_t, t) = e^{-\int_0^t d\tau \boldsymbol{\nabla} \cdot \boldsymbol{w}(\boldsymbol{r}_\tau, \tau)} \; W(\boldsymbol{r}_0, 0) \; . \tag{19}$$

Trahan and Wyatt deduced [13] "*two important non-crossing rules that follow directly from Eq. [(19)]: (i) a trajectory cannot cross a surface on which the density is zero; (ii) the sign of the density riding along the trajectory cannot change.*" [60]

Hudson's theorem [40], however, shows that for anharmonic systems the Wigner distribution can at best be positive everywhere in phase space for one point in time only. Time evolution in an anharmonic potential immediately introduces zero-lines of W somewhere in phase space. At W's zeros the Picard-Lindelöf theorem is violated, integrals (6), (17), (18) and (19) do not exist globally. Therefore, the Lagrangian transport solution and trajectories $\boldsymbol{r}_t$ do not exist across phase space.

In other words, Eq. (19) proves that bounded magnitude of $\boldsymbol{\nabla} \cdot \boldsymbol{w}$ precludes sign changes in W along streamlines of $\boldsymbol{w}$.

This leads to one of our central results: *the singularities of* $\boldsymbol{w}$ *are needed to create the negativities of* W*, i.e., they are needed to create quantum coherences* (Section 5.1).

6.1. The phase space velocity $\boldsymbol{w}$ *is non-linear in* W

In general, an evolution equation with higher order derivatives does not allow for trajectory-based solutions since it is neither of first order in derivatives nor linear in W, see Section 2.1. Forcing such an equation into Lagrangian decomposition (15) leads to equations (16) which burden us with spurious non-linearities in W: while $\boldsymbol{J}(W_a) + \boldsymbol{J}(W_b) = \boldsymbol{J}(W_a + W_b)$, in general $\boldsymbol{w}(W_a) + \boldsymbol{w}(W_b) \neq \boldsymbol{w}(W_a + W_b)$ and left and right hand side of Eq. (15) are also non-linear in W. This argument carries over to evolution equations [61, 62] of other quantum phase space distributions.

7. Short time integration of Eulerian and Lagrangian evolution equations –an analytically solvable case–

We now demonstrate that application of the Lagrangian decomposition (15) creates misleading analytical and numerical results, whereas the Eulerian approach gives correct results.

We use the harmonic oscillator groundstate $W_0(\boldsymbol{r}) = (\hbar\pi)^{-1} \exp[-(x^2 + p^2/\hbar^2)]$ as a globally positive initial state for a quartic oscillator $V(x) = Kx^4$, $K > 0$. Since it is not an energy eigenstate and all states have at least one zero

at infinity, it immediately develops negativities [40].

We find that even in this case, where initially singularities of $\boldsymbol{w}$ and $\boldsymbol{\nabla} \cdot \boldsymbol{w}$ are absent, the Lagrangian approach fails, see Fig. 1.

A first order difference approximation of continuity equation (11), using a finite value for Δt, applied to $W_0(\boldsymbol{r})$, according to the Eulerian equation (13) gives the single-step propagation approximation

$$W(\boldsymbol{r}, \Delta t) \approx W_0(\boldsymbol{r}) \; - \Delta t \;\; \boldsymbol{\nabla} \cdot \boldsymbol{J} \tag{20}$$

$$= \left[1 + \Delta t \left(-\hbar^2 K x \partial_p^3 + \{4Kx^3 \partial_p - \frac{p}{M} \partial_x\}\right)\right] \; W_0(\boldsymbol{r}) \; . \tag{21}$$

Eq. (21) is illustrated in Fig. 1 (a). It confirms the immediate formation of negativities and that even the single-step approximation of the Eulerian equation (13) gives tolerable results. Repeated iteration of Eq. (21) yields successively better approximations of the true dynamics, see Fig. 1 (b).

We now show that the growth of the magnitude $|\boldsymbol{\nabla} \cdot \boldsymbol{w}|$, at small values of W (even if $W_0 > 0$ everywhere), is so explosive that it renders the Lagrangian approach misleading, for any non-zero timestep Δt. We repeat calculation (21) using the transport form (17). In this case, for the same initial state W_0, we get the Lagrangian single-step propagation approximation

$$W(\boldsymbol{r}, \Delta t) \approx W_0(\boldsymbol{r} - \Delta t \; \boldsymbol{w}) \; [1 - \Delta t \; 8\hbar^{-2} K \; x \; p] \; , \tag{22}$$

$$\text{where } \boldsymbol{w} = \begin{pmatrix} p/M \\ -4Kx^3 + \hbar^2 K x \; W^{-1} \; \partial_p^2 W \end{pmatrix} \; . \tag{23}$$

Equation (22) is incorrect, see Fig. 1 (c), it puts the Wigner distribution's negative patches into the wrong sectors in phase space and creates deep gashes in them, see Fig. 1 (d); these violate probability conservation.

We cross-checked these results, see Fig. 1 (b), using standard numerical Schrödinger function solvers, the 'QuTiP' programming suite [63] and a split-operator technique [36], confirming that only the Eulerian equation (21), see Fig. 1 (a), and iterations thereof, see Fig. 1 (b), give acceptable results.

Fig. 1 (d) shows that even for our initially positive state W_0, the behaviour of $\boldsymbol{w}$ is responsible for the stark deviation of the ill-defined Lagrangian transport

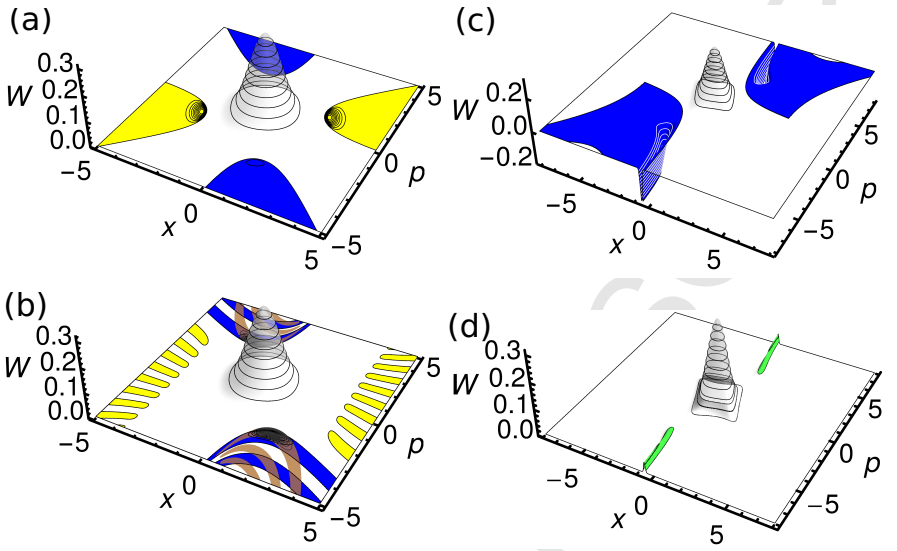

Figure 1: Initially positive Wigner distribution W evolved in Eulerian form (a) and (b) or Lagrangian form (c) and (d). (a), the single step propagation of W_0 with $\hbar = 1, M = 1, V = x^4$, and $\Delta t = 10^{-2}$, using the Eulerian solution (21), shows correct formation of negativities as blue patches in phase space. However, due to the crude nature of the first order difference approximation (20) of the Δt-step employed in this illustration, spurious negative classical transport patches form, shown in yellow. (c), essentially the same scenario as (a) (for explicitness we chose a longer time of $\Delta t = 5 \times 10^{-2}$) is displayed using the Lagrangian transport form (22): deep, unphysical gashes form due to the singularities in $\boldsymbol{w}$ in (23). (b), using a twelve step iteration of the Eulerian solution (21), while reducing the time step per iteration to $10^{-2}/12$, we end up with a better approximation than in (a): W's negativities (blue patches) persist and develop fringes, whereas the unphysical (yellow) classical patches recede. This is confirmed by an exact numerical integration (brown overlay). (d), the transport shift form (18), for the same scenario as (c), displays unphysical formation of humps highlighted in green, their positions confirm that the singularities of $\boldsymbol{w}$ create the deep gashes in (c).

form (17) from the correct Eulerian continuity equation's solution.

8. Misconceptions associated with phase space trajectories

8.1. There are no Wigner trajectories

In reference [1] Lee and Scully consider energy eigenstates (of the Morse potential) and argue that "*In terms of the Wigner distribution, it means that each phase space point should move in such a way that the Wigner distribution does not change in time. This consideration leads to the concept of 'Wigner trajectories', trajectories along which phase space points of the Wigner distribution move. For the case under consideration, Wigner trajectories must be*

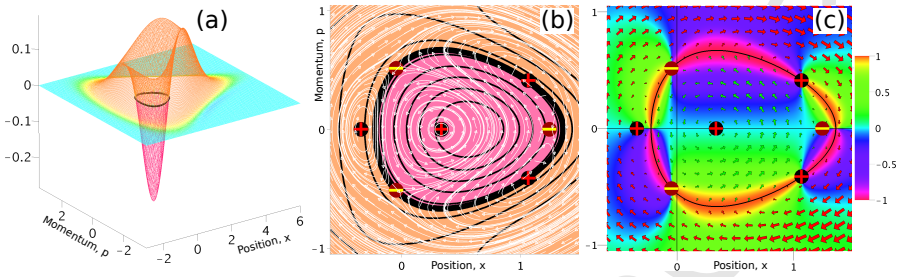

Figure 2: (a) The Wigner distribution for the first excited state of an anharmonic Morse oscillator [64] with potential $U(x) = 3(1 - \exp(-x/\sqrt{6}))^2$ (parameters: $\hbar = 1$ and $M = 1$) is depicted by its black contour lines in (b). W's thick zero contour (black line in (a)) separates the negative central patch from the surrounding positive area in (b): Red crosses and yellow bars mark the locations of $\boldsymbol{J}$'s stagnation points, with Poincaré-Hopf indices [54] $\omega = +1$ and -1, respectively. Integrated fieldlines of $\boldsymbol{J}$ are depicted as thin white lines, displayed together with normalized current $\boldsymbol{J}/J$ (white arrows). $\boldsymbol{J}$-fieldlines, cut across the Wigner distribution's contours and enter and leave the negative area. (c) shows $\frac{2}{\pi}\arctan|\boldsymbol{\nabla}\cdot\boldsymbol{w}|$ and illustrates that $\boldsymbol{w}$ is Liouvillian only on lines in phase space (cyan coloring) while featuring singular behaviour where $W = 0$ (thin black line). Red arrows depict regular and green arrows inverted [54] current $\boldsymbol{J}$.

trajectories along the surfaces on which the Wigner distribution takes on the same value, i. e., trajectories along the equi-Wigner surfaces. These Wigner trajectories are 'quantum-mechanical' trajectories in the sense that they represent paths of phase space points that move according to the quantum-mechanical equation of motion. They describe the exact quantum-mechanical dynamics in a phase space, whereas classical trajectories obviously yield only an approximate description of quantum dynamics" [1].

It has been suspected before that this concept might be flawed, see e.g. [6, 23], here we provide a simple proof and a counterexample.

To disprove Lee and Scully's assertion that for energy eigenstates of quantum systems $\boldsymbol{J}\cdot\boldsymbol{\nabla}W = 0$, note that for eigenstates $\boldsymbol{\nabla}\cdot\boldsymbol{J} = -\partial_t W = 0$, so, with $\boldsymbol{w} = \boldsymbol{J}/W$

$$\boldsymbol{\nabla}\cdot\boldsymbol{w} = \frac{W\boldsymbol{\nabla}\cdot\boldsymbol{J} - \boldsymbol{J}\cdot\boldsymbol{\nabla}W}{W^2} = -\frac{\boldsymbol{J}\cdot\boldsymbol{\nabla}W}{W^2}\,. \tag{24}$$

Therefore Lee and Scully implicitly assume that the flow is Liouvillian which we showed previously [51] to imply that no quantum terms are present in Eq. (12) for $\boldsymbol{J}$. This is incorrect for the Morse oscillator they studied [1].

We confirm our conclusion by a plot of fieldlines of $\boldsymbol{J}$ (to which the velocity

field $\boldsymbol{w}$, where it exists, is tangential) in Fig. 2 (b). This shows that Wigner current crosses W's contours, in other words, $\boldsymbol{J} \cdot \boldsymbol{\nabla} W \neq 0$.

8.2. The Non-Crossing Rules do not apply

We have shown in Section 6 that the non-crossing rules by Trahan and Wyatt are artefacts of the use of the Lagrangian form (15).

Daligault also seems to invoke non-crossing rules when he states that for a region V_0 where the Wigner distribution has negative polarity, and $\boldsymbol{\nabla} \cdot \boldsymbol{w} < 0$, *"the trajectories lying in this volume would condense and eventually collapse into a volume of zero volume. From the practical viewpoint, the set of initial trajectories modelling the whole initial region V_0 would eventually describe a tiny volume."* [12]

Lee and Scully's argument [1] for 'Wigner trajectories', see section 8.1 above, also amounts to invocation of a non-crossing rule.

Section 8.1 and Fig. 2 (b) prove assertions based on Liouvillian flow and non-crossing rules incorrect. Instead of trajectories-based on the velocity field $\boldsymbol{w}$, fieldlines of Wigner current $\boldsymbol{J}$ should be used, they are singularity-free and cross zero-contours of W [54, 55].

8.3. Misconceptions due to incorrect decomposition of the continuity equation

In equation (12) for $\boldsymbol{J}$ the $l = 0$-term is the classical force term rendering the dynamics, if truncated here, Liouvillian ($\boldsymbol{\nabla} \cdot \boldsymbol{w} = 0$). The classical form also is *degenerate* in the sense that the current is zero wherever W is zero [55].
In the anharmonic quantum case this is typically not the case, since (lines of) zeros of the Wigner distribution do not imply that the current stagnates. Instead, this degeneracy in $\boldsymbol{J}$ is lifted due to the quantum terms, of order $l \geq 1$ [55]. This implies that zeros of W are zeros of J_x but not of J_p. The quantum terms in (12) shift the lines of zero of J_p away from those of J_x. Only where those lines intersect do stagnation points of the current exist [55], see Fig. 2 (b) and (c). The stagnation points of the current therefore straddle the boundaries of negative regions of W where the current gets inverted [54, 55]. These stagnation points have special importance because they are topologically protected [54], and they

display very large local variations of the direction of the current for non-zero values of the momentum p, a feature alien to classical Hamiltonian flows. These aspects of the stagnation points of Wigner current were found recently [54, 55] although precursors were observed in quantum phase space studies of Husimi's function [19].

Incorrect use of Newton trajectories. In reference [15] continuity equation (11) is decomposed into its classical term [with $\boldsymbol{v}$ from Eq. (7)] and quantum term Q

$$\partial_t W + \boldsymbol{v} \cdot \boldsymbol{\nabla} W = -\partial_p J_p - \partial_p W \partial_x V = Q \, . \tag{25}$$

This is an incorrect decomposition, the correct Lagrangian decomposition is given in equation (15). The authors then formally integrate this equation propagating their solutions along classical Newtonian trajectories (6), supposedly fully taking into account all quantum effects [15, 16]. This is only correct for quantum-mechanical cases whose hamiltonians have potentials up to second order in position x [44, 41, 15, 54, 59], in which case $Q = 0$. In the anharmonic case, the approach of references [15, 16] does not allow for the directional modifications of the current that is so characteristic for quantum dynamics (see [54, 55] and Fig. 2): the Newton trajectory approach is incorrect.

Incorrect total derivative decomposition. Carruthers and Zachariasen [2] decomposed Wigner current according to $\frac{dW}{dt} = -\partial_p J_p$, the correct expression is $\frac{dW}{dt} = -W \partial_p w_p$, see equation (15).

The $\dot{p} = \partial_p J_p / \partial_p W$ decomposition error. Lee [5] and Lee and Scully [1, 3, 8] incorrectly decomposed $\boldsymbol{J}$ using the analogy with classical physics. Imposing the Liouvillian form

$$\partial_t W + \frac{p}{M} \, \partial_x W + \dot{p} \, \partial_p W = 0 \, , \tag{26}$$

they concluded that, in the quantum case, $\dot{p} = \partial_p J_p / \partial_p W$. Their formal integration of this equation leads to incorrect results such as those detailed in Section 8.1.

This decomposition was criticised by Daligault [12], criticised and yet adopted by Sala *et al.* [6] and by Henriksen *et al.* [4] (who later concluded though that, based on numerical work, *"These studies showed a fatal degradation of the distribution function"* [32]). Decomposition (26) was also adopted by, e.g., Muga *et al.* [7], Razavy [9, 11], Dias and Prata [10], Zhang and Zheng [14], and reported by Landauer [21].

8.4. Can the non-zero divergence of the current be transformed away?

In Reference [51] we established that Wigner current obeys Liouville's theorem only for systems with potentials at most quadratic in x.

Daligault asks whether one can find a transformation *"that would render Hamiltonian* [divergence-free] *quantum fluid dynamics in phase space"* [12]. Reference [51] proves this is not possible. Here we give an additional argument:

The idea of 'transforming away' the divergence in $\boldsymbol{w}$ amounts to transforming away the quantum terms in $\boldsymbol{J}$ [51] and is ill-conceived: according to equation (19), a divergence-free velocity field would not allow for a change of the value of W along a fieldline of $\boldsymbol{J}$. Since fieldlines are defined in all of phase space, negativities and quantum coherences could never form.

Based on an analysis different from Daligault's, Sala *et al.* [6] argue that the 'Wigner trajectories' of Lee and Scully, see section 8.1, exist, that these trajectories follow the contours of W, and that along them $\frac{dW}{dt} = 0$. They modify and reinforce this statement by saying that *"Liouville's theorem in the form of area preservation of a given contour of moving phase points is obeyed as long as the defined contour does not touch any of the singularities. The singularities are not only responsible for "destruction" of trajectories. They can also "create" them."*[6]

We found here that for anharmonic oscillators $\boldsymbol{w}$ is divergence-free only on lines (of measure zero) in phase space, see Fig. 2 (c). In other words, quantum phase space dynamics of anharmonic systems is non-Liouvillian almost everywhere in phase space. We have (other than for harmonic oscillator eigenstates and high-temperature thermal states) not seen evidence of fieldlines of $\boldsymbol{J}$ fol-

lowing W's contours. The reported observation of the "creation or destruction" of trajectories at a singularity of $\boldsymbol{w}$ might be due to careless numerics using an adaptive integrator.

8.5. There are no quantum potentials in phase space

The concept of Wigner trajectories was also used for the introduction of the concept of a "quantum potential" $\tilde{V}$ [5] or "quantum force" $\tilde{F}$ [9, 11]. The underlying idea is to identify the term $\dot{p}$ in Eq. (26) with $\dot{p} = \tilde{F} = -\partial_x \tilde{V}$. Being based on an erroneous identification of terms in Eq. (26), it gives rise to incorrect and peculiar results such as a force with singularities [9, 11].

8.6. What about positive phase space distibutions?

Proof (19) applies to all phase space quantum distributions with negative values, i.e., to the entire continuum of gaussian smeared distributions of which Husimi's Q-function is the (positive semidefinite) limit [38].

Certain technical issues are tamed by using positive distributions such as Husimi's Q-function [65] or some thermal Wigner distributions, but we doubt it changes the fundamental inadmissibility of the trajectory concept for positive distributions: to use trajectories one would have to find a transformation that removes the quantum terms in (12) in order to render the equations first order in their derivatives and linear in W (Section 6.1). But the quantum terms are always present for anharmonic systems [38, 61, 62].

Particular non-trivial anharmonic systems with special states and special symmetries, admitting transformations to Lagrangian forms that simplify treatment, might exist. In general (and in light of failed attempts to find such transformations for W [51]) suggestions [25] that evolution equations of non-negative quantum distributions for anharmonic systems might admit trajectory-based representations appear implausible.

9. Conclusions

Quantum phase space dynamics has frequently been cast into Lagrangian form in order to represent its transport along trajectories. For anharmonic

quantum mechanical systems this leads to a phase space velocity field $\boldsymbol{w}$ with singularities and singular divergence $\boldsymbol{\nabla} \cdot \boldsymbol{w}$. For anharmonic quantum systems transport-solutions, using trajectories, are mathematically ill-defined: trajectory-based approaches have to be avoided.

The occurrence of singularities of $\boldsymbol{\nabla} \cdot \boldsymbol{w}$ in the anharmonic quantum case is *needed and responsible* for the generation of negativities in Wigner's quantum phase space distribution and thus for the generation of quantum coherences. This realization provides a deeper understanding of the differences between quantum and classical phase space dynamics (for which $\boldsymbol{\nabla} \cdot \boldsymbol{w} = 0$). It also explains the frequently reported poor performance of numerical schemes employing trajectories in phase space.

Instead of studying quantum phase space dynamics from a Lagrangian trajectory approach it should primarily be studied from an Eulerian approach centered on Wigner's quantum phase space current $\boldsymbol{J}$. $\boldsymbol{J}$-fieldlines always exist and they reveal intriguing detail [54, 55].

An interesting open question [25] is: how stable are entangled-trajectories methods [33, 66, 23]?

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- Generally there are no trajectories in quantum phase space.
- Previous research employed trajectories in quantum phase space with erroneous results.
- Phase space velocity field singularities create quantum coherences.
- Wigner current instead of trajectories describes quantum dynamics.