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Wigner's representation of quantum mechanics in integral form and its applications

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We consider quantum phase-space dynamics using Wigner's representation of quantum mechanics. We stress the usefulness of the integral form for the description of Wigner's phase-space current \mathbf{J} as an alternative to the popular Moyal bracket. The integral form brings out the symmetries between momentum and position representations of quantum mechanics, is numerically stable, and allows us to perform some calculations using elementary integrals instead of Groenewold star products. Our central result is an explicit, elementary proof which shows that only systems up to quadratic in their potential fulfill Liouville's theorem of volume preservation in quantum mechanics. Contrary to a recent suggestion, our proof shows that the non-Liouvillian character of quantum phase-space dynamics cannot be transformed away.

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I. MOTIVATION AND INTRODUCTION

Wigner's representation of quantum mechanics in phase-space [1] is equivalent to Heisenberg's, Schrödinger's and Feynman's [2]. The description of the time evolution of Wigner's phase-space distribution function W uses Moyal brackets [3], the quantum analog of classical Poisson brackets. The similarity of the Moyal form with classical physics explains its popularity.

Moyal's bracket is defined as an infinite series of derivatives, which can make it cumbersome to use and also numerically unstable. It has limited applications because it assumes that the potential can be Taylor expanded. The integral form of quantum phase-space dynamics [1, 4] is an alternative to Moyal's form, it also applies to piecewise or singular potentials and displays symmetries between momentum and position representation not obvious when using Moyal's formulation only.

We recently showed that in anharmonic quantum systems the violation of Liouville's volume preservation can be so large that quantum phase-space volumes locally change at singular rates [5]. These singularities are of central importance; they are responsible for the generation of quantum coherences.

Here, we investigate a recent suggestion by Daligault [6], who provided a recipe that might enable us to "transform away" the violation of Liouville's theorem in anharmonic quantum-mechanical systems.

We illustrate the power of the integral form of Wigner's representation, which allows us to give an elementary proof that Daligault's suggestion amounts to a specific modification that makes the dynamics classical and is incompatible with his stated aim of finding a Liouvillian system that reproduces quantum dynamics.

Our proof shows that the singularities, reported in Ref. [5], cannot be removed to make quantum phase-space dynamics divergence-free.

II. WIGNER'S DISTRIBUTION AND ITS EVOLUTION

In Wigner's representation of quantum mechanics [1, 7] Wigner's phase-space distribution is the "closest quantum analogue of the classical phase-space distribution" [8]. It is defined as

$$W(x, p, t) = \frac{1}{\pi\hbar} \int dy \varrho(x-y, x+y, t) e^{\frac{2i}{\hbar}py}, \quad (1)$$

$$= \frac{1}{\pi\hbar} \int ds \tilde{\varrho}(p-s, p+s, t) e^{-\frac{2i}{\hbar}xs}; \quad (2)$$

here, $\hbar = h/(2\pi)$ is Planck's constant, integrals run from $-\infty$ to $+\infty$: $\int = \int_{-\infty}^{\infty}$, and ϱ and $\tilde{\varrho}$ are the density operator in position and momentum representation, respectively.

Wigner's distribution W is set apart from other quantum phase-space distributions [7] by the fact that only W simultaneously yields the correct projections in position and momentum ($\varrho(x, x, t) = \int dp W$ and $\tilde{\varrho}(p, p, t) = \int dx W$) as well as state overlaps $|\langle\psi_1|\psi_2\rangle|^2 = 2\pi\hbar \iint dx dp W_1 W_2$, while maintaining its form (1) when evolved in time. Additionally, the Wigner distribution's averages and uncertainties evolve *momentarily* classically [9, 10].

In this work we consider one-dimensional conservative systems in a pure state with quantum-mechanical Hamiltonians

$$\hat{\mathcal{H}}(\hat{x}, \hat{p}) = \frac{\hat{p}^2}{2M} + \hat{V}(\hat{x}). \quad (3)$$

The Wigner function's time evolution arises, in analogy to Eq. (1), from a Wigner-transform [which can be implemented as a fast Fourier transform (FFT)] of the von Neumann equation $i\hbar \frac{\partial \hat{\varrho}}{\partial t} = [\hat{\mathcal{H}}, \hat{\varrho}]$ as [1, 7]

$$\partial_t W = -\frac{p}{M} \frac{1}{\pi\hbar} \int dy \partial_x \varrho(x-y, x+y, t) e^{\frac{2i}{\hbar}py}$$

$$+ \frac{i}{\pi\hbar^2} \int dy [V(x+y) - V(x-y)]$$

$$\times \varrho(x-y, x+y, t) e^{\frac{2i}{\hbar}py}, \quad (4)$$

also known as the quantum Liouville equation.

Throughout, we write partial derivatives as $\frac{\partial^n}{\partial x^n} = \partial_x^n$.

If the potential V can be globally Taylor expanded, the integrals (4) yields the Moyal bracket $\{\{\cdot, \cdot\}\}$ [3]

$$\frac{\partial W}{\partial t} = \{\{\mathcal{H}, W\}\} = \frac{1}{i\hbar} (\mathcal{H} \star W - W \star \mathcal{H}) \quad (5)$$

$$= \frac{2}{\hbar} \mathcal{H} \sin\left(\frac{\hbar}{2} \left(\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x\right)\right) W. \quad (6)$$

Here we use Groenewold star products (\star) [11], defined as $f \star g = f e^{\frac{i\hbar}{2} (\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x)} g$; the arrows indicate whether derivatives are executed on f or g .

Equations (4) or (6) can be written as the continuity equation [1]

$$\partial_t W + \nabla \cdot \mathbf{J} = \partial_t W + \partial_x J_x + \partial_p J_p = 0. \quad (7)$$

Comparing Eqs. (7) and (4), we identify the Wigner current $\mathbf{J} = \begin{pmatrix} J_x \\ J_p \end{pmatrix}$, with position component

$$J_x = \frac{p}{M\pi\hbar} \int dy \varrho(x-y, x+y, t) e^{\frac{2i}{\hbar}py} = \frac{p}{M} W, \quad (8)$$

and momentum component

$$J_p = -\frac{1}{\pi\hbar} \int dy \left[\frac{V(x+y) - V(x-y)}{2y} \right] \times \varrho(x-y, x+y, t) e^{\frac{2i}{\hbar}py}. \quad (9)$$

If the potential can be Taylor expanded, the explicit form of the components of Wigner current \mathbf{J} in Eq. (6) is [1, 12–14]

$$\mathbf{J} = \mathbf{j} + \begin{pmatrix} 0 \\ -\sum_{l=1}^{\infty} \frac{(i\hbar/2)^{2l}}{(2l+1)!} \partial_p^{2l} W \partial_x^{2l+1} V(x) \end{pmatrix}. \quad (10)$$

Here, with $\mathbf{v} = \begin{pmatrix} p/M \\ -\partial_x V \end{pmatrix}$, $\mathbf{j} = W\mathbf{v}$ is the classical and $\mathbf{J} - \mathbf{j}$ are quantum terms.

III. FEATURES AND APPLICATIONS OF THE INTEGRAL FORM

The integral form (4) is more general than the Moyal expression since it does not rely on V being analytic.

A numerical implementation of the integral form can use fast Fourier transforms. In the case of potentials featuring high order Taylor terms, high order numerical derivatives can render Eq. (10) poorly convergent [14].

In Ref. [14] we showed (note typographical errors in Eqs. (4) and (5) of [14]) that the p projection of J_x yields the quantum probability current j in position space,

$$\begin{aligned} \int dp J_x &= \frac{\hbar}{2iM} \int dy \varrho(x-y, x+y, t) \partial_y \delta(y) \\ &= \sum_k P_k \frac{\hbar}{2iM} (\Psi_k^* \partial_x \Psi_k - \Psi_k \partial_x \Psi_k^*) = j(x, t), \end{aligned} \quad (11)$$

where we used Dirac's δ and wrote the density matrix as $\varrho(x, x', t) = \sum_k P_k \Psi_k(x, t) \Psi_k^*(x', t)$, a statistical mixture of pure states. Additionally,

$$\int dx J_x = \frac{p}{M} \int ds \tilde{\varrho}(p-s, p+s, t) \delta(s) = \frac{p}{M} \tilde{\varrho}(p, p, t). \quad (12)$$

Analogously to Eq. (11), the quantum probability current \tilde{j} in momentum space [14], is

$$\begin{aligned} \int dx J_p &= -\frac{1}{\pi\hbar} \iint dy dx \left[\frac{V(x+y) - V(x-y)}{2y} \right] \\ &\quad \times \varrho(x-y, x+y, t) e^{\frac{2i}{\hbar}py} \\ &= \frac{1}{i\sqrt{2\pi\hbar^3}} \int_{-\infty}^p dp' \int dp'' \tilde{V}^*(p'' - p') \tilde{\varrho}(p'', p') \\ &\quad - \tilde{V}(p'' - p') \tilde{\varrho}(p', p'') = \tilde{j}(p, t), \end{aligned} \quad (13)$$

(where $\tilde{V}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int dx V(x) e^{-\frac{i}{\hbar}px}$), while

$$\begin{aligned} \int dp J_p &= -\int dy \left[\frac{V(x+y) - V(x-y)}{2y} \right] \\ &\quad \times \varrho(x-y, x+y, t) \delta(y) \\ &= -\varrho(x, x, t) \frac{dV}{dx}. \end{aligned} \quad (14)$$

We would like to emphasize that the quantum terms of Eq. (10) do not contribute in Eq. (14).

Averaging over Eqs. (12) and (14), reproduces Ehrenfest's theorem [2]

$$\iint dx dp J_x = \frac{\langle \hat{p} \rangle}{M} = \frac{d\langle \hat{x} \rangle}{dt} \quad (15)$$

and

$$\iint dx dp J_p = -\left\langle \frac{d\hat{V}}{dx} \right\rangle = \frac{d\langle \hat{p} \rangle}{dt}. \quad (16)$$

Where applicable, the Moyal bracket formalism [2] yields the same results. Note the various subtleties associated with the interpretation of Ehrenfest's theorem [9, 10].

IV. WHEN IS QUANTUM MECHANICAL TIME EVOLUTION LIOUVILLIAN?

To investigate whether quantum phase-space dynamics is Liouvillian we determine the divergence of its quantum phase-space velocity field \mathbf{w} [6, 13, 15]. \mathbf{w} is the quantum analog of the classical velocity field \mathbf{v} (Eq. (10)):

$$\mathbf{w} = \frac{\mathbf{J}}{W} = \mathbf{v} + \frac{1}{W} \begin{pmatrix} 0 \\ -\sum_{l=1}^{\infty} \frac{(i\hbar/2)^{2l}}{(2l+1)!} \partial_p^{2l} W \partial_x^{2l+1} V \end{pmatrix}. \quad (17)$$

To rephrase the continuity equation (7) in terms of \mathbf{w} , we switch to the Lagrangian decomposition [6, 13, 15]

$$\frac{dW}{dt} = \partial_t W + \mathbf{w} \cdot \nabla W = -W \nabla \cdot \mathbf{w} . \quad (18)$$

Note that \mathbf{w} is singular at zeros of W since, generally, zeros of W do not coincide with zeros of its derivatives. This implies, among other things, that the concept of trajectories in quantum phase-space cannot be applied to the dynamics of anharmonic systems [5].

Problems associated with the singularities have been observed multiple times [15, 16], they badly affect numerical quantum phase-space studies [15].

It would therefore be intriguing to be able to transform such problems away, as suggested by Daligault [6]. He speculated that it might be possible to add an auxiliary field $\delta\mathbf{J}$ to \mathbf{J} in Eq. (7) which would not modify the dynamics since it is assumed to be divergence-free. Yet, this auxiliary field might yield a modification to the velocity field such that their sum fulfills Liouville's theorem: $\nabla \cdot (\mathbf{w} + \delta\mathbf{w}) = 0$. If possible, we could deploy the machinery of classical phase-space transport equations to solve quantum problems.

We now prove that we cannot get rid of the non-Liouvillian character of quantum phase-space dynamics in anharmonic systems in the way Daligault suggested.

To do this, we need to establish when \mathbf{J} obeys Liouville's theorem, i.e., when the divergence of \mathbf{J} 's velocity field vanishes everywhere in phase-space. With $\mathbf{w} = \mathbf{J}/W$ we have

$$\begin{aligned} \nabla \cdot \mathbf{w} &= \partial_x \left(\frac{J_x}{W} \right) + \partial_p \left(\frac{J_p}{W} \right) = \partial_x \left(\frac{p}{M} \right) + \partial_p \left(\frac{J_p}{W} \right) \\ &= \partial_p \left(\frac{J_p}{W} \right) = 0. \end{aligned} \quad (19)$$

Integrating gives us $\int_{-\infty}^p dp' \partial_{p'} \frac{J_p(x, p', t)}{W} = \frac{J_p}{W} = C(x)$ which implies $\int dp J_p = C(x) \int dp W = C(x) \varrho(x, x, t)$. With $-\frac{dV}{dx} \varrho(x, x, t) = C(x) \varrho(x, x, t)$, from (14), it follows that $\nabla \cdot \mathbf{w} = 0$ implies

$$J_p + \delta J_p = -W \frac{\partial}{\partial x} [V(x) + \delta V(x)] . \quad (20)$$

We have shown that the application of Daligault's recipe filters through in a very specific form: the dynamics becomes classical and the shift only affects the potential (since the goal is to not affect the time evolution of W). Strictly speaking, in Eq. (20), we should write $\delta V(x, W(x, p, t))$ to remind ourselves of Daligault's assumption that δJ_p depends on W . But to yield Liouvillian dynamics δV must not depend on p ; hence $\delta V(x, W(x, p, t)) = \delta V(x)$.

For systems in which the potential can be globally Taylor expanded, Eq. (20) shows us that quantum terms must not be present in Eq. (10). To fulfill Liouvillian behavior for all times the potential V might be of "harmonic" form: $V = V_{\text{harmonic}} = \frac{K}{2}x^2 + ax + b$ with arbitrary real K , a , and b and, therefore, $\delta V = 0$.

Alternatively, the auxiliary field has the trivial form $\delta\mathbf{J} = \mathbf{j} - \mathbf{J}$ which subtracts all the quantum parts in Eq. (10), so that the potential assumes the form $V + \delta V = V_{\text{harmonic}}$. This is neither what Daligault intended nor is it helpful, in fact, it is not even permissible since such a field would not fulfill the condition $\nabla \cdot \delta\mathbf{J} = 0$.

One might wonder whether there is some other option, perhaps the anharmonic quantum terms $\mathbf{J} - \mathbf{j}$ in Eq. (10) are present but the initial state W_0 has some special form that cancels all anharmonic terms yet does not force the trivial form $V + \delta V = V_{\text{harmonic}}$ on us.

This cannot be though: if $J_p + \delta J_p$ fulfills Eq. (20), the dynamics is classical and anharmonic, shearing the phase-space distribution. Since a Wigner distribution can be expanded in the coherent-state basis, we assume, without loss of generality, that the initial state W_0 is a coherent state. Classically shearing a phase-space distribution bends it out of shape while keeping it positive, this violates the constraint that a positive Wigner distribution has Gaussian form [17]: anharmonic positivity-preserving classical dynamics is incompatible with quantum phase-space dynamics.

Generalizing Daligault's recipe slightly: might modifications to the J_x component help? We doubt it, if the system is Hamiltonian; even if not quantum *mechanical* but, say, of the classical Kerr-oscillator type, one would, according to Eq. (18), still end up with Liouvillian dynamics: $\frac{d}{dt}W = 0$. W cannot change sign, Daligault's recipe could never give us quantum dynamics, i.e., negativity formation in phase-space [5].

In their monograph on the Wigner representation, Zachos *et al.* [2] argue that anharmonic quantum systems cannot fulfill Liouville's theorem since the difference between the Moyal and Poisson brackets is nonzero for anharmonic quantum systems. In light of Daligault's speculation that a mapping to *another* system might exist, that reproduces the same dynamics and fulfills Liouville's theorem, we feel the above proof with the explicit use of \mathbf{J} is needed to settle the matter.

Figure 1 shows that the divergence $\nabla \cdot \mathbf{w}$ becomes singular when $W = 0$. This follows from Eq. (17). It indicates qualitatively that, since quantum states almost always have zero-lines [17], there will almost always be regions of singularities of $\nabla \cdot \mathbf{w}$. In this sense, the attempt to transform away non-Liouvillian behavior of quantum dynamics appears futile. Instead, such divergences explain certain numerical problems [5] and emphasize how very different quantum and classical phase-space dynamics are: whereas classical dynamics constitute one extreme ($\nabla \cdot \mathbf{w} = 0$ always), quantum dynamics (for anharmonic systems) constitute another ($|\nabla \cdot \mathbf{w}| = \infty$, almost always, somewhere in phase-space).

Since Eq. (7) features singular divergence of the velocity field one should perhaps stress quantum dynamics from the continuity equation point of view rather than referring to quantum Liouville equations.

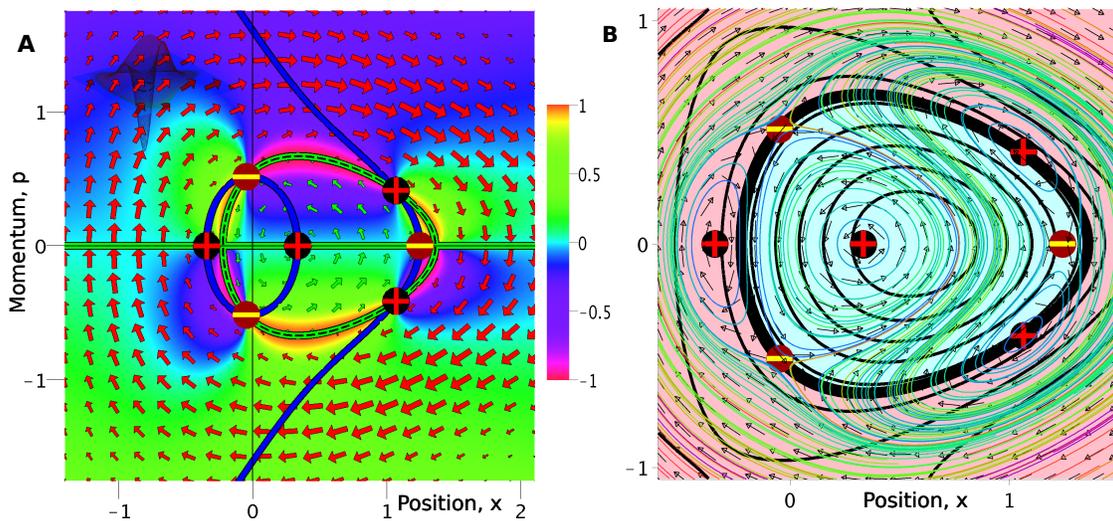


FIG. 1. **A, Singularities of $\nabla \cdot \mathbf{w}$ coincide with zeros of W .** \mathbf{J} depicted by arrows (red for clockwise and green for inverted flow [14]), together with the zeros of the J_x and J_p components (green and blue lines, respectively), is superimposed on top of a colorplot of $\frac{2}{\pi} \arctan(\nabla \cdot \mathbf{w})$. The inset shows the corresponding Wigner distribution for the first excited state of an anharmonic Morse oscillator [18] with potential $V(x) = 3[1 - \exp(-x/\sqrt{6})]^2$. The red crosses and yellow bars mark the locations of the flow's stagnation points, with Poincaré-Hopf indices [14] $\omega = +1$ and -1 . Parameters: $\hbar = 1$ and $M = 1$. The black dashed line marks the zero contour of the Wigner distributions (compare inset); here the divergence $\nabla \cdot \mathbf{w}$ is singular [5].

B, Integrated Fieldlines of \mathbf{J} cross Wigner Distribution Contours. Thin colored lines display fieldlines of \mathbf{J} , displayed together with normalized current $\mathbf{J}/\|\mathbf{J}\|$ (black arrows), and its stagnation points, for the same state as depicted in **A**. W 's zero contour, around the negative (light cyan-colored) patch at the center, is highlighted by a thick black line. Many fieldlines, for this first excited state, cut across the Wigner distribution's contours and enter and leave the negative area.

V. CONCLUSION

We showed that the integral form of Wigner's representation of quantum mechanics should be consulted as an alternative to Moyal's formulation. It is more gen-

eral than Moyal's form. If high order derivatives are present in Moyal's form, the integral form tends to converge better in numerical calculations, which can be implemented as FFTs. It can make mathematical manipulations more transparent than Moyal's form, and it displays symmetries between position and momentum configuration space more clearly.

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