Comment on “Wigner phase space description of a Morse oscillator” [J. Chem. Phys. 77, 4604 (1982)]

Dimitris Kakofengitis, Maxime Oliva and Ole Steurmenagel
School of Physics, Astronomy and Mathematics, University of Hertfordshire, Hatfield, AL10 9AB, UK
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In reference [1] Lee and Scully introduce the concept of trajectories for the study of quantum dynamics in quantum phase space. Specifically, they consider energy eigenstates (of the Morse potential) of the quantum-mechanical Wigner distribution [2, 3].

They state that “the main purpose of our investigation is to obtain physical insights, we consider a rather trivial case when no external force is applied to the oscillator. Then, the oscillator should remain in the same eigenstate throughout. 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 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]

This concept of ‘Wigner trajectories’ was referred to by many and explicitly endorsed by some [4, 5] but also criticised [6, 7]. Specifically, Dittrich et al. consider it meaningless because their semi-classical integration method [6] did not produce ‘Wigner trajectories’. They find their own semi-classical trajectories, starting from classical trajectories, when increasingly refined, at first approach the “Wigner contour [...]. However, they do not approach it asymptotically but continue shifting further past the Wigner contour, indicating that it plays no particular role for quantum time evolution in phase space, not even of eigenstates.” [7]

This still leaves the question whether Lee and Scully are correct?

Here we show that Lee and Scully’s concept of trajectories for energy eigenstates of anharmonic quantum mechanical systems is flawed [8]. Instead, there is a well defined alternative concept: Wigner’s phase space current $J$ [9–11].

This current can always be integrated and yields fieldlines which resemble the ‘trajectories’ Lee and Scully tried to find. The $J$-fieldlines show behaviour very different from what Lee and Scully speculated might happen: the fieldlines neither follow the contours of the Wigner distribution nor are the values of the Wigner distribution along the fieldlines constant.

The time evolution of $W$, Wigner’s quantum phase-space distribution [2, 3], is given by the Eulerian continuity equation [2, 3] (also called the quantum ‘Liouville’ equation, although it is not Liouvillean [11])

$$\partial_t W(r, t) = -\nabla \cdot J(r, t).$$ (1)

Above, partial derivatives (abbreviated as $\partial_t = \partial/\partial t$) are combined to form the divergence $\nabla \cdot J = \partial_x J_x + \partial_p J_p$.

Generally, Wigner current $J$ has an integral representation [2, 3, 12], but for potentials $V(x)$ that can be Taylor-expanded, giving rise to finite forces only, $J$ is of the form [2]

$$J = \left(\begin{array}{c} J_x \\ J_p \end{array}\right) = j + \left( -\sum_{l=1}^{\infty} \frac{(ih/2)^{2l}}{(2l+1)!} \partial_p^{2l} W \partial_x^{2l+1} V \right).$$ (2)

Here, with $v = (bi/M) \cdot \partial_x V$, $j = Wv$ is the classical term and $J - j$ are quantum terms.

Fieldlines of Wigner current are well defined and their depiction has helped to reveal the topological charge conservation of $J$’s stagnation points [9], see Fig. 1.

The concept of trajectories, instead of $J$-fieldlines, originates from phase space transport in Lagrangian form using the total (or comoving) derivative $dW/dt$. To investigate this transport we have to decompose the continuity equation (1) in Lagrangian form [6, 8, 13, 14]

$$\frac{dW}{dt} = \partial_t W + w \cdot \nabla W = -W \nabla \cdot w.$$ (3)

Here, the quantum phase space velocity field $w$ [6, 13, 14], corresponding to the hamiltonian velocity field $v$, is

$$w = \frac{J}{W} = v + \frac{1}{W} \left( -\sum_{l=1}^{\infty} \frac{(ih/2)^{2l}}{(2l+1)!} \partial_p^{2l} W \partial_x^{2l+1} V \right).$$ (4)

$w$ and its divergence

$$\nabla \cdot w = \frac{W \nabla \cdot J - J \cdot \nabla W}{W^2}$$ (5)

are singular at zeros of $W$, since generally zeros of $W$ do not coincide with zeros of its derivatives [8].

Lee and Scully’s assumption that “Wigner trajectories must be trajectories along the surfaces on which the Wigner distribution takes on the same value” formally amounts to the statement that $\nabla \cdot W = 0$. According to Eq. (4) this implies $J \cdot \nabla W = 0$ (if $W \neq 0$). For eigenstates $\nabla \cdot J = -\partial_t W = 0$, the flow is therefore assumed...
to be Liouvillian $\nabla \cdot w = 0$ (see Eq. (3)): “each phase-space point should move in such a way that the Wigner distribution does not change in time”, (formally $\frac{dw}{dt} = 0$, see Eq. (3)).

Both statements are incorrect, as the Morse oscillator is anharmonic, generally $\nabla \cdot w \neq 0$ [11] and $\frac{dW}{dt} \neq 0$.

Elsewhere [8] we have shown that anharmonic quantum mechanical systems do not feature trajectories because the values of $w$ are, according to Eq. (3), singular when $W = 0$. Additionally, the divergence of the velocity field features singularities, see Fig. 1A, which cannot be transformed away [11]. Here, we confirm those abstract conclusions by a plot of the fieldlines of $J$ in Fig. 1B. This shows that Wigner current crosses from positive to negative areas and back. In other words, unlike in the classical case, even for energy eigenstates $\frac{dW}{dt} \neq 0$.

It might seem as if our analysis on the one hand and Lee and Scully’s on the other are each internally consistent. It is therefore worth explaining where exactly Lee and Scully went wrong. Arguably, their starting point is Eq. (3.19) in reference [1]. In our terminology their Eq. (3.19) states that the second component of $w$ has the form $w_p = \partial_x V_{\text{eff}}(x, p) = \frac{J_x}{\partial_x w}$; this is incorrect, the correct form is given in Eq. (4).

Lee and Scully arrived at this incorrect decomposition of $J$ to yield their version of $w_p$ because they have assumed that quantum phase space flow is Liouvillian, i.e., has the form $\frac{\partial t}{\partial t} = -\frac{\partial}{\partial x} V + \partial_x V_{\text{eff}} \partial p W$ (their Eq. (3.13)). But this is inconsistent, since constructing $J = W \cdot w$ from their version of $w_p$ does not yield Eq. (1) as the evolution equation.

Lee and Scully’s decomposition was criticised by Daligault [6], criticised and yet adopted by Sala et al. [15] and by Henriksen et al. [17] (who later concluded though that, based on numerical work, “These studies showed a fatal degradation of the distribution function” [18]). Their decomposition was also adopted by, e.g., Muga et al. [19], Razavy [4, 5], Dias and Prata [20], Zhang and Zheng [21], and reported by Landauer [22].

Confusion persists about the nature of quantum phase space dynamics: confusion about the correct decomposition of the continuity equation, the fact that trajectories do not exist [8], and that the quantum Liouville equation (1) in Lagrangian decomposition (3) features singular divergence of its velocity field $w$ (which cannot be removed [11]).

Wigner current $J$ and its fieldlines are a powerful tool to study the behaviour of quantum phase space dynamics. Particularly, plots like those in Fig. 1 and elsewhere [9, 10] have guided our understanding of quantum phase space dynamics — to share this observation is our main motivation for this comment.
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