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Phase space flow in the Husimi representation

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Abstract

We derive a continuity equation for the Husimi function evolving under a general non-Hermitian Hamiltonian and identify the phase space flow associated with it. For the case of unitary evolution we obtain explicit formulas for the quantum flow, which can be written as a classical term plus quantum corrections. The quantum terms can be expanded in powers of Planck's constant providing a series of semiclassical corrections to the classical flow. We test the exact and semiclassical formulas for a particle in a double well potential and find numerical evidence that the zeros of the Husimi function are always saddle points of the flow. Merging or splitting of stagnation points, reported for the Wigner flow, was not observed.

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(Some figures may appear in colour only in the online journal)

1. Introduction

In classical mechanics the state of a system is often associated with a point in phase space. The initial condition defined by this point specifies a unique trajectory that guides the evolution of the system. This association, however, is not accurate in many situations due to imprecision in assessing the system's state or the statistical nature of the problem at hand. In these cases it is better to work with probability distributions and the associated Liouville equation than with individual trajectories and Hamilton's equations.

In one-dimension the phase space is constructed with a pair of canonically conjugate variables, position x and momentum p, and the general dynamics of a function F(x, p; t) can be written in the form of a continuity equation

$$\frac{\partial F}{\partial t} + \nabla \cdot \mathbf{J} = \sigma, \tag{1}$$

where $\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial p}\right)$, **J** is the current and σ represents the source and sink contributions. In the case of conservative systems driven by a Hamiltonian flow the continuity equation

In the case of conservative systems driven by a Hamiltonian flow the continuity equation is the Liouville equation, for which $\sigma = 0$ and the classical current vector is given by

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$$\mathbf{J}_{cl} = \begin{pmatrix} J_x \\ J_p \end{pmatrix} = \begin{pmatrix} \dot{x}F \\ \dot{p}F \end{pmatrix},\tag{2}$$

where the dots indicate total derivative with respect to time [1]. The characteristic property of this construction is that each point of the phase space on which *F* is evaluated is guided by a well-defined trajectory and the flow lines of the current are just the tangent vectors to these trajectories. The dynamics of the function *F* is thus trivial in the sense that the points just follow the flow, that is, $F(x, p; t) = F(x_0, p_0; 0)$ where x_0 and p_0 are the initial conditions that propagate to *x* and *p* in the time *t*.

In quantum mechanics states are naturally described in terms of probability distributions but, due to the uncertainty principle, phase space representations have interpretations that are different from their classical counterparts. Two of the most used quantum phase space representations are the Wigner and the Husimi functions. The Wigner function W(x, p, t)associated to a state $|\psi\rangle$ has the correct marginal probability distributions when projected into the x or p subspaces, but can be itself negative. The Husimi distribution Q(x, p, t), on the other hand, is positive by definition, but does not project onto the correct marginal distributions. Despite these well-known properties, both representations, and others as well, have been successfully employed in many quantum mechanical treatments [2–6], particularly in the study of the boundary between quantum and classical mechanics [7–14], applications to chemistry [15–23] and to quantum decoherence [24, 25].

If F(x, p; t) is a phase space representation of a quantum state, a natural question to ask is whether it obeys a continuity equation similar to (1), such that a flow can be defined. Because the uncertainty principle forbids the definition of authentic quantum trajectories x(t) and p(t) guiding the dynamics in these representations, the construction of a flow may not seem possible. However, it has been previously shown that the dynamics of the Wigner function can indeed be cast as a continuity-like equation [26–29], thus confirming that for this particular representation a flow is well-defined even though the trajectories in the classical sense are not. In this work we employ the coherent state representation and show that it is also possible to develop a flow formalism for the Husimi function. A continuity equation for the Husimi dynamics has already been demonstrated but only for a particular class of systems [30]. Here we provide a derivation of the Husimi flow that holds for general non-Hermitian Hamiltonian systems. The flow is organized as the associated classical flow plus quantum contribution, that can be expanded in powers of \hbar , providing a series of semiclassical corrections. We show that for Hermitian Hamiltonians there are no source or sink terms, which do appear for non-unitary evolution.

The quantum flow associated with the Wigner function exhibits many interesting nonclassical features, like traveling stagnation points that can merge with or split from other such points, vortices and conservation of the flow winding number [29]. One of our goals is to compare features of the Husimi flow with those of the Wigner flow. Like its Wigner counterpart, non-local features lead to noticeable time-dependent distortions with respect to the classical flow lines, including the displacement and motion of the classical equilibrium (or stagnation) points and inversion of momentum. In [29] it was shown that phase space regions where the Wigner function is negative display flow reversal. Such reversals were also found here, despite the non-negativity of the Husimi function, showing that the negativity is not a necessary condition for the appearance of inversions.

We illustrate the main features of the Husimi flow for a double well potential with the initial state localized in one of the wells. Contrary to the Wigner flow, we did not observe merging or splitting of stagnation points. Interestingly, we found that every zero of the Husimi function is also a saddle point of the flow, with only one extra saddle identified that is not a zero of the Husimi. This association between zeros and saddle points observed in this

example would explain the lack of merging and splitting because of the isolation of the Husimi zeroes. Although the applications considered in this paper are for Hermitian Hamiltonians, our approach also encompasses non-Hermitian operators, which have been the focus of recent research [31–33].

The paper is organized as follows: in section 2 we define the Husimi function and construct the associated continuity equation for general non-Hermitian Hamiltonians. We provide a detailed derivation of the flow and then restrict the calculations to the unitary case. In section 3 we show how to obtain the classical equation of motion given in terms of Poisson brackets from the quantum flow and also derive semiclassical corrections to the classical flow. In section 4 we illustrate these features using as example a one-dimensional double well potential. In section 5 we make some final remarks about the main results.

2. The Husimi flow

2.1. The Husimi function

The coherent states of a harmonic oscillator with mass *m* and frequency Ω are defined as the eigenstates of the annihilation operator $\hat{a} = (\gamma \hat{x} + i \hat{p}/\gamma) / \sqrt{2\hbar}$, where $\gamma = \sqrt{m\Omega}$:

$$\widehat{a}|z\rangle = z|z\rangle. \tag{3}$$

The normalized coherent states can also be written as [2]

$$|z\rangle = e^{-\frac{1}{2}|z|^2} e^{z\widehat{a}^{\tau}} |0\rangle, \tag{4}$$

which will be useful in what follows. Here z is a complex number and $|0\rangle$ is the ground state of the oscillator, which is also the coherent state labeled by z = 0. The coherent states form an over-complete basis and the identity operator is expressed as

$$\widehat{1} = \int d^2 z |z\rangle \langle z|.$$
(5)

These states can also be described as the ground state displaced by z, and because of the ground state $|0\rangle$ is a minimum uncertainty Gaussian wavepacket, the displaced states $|z\rangle$ are minimum uncertainty Gaussian states as well [5, 6]. The relation between z and the mean momentum p and position x of the displaced state is given by

$$z = \frac{1}{\sqrt{2\hbar}} \left(\gamma x + \frac{\mathrm{i}p}{\gamma} \right). \tag{6}$$

The integration measure in equation (5) is given by $d^2 z = dz^* dz/2\pi i = dx dp/2\pi \hbar$, and the star denotes the complex conjugate.

It will be useful to express some of the results both in terms of z and z^* and in terms of x and p. We will refer to the (x, p) plane as Ξ_{xp} and to the complex z plane as Ξ_z .

Given a pure one-particle quantum state $|\psi\rangle$ and its projection $\psi(z^*, z) = \langle z | \psi \rangle$, the Husimi function is the quasi-probability density associated with this wavefunction,

$$Q_{\psi}(z^{\star}, z) = |\psi(z^{\star}, z)|^2 = \operatorname{tr}(|z\rangle\langle z|\widehat{\rho})$$
(7)

where $\hat{\rho} = |\psi\rangle\langle\psi|$ is the density operator. This function is also called the *Q*-representation or *Q*-symbol of the quantum state. The Husimi function is a positive function over Ξ_z , but it is not a probability distribution in the sense that the coordinate and momentum probability densities cannot be retrieved as the marginals distributions from equation (7); also the associated flow cannot be retrieved, unlike in the case of the Wigner flow [29].

2.2. Time-dependent states

Consider a time-dependent quantum state $|\psi; t\rangle$ evolved under the action of a time independent Hamiltonian \hat{H} (which we do not assume to be Hermitian at this point),

$$|\psi;t\rangle = \widehat{K}(t-t_0)|\psi;t_0\rangle,$$

where $\widehat{K}(t) = e^{-i\widehat{H}t/\hbar}$ is the time evolution operator. The Husimi function inherits the time dependence of the state

$$Q_{\psi}(z^{\star}, z; t) = \operatorname{tr}(|z\rangle \langle z|\widehat{\rho}(t)), \tag{8}$$

where $\hat{\rho}(t) = |\psi; t\rangle \langle \psi; t|$, and the equation governing the dynamics of the Husimi function becomes

$$i\hbar \frac{\partial}{\partial t} Q_{\psi} = tr(|z\rangle \langle z|\widehat{H}\widehat{\rho} - \widehat{\rho}\widehat{H}^{\dagger}|z\rangle \langle z|).$$
(9)

Note that for Hermitian Hamiltonians this is just von Neumann's relation cast in the Husimi representation: $i\hbar \frac{\partial}{\partial t}Q_{\psi} = tr(|z\rangle\langle z|[\widehat{H},\widehat{\rho}])$. To further simplify this expression we assume that the Hamiltonian can be expressed as a normal ordered power series on the creation and annihilation operators as

$$\widehat{H} = \sum_{m,n} h_{mn} \widehat{a}^{\dagger m} \widehat{a}^{n}.$$
(10)

If $h_{mn} = h_{nm}^{\star}$ the Hamiltonian is Hermitian. The normalized matrix elements of the Hamiltonian in the coherent states representation become

$$H(z^{\prime\star}, z) = \frac{\langle z^{\prime} | H | z \rangle}{\langle z^{\prime} | z \rangle} = \sum_{m,n} h_{mn} z^{\prime\star m} z^n.$$
(11)

The action of the operators \hat{a}^{\dagger} and \hat{a} on the projector $|z\rangle\langle z|$ is given by its differential algebra on the representation of the coherent states [34–36] and can be derived by applying them to the states as defined in equation (4). The action of a general term of the Hamiltonian is given as

$$\widehat{a}^{\dagger i} \widehat{a}^{j} |z\rangle \langle z| = z^{j} \left(\frac{\partial}{\partial z} + z^{\star}\right)^{i} |z\rangle \langle z|$$
(12)

and

$$|z\rangle\langle z|\widehat{a}^{\dagger j}\widehat{a}^{i} = |z\rangle\langle z|\left(\frac{\overleftarrow{\partial}}{\partial z^{\star}} + z\right)^{i}z^{\star j},\tag{13}$$

where $\overleftarrow{\partial}$ indicates that the derivative acts to the left only. We evaluate the first term inside the trace in equation (9) employing equations (12) and (13) and using the Hamiltonian power series (10). We obtain

$$\operatorname{tr}(|z\rangle\langle z|\widehat{H}\widehat{\rho}) = \operatorname{tr}\left(|z\rangle\langle z|\sum_{m,n}h_{mn}\widehat{a}^{\dagger m}\widehat{a}^{n}\widehat{\rho}\right)$$
$$= \operatorname{tr}(|z\rangle\langle z|\widehat{\rho})\sum_{m,n}h_{mn}\left[\left(\frac{\overleftarrow{\partial}}{\partial z^{\star}} + z\right)^{n}z^{\star m}\right]$$
$$= \sum_{m,n}h_{mn}z^{\star m}\left(\frac{\partial}{\partial z^{\star}} + z\right)^{n}Q_{\psi}.$$

The passing from the first to the second line can be accomplished by the linearity of the trace, and from the second to the third line a rearrangement of the factors was performed, putting the

derivative operator acting to the right as usual. A similar calculation can be done for the second term inside the trace in equation (9). After gathering all the terms the resulting equation is

$$i\hbar\frac{\partial}{\partial t}Q_{\psi} = \sum_{m,n} h_{mn} z^{\star m} \left(\frac{\partial}{\partial z^{\star}} + z\right)^{n} Q_{\psi} - \sum_{m,n} h_{mn}^{\star} z^{m} \left(\frac{\partial}{\partial z} + z^{\star}\right)^{n} Q_{\psi}.$$
 (14)

Since the Husimi is a real function, $\frac{\partial}{\partial z^*}Q_{\psi} = \left(\frac{\partial}{\partial z}Q_{\psi}\right)^*$. Therefore, although the dynamical equation for Q_{ψ} is the sum of two complex functions, its time evolution remains real as it should be.

2.3. Continuity equation and flow

In order to write the equation (14) as a continuity equation all the derivatives with respect to z^* and z must be put to the left, so that we can single out terms of the form $\frac{\partial}{\partial z^*}J_z$ and $\frac{\partial}{\partial z^*}J_{z^*}$, identifying in this way the Husimi currents J_z and J_{z^*} . The relation between these complex currents in Ξ_z and the real currents J_x and J_p in Ξ_{xp} can be obtained using equation (6) and its complex conjugate :

$$\frac{\partial}{\partial z} = \frac{\sqrt{\hbar/2}}{\gamma} \frac{\partial}{\partial x} - i\gamma \sqrt{\hbar/2} \frac{\partial}{\partial p}, \qquad \frac{\partial}{\partial z^{\star}} = \frac{\sqrt{\hbar/2}}{\gamma} \frac{\partial}{\partial x} + i\gamma \sqrt{\hbar/2} \frac{\partial}{\partial p}.$$
 (15)

We obtain

$$J_x = \frac{\sqrt{\hbar/2}}{\gamma} (J_{z^*} + J_z), \qquad J_p = i\gamma \sqrt{\hbar/2} (J_{z^*} - J_z). \tag{16}$$

To put derivatives to the left in (14), we need to change the position of the terms $\left(\frac{\partial}{\partial z^*} + z\right)^j$ and $\left(\frac{\partial}{\partial z} + z^*\right)^j$ with that of the terms z^{*i} and z^i , respectively. A concise way to express both changes is to define

$$\begin{cases} X = z^{\star} & \text{and} \quad D = \left(\frac{\partial}{\partial z^{\star}} + z\right) \\ & \text{or} \\ X = z & \text{and} \quad D = \left(\frac{\partial}{\partial z} + z^{\star}\right). \end{cases}$$

In both cases, XD = DX - 1, and we need to express the X^iD^j term as a combination of those with the opposite ordering. This calculation can be done by induction and the swapping of factors results

$$X^{i}D^{j} = \sum_{k=0}^{\min(i,j)} r_{i,j,k}D^{j-k}X^{i-k},$$

where

$$r_{i,j,k} = \frac{(-1)^k i! j!}{k! (i-k)! (j-k)!}$$

Substituting the series above for the commutation of derivatives and functions in equation (14) and expanding the binomials inside the definition of D, we end up with

$$\frac{\partial}{\partial t}Q_{\psi} = \frac{1}{i\hbar} \sum_{m,n} \sum_{k=0}^{\min(m,n)} \sum_{l=0}^{n-k} h_{mn} r_{m,n,k} \frac{(n-k)!}{(n-k-l)!l!} \frac{\partial^{l}}{\partial z^{\star l}} z^{n-k-l} z^{\star m-k} Q_{\psi} - \frac{1}{i\hbar} \sum_{m,n} \sum_{k=0}^{\min(m,n)} \sum_{l=0}^{n-k} h_{mn}^{\star} r_{m,n,k} \frac{(n-k)!}{(n-k-l)!l!} \frac{\partial^{l}}{\partial z^{l}} z^{\star n-k-l} z^{m-k} Q_{\psi}.$$
(17)

Before we factor out the derivatives identifying the currents we notice that in each summation there is a collection of terms having no derivatives at all, that is, l = 0. This set of terms plays the role of sources and sinks σ in the continuity equation. Its explicit expression is

$$\sigma = \frac{1}{\mathrm{i}\hbar} \sum_{m,n} \sum_{k=0}^{\min(m,n)} r_{m,n,k} (h_{mn} z^{n-k} z^{\star m-k} - \mathrm{c.c.}) Q_{\psi},$$

where c.c. stands for complex conjugate. If the Hamiltonian is Hermitian it can be shown, using the fact that the coefficients $r_{i,j,k}$ are symmetric in the *i* and *j* indexes, that σ vanishes, which is expected for the unitary evolution.

From now on we assume that the Hamiltonian *is* Hermitian and drop the source and sink terms. Taking out to the left one derivative of the expression (17) we can write at last

$$\frac{\partial}{\partial t}Q_{\psi} = -\frac{\partial}{\partial z}J_z - \frac{\partial}{\partial z^{\star}}J_{z^{\star}},\tag{18}$$

where the currents are given by

$$J_{z} = \frac{1}{\mathrm{i}\hbar} \sum_{m,n} \sum_{k=0}^{\min(m,n)} \sum_{l=1}^{n-k} h_{nm} r_{m,n,k} \frac{(n-k)!}{(n-k-l)!l!} \frac{\partial^{l-1}}{\partial z^{l-1}} z^{\star n-k-l} z^{m-k} Q_{\psi}, \qquad (19)$$

$$J_{z^{\star}} = -\frac{1}{\mathrm{i}\hbar} \sum_{m,n} \sum_{k=0}^{\min(m,n)} \sum_{l=1}^{n-k} h_{mn} r_{m,n,k} \frac{(n-k)!}{(n-k-l)!l!} \frac{\partial^{l-1}}{\partial z^{\star l-1}} z^{n-k-l} z^{\star m-k} Q_{\psi}.$$
 (20)

It can be readily checked that $J_{z^{\star}} = J_{z}^{\star}$, even for non-Hermitian Hamiltonians, and our expectation about the existence of real currents (16) on Ξ_{xp} is met and the following relations hold:

$$J_x = \frac{\sqrt{2\hbar}}{\gamma} \operatorname{Re}(J_z), \qquad J_p = \gamma \sqrt{2\hbar} \operatorname{Im}(J_z).$$

The currents J_z and $J_{z\star}$ define the flow of the Husimi function Q_{ψ} in Ξ_z . The non-local character of the currents is expressed by the derivatives of Q_{ψ} present in their definition and is responsible for non-classical features of the flow.

3. Classical limit and semiclassical corrections

3.1. Classical currents

We expect that in the limit $\hbar \to 0$ the currents given by equations (19) and (20) should reduce to the classical Liouville currents equation (2). A complication that arises in the investigation of this limit is that not only the equations (19) and (20) depend explicitly on \hbar but also the Hamiltonian function $H \equiv H(z^*, z)$ itself involves terms of order \hbar or higher. An expansion of the equations in powers of \hbar should take all these terms into account order by order.

As an example consider

$$\widehat{H} = \frac{\widehat{p}^2}{2m} - \frac{k}{2}\widehat{x}^2 + \lambda\widehat{x}^4 + V_0 \tag{21}$$

for which we find

$$H = -\frac{\hbar\Omega}{4}(z - z^{\star})^{2} - \frac{k\hbar}{4m\Omega}(z + z^{\star})^{2} + \frac{\lambda\hbar^{2}}{4m^{2}\Omega^{2}}(z + z^{\star})^{4} + V_{0} + \frac{\hbar\Omega}{4} - \frac{k\hbar}{4m\Omega} + \frac{3\hbar^{2}\lambda}{4m^{2}\Omega^{2}} + \frac{3\hbar^{2}\lambda}{2m^{2}\Omega^{2}}(z + z^{\star})^{2}.$$
(22)

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In terms of x and p, we obtain

$$\tilde{H} = \frac{p^2}{2m} - \frac{kx^2}{2} + \lambda x^4 + V_0$$
$$+ \frac{\hbar\Omega}{4} - \frac{\hbar k}{4m\Omega} + \frac{3\hbar\lambda x^2}{m\Omega} + \frac{3\hbar^2\lambda}{4m^2\Omega^2}$$
(23)

where the tilde identifies functions written in the Ξ_{xp} variables x and p. In both expressions (22) and (23), the first line corresponds to the *classical* Hamiltonian and is \hbar independent. The second lines contain the corrections that appear due to the ordering process. When the $\hbar \rightarrow 0$ limit is performed on these Hamiltonian functions, the classical Hamiltonian (21) is retrieved.

In what follows we will not expand the Hamiltonian, only the dynamical equations, in powers of \hbar . We will see that using the full Hamiltonian H and keeping only terms of order \hbar^0 in the dynamical equations leads to the Liouville equation for H. This corresponds to the classical flow for a modified Hamiltonian that includes quantum corrections coming from normal ordering the operators in \hat{H} as shown above. Not expanding the Hamiltonian makes the procedure simpler and highlights the dynamical features of the continuity equation. Although a complete expansion could be performed, it is much more complicated and does not bring any extra insight into the structure of the flow. The non-classical flow features, such as momentum inversion or motion of the stagnation points, only appear when higher order \hbar corrections are included in the equations.

In order to select the correct \hbar^0 terms of the dynamical equation (18) we first note that the variables *z* and *z*^{*} in equation (6) are proportional to $\hbar^{-1/2}$, and in turn the derivatives $\partial/\partial z$ and $\partial/\partial z^*$ are proportional to $\hbar^{1/2}$; therefore, we must look for the current terms of order $\hbar^{-1/2}$. One way to do it is to set l = q - k + 1 and rewrite equation (19) as

$$J_{z} = \frac{1}{\mathrm{i}\hbar} \sum_{m,n} \sum_{k=0}^{\min(m,n-1)} \sum_{q=k}^{n-1} h_{nm} r_{m,n,k} \frac{(n-k)!}{(q-k+1)!(n-q-1)!} \frac{\partial^{q-k}}{\partial z^{q-k}} z^{\star n-q-1} z^{m-k} Q_{\psi}$$
(24)

It can be checked that the \hbar order of the terms in the previous summations is $q - \frac{1}{2}$, and the highest order is $n - \frac{3}{2}$. Now the limit $\hbar \to 0$ can be taken by selecting the term q = k = 0 in this summation, which is the only one with the $\hbar^{-1/2}$ dependence, as can be readily verified. The result is

$$J_{z} = \frac{1}{\mathrm{i}\hbar} \sum_{m,n} nh_{nm} z^{\star n-1} z^{m} Q_{\psi} = \frac{1}{\mathrm{i}\hbar} \frac{\partial H}{\partial z^{\star}} Q_{\psi}.$$
(25)

Analogously,

$$J_{z^{\star}} = -\frac{1}{\mathrm{i}\hbar} \frac{\partial H}{\partial z} Q_{\psi}.$$
(26)

In terms of x and p we obtain, using (25) and (26),

$$J_x = \frac{\partial H}{\partial p} \tilde{Q}_{\psi}, \qquad J_p = -\frac{\partial H}{\partial x} \tilde{Q}_{\psi}.$$
(27)

By direct comparison of equations (2) and (27) we can extract the classical equations of motion in the phase space

$$\dot{x} = \frac{\partial \tilde{H}}{\partial p}, \qquad \dot{p} = -\frac{\partial \tilde{H}}{\partial x}.$$

Notice that we have not made any assumptions regarding trajectories being guided by a Hamiltonian. The classical structure emerges naturally from the quantum case. The dynamics of the Husimi function in the classical limit is governed by the equation

$$\frac{\partial}{\partial t}\tilde{Q}_{\psi} = -\frac{\partial}{\partial x}\left(\frac{\partial\tilde{H}}{\partial p}\tilde{Q}_{\psi}\right) - \frac{\partial}{\partial p}\left(-\frac{\partial\tilde{H}}{\partial x}\tilde{Q}_{\psi}\right) = \{\tilde{H},\tilde{Q}_{\psi}\}_{[x,p]},$$

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where $\{\cdot, \cdot\}_{[x,p]}$ is the Poisson bracket in the coordinates x and p. The additional terms in equation (24), of higher order in \hbar , lead to quantum deviations from the classical flow.

Note that if we take the limit $\hbar \to 0$ in the Hamiltonian function, all the ordering factors disappear and the usual classical flow is obtained with the original classical Hamiltonian.

3.2. Semiclassical corrections

The first quantum corrections to the classical dynamics are given by the q = 1 terms in equation (24). In this case two contributions arise, from k = 0 and k = 1. For J_z and J_{z^*} this amounts to

$$\begin{split} J_{z}|_{q\leqslant 1} &= \frac{1}{\mathrm{i}\hbar} \frac{\partial H}{\partial z^{\star}} Q_{\psi} + \frac{1}{\mathrm{i}\hbar} \frac{1}{2} \frac{\partial^{2} H}{\partial z^{\star 2}} \frac{\partial}{\partial z} Q_{\psi} - \frac{1}{\mathrm{i}\hbar} \frac{1}{2} \frac{\partial^{3} H}{\partial z^{\star 2} \partial z} Q_{\psi}, \\ J_{z^{\star}}|_{q\leqslant 1} &= -\frac{1}{\mathrm{i}\hbar} \frac{\partial H}{\partial z} Q_{\psi} - \frac{1}{\mathrm{i}\hbar} \frac{1}{2} \frac{\partial^{2} H}{\partial z^{2}} \frac{\partial}{\partial z^{\star}} Q_{\psi} + \frac{1}{\mathrm{i}\hbar} \frac{1}{2} \frac{\partial^{3} H}{\partial z^{2} \partial z^{\star}} Q_{\psi}. \end{split}$$

With these corrections the flow becomes exact for Hamiltonians quadratic in the operators \hat{a}^{\dagger} and \hat{a} and therefore may be termed the first-order semiclassical approximation for the current. Substituting these expressions into equation (18) we find

$$\frac{\partial}{\partial t}Q_{\psi}|_{q\leqslant 1} = \frac{1}{\mathrm{i}\hbar}\{H, Q_{\psi}\}_{[z,z^{\star}]} + \frac{1}{\mathrm{i}\hbar}\frac{1}{2}\frac{\partial^{2}H}{\partial z^{2}}\frac{\partial^{2}}{\partial z^{\star 2}}Q_{\psi} - \frac{1}{\mathrm{i}\hbar}\frac{1}{2}\frac{\partial^{2}H}{\partial z^{\star 2}}\frac{\partial^{2}}{\partial z^{2}}Q_{\psi}$$

which is an anisotropic diffusion equation. Two simple examples are:

(1) The harmonic oscillator of mass m and frequency Ω . The Hamiltonian is

$$H = \hbar\Omega\left(z^{\star}z + \frac{1}{2}\right),\,$$

the diffusive corrections are zero and the Husimi function follows the classical flow. For a harmonic oscillator with frequency $\omega \neq \Omega$ the corrections would not be zero, corresponding to the motion of a squeezed state.

(2) The free particle with mass m,

$$H = -\frac{\hbar\Omega}{4}[(z - z^{\star})^2 - 1],$$

and the diffusive correction leads to

$$\frac{\partial}{\partial t}\tilde{Q}_{\psi}|_{q\leqslant 1} = -\frac{p}{m}\frac{\partial}{\partial x}\tilde{Q}_{\psi} + \frac{\hbar\Omega}{2}\frac{\partial^2}{\partial x\partial p}\tilde{Q}_{\psi}$$

where it is possible to identify the classical velocity p/m and the diffusion coefficient $\hbar\Omega$, which depends on parameters of the coherent states used in the representation.

4. Husimi flow for a particle in a double well

In this section we illustrate the main features of the Husimi flow with a numerical example. Although the currents are defined by an *a priori* infinite series of terms, comprising the Taylor expansion of the Hamiltonian, the series truncate for polynomial potentials. In order to obtain exact results we choose as toy-model the Hamiltonian (21) describing a particle in a symmetric double well potential:

$$\widehat{H} = \frac{\widehat{p}^2}{2m} + \lambda \widehat{x}^4 - \frac{k}{2}\widehat{x}^2 + V_0.$$

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Figure 1. Husimi flow at t = 3.5 for the double well potential. The unit arrows indicate the direction of the current, regardless of the intensity. Upper left: \hbar^0 (classical flow); upper right: \hbar^1 correction; lower left: \hbar^2 correction; lower right: \hbar^3 correction (exact Husimi flow). The red stars mark the zeros of the Husimi function (plotted as background in the last image).

The Hamiltonian function can be rearranged as

$$H(z^{\star}, z) = -\frac{\hbar\Omega}{2}(z^{\star 2} + z^2) + \frac{\lambda\hbar^2}{4m^2\Omega^2}(z^{\star} + z)^4,$$
(28)

or

$$\tilde{H}(x,p) = \frac{p^2}{2m} - \frac{m\Omega^2}{2}x^2 + \lambda x^4$$
(29)

where the parameters of the potential were chosen to be $k = (m\Omega^2 + \frac{6\lambda\hbar}{m\Omega})$ and $V_0 = \frac{3\lambda\hbar^2}{2m^2\Omega^2}$. The classical currents for the Hamiltonian H(x, p) have three stationary points, all of them with p = 0: one saddle at x = 0 and two clockwise centers at $x = \pm \sqrt{m\Omega^2/4\lambda}$ as shown in figure 1 (upper left corner).

For the numerical calculations we used $2m = 3\lambda = \Omega/2 = \hbar = 1$, and the initial wavepacket is a coherent state $|z_0\rangle$ centered at $x_0 = \sqrt{3/2} \approx 1.225$, $p_0 = 1.305$, corresponding to the center of the left well with energy equal to about twice the classical barrier height V_0 . We computed the time evolution of the wave packet with the Split-Time-Operator method [37], obtained the Husimi function using equation (8) and the flow using equations (19) and (20).

Figure 1 shows the direction of the flow at time t = 3.5 using increasingly accurate approximations for the dynamical equations (18)–(20). For the Hamiltonian (28) the highest \hbar



Figure 2. Logarithmic plot of the Husimi function for the double well potential superposed with the current unit vectors. Upper left t = 1.0, upper right t = 2.0, lower left t = 3.0 and lower right t = 4.0. The zeros are shown by the white spots. The shifted classical centers (blue circles) and saddle (square) are also indicated. Except for the displaced classical saddle, all the others are followed by a flow center (blue triangles).

power in the flow series (24) is q = 3. The panels show the classical flow q = 0, the first order semiclassical correction q = 1, the next order q = 2 and the exact result corresponding to q = 3, for which the Husimi function is also shown as a gray scale contour plot. The corrections in increasing powers of \hbar change the overall structure of the current portraits and, except for some small displacements, the \hbar^1 correction, in this weakly perturbed system, almost mimics the exact quantum flow. The center stationary points of the classical flow, where the flow circulates around the critical point, are displaced from their locations both in momentum and position. The saddle point at x = p = 0 is also displaced and is located at a zero of the Husimi function (marked with a star). It can also be seen that additional saddle points appear, one for each extra zero of the Husimi function. Each of these extra saddle points are accompanied by a center point, indicating the conservation of the overall flow winding number [29]. Indeed it was observed that, except for the two centers and one saddle corresponding to the classical stagnation points (see figure 2), all zeros of the Husimi function are saddles followed by a center.

Any state can be completely characterized by the zeros of its Husimi function [38–41] and, in the particular case of eigenstates, they are fixed on the phase space, forming the so called the stellar representation. For non-stationary states the zeros of the Husimi function



Figure 3. Comparison between the Husimi (left) and Wigner (right) flow vectors for the double well potential for t = 3.5.

display a non-trivial dynamics that is neither governed by the classical equations of motion, nor driven by the Husimi flow, since they are saddle points of the flow.

Figure 2 shows the dynamics of the stagnation points of the flow. At t = 0, because the initial state is Gaussian, there are no zeros of the Husimi function and the saddle point of the classical flow at x = p = 0 is not present. However, for very short times the saddle moves from infinity to the area of its classical position (t = 1.0) and stays in the region where the Husimi is significant. All other zeroes that develop at later times are saddles followed by a center.

Figure 3 shows a comparison between the Husimi and Wigner flows at t = 3.5. One of the features of the Wigner flow described in [29] is the inversion of the flow orientation along the *x* direction. This phenomenon happens because the negativity of the Wigner function changes the sign of the *x* component of the current (see the yellow shaded areas in figure 3). The inversion of the orientation of the *x* component of the flow was also observed in the Husimi flow, where J_x becomes negative for p > 0 and vice-versa. Therefore, the negativity of the function is not a necessary condition for the occurrence of inversion.

5. Final remarks

In this work we constructed the phase space flow for the Husimi representation of a one-particle quantum state. The formulas were tested for a particle in a double well potential. We showed that the flow lines differ substantially from its corresponding classical structure, displacing the stagnation points and modifying their quantity. The counter-classical orientation of the flow lines is also observed in the Husimi representation. For the Wigner flow such orientation reversals are associated with the negativity of the function in the phase space [29]. Therefore, the existence of regions with counter orientation seems to be a more general feature of phase space representations of quantum states, regardless of negativity.

Contrary to the Wigner flow [29], the Husimi flow did not show birth or merging of critical points for the example studied. We found that critical points of the flow are the three classical ones (two centers and a saddle) plus pairs composed of a center and a saddle, so that the winding number of the global flow is conserved. We also found that the zeros of the Husimi function are always saddle points of the flow. The association between saddle points

of the flow and the zeros of the Husimi function explains the lack of birth or merging of the saddle-center pairs, because the zeros of the Husimi function cannot disappear [38], although they can merge with other zeros or split. For small propagation times the zeros move from infinity into the region where the Husimi function is significant and remain there without bifurcating.

Finally we note that the continuity equation could in principle be used directly to compute the time evolution of the Husimi distribution. This procedure, however, involves the solution of a partial differential equation containing several derivatives of the Husimi function and turns out to be numerically difficult to handle. On the other hand, the method would provide a novel way to integrate Schroedinger's equation that is naturally arranged as a classical evolution plus semiclassical corrections. Work in this direction is under way.

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References

- [1] Abraham R and Marsden J E 1997 Foundations of Mechanics 2nd edn (Reading, MA: Addison-Wesley)
- [2] Glauber R J 1963 Phys. Rev. 131 2766
- [3] Cohen L 1966 J. Math. Phys. 7 781
- [4] Hillery M, O'Connel R F, Scully M O and Wigner E P 1984 Phys. Rep. 106 121
- [5] Klauder J R and Skagerstam B S 1985 Coherent States Applications in Physics and Mathematical Physics (Singapore: World Scientific)
- [6] Perelomov A M 1986 Generalized Coherent States and Their Application (Berlin: Springer)
- [7] Heller E J 1975 J. Chem. Phys. 62 1544
- [8] Herman M F and Kluk E 1984 Chem. Phys. 91 27
- [9] Berry M V 1989 Proc. R. Soc. Lond. A 423 219
- [10] Kurchan J, Leboeuf P and Saraceno M 1989 Phys. Rev. A 40 6800
- [11] Xavier A L Jr and de Aguiar M A M 1997 Phys. Rev. Lett. 79 3323
- [12] de Almeida A M O 1998 Phys. Rep. 295 265
- [13] Baranger M, de Aguiar M A M, Keck F, Korsch H J and Schellhaas B 2001 J. Phys. A: Math. Gen. 34 7227
- [14] Ribeiro A D, de Aguiar M A M and Baranger M 2004 Phys. Rev. E 69 066204
- [15] Kay K G 1994 J. Chem. Phys. 100 4377
- [16] Kay K G 1994 J. Chem. Phys. 100 4432
- [17] Miller W H 2001 J. Phys. Chem. A 105 2942
- [18] Pollak E and Shao J 2003 J. Phys. Chem. A 107 7112
- [19] Shalashilin D V and Child M S 2004 Chem. Phys. 304 103
- [20] Shalashilin D V and Burghardt I 2008 J. Chem. Phys. 129 084104
- [21] de Aguiar M A M, Vitiello S A and Grigolo A 2010 Chem. Phys. 370 42
- [22] Viscondi T F and de Aguiar M A M 2011 J. Math. Phys. 52 052104
- [23] Viscondi T F and de Aguiar M A M 2011 J. Chem. Phys. 134 234105
- [24] Ribeiro A D and Angelo R M 2010 Phys. Rev. A 82 052335
- [25] Ribeiro A D and Angelo R M 2012 Phys. Rev. A 85 052312
- [26] Wigner E P 1932 Phys. Rev. 40 749
- [27] Donoso A, Zheng Y and Martens C C 2003 J. Chem. Phys. 119 5010
- [28] Bauke H and Itzhak N R 2011 arXiv:1101.2683v1
- [29] Steuernagel O, Kakofengitis D and Ritter G 2013 Phys. Rev. Lett. 110 030401
- [30] Skodje R T, Rohrs H W and VanBuskirk J 1989 Phys. Rev. A 40 2894
- [31] Graefe E-M, Höning M and Korsch H J 2010 J. Phys. A: Math. Theor. 43 075306
- [32] Graefe E-M and Schubert R 2011 Phys. Rev. A 83 060101
- [33] Graefe E-M and Schubert R 2012 J. Phys. A: Math. Theor. 45 244033
- [34] Gilmore R, Bowden C M and Narducci L M 1975 Phys. Rev. A 12 1019

- [35] Zhang W-M, Feng D H and Gilmore R 1990 Rev. Mod. Phys. 62 867
- [36] Trimborn F, Witthaut D and Korsch H J 2008 Phys. Rev. A 77 043631
- [37] Bandrauk A D and Shen H 1993 J. Chem. Phys. 99 1185
- [38] Leboeuf P and Voros A 1990 J. Phys. A: Math. Gen. 23 1765
- [39] Cibils M B, Cuche Y, Leboeuf P and Wreszinski W F 1992 Phys. Rev. A 46 4560
- [40] Nonnenmacher S and Voros A 1997 J. Phys. A: Math. Gen. 30 295
- [41] Korsch H J, Muller C and Wiescher H 1997 J. Phys. A: Math. Gen. 30 L677