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Operator equation of motion in phase space: Application to time-dependent systems possessing invariants

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We have derived an equation of motion for a Wigner operator in phase space, which is the phase-space analog of the Heisenberg equation of motion for a quantum-mechanical operator. An application of this operator equation to time-dependent systems possessing invariants is considered, and the solution for the corresponding Wigner phase-space distribution function is obtained.

I. INTRODUCTION

The phase-space distribution function, originally introduced by Wigner[1] and subsequently generalized by Moyal,[2] Cohen,[3] and others,[4] provides a means to calculate the quantum-mechanical expectation values using classical-like phase-space (PS) integration, where position and momentum are treated as ordinary variables rather than as operators. In the PS picture, the quantum corrections become transparent, and a smooth transition from quantum to classical physics is encountered. It is particularly suitable for obtaining quantum-mechanical (QM) results in situations where a good initial approximation comes from the classical result and also for deriving classical limits of quantal processes. The strength of the PS framework is also revealed by its ability to provide a unified treatment of states and transitions by associating PS functions to quantum states as well as quantum transitions. Also, both pure and mixed states can be discussed using the same framework.

The Wigner PS function is the Weyl transform of the density operator and is a particular representation of the density matrix. There also results another meaningful picture of the Wigner function when it is interpreted as the expectation value of the parity operator.[5]

The calculation of the Wigner function from the wave function in coordinate space as the starting point is met with difficulties. Even for the hydrogen atom, one has to take recourse to either expansion in terms of the Gaussians[6] or exploit the hydrogen-atom–oscillator connection.[7] The equation governing the time evolution of the PS function has therefore been employed directly in a variety of problems, such as collisions,[8] intramolecular energy transfer,[9] photodissociation,[10] and other semiclassical applications.[11] Recently, the PS distribution function has also been useful in discussing quantum chaos,[12,13] quantum fluid dynamics[14] and some aspects of density-functional theory.[15] The creation and annihilation operators have also been defined in phase space[16] (see Kim and Zachary[17] for a variety of applications of the physics of phase space).

The PS formalisms have mostly been centered around the distribution functions. However, operators known as Wigner operators (which are essentially Bopp operators) have also been defined[4,18] in phase space. Although the Wigner operators are not needed for evaluating the expectation values, they appear in the equations determining the PS distribution functions. While these equations involving the PS function have been studied extensively, the equations of motion for the Wigner operators themselves have not attracted sufficient attention. In the present work, we aim at obtaining the equation of motion for the Wigner operators in phase space, which will be the PS analog of Heisenberg equation of motion for a quantum-mechanical operator.

The equation for the time evolution of the PS function is not a differential equation with simple order but involves series expansion in the derivatives with respect to position as well as momentum coordinates. It is therefore of utmost importance to have methods of solution for these equations. We exploit the operator equations derived here to obtain solutions for the PS distribution for a certain class of time-dependent (TD) problems, viz., those associated with TD invariants,[19] which includes problems involving a TD harmonic oscillator or a charged particle moving in a TD magnetic field.

In what follows, a brief review of Wigner distribution functions is presented in Sec. II. The operator equation of motion is then derived in Sec. III. The solution for the PS function through the operator equation is obtained in Sec. IV for general TD systems possessing invariants and the TD harmonic oscillator as a special case. Finally, we offer a few concluding remarks in Sec. V.

II. WIGNER DISTRIBUTION FUNCTION IN PHASE SPACE AND RELATED EQUATIONS

The Wigner distribution function $f(q,p)$ is defined through the partial Fourier transform of the off-diagonal elements of the density matrix, viz.,

$$f(q,p)=(2\pi\hbar)^{-1}\int dy \exp\left[\frac{ipy}{\hbar}\right]\times\langle q-y/2|\hat{\rho}|q+y/2\rangle\ , \tag{1}$$

or an equivalent expression

$$f(q,p)=(2\pi\hbar)^{-1}\int dk \exp\left[\frac{-iqk}{\hbar}\right]\times\langle p-k/2|\hat{\rho}|p+k/2\rangle\ , \tag{2}$$

and clearly satisfies the following properties:

$$\begin{aligned}&\int dq\, f(q,p)=\langle p|\hat{\rho}|p\rangle\ ,\\ &\int dp\, f(q,p)=\langle q|\hat{\rho}|q\rangle\ ,\\ &\int dq\int dp\, f(q,p)=1\ .\end{aligned} \tag{3}$$

These results, written for a single particle in one dimension, can easily be generalized to higher dimensions and many-particle systems. Another more general scheme is the Wigner-Moyal transform, which yields the PS function $A_s(q,p)$ corresponding to a QM operator $A(q,p)$ and is given by[2,18,20,21]

$$A_s(q,p)=\int dy \exp\left[\frac{ipy}{\hbar}\right]\langle q-y/2|\hat{A}|q+y/2\rangle\ . \tag{4}$$

Clearly, Eq. (1) is a special case of Eq. (4) for the density operator, i.e., $\hat{A}=\hat{\rho}$ and $f(q,p)=(2\pi\hbar)^{-1}\rho_s$. The PS function $A_s(q,p)$ is known as the Wigner equivalent of operator $\hat{A}$ and the transformation given by Eq. (4) can be recast in several other equivalent forms.[18] From Eqs. (1) and (4), it also follows that

$$\mathrm{Tr}(\hat{\rho}\hat{A})=\int dq\int dp\ A_s(q,p)f(q,p)\ , \tag{5}$$

which implies a classical-like procedure for the evaluation of expectation values. One also has the generalization of Eq. (5), viz.,

$$\mathrm{Tr}(\hat{A}\hat{B})=(2\pi\hbar)^{-1}\int dq\int dp\ A_s(q,p)B_s(q,p)\ . \tag{6}$$

The Wigner equivalent of the product of operators can be expressed in terms of the Wigner equivalents of the individual operators. Thus, for $\hat{F}=\hat{A}\hat{B}$, one has

$$\begin{aligned}F_s(q,p)&=A_s(q,p)\exp\left[\frac{\hbar\Lambda}{2i}\right]B_s(q,p)\\ &=B_s(q,p)\exp\left[\frac{-\hbar\Lambda}{2i}\right]A_s(q,p)\ ,\end{aligned} \tag{7}$$

where Λ (essentially the Poisson bracket operator) is given by

$$\Lambda=\left[\frac{\overleftarrow{\partial}}{\partial p}\right]\left[\frac{\overrightarrow{\partial}}{\partial q}\right]-\left[\frac{\overleftarrow{\partial}}{\partial q}\right]\left[\frac{\overrightarrow{\partial}}{\partial p}\right]\ , \tag{8}$$

with the arrows indicating the direction in which the derivatives act. In the general multidimensional case, Eq. (8) involves a multidimensional scalar product.

The Wigner equivalent of the commutator $[\hat{A},\hat{B}]_-$ and the anticommutator $[\hat{A},\hat{B}]_+$ now follow directly:

$$([\hat{A},\hat{B}]_-)_s=-2iA_s[\sin(\hbar\Lambda/2]B_s\ , \tag{9a}$$

$$([\hat{A},\hat{B}]_+)_s=2A_s[\cos(\hbar\Lambda/2)]B_s\ . \tag{9b}$$

The classical limits ($\hbar\to 0$) of Eqs. (9) yield the desired result:

$$(i\hbar)^{-1}([\hat{A},\hat{B}]_-)_s\to\{A_sB_s\}_{\mathrm{PB}}\ , \tag{10a}$$

$$(\tfrac{1}{2})([\hat{A},\hat{B}]_+)_s\to A_sB_s\ , \tag{10b}$$

where $\{\ \}_{\mathrm{PB}}$ denotes the Poisson bracket.

One can thus obtain the Wigner equivalent PS function corresponding to any QM operator using Eq. (4). The reverse process of obtaining a QM operator equivalent of a classical PS function is via the Weyl transform. One can also define operators in phase space, known as Wigner operators. Thus, corresponding to a PS function $A_s(q,p)$, the differential operator $\hat{A}_w(q,p)$ is defined as

$$\hat{A}_w(q,p)=A_s(\hat{Q},\hat{P})\ , \tag{11}$$

where $\hat{Q}$ and $\hat{P}$ are the Bopp operators[22] and are given[4,18] by

$$\begin{aligned}\hat{Q}&=q-\left[\frac{\hbar}{2i}\right]\left[\frac{\partial}{\partial p}\right]\ ,\\ \hat{P}&=p+\left[\frac{\hbar}{2i}\right]\left[\frac{\partial}{\partial q}\right]\ .\end{aligned} \tag{12}$$

The PS operator $\hat{A}_w(q,p)$ can be rewritten as

$$\hat{A}_w=A_s(q,p)\exp\left[\frac{\hbar\Lambda}{2i}\right] \tag{13a}$$

$$=\exp\left[(\hbar/2i)\left[\frac{\partial}{\partial p_A}\right]\left[\frac{\partial}{\partial q}\right]-\left[\frac{\partial}{\partial q_A}\right]\left[\frac{\partial}{\partial p}\right]\right]A_s(q,p)\ , \tag{13b}$$

where $(\partial/\partial p_A)$ and $(\partial/\partial q_A)$ operate on A_s, while $(\partial/\partial q)$ and $(\partial/\partial p)$ are free and are to operate on the function that follows A_s. One can thus obtain the PS operator $\hat{A}_w$ corresponding to any QM operator $\hat{A}$ or the Wigner equivalent PS function $A_s(q,p)$ using Eqs. (11)–(13). The reverse transformation of the PS operator $\hat{A}_w$ into the PS function $A_s(q,p)$ is by operating on unity, viz.

$$\hat{A}_w(\hat{Q},\hat{P})1=\hat{A}_w(\hat{Q}^*,\hat{P}^*)1=A_s(q,p)\ , \tag{14}$$

where $\hat{Q}^*$ and $\hat{P}^*$ are complex conjugates of $\hat{Q}$ and $\hat{P}$ of Eq. (12). $\hat{A}_w(Q,P)$ is an operator not on the Hilbert space on which $\hat{A}(\hat{q},\hat{p})$ is an operator, but it acts on functions in PS. It also follows from Eqs. (7) and (13) that corresponding to the product of QM operators, $\hat{F}=\hat{A}\hat{B}$, one has

$$F_s(q,p)=\hat{A}_w\hat{B}_w1=\hat{A}_wB_s(q,p) \tag{15a}$$

$$=\hat{B}^*_w\hat{A}_w1=\hat{B}^*_wA_s(q,p)\ , \tag{15b}$$

where $\hat{B}_w^*$ denotes $\hat{B}_w(\hat{Q}^*,\hat{P}^*)$. The expectation values can also be expressed in terms of the Wigner operators, viz.,

$$\mathrm{Tr}(\hat{A}\hat{B})=(2\pi\hbar)^{-1}\int dq\int dp\ A_s(q,p)B_s(q,p)$$
$$=(1/\hbar)\int dq\int dp\ \hat{A}_w B_s(q,p) \quad (16a)$$
$$=(1/\hbar)\int dq\int dp\ \hat{B}_w A_s(q,p)\ , \quad (16b)$$

and the expectation value $\langle \hat{A}\rangle$ is given by [compare Eq. (5)]

$$\langle \hat{A}\rangle=\mathrm{Tr}(\hat{\rho}\hat{A})=\int dq\int dp\ \hat{A}_w f(q,p)\ . \quad (17)$$

One also has the commutator relation

$$\hat{A}_w\hat{B}_w^*=\hat{B}_w^*\hat{A}_w\ . \quad (18)$$

With the help of the interconnections among the QM operator $\hat{A}(\hat{q},\hat{p})$, the classical PS function $A_s(q,p)$ and the PS (Wigner) operator $\hat{A}_w$, the equation of motion for the density operator, viz.

$$i\hbar\left[\frac{\partial\hat{\rho}}{\partial t}\right]=[\hat{H},\hat{\rho}]\ , \quad (19)$$

will have the following form in the Wigner representation:

$$\hbar\left[\frac{\partial f}{\partial t}\right]=-2H_s(q,p)\sin\left[\frac{\hbar\Lambda}{2}\right]f(q,p,t)\ , \quad (20a)$$

which can be rewritten as

$$\frac{\partial f}{\partial t}=(i\hbar)^{-1}(\hat{H}_w-\hat{H}_w^*)f(q,p,t)=i\hat{L}f(q,p,t)\ , \quad (20b)$$

where $\hat{L}$ is the quantum Liouville operator defined in terms of the Wigner operator $\hat{H}_w$ and $\hat{H}_w^*$ corresponding to the Hamiltonian $\hat{H}$, viz.,

$$i\hat{L}=(i\hbar)^{-1}(\hat{H}_w-\hat{H}_w^*)\ . \quad (21)$$

Equation (21) is the quantum Liouville equation and determines the time evolution of the PS distribution function. Expansion in power series of $\hbar$ using Eq. (13) shows that the zeroth-order term in Eq. (20) corresponding to the classical Liouville equation and the terms of even order in $\hbar$ represent the quantum corrections.

Equation (20) governs the time evolution of $f(q,p)$, which is the Wigner equivalent of the density operator. The equation of motion for a general operator $\hat{A}(\hat{q},\hat{p})$, viz.,

$$\left[\frac{d}{dt}\right]\hat{A}(q(t),p(t),t)=\left[\frac{\partial}{\partial t}\right]\hat{A}(q(t),p(t),t)+(i\hbar)^{-1}[\hat{A}(q,p,t),\hat{H}(q,p,t)] \quad (22)$$

can also be transformed into the PS equation:

$$\left[\frac{d}{dt}\right]A_s(q(t),p(t),t)=\left[\frac{\partial}{\partial t}\right]A_s(q(t),p(t),t)-i\hat{L}(q(t),p(t))A_s(q(t),p(t))\ , \quad (23)$$

which yields the classical Liouville equation in the classical limit $\hbar\to 0$. For Hamiltonians of the type

$$H(q,p,t)=p^2/2m+V(q,t)\ , \quad (24)$$

with $V(q,t)$ linear or quadratic in q, the equation of motion is the classical Liouville equation. For a general potential, however, Eq. (20) or (24) does not represent a differential equation of simple order and involves a power series. The formalisms presented in subsequent sections would provide schemes for solving the quantum Liouville equation.

III. OPERATOR EQUATION OF MOTION IN PHASE SPACE

While the equation for the PS function [Eqs. (20) and (23)] corresponds to the Schrödinger picture of QM, an analog of the Heisenberg picture can be established through the PS equation corresponding to the QM operator equation (22). Since the equation of motion for the Wigner operator $\hat{A}_w$ does not seem to have been studied earlier, we first present a derivation of this equation.

The time dependence of $\hat{A}_w$ can be obtained from Eq. (23) for the corresponding PS function A_s through the operator correspondence [Eqs. (11)–(13)]. Since Eq. (13) can also be written[18] in the form

$$\hat{A}_w=\frac{\hbar}{2\pi}\int\int d\xi\, d\eta\, G_A(\xi,\eta)\exp\left[i\left\{\xi\left[p+\left[\frac{\hbar}{2i}\right]\left[\frac{\partial}{\partial q}\right]\right]+\eta\left[q-\left[\frac{\hbar}{2i}\right]\left[\frac{\partial}{\partial p}\right]\right]\right\}\right]\ , \quad (25a)$$

$$\hat{A}_w^*=\frac{\hbar}{2\pi}\int\int d\xi\, d\eta\, G_A(\xi,\eta)\exp\left[-i\left\{\xi\left[p-\left[\frac{\hbar}{2i}\right]\left[\frac{\partial}{\partial q}\right]\right]+\eta\left[q+\left[\frac{\hbar}{2i}\right]\left[\frac{\partial}{\partial p}\right]\right]\right\}\right]\ , \quad (25b)$$

where

$$G_A(\xi,\eta)=\frac{1}{\hbar}\int\int dq\, dp\ A_s(q,p)\exp[-i(\xi p+\eta q)]\ , \quad (26)$$

one obtains the equation for $\hat{A}_w$ from Eq. (23), viz.,

$$\left[\frac{d}{dt}\right]A_s=\left[\frac{\partial}{\partial t}\right]A_s-(i\hbar)^{-1}(\hat{H}_w A_s-\hat{A}_w H_s)\ , \tag{27}$$

by multiplying with the exponential terms of Eqs. (25) and (26) followed by integrations over ξ, η, q, and p variables.

The term $\hat{H}_w A_s$ is the Wigner equivalent of the QM operator product $\hat{H}\ \hat{A}$ and can be expressed as

$$F_s=(\hat{H}\hat{A})_s=\hat{H}_w A_s=(\hbar/2\pi)^2\int\int\int\int d\xi_1 d\eta_1 d\xi_2 d\eta_2 G_H(\xi_1,\eta_1)G_A(\xi_2,\eta_2)$$
$$\times\exp\{i[(\xi_1+\xi_2)p+(\eta_1+\eta_2)q]+(i\hbar/2)(\xi_1\eta_2-\eta_1\xi_2)\}\ , \tag{28}$$

and therefore the corresponding Wigner operator is given by

$$\hat{F}_w=\left[\frac{\hbar}{2\pi}\right]^3(1/\hbar)\int\int\int\int\int\int d\xi\, d\eta\, d\xi_1 d\eta_1 d\xi_2 d\eta_2 dq'dp' G_H(\xi_1,\eta_1)G_A(\xi_2,\eta_2)$$
$$\times\exp[(i\hbar/2)(\xi_1\eta_2-\eta_1\xi_2)]\exp\{i[(\xi_1+\xi_2-\xi)p'+(\eta_1+\eta_2-\eta)q']\}$$
$$\times\exp\left[i\left\{\xi\left[p+\left[\frac{\hbar}{2i}\right]\left[\frac{\partial}{\partial q}\right]\right]+\eta\left[q-\left[\frac{\hbar}{2i}\right]\left[\frac{\partial}{\partial p}\right]\right]\right\}\right]\ , \tag{29}$$

where use has been made of the identities

$$\exp\left[i\left\{\xi_1\left[p+\left[\frac{\hbar}{2i}\right]\left[\frac{\partial}{\partial q}\right]\right]+\eta_1\left[q-\left[\frac{\hbar}{2i}\right]\left[\frac{\partial}{\partial p}\right]\right]\right\}\right]\exp\left[i\left\{\xi_2\left[p+\left[\frac{\hbar}{2i}\right]\left[\frac{\partial}{\partial q}\right]\right]+\eta_2\left[q-\left[\frac{\hbar}{2i}\right]\left[\frac{\partial}{\partial p}\right]\right]\right\}\right]$$
$$=\exp\left[i\left\{(\xi_1+\xi_2)\left[p+\left[\frac{\hbar}{2i}\right]\left[\frac{\partial}{\partial q}\right]\right]+(\eta_1+\eta_2)\left[q-\left[\frac{\hbar}{2i}\right]\left[\frac{\partial}{\partial p}\right]\right]\right\}\right]\exp[(i\hbar/2)(\xi_1\eta_2-\eta_1\xi_2)]\ . \tag{30}$$

Since the integral over the p' and q' variables of the second exponential term in Eq. (29) gives a δ function, one readily obtains

$$\hat{F}_w=\hat{H}_w\hat{A}_w\ . \tag{31}$$

Analogously, the term $\hat{H}^*_w A_s$ is equal to $\hat{A}_w H_s$ by Eq. (15), and hence the corresponding Wigner operator is $\hat{A}_w\hat{H}_w$. The equation of motion for the Wigner operator is therefore given by

$$\left[\frac{d}{dt}\right]\hat{A}_w=\left[\frac{\partial}{\partial t}\right]\hat{A}_w+(i\hbar)^{-1}(\hat{H}_w\hat{A}_w-\hat{A}_w\hat{H}_w)\ , \tag{32}$$

which is analogous to the Heisenberg equation of motion for a quantum-mechanical operator.

IV. TIME-DEPENDENT INVARIANTS AND SOLUTION FOR THE PHASE-SPACE DISTRIBUTION FUNCTION

Consider the TD system characterized by the Hamiltonian of the form of Eq. (24) and the resulting equation for the PS distribution given by Eq. (20). Now, assume that there exists an invariant $I(q,p,t)$ for this TD problem. The Wigner operator $\hat{I}_w$ corresponding to this invariant satisfies

$$\left[\frac{d}{dt}\right]\hat{I}_w=\left[\frac{\partial}{\partial t}\right]\hat{I}_w-(i\hbar)^{-1}(\hat{H}_w\hat{I}_w-\hat{I}_w\hat{H}_w)=0\ . \tag{33}$$

Now, operating $(\partial\hat{I}_w/\partial t)$ on $f(q,p,t)$ and using Eqs. (33) and (20) and the commutator condition $(\hat{H}_w\hat{I}^*_w=\hat{I}^*_w\hat{H}_w)$ [see Eq. (18)], one obtains

$$(i\hbar)\left[\frac{\partial}{\partial t}\right](\hat{I}_w f)=(\hat{H}_w-\hat{H}^*_w)(\hat{I}_w f)\ . \tag{34}$$

Hence, $(\hat{I}_w f)$ also satisfies the same Wigner-Moyal-type equation (20). We now make use of the properties of this invariant to solve for the PS function $f(q,p,t)$ from Eq. (20).

The solution involves an expansion in terms of the PS eigenstates of the invariant operator, given by

$$(1/\hbar)(\hat{I}_w-\hat{I}^*_w)f_{n,m}(q,p,t)=a_{nm}f_{n,m}(q,p,t)\ . \tag{35}$$

The definition of the PS eigenfunctions $f_{n,m}$ for stationary states follows from the generalization of Eq. (1) for the PS distribution function, viz.,

$$f_{n,m}=(2\pi\hbar)^{-1}\int dy\,\exp\left[\frac{ipy}{\hbar}\right]$$
$$\times\langle q-y/2|\hat{\rho}_{n,m}|q+y/2\rangle\ , \tag{36}$$

corresponding to the density matrix operator $\hat{\rho}_{n,m}=|n\rangle\langle m|$. Here, $\hat{\rho}_{n,m}$ $(=\psi_n\otimes\psi_m)$ characterizes the nth and mth eigenstates corresponding to the eigenvalue problem in the Hilbert space of the wave function, viz.,

$$\hat{I}\psi_n=a_n\psi_n\ . \tag{37}$$

The two eigenvalue equations[23] obeyed by the PS functions $f_{n,m}(q,p)$ are

$$(1/\hbar)([\hat{I},\hat{\rho}_{nm}]_-)_s=(1/\hbar)(\hat{I}_w-\hat{I}^*_w)f_{n,m}(q,p)$$
$$=-2(i/\hbar)I(q,p,t)\sin(\hbar\Lambda/2)f_{n,m}$$
$$=a_{nm}f_{n,m}(q,p)\ , \tag{38a}$$
$$\tfrac{1}{2}([\hat{I},\hat{\rho}_{nm}]_+)_s=I(q,p,t)\cos(\hbar\Lambda/2)f_{n,m}$$
$$=a'_{nm}f_{n,m}\ , \tag{38b}$$

where the eigenvalues a_{nm} and a'_{nm} are related to the QM eigenvalues by

$$a_{nm}=(1/\hbar)(a_n-a_m)\ , \tag{39a}$$

$$a'_{nm}=\tfrac{1}{2}(a_n+a_m)\ . \tag{39b}$$

Since the Bopp operators $\hat{Q}$ and $\hat{P}$ defined in Eq. (12) as well as the operators $\hat{Q}^*$ and $\hat{P}^*$ are Hermitian, any real function of these operators is also Hermitian. Since $I_s(q,p)$ is a real function of its arguments, the operator $(\hat{I}_w-\hat{I}^*_w)$ is clearly Hermitian and the eigenvalues $\{a_{nm}\}$ are real. Also since $\{\psi_n\}$ form an orthonormal set, the PS eigenfunctions $\{f_{nm}\}$ also form an orthonormal complete set, i.e., they satisfy

$$(2\pi\hbar)^{-1}\int\int dq\,dp\,f_{n,m}f^*_{n',m'}=\delta_{nn'}\delta_{mm'} \tag{40a}$$

and also the "self-orthogonality" relation

$$\int\int dq\,dp\,f_{n,m}=\delta_{nm}\ . \tag{40b}$$

The functions $f_{n,m}$ form a Hermitian matrix with respect to their subscripts n and m, i.e.,

$$f_{n,m}(q,p,t)=f^*_{m,n}(q,p,t)\ . \tag{41}$$

We now proceed first to prove that the eigenvalues $a_{n,m}$ are not explicitly time dependent. Differentiating Eq. (38a) with respect to time, one obtains

$$\left[\frac{1}{\hbar}\right]\left[\left[\frac{\partial}{\partial t}\right]\hat{I}_w-\left[\frac{\partial}{\partial t}\right]\hat{I}^*_w\right]f_{n,m}+\left[\frac{1}{\hbar}\right](\hat{I}_w-\hat{I}^*_w)\left[\frac{\partial}{\partial t}\right]f_{n,m}=\left[\frac{\partial a_{nm}}{\partial t}\right]f_{n,m}+a_{nm}\left[\frac{\partial f_{n,m}}{\partial t}\right]\ . \tag{42}$$

Now, allowing Eq. (33) to operate on $f_{n,m}$ and the equation of $\hat{I}^*_w$ corresponding to Eq. (33) on $f_{n,m}$ and subtracting, one obtains

$$\left[\left[\frac{\partial}{\partial t}\right]\hat{I}_w-\left[\frac{\partial}{\partial t}\right]\hat{I}^*_w\right]f_{n,m}+\left[\frac{1}{i\hbar}\right][(\hat{H}_w-\hat{H}^*_w)(\hat{I}_w-\hat{I}^*_w)-(\hat{I}_w-\hat{I}^*_w)(\hat{H}_w-\hat{H}^*_w)]f_{n,m}=0\ . \tag{43}$$

From Eqs. (42) and (43), one obtains

$$[(\hat{I}_w-\hat{I}^*_w)-\hbar a_{nm}]\left[i\hbar\left[\frac{\partial}{\partial t}\right]-(\hat{H}_w-\hat{H}^*_w)\right]f_{n,m}$$
$$=i\hbar\left[\frac{\partial}{\partial t}\right](\hbar a_{n,m})f_{n,m}\ . \tag{44}$$

Taking the scalar product with $f^*_{n',m'}$ and using the orthogonality property of $f_{n,m}$ [see Eq. (40)], we get

$$\hbar(a_{n'm'}-a_{nm})\left[f_{n',m'},\left[i\hbar\left[\frac{\partial}{\partial t}\right]-(\hat{H}_w-\hat{H}^*_w)\right]f_{n,m}\right]$$
$$=i\hbar\left[\frac{\partial}{\partial t}\right](\hbar a_{n,m})\delta_{nn'}\delta_{mm'}\ , \tag{45}$$

which implies that

$$\left[\frac{\partial}{\partial t}\right]a_{n,m}=0\ , \tag{46}$$

indicating that the eigenvalues of the invariant operator have no explicit time dependence.

Equation (45) for the off-diagonal case implies that

$$\left[f_{n',m'},\left[i\hbar\left[\frac{\partial}{\partial t}\right]-(\hat{H}_w-\hat{H}^*_w)\right]f_{n,m}\right]=0\ . \tag{47}$$

The objective now is to find a solution to Eq. (20b) through the eigenfunctions $f_{n,m}$ of the invariant operator. Since $\{f_{n,m}\}$ form a complete set, $f(q,p,t)$ can be written as

$$f(q,p,t)=\sum_{n,m}C_{n,m}(t)f_{n,m}(q,p,t)\ . \tag{48}$$

Substituting Eq. (48) into Eq. (20), taking the inner product with $f_{n',m'}$, and using Eq. (47), one obtains

$$i\hbar\left[\frac{\partial C_{n',m'}}{\partial t}\right]+\hbar\left[\frac{\partial\alpha_{n',m'}}{\partial t}\right]C_{n',m'}=0\ , \tag{49}$$

where

$$\hbar\left[\frac{\partial\alpha_{n',m'}}{\partial t}\right]$$
$$=\left[f_{n',m'},\left[i\hbar\left[\frac{\partial}{\partial t}\right]-(\hat{H}_w-\hat{H}^*_w)\right]f_{n',m'}\right]\ . \tag{50}$$

Therefore, the time-dependent coefficients $C_{n',m'}(t)$ are given by

$$C_{n',m'}(t)=\exp\{i[\alpha_{n',m'}(t)-\alpha_{n',m'}(t')]\}C_{n',m'}(t')\ , \tag{51}$$

which on substitution in Eq. (48) leads to

$$f(q,p,t)=\sum_{n,m}\exp[-i\alpha_{nm}(t')]\left[\int\int dq'dp'\,f^*_{n,m}(q',p',t')f_0(q',p',t')\right]\exp[i\alpha_{nm}(t)]f_{n,m}(q,p,t)\ . \quad (52)$$

Equation (52) enables one to obtain $f(q,p,t)$ from the eigenfunctions $f_{n,m}$ and the boundary condition for $f(q,p,t)$ at $t=t'$.

As an example, we now consider the case of a time-dependent harmonic oscillator described by the Hamiltonian

$$H=p^2/2+\tfrac{1}{2}\omega^2(t)q^2\ . \quad (53)$$

The time-dependent invariant $I(t)$ associated with this system is given by[19]

$$I(p,q,t)=\tfrac{1}{2}[(\rho p-\dot{\rho}q)^2+k(q/\rho)^2]\ , \quad (54)$$

where k is a constant and $\rho(t)$ satisfies

$$\ddot{\rho}+\rho w^2(t)=k/\rho^3\ . \quad (55)$$

Our objective is to obtain the solution of Eq. (20b) for this system in terms of the eigenfunctions of the invariant operator (54). The latter can be expressed in the simple form

$$I=\tfrac{1}{2}(P^2+kQ^2) \quad (56)$$

in terms of the new variables Q and P obtained through the canonical transformations

$$Q=q/\rho,\quad P=\rho p-\dot{\rho}q\ . \quad (57)$$

Equation (56) suggests that the invariant in the transformed variable plays the role of Hamiltonian for a time-independent harmonic oscillator.

For the phase-space considerations of the oscillator problem, we have

$$(\hat{H}_w-\hat{H}^*_w)=-ip\left[\frac{\partial}{\partial q}\right]+i\omega^2(t)q\left[\frac{\partial}{\partial p}\right]\ , \quad (58)$$

$$(\hat{I}_w-\hat{I}^*_w)=-i(\rho p-\dot{\rho}q)\left[\rho\left[\frac{\partial}{\partial q}\right]+\dot{\rho}\left[\frac{\partial}{\partial p}\right]\right]+i\left[\frac{k}{\rho^2}\right]q\left[\frac{\partial}{\partial p}\right]\ . \quad (59)$$

The second expression when reexpressed in terms of the new variables Q and P takes the form

$$(\hat{I}_w-\hat{I}^*_w)=-iP\left[\frac{\partial}{\partial Q}\right]+ikQ\left[\frac{\partial}{\partial P}\right]\ . \quad (60)$$

Equation (60) suggests that the eigenfunctions in Eq. (38a) would be functions of Q and P, i.e.,

$$f_{n,m}(q,p,t)=f_{n,m}(q/\rho,\rho p-\dot{\rho}q)\ . \quad (61)$$

Using this knowledge of the functional dependence of $f_{n,m}$ on q and p, one can easily solve Eq. (50), rewritten as

$$\hbar\left[\frac{\partial\alpha_{n,m}}{\partial t}\right]=\left[f_{n,m},\left[i\hbar\left[\frac{\partial}{\partial t}\right]-(\hat{H}_w-\hat{H}^*_w)\right]f_{n,m}\right]=-\rho^{-2}(f_{n,m},\hbar(\hat{I}_w-\hat{I}^*_w)f_{n,m})\ , \quad (62)$$

to obtain the phase factor given by

$$\alpha_{n,m}(t)=-\hbar a_{n,m}\int^t dt\,\rho^{-2}\ . \quad (63)$$

Once we identify $(\hat{I}_w-\hat{I}^*_w)$ with $(\hat{H}_w-\hat{H}^*_w)$ of the time-independent harmonic oscillator, the eigenfunctions $f_{n,m}$ can be obtained from standard results.[21] Therefore, one has all the necessary quantities to obtain the distribution function $f(q,p,t)$ from Eq. (52) when the initial function $f_0(q,p,t')$ is known.

V. CONCLUDING REMARKS

The evolution of phase-space formalisms in quantum mechanics has been driven by a desire to obtain a classical conceptual framework for discussing quantum phenomena. It not only provides an enhanced view of the interpretive aspects, but it also enables one to employ the various methods of approximation or expansion used in classical cases to the problems of quantum domain.[24]

The operator equation in phase space that has been proposed here supplements the analogous equation-of-motion approach for the quantum chemical calculations. Invariance plays an important role[19] in obtaining the solution for the time-dependent harmonic oscillator and to obtain the phase-space distribution function, the operator equation for the invariant operator is essential. Using the operator equation derived here, a time-dependent density-functional theory[25] can be developed in phase space. A master-equation approach for open quantum systems can also be developed using the operator equation. It is also of interest to obtain a path-integral solution[26] to the phase-space function and show its interconnection with the Bohm's quantum-fluid-dynamical approach.[14,24]

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