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State operator, constants of the motion, and Wigner functions: The two-dimensional isotropic harmonic oscillator

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For a closed quantum system the state operator must be a function of the Hamiltonian. When the state is degenerate, additional constants of the motion enter the play. But although it is the Weyl transform of the state operator, the Wigner function is not necessarily a function of the Weyl transforms of the constants of the motion. We derive conditions for which this is actually the case. The Wigner functions of the energy eigenstates of a two-dimensional isotropic harmonic oscillator serve as an important illustration.

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I. INTRODUCTION

A convenient formulation of quantum mechanics is the Weyl-Wigner phase-space representation, in which the state operator is represented by the Wigner function. A key model of a quantum-mechanical system is the harmonic oscillator. It is well known that for the one-dimensional harmonic oscillator the phase-space variables enter into the stationary-state Wigner functions only through the phase-space Hamiltonian.

In the present Brief Report we give the reason for this. Subsequently, we show that for the two-dimensional isotropic harmonic oscillator the phase-space variables enter into the stationary-state Wigner functions only through the constants of the motion, including the Hamiltonian. Working within the Weyl-Wigner representation, we derive expressions for these functions by actually solving the dynamical phase-space equations that define them. These equations are coupled differential equations.

This Brief Report is organized as follows. In Sec. II we briefly recall the form of the dynamical phase-space equations and discuss the stationary-state Wigner functions for the one-dimensional harmonic oscillator. In Sec. III we discuss the constants of the motion of the two-dimensional isotropic harmonic oscillator. We determine the generic form of the Wigner function by actually solving the dynamical equations defined by the energy and an unspecified constant of the motion. Finally, we present the form of the Wigner function for specific constants of the motion. Section IV contains our conclusions.

II. LIOUVILLE SPACE AND PHASE SPACE

Consider a closed physical system with Hamiltonian $\hat{H}$ and a Hilbert space spanned by the normalized kets $|\psi_i\rangle$. The position and momentum representatives of $|\psi_i\rangle$ are the wave functions $\psi_i(q)$ and $\phi_i(p)$, respectively. Liouville space is the space formed by $\hat{H}$ and other operators acting on Hilbert space. These operators include the state operators, or density operators,

$$\hat{\rho}_i \equiv \hat{\rho}_{ii} = |\psi_i\rangle\langle\psi_i|. \tag{1}$$

Assume that $|\psi_i\rangle$ describes a stationary state. It is an eigenvector of $\hat{H}$ with energy E_i. The state operator $\hat{\rho}_i$ obviously commutes with the Hamiltonian. It is a projection operator,

$$\hat{\rho}_i \sum_j c_j|\psi_j\rangle = c_i|\psi_i\rangle, \quad \hat{\rho}_i^2 = \hat{\rho}_i. \tag{2}$$

In the absence of degeneracies it equals the energy projection operator [1,2],

$$\hat{\rho}(E_i) = \prod_{j\neq i} \frac{\hat{H}-E_j}{E_i-E_j}. \tag{3}$$

In the presence of degeneracies, the energy projection operator may not suffice to uniquely determine $\hat{\rho}_i$. It will usually have to be multiplied by additional projection operators corresponding to other dynamical variables. To preserve the energy, such operators must be Hermitian and commute with the Hamiltonian; that is, they must be constants of the motion.

Expression (3) defined by the Hamiltonian, together with similar expressions defined by additional constants of the motion, shows that the state operator is a function of the Hamiltonian and the other constants of the motion. How is this displayed in phase space?

Quantum mechanics in phase space may be considered a mapping of quantum mechanics as formulated in Liouville space [3,4]. In particular, the Liouville space operators $\hat{A}$ are mapped into phase-space functions $a(q,p)$, with q and p being the position and momentum variables, respectively. The mapping from Liouville space to phase space may be expressed by the Weyl transformation,

$$a(q,p) = \int_{-\infty}^{\infty} dy \langle q+y/2|\hat{A}|q-y/2\rangle e^{-ipy/\hbar}, \tag{4}$$

in a notation which, for simplicity, refers to a single dimension. Choosing $\hat{A}$ as the state operator $\hat{\rho}_i$ divided by Planck's constant gives the Wigner function,

$$W_i(q,p) = \frac{1}{h}\int_{-\infty}^{\infty} dy\, \psi_i^*(q-y/2)\psi_i(q+y/2)e^{-ipy/\hbar}. \tag{5}$$

We also note that an operator of the form $F(\hat{q})+G(\hat{p})$ is mapped into the phase-space function $F(q)+G(p)$.

Let $a(q,p)$ and $b(q,p)$ be the phase-space functions corresponding to the operators $\hat{A}$ and $\hat{B}$, respectively. The phase-space function $c(q,p)$ corresponding to the operator product $\hat{C}=\hat{A}\hat{B}$ is then given by the star product $c(q,p)=a(q,p)\star b(q,p)$. Explicitly, the star product may be written in various equivalent forms. Here we use

$$c(q,p) = a(\hat{Q},\hat{P})b(q,p) = b(\hat{Q}^*,\hat{P}^*)a(q,p), \tag{6}$$

where $\hat{Q}$ and $\hat{P}$ are Bopp operators [3,5],

$$\hat{Q} = q + \frac{i\hbar}{2}\frac{\partial}{\partial p}, \quad \hat{P} = p - \frac{i\hbar}{2}\frac{\partial}{\partial q}, \tag{7}$$

and $\hat{Q}^*$ and $\hat{P}^*$ are their complex conjugates.

Assume now that a ket $|\psi\rangle$ is eigenvector of the operator $\hat{A}$ with eigenvalue α. Exploiting Eq. (6) gives the dynamical equations [6–10],

$$\frac{1}{2}[a(\hat{Q},\hat{P}) + a(\hat{Q}^*,\hat{P}^*)]W(q,p) = \alpha W(q,p), \tag{8}$$

$$[a(\hat{Q},\hat{P}) - a(\hat{Q}^*,\hat{P}^*)]W(q,p) = 0. \tag{9}$$

To determine the Wigner function one must construct and solve the dynamical equations for the relevant constants of the motion.

Let us consider the one-dimensional harmonic oscillator defined by the Hamiltonian

$$\hat{H}_1 = \frac{1}{2M}\hat{p}_\xi^2 + \frac{1}{2}M\omega^2\hat{\xi}^2, \tag{10}$$

where M is the mass of the oscillator and ω is the angular frequency. We introduce different variables ($\hat{x}=\sqrt{M\omega}\hat{\xi}$, $\hat{p}=\hat{p}_\xi/\sqrt{M\omega}$, and $\hat{H}=\hat{H}_1/\omega$) and get the reduced Hamiltonian

$$\hat{H} = \frac{1}{2}(\hat{p}^2 + \hat{x}^2). \tag{11}$$

The Wigner functions for the stationary states of the oscillator may be constructed by inserting the well-known wave function

$$\psi_n(x) = \left\{\frac{1}{2^n n!\,\sqrt{\pi\hbar}}\right\}^{1/2} H_n(x/\sqrt{\hbar})e^{-(1/2)(x^2/\hbar)} \tag{12}$$

into Eq. (5), or it may be determined by solving Eqs. (8) and (9) with a being the Weyl transform $h(x,p)$ of Hamiltonian (11), namely, $h(x,p)=\frac{1}{2}(p^2+x^2)$. The result is [3]

$$W_n(x,p) = \frac{(-1)^n}{\pi\hbar}L_n(4h(x,p)/\hbar)e^{-2h(x,p)/\hbar},$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar, \quad n = 0,1,2, \ldots . \tag{13}$$

In the above equations, $H_n(z)$ is a Hermite polynomial and $L_n(z)$ is a Laguerre polynomial [11].

As emphasized in Sec. I, Wigner function (13) only depends on x and p through the phase-space representative $h(x,p)$ of the Hamiltonian. To rationalize this, we recall that $W_n(x,p)$ is the Weyl transform of the state operator which in turn is a function of $\hat{H}$. Assume that this function may be written in terms of powers of $\hat{H}$. We may then form its phase-space equivalent, that is, the Wigner function by calculating the phase-space image $(h(x,p)*)^n$ of $\hat{H}^n$ for all n. In general, we will find that $(h(x,p)*)^n$ cannot be written as an ordinary function of $h(x,p)$. If so, the Wigner function is not just a function of $h(x,p)$ alone.

The condition for $(h(x,p)*)^n$ to be an ordinary function of $h(x,p)$ for any n is that $h(x,p)*f(h(x,p))$ be a function of $h(q,p)$ for an arbitrary function f. This condition is found to be fulfilled for the harmonic oscillator. One finds in fact [12] that

$$h * f(h) = hf(h) - \frac{\hbar^2}{4}\frac{df}{dh} - \frac{\hbar^2}{4}h\frac{d^2f}{dh^2}. \tag{14}$$

Thus we understand why the Wigner function for the harmonic oscillator merely depends on q and p through $h(x,p)$. It is easy to see that a relation similar to that of Eq. (14) does not exist for a Hamiltonian of the form $\hat{H}=\frac{1}{2}\hat{p}^2+a\hat{q}^n$ for n larger than 2.

III. ISOTROPIC HARMONIC OSCILLATOR

We now turn to the two-dimensional isotropic harmonic oscillator with the reduced Hamiltonian

$$\hat{H} = \frac{1}{2}(\hat{p}_x^2 + \hat{p}_y^2 + \hat{x}^2 + \hat{y}^2). \tag{15}$$

This is a system with high degeneracy. The degeneracy is due to the high symmetry of the Hamiltonian which is invariant not just under rotations in the x-y plane (geometrical symmetry), but also under rotations that mix coordinates and momenta (dynamical symmetry). One realizes that the following three operators are constants of the motion [13–15]:

$$\hat{T}_1 = \frac{1}{2}(\hat{x}\hat{y} + \hat{p}_x\hat{p}_y), \tag{16}$$

$$\hat{T}_2 = \frac{1}{2}(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x), \tag{17}$$

$$\hat{T}_3 = \frac{1}{4}(\hat{x}^2 - \hat{y}^2 + \hat{p}_x^2 - \hat{p}_y^2). \tag{18}$$

They obey the mutual commutation relations

$$[\hat{T}_i,\hat{T}_j] = i\hbar\sum_k \epsilon_{ijk}\hat{T}_k. \tag{19}$$

The operator

$$\hat{T}^2 \equiv \hat{T}_1^2 + \hat{T}_2^2 + \hat{T}_3^2 = \frac{1}{4}(\hat{H}^2 - 1) \tag{20}$$

commutes with each $\hat{T}_i$. It is the Casimir operator of the problem.

The commutation relations show that the operators $\hat{T}_1$, $\hat{T}_2$, and $\hat{T}_3$ are the generators of an SU(2) Lie algebra. This is the algebra which is so familiar from angular-momentum theory [16]. The possible eigenvalues of $\hat{T}^2$ are $j(j+1)\hbar^2$, where $j=0,\frac{1}{2},1,\frac{3}{2},\ldots$. For a fixed value of j, the possible eigenvalues of a preferred $\hat{T}_k$ $(k=1,2,3)$ are $m\hbar$, with $m=j,j-1,\ldots,-j$. Thus the degeneracy in j is $2j+1$. This is also the degeneracy of the energy levels. Equation (20) shows that $j(j+1)\hbar^2=\frac{1}{4}(E^2-1)$, from which we get that

$$E_j=(2j+1)\hbar, \quad j=0,\frac{1}{2},1,\frac{3}{2},\ldots . \tag{21}$$

Let us now consider the state operator corresponding to selected values of j and m, with $m\hbar$ being the eigenvalue of $\hat{T}_k$. The only operators that commute with this state operator are $\hat{H}$ and $\hat{T}_k$. Hence, the state operator must be a function of those two operators. In light of the discussion in Sec. II, we expect the corresponding Wigner function to be a function of the phase-space representatives of $\hat{H}$ and $\hat{T}_k$. We denote the phase-space functions corresponding to $\hat{H}$, $\hat{T}_1$, $\hat{T}_2$, and $\hat{T}_3$ by t_0, t_1, t_2, and t_3, respectively, and find easily that each t_k originates from the expression for the corresponding operator by simply removing the operator symbols.

Assume now that F is an arbitrary function of t_0 and a preferred t_k. We then find, after some tedious algebra, in which the derivatives with respect to x, y, p_x, and p_y are converted to derivatives with respect to t_0 and t_k,

$$t_0 * F = t_0F-\frac{\hbar^2}{4}\left[2\frac{\partial F}{\partial t_0}+t_0\left(\frac{\partial^2 F}{\partial t_0^2}+\frac{1}{4}\frac{\partial^2 F}{\partial t_k^2}\right)+2t_k\frac{\partial^2 F}{\partial t_0\,\partial t_k}\right], \tag{22}$$

$$t_k * F = t_kF-\frac{\hbar^2}{16}\left[2\frac{\partial F}{\partial t_k}+t_k\left(4\frac{\partial^2 F}{\partial t_0^2}+\frac{\partial^2 F}{\partial t_k^2}\right)+2t_0\frac{\partial^2 F}{\partial t_0\,\partial t_k}\right]. \tag{23}$$

These equations show that t_0*F and t_k*F are ordinary functions of t_0 and t_k whenever F is. We may accordingly conclude that the above Wigner function is in fact an ordinary function of t_0 and t_k. We shall now determine its analytical form by solving the dynamical equations corresponding to Eqs. (8) and (9). We have that the state operator $\hat{\rho}$ leading to W is a function of $\hat{H}$ and $\hat{T}_k$, while the operator $\hat{A}$ leading to a is either $\hat{H}$ or $\hat{T}_k$. Then $\hat{A}$ and $\hat{\rho}$ commute and the second equation is automatically satisfied. But with that equation satisfied, the first equation reads $a(\hat{Q},\hat{P})W(q,p)=\alpha W(q,p)$ or $a(q,p)*W(q,p)=\alpha W(q,p)$.

Let us now use the above expressions to determine the Wigner function W_{jm} corresponding to the eigenvalues $\epsilon\hbar$ and $m\hbar$ for the Hamiltonian and the operator $\hat{T}_k$, respectively, with $|m|\leq j$. The eigenvalue equations are

$$t_0 * W=\epsilon\hbar W, \quad t_k * W = m\hbar W, \tag{24}$$

that is,

$$-\frac{\hbar^2}{4}\left[2\frac{\partial W}{\partial t_0}+t_0\left(\frac{\partial^2 W}{\partial t_0^2}+\frac{1}{4}\frac{\partial^2 W}{\partial t_k^2}\right)+2t_k\frac{\partial^2 W}{\partial t_0\,\partial t_k}\right]+t_0W=\epsilon\hbar W, \tag{25}$$

$$-\frac{\hbar^2}{16}\left[2\frac{\partial W}{\partial t_k}+t_k\left(4\frac{\partial^2 W}{\partial t_0^2}+\frac{\partial^2 W}{\partial t_k^2}\right)+2t_0\frac{\partial^2 W}{\partial t_0\,\partial t_k}\right]+t_kW=m\hbar W. \tag{26}$$

To solve these equations, we introduce the different variables $u=(2t_0+4t_k)\hbar$ and $v=(2t_0-4t_k)/\hbar$ and separate variables by writing $W(u,v)=W_1(u)W_2(v)$. The equations for W_1 and W_2 are

$$u\frac{\partial^2 W_1}{\partial u^2}+\frac{\partial W_1}{\partial u}-\frac{1}{4}uW_1+\frac{\epsilon+2m}{2}W_1=0, \tag{27}$$

$$v\frac{\partial^2 W_2}{\partial v^2}+\frac{\partial W_2}{\partial v}-\frac{1}{4}vW_2+\frac{\epsilon-2m}{2}W_2=0. \tag{28}$$

These equations have acceptable solutions when $(\epsilon+2m)/2=n_1+1/2$ and $(\epsilon-2m)/2=n_2+1/2$ with n_1 and n_2 taking the values $0,1,2,\ldots$. The solutions are

$$W_1(u)=\frac{(-1)^{n_1}}{\pi\hbar}L_{n_1}(u)e^{-u/2}, \tag{29}$$

$$W_2(v)=\frac{(-1)^{n_2}}{\pi\hbar}L_{n_2}(v)e^{-v/2}. \tag{30}$$

The admissible values of the energy, $E=\epsilon\hbar$, and the quantum number m become

$$E=(n_1+n_2+1)\hbar, \quad m=(n_1-n_2)/2. \tag{31}$$

By introducing the quantum number j by the definition $j=(n_1+n_2)/2$ we may write the energy as in Eq. (21), that is,

$$E=(2j+1)\hbar, \quad j=0,1/2,1,3/2,\ldots . \tag{32}$$

By combining the functions of Eqs. (29) and (30) we finally get the complete expression for the generic Wigner function,

$$W_{j,m}(t_0,t_k)=\frac{(-1)^{2j}}{\pi^2\hbar^2}L_{j+m}((2t_0+4t_k)/\hbar)\times L_{j-m}((2t_0-4t_k)/\hbar)e^{-2t_0/\hbar} \tag{33}$$

with $k=1,2,3$. We obtain specific expressions by inserting the form of t_0 and t_k for each k.

We first set $k=3$. Substituting $j=(n_1+n_2)/2$ and $m=(n_1-n_2)/2$ leads to the function

$$W_{n_1,n_2}(t_0,t_3)=W_{n_1}(x,p_x)W_{n_2}(y,p_y), \tag{34}$$

where $W_n(x,p)$ is given by Eq. (13). This Wigner function is the product of two Wigner functions corresponding to independent motions in the x and y directions. It is, of course, well known that the Hamiltonian of Eq. (15) allows us to separate the x and y variables. The position-space wave function in the Schrödinger picture is

$$\Psi_{n_1 n_2}(x,y) = \psi_{n_1}(x)\psi_{n_2}(y), \tag{35}$$

with ψ_n as given by Eq. (12).

The $k=1$ case is found to be completely analogous to the $k=3$ case, but the separation of variables must be performed in a coordinate system obtained by rotating the original system through an angle of $\pi/4$. The $k=2$ case is different, however. The function $2t_2 = xp_y - yp_x$ is the angular momentum of the system. In the Schrödinger picture, the motion separates in polar coordinates, $(x,y) = r(\cos\varphi, \sin\varphi)$. The position-space wave function is eigenfunction of the Hamiltonian and the angular-momentum operator $2\hat{T}_2$, where $\hat{T}_2$ is given by Eq. (17). It has the form [17]

$$\Psi_{jm}(r,\varphi) = \left\{ \frac{1}{\pi\hbar} \frac{(j-|m|)!}{(j+|m|)!} \right\}^{1/2} \left(\frac{r}{\sqrt{\hbar}} \right)^{2|m|} \times L_{j-|m|}^{2|m|}\left(\frac{r^2}{\hbar} \right) e^{-r^2/2\hbar} e^{2im\varphi}. \tag{36}$$

The two wave functions, $\Psi_{n_1 n_2}(x,y)$ of Eq. (35) and $\Psi_{jm}(r,\varphi)$ of Eq. (36), corresponding to two different separations of variables, look quite different. Yet the Wigner functions are similar. This surprising similarity was first recognized by Simon and Agarwal [18]. They connected the $k=2$ and $k=3$ cases by performing intelligent rotations in phase space.

IV. CONCLUSIONS

The two-dimensional isotropic harmonic oscillator appears in many areas of chemistry and physics. Its stationary states are highly degenerate. Hence a specific function is defined not only by its energy, but also by the values of other constants of the motion. We have shown that not only are the Wigner functions parametrized by the energy and the other constants of the motion, they are genuine functions of them. This has allowed us to derive one generic expression for all stationary-state Wigner functions. Inserting the form of the different constants of the motion into this expression leads to specific Wigner functions. A brief look at the Schrödinger wave functions for the stationary states shows that they are much less suited to give a united picture of this complex system.

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