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Phase-space formulation of quantum mechanics under phase-space transformations: Wigner functions of an oscillator system in crossed magnetic and electric fields

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(Received 29 September 1989)

We give a rigorous proof for the following result that combines those discussed earlier by Krüger and Poffyn [Physica 85A, 84 (1976)] and by Springborg [J. Phys. A 16, 535 (1983)]. The Wigner correspondence of a quantum operator can be obtained by simple substitutions under an arbitrary linear phase-space transformation. This property cannot be generalized to any other transformations or rules of phase-space correspondence. As an application of this result, the Wigner distribution functions of an anisotropic harmonic-oscillator system in crossed magnetic and electric fields are obtained.

I. INTRODUCTION

A. Brief review of the phase-space representation of quantum mechanics

Wigner proposed a quantum distribution function

\[ P^{(w)}(q,p) = \frac{1}{(2\pi)^n} \int d^n\psi^*(q+y)\psi(q-y)e^{2ip\cdot y/n} \]

(1)

for a pure state described by wave function \( \psi(q) \), where \( n \) is the number of dimensions, \( d^n y = dy_1 \cdots dy_n \), \( y_1, \ldots, y_n \) are the components of \( y \), and likewise for other vectors. It is a real function and satisfies the following properties that are usually required for probability distributions:

\[ \int d^n p P^{(w)}(q,p) = |\psi(q)|^2, \]

(2a)

\[ \int d^n q P^{(w)}(q,p) = |\phi(p)|^2, \]

(2b)

with

\[ \phi(p) = (2\pi)^{-n/2} \int d^n q e^{iq\cdot p/n}\psi(q), \]

(2c)

and

\[ \int d^n q d^n p P^{(w)}(q,p) = 1. \]

(2d)

The range of integration in this paper is always from \(-\infty \) to \(+\infty \). For clearness we use a hat to denote an operator. If one associates a Wigner correspondence

\[ A^{(w)}(q,p) = \int d^n z e^{ip\cdot z/n} \langle q - \frac{1}{2} z | \hat{A} | q + \frac{1}{2} z \rangle \]

(3)

with an arbitrary operator \( \hat{A} \), one can evaluate the quantum-mechanical average of \( \hat{A} \) through a phase-space integration:

\[ \langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle = \int d^n q d^n p P^{(w)}(q,p) A^{(w)}(q,p). \]

(4)

Similar results hold for mixed states. In addition to the Wigner distribution function, other quantum distribution functions (QDF's) have been introduced. For example, there are the Kirkwood \(^5\) (antistandard), the standard-ordered, \(^4\) the Husimi \(^3\) (anti-normal-ordered), the \( P \) (Ref. 6) (normal-ordered), and the symmetric-ordered \(^7\) distribution functions. They can be calculated from each other by differentiations. \(^8\) Each QDF corresponds to a particular rule of associating phase-space functions with quantum-mechanical operators. \(^9\) In general, the superscripts \( (w) \) in Eq. (4) may be replaced by an arbitrary correspondence \( (\Omega) \). \(^10\) A QDF is simply the phase-space correspondence (PSC) of the density operator through the conjugate rule \( (\Omega) \), apart from a factor of \( (2\pi)^{-n} \). \(^1\) The Wigner PSC is the only one that has the property \( \Omega = \Omega = \omega \), i.e., both the Wigner QDF and the Wigner PSC can be obtained from the same Weyl rule. \(^9\)

B. Phase-space transformations

Coordinate transformations are frequently encountered. For instance, as a remarkable development in quantum optics, O'Connell \(^11\) has proposed the use of the Wigner distribution function for squeezed states \(^12\) through coordinate transformations. This idea has been enhanced by other authors and much work has been done in line with this new trend. \(^13\)

Let us now consider an arbitrary phase-space transformation:
\[
q = q(q', p'), \quad p = p(q', p'), 
\]
which is an abbreviation of
\[
q_i = q_i(q^1, \ldots, q^n, p^1, \ldots, p^n), \\
p_i = p_i(q^1, \ldots, q^n, p^1, \ldots, p^n),
\]
where \(i = 1, 2, \ldots, n\). Given the QDF \(P^{(1)}(q, p)\) and the PSC \(A^{(1)}(q, p)\) of an operator \(\hat{A}\) in one phase space \((q, p)\), one may ask the following question: is it true that the QDF \(P^{(1)}(q', p')\) and the PSC \(A^{(1)}(q', p')\) of the operator \(\hat{A}\) in phase space \((q', p')\) can be obtained simply by substituting Eq. \(5\) into \(P^{(1)}(q, p)\) and \(A^{(1)}(q, p)\)? Considering the complexity in the definitions of QDF's and PSC's, the answer is not obvious.

Krüger and Poffyn\textsuperscript{14} have first shown that the answer to the above question is positive only to the Wigner PSC rule when the phase-space transformation considered is one of the Galilean transformations, i.e., rigid displacement, uniform translation, space reflection and rotation. Springborg\textsuperscript{15} has shown that the Wigner PSC rule is the only one to remain invariant after a canonical phase-space transformation. But further restrictions on the canonical transformation, i.e., Eq. \(25\) in Ref. 15, have been used in Springborg’s proof of this result.

We shall prove rigorously in this paper that the invariance of any given QDF and PSC is guaranteed only in the case where the Wigner PSC rule is used \((\Omega = u)\) and the transformation is a linear transformation, i.e.,
\[
\left[ \begin{array}{c} q \\ p \end{array} \right] = \left[ \begin{array}{cc} a & b \\ c & d \end{array} \right] \left[ \begin{array}{c} q' \\ p' \end{array} \right] + \left[ \begin{array}{c} e \\ f \end{array} \right],
\]
where \(a, b, c, d\) are \(n \times n\) matrices. This result combines those discussed in Refs. 14 and 15 [i.e., rigid displacement \(e\), uniform translation \(f\), and canonical transformations including reflection and rotation given by the \(2n \times 2n\) matrix in Eq. \(25\)].

C. Oscillator systems in crossed \(E\) and \(B\) fields

As an application of the general discussions on phase-space transformations, we shall derive the Wigner distribution functions in different phase spaces for an anisotropic harmonic-oscillator system in crossed magnetic and electric fields, where coordinate transformations are necessary. There are two additional reasons for these derivations.

First of all, the model is a few exactly soluble models and has enjoyed enormous applications in both physics and physical chemistry.\textsuperscript{16-26} The Schrödinger equations for both isotropic and anisotropic harmonic oscillators either without or with magnetic field have been solved exactly for some time.\textsuperscript{19-22} Recently there has been renewed interest in various questions related to the harmonic oscillator. In particular, the Bloch density matrix,\textsuperscript{23} the propagator,\textsuperscript{24} the lattice effect\textsuperscript{25} of a harmonic oscillator in a magnetic field, as well as the free energy of a Fermionic ensemble of such systems,\textsuperscript{26} have been evaluated exactly. Hence derivations of the Wigner distribution functions for an anisotropic oscillator system in crossed magnetic and electric fields can be considered as a supplement to the works mentioned above.

Secondly, there have been extensive applications of quantum distribution functions and the Wigner-Kirkwood expansions in physics and physical chemistry.\textsuperscript{27} In particular, Dickman and O’Connell\textsuperscript{27(k)} have recently developed a useful perturbation expansion for quantum correlation functions via Wigner distribution functions (WDF’s), for a system with Hamiltonian \(H = H_0 + \lambda H'\), where the WDF corresponding to \(H_0\) is known exactly. This formulation has been applied to calculate phonon frequency shifts in an anharmonic lattice, where \(H_0\) is a harmonic-oscillator Hamiltonian, in the absence of external fields.\textsuperscript{27(k)} Hence the present work is needed for a possible generalization of the Dickman-O’Connell expansion to include electric and magnetic fields.

II. QUANTUM DISTRIBUTION FUNCTIONS AND PHASE-SPACE CORRESPONDENCES UNDER PHASE-SPACE TRANSFORMATIONS

We start by considering a definition for the Wigner PSC that is equivalent to Eq. \(3\). For an operator in the following Weyl form:\textsuperscript{1,2}
\[
\hat{A} = \hat{A}(\hat{q}, \hat{p}) = \int d\sigma d\tau e^{i/\hbar (\sigma \hat{q} + \tau \hat{p})} \alpha(\sigma, \tau),
\]
its Wigner PSC is simply
\[
A^{(1)}(q, p) = \int d\sigma d\tau e^{i/\hbar (\sigma q + \tau p)} \alpha(\sigma, \tau).
\]
Here \(\alpha(\sigma, \tau)\) is frequently called the characteristic function. After phase-space transformation given by Eq. \(25\), the operator \(\hat{A}\) becomes
\[
\hat{A} = \hat{A}(\hat{q}', \hat{p}') = \int d\sigma' d\tau' e^{i/\hbar (\sigma' \hat{q}' + \tau' \hat{p}')} \alpha'(\sigma', \tau'),
\]
where we have defined
\[
\left[ \begin{array}{c} \sigma' \\ \tau' \end{array} \right] = \left[ \begin{array}{cc} \sigma \\ \tau \end{array} \right] = \left[ \begin{array}{cc} a & c \\ b & d \end{array} \right] \left[ \begin{array}{c} \sigma \\ \tau \end{array} \right],
\]
\[a' = \begin{vmatrix} a & c \\ b & d \end{vmatrix}^{-1} \left[ \begin{array}{c} \sigma' \\ \tau' \end{array} \right],
\]
and
\[
\alpha'(\sigma', \tau') = \alpha(\sigma(\sigma', \tau'), \tau(\sigma', \tau')) |J| \times e^{i/\hbar (\sigma(\sigma', \tau') \sigma + \tau(\sigma', \tau') \tau + f)},
\]
where \(|J|\) is the Jacobian determinant of the transformation given in Eq. \(25\).

Since Eq. \(10\) is still in the form of Eq. \(8\), the Wigner PSC of operator \(\hat{A}\) in phase space \((q', p')\) is therefore, according to Eq. \(9\),
$$\mathcal{A}^{(\omega)}(q',p') = \int d^n\sigma d^n\tau e^{i/\hbar(\sigma q' + \tau p')} \alpha(\sigma',\tau') \mathcal{A}^{(\omega)}(q,p)$$

$$= \mathcal{A}^{(\omega)}(q'q',p'p')$$

Hence we have proven that the Wigner PSC of an operator in a new phase space after a transformation can be obtained from that in the original phase space by a simple substitution [see Eq. (13)] provided the transformation is a linear one.

It is easy to see from the above proof that this result does not hold for any nonlinear phase-space transformations. For correspondence rules other than the Wigner one, the PSC can be calculated from the Wigner PSC (Ref. 10),

$$A^{(\omega)}(q',p') = \gamma^{(\omega)}(q,p) A^{(\omega)}(q,p)$$

$$= \int d^n\sigma d^n\tau e^{i/\hbar(\sigma q' + \tau p')} \alpha(\sigma',\tau') \gamma^{(\omega)}(\sigma',\tau') .$$

where in the second equality we have used Eq. (13). Comparing Eqs. (17) and (19), since \( \gamma^{(\omega)} \neq \gamma^{(\omega)} \), if \( \gamma^{(\omega)} \neq 1 \), which can be readily checked out through the example given by Eq. (15), we conclude

$$A^{(\omega)}(q',p') \neq A^{(\omega)}(q'q',p'p')$$

if \( \gamma^{(\omega)} \neq 1 \) (or \( \Omega \neq w \)).

In other words, the Wigner PSC rule is the only one with the property that under linear phase-space transformation the PSC can be obtained through a simple substitution [see Eq. (13)].

We comment that a conclusion has been reached in Ref. 15 that the Wigner PSC rule and QDF are the only ones to remain invariant under canonical phase-space transformations, which is a special class of linear transformations; however, the proof given in Ref. 15 for the inequality stated by our Eq. (20) makes explicit use of a particular canonical transformation, i.e., \( q' = p \) and \( p' = -q \), as well as the properties of the eigenstates of coordinate and momentum operators. A direct generalization of this proof to the case of an arbitrary canonical transformation does not seem obvious.

III. WIGNER DISTRIBUTION FUNCTIONS
OF AN OSCILLATOR SYSTEM IN CROSSED FIELDS

As an application of the general discussions in Sec. II, we derive the Wigner distribution functions for a harmonic-oscillator system in crossed magnetic and electric fields, where phase-space transformations are unavoidable.

A. Phase-space transformations

The Hamiltonian that we work with is

$$\hat{H} = \frac{1}{2M} \left( \hat{\mathbf{p}} - \frac{e}{c} \mathbf{A} \right)^2 + \frac{1}{2} M (\omega_1^2 \hat{\mathbf{r}}^2 + \omega_2^2 \hat{\mathbf{y}}^2 + \omega_3^2 \hat{\mathbf{z}}^2)$$

$$- e (E_x \hat{\mathbf{r}} + E_y \hat{\mathbf{y}} + E_z \hat{\mathbf{z}}) ,$$

where \( M \) and \( e \) are the mass and charge of the particle, which has been assumed to be spinless. We have chosen the direction of the magnetic field as the \( \mathbf{Z} \) direction and

$$\mathbf{A} = B \left( -\omega_2 y + \omega_1 x \right)/(\omega_1 + \omega_2) .$$

We can simplify the Hamiltonian (21) by the following definitions:

$$\hat{x} = \hat{\mathbf{r}} - \frac{eE_1}{M\omega_1^2}$$

$$\hat{y} = \hat{\mathbf{y}} - \frac{eE_2}{M\omega_2^2}$$

$$\hat{z} = \hat{\mathbf{z}} - \frac{eE_3}{M\omega_3^2} ,$$

For instance, for the standard-ordering rule

$$\gamma^{(\omega)}(\sigma,\tau) = e^{-i\hbar \sigma \cdot \tau / 2} ,$$

and

$$A^{(\omega)}(q,p) = \exp \left[ \frac{i\hbar}{2} \frac{\partial^2}{\partial q \partial p} \right] A^{(\omega)}(q,p) .$$

Substituting Eq. (7) into Eq. (14), we obtain

$$A^{(\omega)}(q',p',p(q',p')) = \int d^n\sigma d^n\tau e^{i/\hbar(\sigma q' + \tau p')} \alpha(\sigma',\tau') \gamma^{(\omega)}(\sigma',\tau') ,$$

where we have defined

$$\gamma^{(\omega)}(\sigma',\tau') = \gamma^{(\omega)}(\sigma(\sigma',\tau'),\tau(\sigma',\tau') .$$

However, by definition [Eq. (14)], the \( \Omega \) PSC of operator \( A \) in the new representation should be
\[ \hat{p} = \hat{p}_x i + \hat{p}_y j + \hat{p}_z k = \hat{P} \]  
(23b)

The Hamiltonian now takes the form
\[ \hat{H} = \frac{1}{2M} \left( \hat{p} - \frac{e}{c} \mathbf{A} \right)^2 + \frac{1}{2} M (\omega_1^2 \hat{q}_1^2 + \omega_2^2 \hat{q}_2^2 + \omega_3^2 \hat{q}_3^2) - \epsilon_0 , \]
(24)

where
\[ \epsilon_0 = \frac{e^2}{2M} \left( \frac{E_1}{\omega_1} \right)^2 + \frac{1}{2} \left( \frac{E_2}{\omega_2} \right)^2 + \left( \frac{E_3}{\omega_3} \right)^2 . \]
(25)

The Hamiltonian given in Eq. (24) can be diagonalized through the two transformations used by Datta and Richardson. The first one is the standard definition for the annihilation operators:
\[ \hat{a} = \left( \frac{M \omega_x}{2\hbar} \right)^{1/2} \hat{x} + i (2M \hbar \omega_x)^{-1/2} \hat{p}_x , \]
(26)
and
\[ \hat{b} = \left( \frac{M \omega_y}{2\hbar} \right)^{1/2} \hat{y} + i (2M \hbar \omega_y)^{-1/2} \hat{p}_y , \]
(27)

where
\[ \omega_x = K \omega_1, \quad \omega_y = K \omega_2, \]
(28)
\[ K = \left[ 1 + 4 \omega_1^2 / (\omega_1 + \omega_2)^2 \right]^{1/2}, \]
(29)
\[ \omega_L = eB / 2Mc \quad \text{(Larmor frequency)} . \]
(30)

After this transformation, the Hamiltonian consists of diagonal terms \( \hat{a} \hat{a}^\dagger \) and \( \hat{b} \hat{b}^\dagger \) and crossing terms of the form \( \hat{a} \hat{b}^\dagger \) or \( \hat{b} \hat{a}^\dagger \). To eliminate the latter, Datta and Richardson used another transformation,\(^{22}\) which we note is identical to a prescription in the theory of antiferromagnetism:  
\[ \hat{\alpha} = (\cos \phi) \hat{a} - i (\sin \phi) \hat{b} , \]
(31)
and
\[ \hat{\beta} = (\sin \phi) \hat{a} + i (\cos \phi) \hat{b} , \]
(32)

where
\[ \tan \phi = \left( 16 \omega_1^2 \omega_x \omega_y \right)^{-1/2} \left\{ \left( \omega_x^2 - \omega_y^2 \right)^2 + 16 \omega_1^2 \omega_x \omega_y \right\}^{1/2} \]
(33)

The operators thus defined obey the following commutation relations:\(^{22}\)
\[ [\hat{a}, \hat{a}^\dagger] = [\hat{b}, \hat{b}^\dagger] = [\hat{a}, \hat{b}^\dagger] = [\hat{a}^\dagger, \hat{b}] = 1 , \]
(34)
and
\[ [\hat{a}, \hat{b}] = [\hat{a}, \hat{b}^\dagger] = [\hat{a}^\dagger, \hat{b}] = [\hat{a}^\dagger, \hat{b}^\dagger] = 0 . \]
(35)

The Hamiltonian is now simply
\[ \hat{H} = \hat{H}_1 + \hat{H}_3 - \epsilon_0 , \]
(36)
with
\[ \hat{H}_1 = (\hat{a}^\dagger \hat{a} + \hat{b}^\dagger \hat{b} + \hat{\alpha}^\dagger \hat{\alpha})/2 + (\hat{\alpha}^\dagger \hat{\alpha} + \hat{\beta}^\dagger \hat{\beta})/2 \]
(37)

\[ \hat{H}_3 = \frac{\hat{p}_z^2}{2M} + \frac{\omega_L^2 \omega_z^2}{2M} \]
(38)

and
\[ \hat{H}_3 = (\hat{\alpha}^\dagger \hat{\alpha} + \hat{\beta}^\dagger \hat{\beta} + \hat{\alpha}^\dagger \hat{\beta})/2 \]
(39)

The energy spectrum is
\[ \epsilon_{mn} = (l + \frac{1}{2}) \hbar \Omega_\alpha + (m + \frac{1}{2}) \hbar \Omega_\beta + (n + \frac{1}{2}) \hbar \Omega_3 - \epsilon_0 , \]
(40)

where \( l, m, \) and \( n \) can be 0, 1, 2, . . . .

In order to derive the WDF's, we wish to use coordinates and momenta (phase space) instead of annihilation and creation operators. We now introduce a new set of operators \( \hat{x}', \hat{p}_x, \hat{y}', \) and \( \hat{p}_y \) by
\[ \hat{a} = \left( \frac{M \Omega_\alpha}{2\hbar} \right)^{1/2} \hat{x}' + i (2M \hbar \Omega_\alpha)^{-1/2} \hat{p}_x' , \]
(42a)
and
\[ \hat{b} = \left( \frac{M \Omega_\beta}{2\hbar} \right)^{1/2} \hat{y}' + i (2M \hbar \Omega_\beta)^{-1/2} \hat{p}_y' . \]
(42b)

By making use of Eqs. (34) and (35), we can verify the following commutation rules obeyed by those new operators:
\[ \hat{x}' = \hat{a}^\dagger \hat{a} \quad \hat{y}' = \hat{b}^\dagger \hat{b} \]
(43a)
and
\[ \hat{x}' = \hat{a} \quad \hat{y}' = \hat{b} . \]
(43b)

Furthermore, we are able to show that those new operators are Hermitian. To achieve this purpose, we obtain the relationship between \( \hat{x}', \hat{p}_x, \hat{y}', \) and \( \hat{p}_y \) by substituting (26) and (27) into (31) and (32), then comparing with (42). We find
\[ \hat{x}' = (\cos \phi) \hat{x} + \left( \frac{\omega_x}{\Omega_\alpha} \right)^{1/2} \hat{p}_x + \frac{\sin \phi}{M} \left( \frac{\omega_x \Omega_\alpha}{\omega_x} \right)^{1/2} \hat{p}_y , \]
(44)
\[ \hat{p}_x' = (\cos \phi) \hat{p}_x - \frac{\sin \phi}{M} \left( \frac{\omega_x \Omega_\alpha}{\omega_x} \right)^{1/2} \hat{p}_y , \]
(45)
\[ \hat{y}' = (\sin \phi) \hat{y} - \left( \frac{\omega_y}{\Omega_\beta} \right)^{1/2} \hat{p}_x + \frac{\cos \phi}{M} \left( \frac{\omega_y \Omega_\beta}{\omega_y} \right)^{1/2} \hat{p}_y , \]
(46)
\[ \hat{p}_y' = (\sin \phi) \hat{p}_y + \frac{\cos \phi}{M} \left( \frac{\omega_y \Omega_\beta}{\omega_y} \right)^{1/2} \hat{p}_x . \]
(47)

It is therefore transparent that \( \hat{x}', \hat{p}_x, \hat{y}', \) and \( \hat{p}_y' \) are indeed Hermitian operators, which, in combination with
Eq. (43), enables us to conclude that \(\hat{x}', \hat{p}_x, \hat{y}', \hat{p}_y\) are coordinate and momentum operators.

In the light of the above results, it is readily proven that the Hamiltonian can now be cast into that of an anisotropic harmonic oscillator, with nature frequencies \(\Omega_\alpha, \Omega_\beta\) and \(\omega_3\), in the absence of external fields:

\[
\hat{H} = \frac{1}{2M}(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2)
+ \frac{1}{2}M(\Omega_\alpha^2 \hat{x}^2 + \Omega_\beta^2 \hat{y}^2 + \omega_3^2 \hat{z}^2) - \epsilon_0 .
\]

(48)

B. Wigner distribution functions

The Wigner distribution functions for the pure state corresponding to the eigenenergy given by Eq. (41) in the representation of \((x', y', z)\) can be readily deduced from that in the absence of external fields:

\[
P_m(x', y', z, \hat{p}_x, \hat{p}_y, \hat{p}_z) = P_m(x', \hat{p}_x, \Omega_\alpha)P_m(y', \hat{p}_y, \Omega_\beta)P_m(z, \hat{p}_z, \omega_3),
\]

(49)

where

\[
P_m(q, p, \omega) = \frac{1}{\pi \hbar} (-1)^n e^{-2H/\hbar \omega} L_n(4H/\hbar \omega),
\]

(50)

\[
H = p^2/2M + M\omega_3^2 \hat{z}^2/2,
\]

(51)

and \(L_n\) is the \(n\)th Laguerre polynomial.

Similarly, we generalize the WDF for an ensemble of oscillators at temperature \(T\) without external fields\(^{30}\) to our present case, i.e., with crossed magnetic and electric fields:

\[
\Lambda'(x', y', z, \hat{p}_x, \hat{p}_y, \hat{p}_z) = \Lambda(x', \hat{p}_x, \Omega_\alpha)\Lambda(y', \hat{p}_y, \Omega_\beta)\Lambda(z, \hat{p}_z, \omega_3),
\]

(52)

where

\[
\Lambda(q, p, \omega) = \text{sech}(\hbar \omega \beta/2)
\times \exp[-(2H/\hbar \omega) \tanh(\hbar \omega \beta/2)],
\]

(53)

and \(\beta = 1/kT\) is the inverse temperature.

We note that the WDF given by (52) and (53) is not normalized. Instead,

\[
P_T(x', y', z, \hat{p}_x, \hat{p}_y, \hat{p}_z) = [(2\pi \hbar)^3 Z(\beta)]^{-1/2} \Lambda'(x', y', z, \hat{p}_x, \hat{p}_y, \hat{p}_z)
\]

(54)

satisfies

\[
\int dx'dy'dz \ dp_x dp_y dp_z P_T(x', y', z, \hat{p}_x, \hat{p}_y, \hat{p}_z) = 1 .
\]

(55)

Here the partition function of the system is obtained by a phase-space integration:

\[
Z(\beta) = \text{Tr}(e^{-\beta \hat{H}})
= (2\pi \hbar)^{-3} \int dx'dy'dz \ dp_x dp_y dp_z \times \Lambda'(x', y', z, \hat{p}_x, \hat{p}_y, \hat{p}_z)
= Z(\beta, \Omega_\alpha)Z(\beta, \Omega_\beta)Z(\beta, \omega_3),
\]

(56)

where

\[
Z(\beta, \omega) = \left[ 2 \sinh \left( \frac{\hbar \omega \beta}{2} \right) \right]^{-1} .
\]

(57)

One of the important applications of WDF’s is to calculate quantum-mechanical averages through classical phase-space integrations.\(^{27}\) This approach is especially powerful in the case of mixed states when the infinite summation over all quantum states cannot be performed easily, whereas an approximate form for the WDF, e.g., the Wigner-Kirkwood expansion, can be obtained. In this section we present a simple demonstration of applications of WDF’s by calculating the mean-squared displacement \(\langle \hat{R}^2 \rangle = \langle \hat{X}^2 + \hat{Y}^2 + \hat{Z}^2 \rangle\) by using the WDF’s derived. We take the inverse of Eqs. (44)–(47) as follows:

\[
\hat{X} = (\cos \phi) \left( \frac{\Omega_\alpha}{\omega_x} \right)^{1/2} \hat{x}' + (\sin \phi) \left( \frac{\Omega_\beta}{\omega_x} \right)^{1/2} \hat{y}',
\]

(58)

\[
\hat{p}_x = (\cos \phi) \left( \frac{\omega_x}{\Omega_\alpha} \right)^{1/2} \hat{p}_x' + (\sin \phi) \left( \frac{\omega_x}{\Omega_\beta} \right)^{1/2} \hat{p}_y',
\]

(59)

\[
\hat{Y} = -\sin \phi \left( \frac{\Omega_\alpha \omega_y}{M} \right)^{-1/2} \hat{p}_x' + \frac{\cos \phi \Omega_\beta}{M} \left( \Omega_\beta \omega_y \right)^{-1/2} \hat{p}_y',
\]

(60)

\[
\hat{p}_y = (\sin \phi) \left( \frac{\Omega_\alpha \omega_y}{M} \right)^{1/2} \hat{x}' - (\cos \phi) \left( \frac{\Omega_\beta \omega_y}{M} \right)^{1/2} \hat{y}'.
\]

(61)

By also using Eq. (23a), we obtain

\[
\langle \hat{R}^2 \rangle_T = \text{Tr}(e^{-\beta \hat{R}^2})
= \langle \hat{R}^2 \rangle + L^2,
\]

(62)

where

\[
\langle \hat{R}^2 \rangle_T = \frac{1}{2 \tanh(\beta \hbar \Omega_\alpha/2)} \left[ \cos^2 \phi \left( \frac{\hbar}{M \omega_x} \right) + \sin^2 \phi \left( \frac{\hbar}{M \omega_y} \right) \right]
+ \frac{1}{2 \tanh(\beta \hbar \Omega_\beta/2)} \left[ \sin^2 \phi \left( \frac{\hbar}{M \omega_x} \right) + \cos^2 \phi \left( \frac{\hbar}{M \omega_y} \right) \right]
+ \frac{1}{2 \tanh(\beta \hbar \omega_3/2)} \left( \frac{\hbar}{M \omega_3} \right),
\]

(63a)

and

\[
L^2 = \frac{E}{M} \left[ \frac{E_1}{\omega_1^2} + \frac{E_2}{\omega_2^2} + \frac{E_3}{\omega_3^2} \right].
\]

(63b)
We denote phase spaces $(X, Y, Z, P_X, P_Y, P_Z)$, $(x, y, z, p_x, p_y, p_z)$, and $(x', y', z', p_{x'}, p_{y'}, p_{z'})$ by $\Delta$, $\delta$, and $\delta'$, respectively. In other words, the transformation combining Eqs. (23), (44)–(47) can be expressed by

$$\delta' = \delta'\left(\delta(\Delta)\right).$$

(64)

So far we obtained the WDF's in the $\delta'$ coordinate. Since the transformation is linear, the general result obtained in Sec. II enables us to conclude that the WDF's and the Wigner correspondence in the $\Delta$ representation, which is the original real coordinate, can be derived from those in the $\delta'$ representation, i.e., $P'$ and $A'$, simply by substituting (64):

$$P'(X, Y, Z, P_X, P_Y, P_Z) = P'_0(\delta'(\delta(\Delta))),$$

(65)

$$A'(X, Y, Z, P_X, P_Y, P_Z) = A'(\delta'(\delta(\Delta))).$$

(66)

In (65) the subscript $o$ may be $lmn$ (pure state) or $T$ (canonical ensemble).

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28. The vector potential given by Eq. (9) of Ref. 22 is erroneous.