PAPERS | OCTOBER 01 2008

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William B. Case

Am. J. Phys. 76, 937–946 (2008)
https://doi.org/10.1119/1.2957889

Wigner functions and Weyl transforms for pedestrians

William B. Case[a)]
Department of Physics, Grinnell College, P.O. Box 805, Grinnell, Iowa 50112

(Received 28 February 2007; accepted 24 June 2008)

Wigner functions and Weyl transforms of operators offer a formulation of quantum mechanics that is equivalent to the standard approach given by the Schrödinger equation. We give a short introduction and emphasize features that give insight into the nature of quantum mechanics and its relation to classical physics. A careful discussion of the classical limit and its difficulties is also given. The discussion is self-contained and includes complete derivations of the results presented.

[DOI: 10.1119/1.2957889]

I. INTRODUCTION: WHY WIGNER FUNCTIONS?

In the standard formulation of quantum mechanics the probability density $\rho(x)$ in position space x is given by the square of the magnitude of the wave function, $\rho(x)=|\psi(x)|^2$. Thus knowing $\psi(x)$ it is easy to visualize the distribution $\rho(x)$. Obtaining the distribution in momentum p is also straightforward. The wave function in p is found by

$$\varphi(p)=\frac{1}{\sqrt{h}}\int e^{-ixp/\hbar}\psi(x)dx=\langle p|\psi\rangle, \tag{1}$$

where all integrations are understood to be over the entire space. The quantity $|\varphi(p)|^2$ gives the probability density in the momentum variable. Although straightforward, the momentum distribution is difficult to visualize if one only has $\psi(x)$. It would be desirable to have a function that displays the probability distribution simultaneously in the x and p variables. The Wigner function, introduced by Wigner in 1932,[1] does just that. Wigner's original goal was to find quantum corrections to classical statistical mechanics where the Boltzmann factors contain energies which in turn are expressed as functions of both x and p. As is well known from the Heisenberg uncertainty relation, there are constraints on this distribution and thus on the Wigner function.

Another reason for a representation of a quantum state in phase space is to examine the connection between quantum and classical mechanics. Quantum mechanics inherently deals with probabilities, while classical mechanics deals with trajectories in phase space. If we wish to compare the two, we can consider ensembles of trajectories in phase space for the classical case and density distributions in x and p or Wigner functions for the quantum case.

Given the wave function ψ the standard way to obtain the expectation value of a quantity A is by

$$\langle A\rangle=\int\psi^*(x)\hat{A}\psi(x)dx=\langle\psi|\hat{A}|\psi\rangle, \tag{2}$$

where $\hat{A}$ is the operator corresponding to A. The operator $\hat{A}$ is a function of the position and momentum operators $\hat{x}$ and $\hat{p}$, $\hat{A}=A(\hat{x},\hat{p})$. We would like to think of the state $\psi(x)$ as describing some probability distribution in phase space, call it $P(x,p)$, which is everywhere positive and such that $\int\int P(x,p)A(x,p)dxdp$ gives the expectation value of $A(x,p)$. In general, it is not possible to find such a probability distribution in quantum mechanics,[2] and so the Wigner function cannot be a simple probability distribution. For this reason, it is often called a quasidistribution. Of course, a simple probability distribution determining expectation values is possible in the classical world.

A main goal of quantum mechanics is to obtain expectation values for physical observables. If the Wigner function is to be a complete formulation of quantum mechanics, it must also be able to reproduce these expectation values of all functions of x and p. When using Wigner functions the expectation values are obtained in conjunction with the closely associated Weyl transforms of the operators corresponding to physical observables. As shown in Sec. IV the correct Weyl transform is critical for obtaining the spread of the energy of a state; without it, the Wigner function is little more than a visual aid for understanding quantum states.

The literature on Wigner functions is extensive. There are several fine review articles[2,3] and chapters in books[4,5] on the Wigner function, Weyl transforms, and related distributions. Several articles on the Wigner function alone without the accompanying Weyl transform have appeared in this journal.[6–8] A paper by Snygg[9] is similar in approach to the present paper, but more formal and abstract. My goal is to give a shorter and more focused presentation of these topics with an eye on the relation between quantum and classical physics. I will also point out a few features that have not been emphasized previously. Special emphasis will also be given to the Wigner–Weyl description's ability to shed light on the classical limit of quantum mechanics.

The Weyl transform and Wigner function are introduced in Sec. II. Other characteristics are examined in Sec. III. Section IV considers the harmonic oscillator as an example and also contains some warnings. In Sec. V we find the time dependence of the Wigner function. Up to this point the presentation is devoted to pure states. Section VI considers the generalization to mixed states. The relation between the Wigner–Weyl formulation and other distributions is also discussed. Section VII examines the classical limit of the Wigner–Weyl description of quantum mechanics. Finally, Sec. VIII discusses the advantages and disadvantages of the Wigner–Weyl description in comparison to the standard Schrödinger equation approach. The Appendix contains a few derivations to allow the main points of the presentation to flow more freely.

II. THE WEYL TRANSFORM AND THE WIGNER FUNCTION

The Weyl transform $\widetilde{A}$ of an operator $\hat{A}$ is defined by[10]

$$\widetilde{A}(x,p) = \int e^{-ipy/\hbar} \langle x + y/2 | \hat{A} | x - y/2 \rangle dy, \tag{3}$$

where the operator has been expressed in the x basis as the matrix $\langle x' | \hat{A} | x \rangle$. The Weyl transform will be indicated by a tilde. The Weyl transform converts an operator into a function of x and p. As shown in the Appendix it can also be expressed in terms of matrix elements of the operator in the momentum basis,

$$\widetilde{A}(x,p) = \int e^{ixu/\hbar} \langle p + u/2 | \hat{A} | p - u/2 \rangle du. \tag{4}$$

A key property of the Weyl transform is that the trace of the product of two operators $\hat{A}$ and $\hat{B}$ is given by the integral over phase space of the product of their Weyl transforms,

$$\mathrm{Tr}[\hat{A}\hat{B}] = \frac{1}{h} \int \int \widetilde{A}(x,p) \widetilde{B}(x,p) dx\, dp. \tag{5}$$

The derivation of Eq. (5) is straightforward, but is left for the Appendix.

To represent the state, we introduce the density operator $\hat{\rho}$. For a pure state $|\psi\rangle$ it is given by

$$\hat{\rho} = |\psi\rangle\langle\psi|, \tag{6}$$

which expressed in the position basis is

$$\langle x | \hat{\rho} | x' \rangle = \psi(x) \psi^*(x'). \tag{7}$$

One of the virtues of the density operator and thus the Wigner function is that it is easily generalized to mixed states. If we form the trace of $\hat{\rho}$ with the operator corresponding to the observable A, we have for the expectation value

$$\mathrm{Tr}[\hat{\rho}\hat{A}] = \mathrm{Tr}[|\psi\rangle\langle\psi|\hat{A}] = \langle\psi|\hat{A}|\psi\rangle = \langle A \rangle. \tag{8}$$

Thus using Eq. (5) we have

$$\langle A \rangle = \mathrm{Tr}[\hat{\rho}\hat{A}] = \frac{1}{h} \int \widetilde{\rho}\widetilde{A} dx\, dp. \tag{9}$$

The Wigner function is defined as

$$W(x,p) = \widetilde{\rho}/h = \frac{1}{h} \int e^{-ipy/\hbar} \psi(x + y/2) \psi^*(x - y/2) dy, \tag{10}$$

and the expectation value of A is given by

$$\langle A \rangle = \int \int W(x,p) \widetilde{A}(x,p) dx\, dp. \tag{11}$$

We see that the expectation value of A has been obtained by what looks like the average of the physical quantity represented by $\widetilde{A}(x,p)$ over phase space with probability density $W(x,p)$ characterizing the state.

If the Wigner function is integrated over p alone and use is made of $\int e^{ipx/\hbar} dp = h\delta(x)$, we have

$$\int W(x,p) dp = \psi^*(x) \psi(x). \tag{12}$$

Equation (12) gives the probability distribution for x. A similar integral over x gives

$$\int W(x,p) dx = \varphi^*(p) \varphi(p). \tag{13}$$

Equation (13) gives the probability distribution for the momentum variable.

Thus we seemed to have achieved our goal. The Wigner function represents the distribution in phase space represented by $\psi(x)$. The projection of $W(x,p)$ onto the x axis gives the probability distribution in x, and the projection on the p axis gives the distribution in p. Expectation values of physical quantities are obtained by averaging $\widetilde{A}(x,p)$ over phase space. We will see that the interpretation of $W(x,p)$ as a simple probability distribution is spoiled by a number of features.

III. CHARACTERISTICS OF THE WEYL TRANSFORMATION AND WIGNER FUNCTION

A direct consequence of the definition of the Wigner function in Eq. (10) is that it is real, as can be seen by taking the complex conjugate of Eq. (10) and changing the variable of integration from y to $-y$.

Using Eq. (4) we can also express the Wigner function in terms of the momentum representation of $|\psi\rangle$,

$$W(x,p) = \widetilde{\rho}/h = \frac{1}{h} \int e^{ixu/\hbar} \langle p + u/2 | \psi \rangle \langle \psi | p - u/2 \rangle du \tag{14a}$$

$$= \frac{1}{h} \int e^{ixu/\hbar} \varphi^*(p + u/2) \varphi(p - u/2) du. \tag{14b}$$

The Weyl transform of the identity operator $\hat{1}$ is 1 because

$$\widetilde{1} = \int e^{-ipy/\hbar} \langle x + y/2 | \hat{1} | x - y/2 \rangle dy$$

$$= \int e^{-ipy/\hbar} \delta(x + y/2 - (x - y/2)) dy = 1. \tag{15}$$

We use Eqs. (15), (10), and (5) and find that

$$\int \int W(x,p) dx dp = \mathrm{Tr}[\hat{\rho}] = 1. \tag{16}$$

Thus $W(x,p)$ is normalized in x,p space. Also from the definition of the density operator we see that for pure states $\hat{\rho}^2 = \hat{\rho}$, and thus $\mathrm{Tr}[\hat{\rho}^2] = \mathrm{Tr}[\hat{\rho}] = 1$. From this relation and Eqs. (5) and (10) we see that

$$\int \int W(x,p)^2 dx\, dp = h^{-1}. \tag{17}$$

The Wigner functions have a reasonable translation property. If the wave function $\psi(x)$ gives the Wigner function $W(x,p)$, then the wave function $\psi(x-b)$ will give $W(x-b,p)$. Shifts in the wave function lead to corresponding shifts in the Wigner function in the position variable x. Also, if the original wave function is replaced with

$\psi(x)\exp(ixb_p/\hbar)$, the new Wigner function becomes $W(x,p-b_p)$. Shifts in momentum of the original wave function lead to corresponding shifts of the Wigner function in the momentum variable p. Both of these properties follow directly from the definition of the Wigner function, Eq. (10). The signs in these shifts might be a little disturbing. If $\psi(x)$ is concentrated about x_0, then $\psi(x-b)$ will be concentrated about x_0+b. If $\psi(x)$ has a certain momentum distribution, then $\psi(x)\exp(ixb_p/\hbar)$ will have the same distribution shifted by $+b_p$. Each of the shifts shift their respective distribution by $+b$ or $+b_p$, respectively.

Consider two density operators, $\hat{\rho}_a$ and $\hat{\rho}_b$, from different states ψ_a and ψ_b, respectively. We can form the combination

$$\mathrm{Tr}[\hat{\rho}_a\hat{\rho}_b] = |\langle\psi_a|\psi_b\rangle|^2. \tag{18}$$

The Weyl transform of Eq. (18) using Eqs. (5) and (10) is

$$\int\int W_a(x,p)W_b(x,p)dx\,dp = h^{-1}|\langle\psi_a|\psi_b\rangle|^2. \tag{19}$$

The product of Wigner functions integrated over phase space is the square of the inner product of the original wave functions divided by h. The left-hand side of Eq. (19) acts as a positive inner product of the original states. If we now consider orthogonal states where $\langle\psi_a|\psi_b\rangle=0$, we have

$$\int\int W_a(x,p)W_b(x,p)dx\,dp = 0. \tag{20}$$

Thus some and indeed most Wigner functions must be negative for some regions of x,p space.

The definition of the Wigner function, Eq. (10), can be expressed as the inner product of two wave functions. First, note that

$$\int \psi(x-y/2)\psi^*(x-y/2)dy$$
$$= 2\int \psi(x-y/2)\psi^*(x-y/2)d(y/2) = 2. \tag{21}$$

Thus we may define the two normalized functions of y, $\psi_1(y)=e^{-ipy/\hbar}\psi(x+y/2)/\sqrt{2}$ and $\psi_2(y)=\psi(x-y/2)/\sqrt{2}$, and express the Wigner function as

$$W(x,p) = (2/h)\int \psi_1(y)\psi_2^*(y)dy. \tag{22}$$

Thus

$$|W(x,p)| \leqslant 2/h, \tag{23}$$

and the distribution $W(x,p)$ cannot take on arbitrarily large values as would be allowed in a classical distribution in phase space. From the definition of the Wigner function in Eq. (10) we see that all even wave functions reach $+2/h$ at $(x,p)=(0,0)$, and all odd wave functions reach $-2/h$ at the same point. Thus a symmetric wave function with widely separated peaks will have a Wigner function with the maximum possible value, $+2/h$, at $(x,p)=(0,0)$. A similar antisymmetric wave function will give $-2/h$ at the same point. The Wigner function will take on these extreme values even if the original wave function is zero in the region of $x=0$.

Given the Wigner function $W(x,p)$ we can recover the original wave function $\psi(x)$.[11] We multiply the definition of the Wigner function in Eq. (10) by $e^{ipx'/\hbar}$ and integrate over p to obtain

$$\int W(x,p)e^{ipx'/\hbar}dp = \psi^*(x-x'/2)\psi(x+x'/2). \tag{24}$$

We set $x=x/2$ and then $x'=x$ in Eq. (24) and recover $\psi(x)$ up to an overall constant with

$$\psi(x) = \frac{1}{\psi^*(0)}\int W(x/2,p)e^{ipx/\hbar}dp. \tag{25}$$

The constant represented by $\psi^*(0)$ can be determined up to a phase by normalization of $\psi(x)$. Note that not all functions of x and p which obey the previously listed constraints given in Eqs. (16), (17), and (23) are acceptable Wigner functions. For pure states a test would be to first use the $W(x,p)$ to find the wave function $\psi(x)$ using Eq. (25). Then use this $\psi(x)$ in Eq. (10) to determine if the original Wigner function $W(x,p)$ is recovered.

Now consider the Weyl transform of the operators corresponding to the observables. Suppose that the operator $\hat{A}$ is only a function of the operator $\hat{x}$, which allows us to write $\hat{A}=A(\hat{x})$. The Weyl transform in this case is particularly simple. From Eq. (3) we have

$$\tilde{A} = \int e^{-ipy/\hbar}\langle x+y/2|\hat{A}(\hat{x})|x-y/2\rangle dy$$
$$= \int e^{-ipy/\hbar}A(x-y/2)\delta(y)dy = A(x). \tag{26}$$

We see that if the operator $\hat{A}$ is purely a function of $\hat{x}$, then its Weyl transform is just the original function with the operator with $\hat{x}$ replaced by x. If we start with an operator dependent only on the momentum operator $\hat{p}$ and Eq. (4), we find a similar result. If the operator $\hat{B}$ is purely a function of $\hat{p}$, then its Weyl transform is simply the original function with the operator with $\hat{p}$ replaced by p. We can extend this argument to sums of operators where each term is purely a function of $\hat{x}$ or $\hat{p}$. Thus the Weyl transform of the Hamiltonian operator $\hat{H}(\hat{x},\hat{p})=\hat{T}(\hat{p})+\hat{U}(\hat{x})$ becomes $H(x,p)=T(p)+U(x)$, where T and U are the kinetic and potential energies. The expectation values of x, p, T, U, and H are given by

$$\langle x\rangle = \int\int W(x,p)x\,dx\,dp, \tag{27a}$$

$$\langle p\rangle = \int\int W(x,p)p\,dx\,dp, \tag{27b}$$

$$\langle T\rangle = \int\int W(x,p)T(p)dx\,dp, \tag{27c}$$

$$\langle U\rangle = \int\int W(x,p)U(x)dx\,dp, \tag{27d}$$

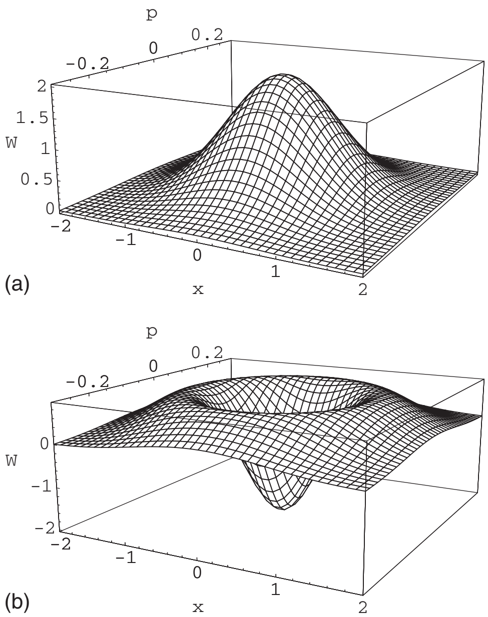

Fig. 1. Plots of the Wigner functions for the two lowest energy states of the harmonic oscillator; (a) $n=0$ and (b) $n=1$. For these plots a and h are set equal to 1.

$$\langle H\rangle = \int\int W(x,p)H(x,p)dx\,dp. \tag{27e}$$

These results could also have been obtained from Eqs. (12) and (13). The Wigner function acts like a probability distribution in phase space except for the fact that W can be negative. The expectation values of other quantities will not be as simple.

IV. AN EXAMPLE: THE HARMONIC OSCILLATOR

We apply the developments in the previous two sections to the harmonic oscillator. Its Hamiltonian and two lowest energy states are given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2, \tag{28}$$

$$\psi_0(x) = \frac{1}{\sqrt[4]{\pi}\sqrt{a}}e^{-x^2/(2a^2)}, \tag{29}$$

$$\psi_1(x) = \frac{1}{\sqrt[4]{\pi}}\sqrt{\frac{2}{a}}\frac{x}{a}e^{-x^2/(2a^2)}, \tag{30}$$

where $a^2=\hbar/(m\omega)$. The corresponding Wigner functions for ψ_0 and ψ_1 can be found using Eq. (10),

$$W_0(x,p) = \frac{2}{h}\exp(-a^2p^2/\hbar^2 - x^2/a^2), \tag{31}$$

$$W_1(x,p) = \frac{2}{h}(-1 + 2(ap/\hbar)^2 + 2(x/a)^2)\exp(-a^2p^2/\hbar^2 - x^2/a^2). \tag{32}$$

Plots of W_0 and W_1 with $a=1$ and $h=1$ are shown in Fig. 1. We see that both functions obey the inequality in Eq. (23). W_0 equals $+2$ at $(x,p)=(0,0)$ and W_1 equals -2 at the same point.

We now take a closer look at the lowest energy state, Eq. (31). The expectation value of the energy can be determined using Eq. (27e), and we find

$$\langle H\rangle = \int\int W_0(x,p)\left(\frac{p^2}{2m} + \frac{m\omega^2x^2}{2}\right)dx\,dp = \frac{\hbar\omega}{2}. \tag{33}$$

Although Eq. (33) is correct, the way it is obtained is a little disturbing. This result should shout out $\hbar\omega/2$ because this value is the only value the energy can take. We would expect all of the nonzero points of the distribution in phase space to lie on an ellipse corresponding to the energy $\hbar\omega/2$. However, the expectation value is obtained by taking an average of combinations of x and p corresponding to different energies with probability $W_0(x,p)$. We would expect such a distribution to imply a spread in energy leaving us with an apparent contradiction. The energy spread Δ is determined by $\Delta^2=\langle H^2\rangle-\langle H\rangle^2$. The second term is $(\hbar\omega/2)^2$; for the first term we must have

$$\langle H^2\rangle = \int\int W_0(x,p)\widetilde{\hat{H}^2}dx\,dp. \tag{34}$$

The Weyl transform of $\hat{H}^2$ will not simply be $H^2(x,p)$ because $\hat{H}^2$ is no longer a sum of terms purely dependent on $\hat{x}$ or $\hat{p}$, but involves cross terms. The Weyl transform is given by

$$\widetilde{\hat{H}^2} = \widetilde{\hat{p}^4}/(2m)^2 + m^2\omega^4\widetilde{\hat{x}^4}/4 + \omega^2(\widetilde{\hat{x}^2\hat{p}^2} + \widetilde{\hat{p}^2\hat{x}^2})/4. \tag{35}$$

The first two terms on the right are $p^4/(2m)^2+m^2\omega^4x^4/4$. The last term is determined with the help of

$$\widetilde{\hat{x}^2\hat{p}^2} + \widetilde{\hat{p}^2\hat{x}^2} = 2x^2p^2 - \hbar^2, \tag{36}$$

which is derived in the Appendix. When this expression is included we find

$$\widetilde{\hat{H}^2} = H^2(x,p) - \frac{(\hbar\omega)^2}{4}. \tag{37}$$

Thus we find after carrying out the integration that

$$\langle H^2\rangle = \left(\tfrac{1}{2}\hbar\omega\right)^2, \tag{38}$$

and the resulting spread Δ is equal to zero as it should.

We see that even for the Wigner function of Eq. (31), which is positive everywhere, quantum behavior is still present. It is the way the physical results are extracted, using not only the Wigner function, but also the Weyl transform of the desired operator, which give this system its quantum behavior. It is widely believed that a Wigner function which is positive everywhere can exhibit only classical phenomena.[12] As we see from this example, this belief is incorrect.

V. TIME DEPENDENCE OF THE WIGNER FUNCTION

By taking the derivative of Eq. (10) with respect to time we have

$$\frac{\partial W}{\partial t} = \frac{1}{h}\int e^{-ipy/\hbar}\left[\frac{\partial \psi^*(x-y/2)}{\partial t}\psi(x+y/2) + \frac{\partial \psi(x+y/2)}{\partial t}\psi^*(x-y/2)\right]dy. \tag{39}$$

The partial derivatives on the right-hand side can be expressed using the Schrödinger equation,

$$\frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar}{2im}\frac{\partial^2 \psi(x,t)}{\partial x^2} + \frac{1}{i\hbar}U(x)\psi(x,t). \tag{40}$$

We use Eq. (40) to write Eq. (39) as

$$\frac{\partial W}{\partial t} = \frac{\partial W_T}{\partial t} + \frac{\partial W_U}{\partial t}, \tag{41}$$

where

$$\frac{\partial W_T}{\partial t} = \frac{1}{4\pi i m}\int e^{-ipy/\hbar}\left[\frac{\partial^2 \psi^*(x-y/2)}{\partial x^2}\psi(x+y/2) - \psi^*(x-y/2)\frac{\partial^2 \psi(x+y/2)}{\partial x^2}\right]dy, \tag{42}$$

$$\frac{\partial W_U}{\partial t} = \frac{2\pi}{ih^2}\int e^{-ipy/\hbar}[U(x+y/2) - U(x-y/2)]\psi^*(x-y/2) \times \psi(x+y/2)dy. \tag{43}$$

We consider each of these terms in the Appendix and find

$$\frac{\partial W_T}{\partial t} = -\frac{p}{m}\frac{\partial W(x,p)}{\partial x}, \tag{44a}$$

$$\frac{\partial W_U}{\partial t} = \sum_{s=0}(-\hbar^2)^s\frac{1}{(2s+1)!}\left(\frac{1}{2}\right)^{2s}\frac{\partial^{2s+1}U(x)}{\partial x^{2s+1}} \times \left(\frac{\partial}{\partial p}\right)^{2s+1}W(x,p). \tag{44b}$$

Equation (41) with Eq. (44) is equivalent to solving the Schrödinger equation, as can be seen by the following argument: Consider the wave function $\psi(x,0)$ and its corresponding Wigner function $W(x,p,0)$. As we saw in Eq. (25) the relation between ψ and W is one to one except for an overall constant phase. We then use the Schrödinger equation to determine $\psi(x,t)$ and Eqs. (41) and (44) to find $W(x,p,t)$. Because both equations are linear and first order in t, these solutions will be unique once the initial functions are given. Since Eqs. (41) and (44) were derived from the Schrödinger equation, these solutions must have the same one-to-one relation as the original wave function and Wigner function. Thus the two methods must be equivalent.

Note that the result in Eq. (44a) is entirely classical in that it contains no $\hbar$, while Eq. (44b) is more complicated. If all derivatives of $U(x)$ higher than the second order are zero, as for a free particle, a constant force, and a harmonic oscillator, then Eq. (44b) becomes

$$\frac{\partial W_U}{\partial t} = \frac{\partial U(x)}{\partial x}\frac{\partial W(x,p)}{\partial p}. \tag{45}$$

With this assumption the expression governing the evolution of the Wigner function becomes

$$\frac{\partial W(x,p)}{\partial t} = -\frac{p}{m}\frac{\partial W(x,p)}{\partial x} + \frac{\partial U(x)}{\partial x}\frac{\partial W(x,p)}{\partial p}. \tag{46}$$

Equation (46) is the classical Liouville equation. In such a regime the motion of the Wigner function in phase space is exactly that of classical physics under the influence of the potential $U(x)$. If higher derivatives of $U(x)$ are present, then the additional terms will give a diffusion-like behavior.

For a harmonic oscillator the motion in x,p space is purely classical. The time evolution of the classical harmonic oscillator is described by

$$x_0 = x\cos(\omega t) - \frac{p}{m\omega}\sin(\omega t), \tag{47a}$$

$$p_0 = p\cos(\omega t) + m\omega x\sin(\omega t), \tag{47b}$$

where x and p are the values of the position and momentum at time t, and x_0 and p_0 are the values at $t=0$. We need only to require that each point of the Wigner function moves in elliptical paths in phase space. Thus if the Wigner function at time $t=0$ is $W(x,p,0)$, the Wigner function at a future time t is given by

$$W(x,p,t) = W\left(x\cos(\omega t) - \frac{p}{m\omega}\sin(\omega t), p\cos(\omega t) + m\omega x\sin(\omega t), 0\right). \tag{48}$$

For the harmonic oscillator all the analysis with Hermite polynomials and exponentials has only to do with the sort of state that can be prepared and not with the physics of its time evolution.

As an application of the time evolution of a harmonic oscillator state we take the Wigner function at time $t=0$ to be the lowest energy state of the harmonic oscillator shifted by b in the x direction. If we use the rule for translation given in Sec. III, $W(x,p,0)$ is easily obtained from Eq. (31),

$$W(x,p,0) = \frac{2}{h}\exp(-a^2p^2/\hbar^2 - (x-b)^2/a^2). \tag{49}$$

From the previous discussion we see that the time evolution of the state is motion in an ellipse in the (x,p) plane centered about (0,0). The Wigner function at other times becomes

$$W(x,p,t) = \frac{2}{h}\exp\left[-\frac{a^2}{\hbar^2}(p\cos(\omega t) + m\omega x\sin(\omega t))^2 - \frac{1}{a^2}\left(x\cos(\omega t) - \frac{p}{m\omega}\sin(\omega t) - b\right)^2\right]. \tag{50}$$

We note that although the source of the Wigner function was the ground state of the harmonic oscillator and thus a proper Wigner function, the oscillator dictating the motion may be a different one; the a in Eq. (50) can be taken as arbitrary and need not be constrained by the relation $a^2=\hbar/(m\omega)$. If we do add the requirement that this state be the shifted ground state of the same oscillator, we may use $a^2=\hbar/(m\omega)$ and find

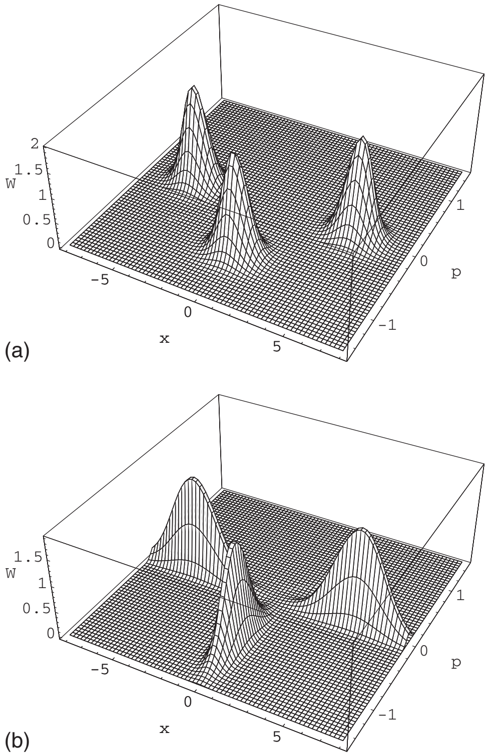

Fig. 2. Plots of the Wigner functions of a (a) coherent state and a (b) squeezed state. The state starts at the right and moves in a clockwise fashion about (0,0). Both are shown at times $t=0$, $t=T/4$, and $t=T/2$, where T is the period for the harmonic oscillator. In generating these plots the following values were used: $h=1$, $\omega=1$, $m=2\pi$, $b=5$; for the coherent state, $a=1$ as follows from $a^2=\hbar/(m\omega)$. For the squeezed state, $a=2$.

$$W(x,p,t) = \frac{2}{h}\exp\left[-\frac{a^2}{\hbar^2}\left(p+\frac{b\hbar}{a^2}\sin(\omega t)\right)^2 - \frac{1}{a^2}(x-b\cos(\omega t))^2\right]. \tag{51}$$

Because the x and p dependencies have now factored, we see that $\psi^*\psi=\int W\,dp$ will be a Gaussian of constant width a moving back and forth with amplitude b and angular frequency ω. This state is the coherent state. Coherent states were introduced by Glauber[13,14] in the study of quantum optics as the closest quantum description of a classical electromagnetic wave. These states play a parallel role in the study of the harmonic oscillator. As the Wigner function moves around its path in phase space, its projection on the x axis moves back and forth with unchanging profile.

We now return to Eq. (50) and consider its implications without the restriction on a, $a^2=\hbar/(m\omega)$. The initial state is no longer the shifted ground state of the harmonic oscillator describing the motion. It will have a different ratio of spread in the x and p directions from the coherent state. This state is the squeezed state.[14] Equation (50) now describes the time evolution of this state where m and ω refer to the harmonic oscillator. Based on this evolution in phase space we can imagine how this state will evolve and how its projection on the x axis will differ from that of the coherent state. Although it will still oscillate with angular frequency ω, its width in x will vary during the motion. The coherent state and the squeezed states are shown in Fig. 2 at $t=0$, $t=T/4$, and $t=T/2$, where T is the period of the oscillator.

A similar treatment can be given of the free particle. Here each point would move in a straight line parallel to the x axis in phase space as dictated by its position and momentum. The Wigner function evolves as

$$W(x,p,t) = W\left(x-\frac{p}{m}t,p,0\right). \tag{52}$$

Equation (52) corresponds to a shear of the distribution. Parts of the Wigner function above the x axis move to the right in proportion to how far above the x axis they lie. Points below the axis move to the left in a similar fashion. Many of these results would be difficult to obtain starting from the Schrödinger equation.

VI. MIXED STATES AND OTHER DISTRIBUTION FUNCTIONS

There is an interesting complementarity between classical physics and quantum physics. In quantum mechanics, linear combinations of wave functions $\psi(x,t)$ that satisfy the Schrödinger equation are also solutions to the Schrödinger equation. This property is the usual linearity of quantum mechanics. When the transformation is made to the corresponding Wigner functions and the x,p space, this linearity is lost. Suppose that $\psi=\psi_\alpha+\psi_\beta$. As can be seen from Eq. (10), we will not have $W_\psi=W_\alpha+W_\beta$. For classical systems there is linearity in phase space. If we have one distribution $D_a(x,p)$ and add another $D_b(x,p)$, we obtain the proper representation of the sum of the two by taking $D(x,p)=(D_a(x,p)+D_b(x,p))/2$. Classical distributions are linear in phase space.

For mixed states the definition of the density operator, Eq. (6), is generalized by replacing it with

$$\hat{\rho} = \sum_j P_j|\psi_j\rangle\langle\psi_j|. \tag{53}$$

The probability of each state P_j will be positive and $\Sigma_j P_j=1$. The expectation values will still be given by $\langle A\rangle=\mathrm{Tr}[\hat{\rho}\hat{A}]$. The Wigner function is calculated as before with Eqs. (10) and (3),

$$W(x,p) = \tilde{\rho}/h = \sum_j P_j W_j(x,p), \tag{54}$$

where $W_j(x,p)$ is the Wigner function obtained for $|\psi_j\rangle$ alone. Thus there is a linearity of mixed states in phase space. In this way, the quantum system of mixed states takes on some of the character of a classical system. Of the relations that were found in Sec. III only Eq. (17), which depends upon $\hat{\rho}^2=\hat{\rho}$, is no longer applicable. The Wigner function can be inverted along the lines of Eq. (25) to recover the density operator if it exists.

We now give an example comparing pure and mixed states. For the pure state we take the sum of two coherent states, one centered at $x=+b$, the other at $x=-b$. This state can be formed from two ground states of the harmonic oscillator in Eq. (29) shifted by a distance b in opposite directions in x,

$$\psi = A[\psi_0(x-b)+\psi_0(x+b)], \tag{55}$$

where A is a normalization constant. The Wigner function for this state can be found using Eq. (10) giving

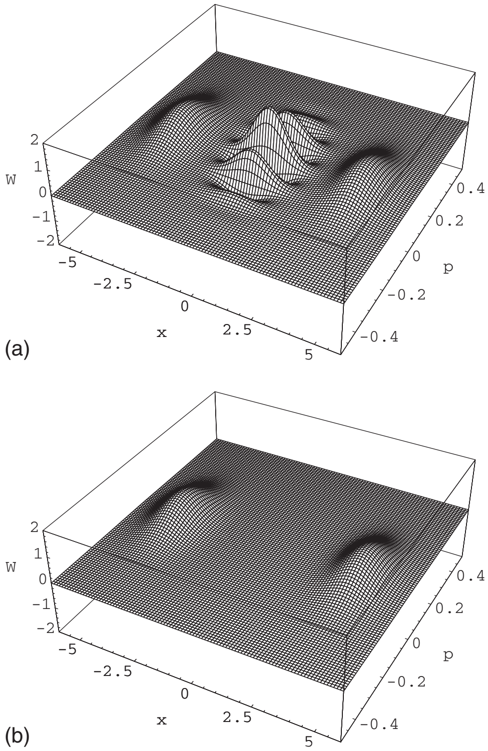

Fig. 3. Plots of the Wigner functions for a (a) pure state and a (b) mixed state consisting of two coherent states. In generating these plots the following values were used: $h=1$, $a=1$, and $b=4$.

$$W(x,p) = \frac{1}{h(1+e^{-b^2/a^2})} e^{-(ap)^2/\hbar^2} [e^{-(x-b)^2/a^2} + e^{-(x+b)^2/a^2} + 2e^{-x^2/a^2}\cos(2bp/\hbar)]. \tag{56}$$

For the mixed state of the same two coherent states we can just sum the Wigner functions of the shifted ground states, Eq. (31), inserting a factor of $1/2$ representing the equal probability of obtaining each,

$$W(x,p) = \frac{1}{2}[W_0(x-b,p) + W_0(x+b,p)] \tag{57a}$$

$$= \frac{1}{h} e^{-a^2p^2/\hbar^2} [e^{-(x-b)^2/a^2} + e^{-(x+b)^2/a^2}]. \tag{57b}$$

The Wigner functions given in Eqs. (56) and (57b) are shown in Fig. 3. As we can see, the mixed state has two peaks centered at $x=\pm b$, and the pure state is similar to the mixed state with nonclassical behavior between the two peaks where the wave function is small. This behavior near (0,0) for symmetric or antisymmetric states was discussed in Sec. III.

As was indicated in Sec. I, the Weyl transform and the Wigner function can be easily generalized to many dimensions. For the Weyl transform of operator $\hat{A}$ we replace Eq. (3) with

$$\tilde{A}(x_1,x_2,\ldots,p_1,p_2,\ldots) = \int\int\cdots e^{-i(p_1y_1+p_2y_2+\cdots)/\hbar} \times\langle x_1+y_1/2,x_2+y_2/2,\ldots|\hat{A}|x_1 - y_1/2,x_2-y_2/2,\ldots\rangle dy_1dy_2\cdots . \tag{58}$$

The defining equation for the Wigner function for a pure state $\psi(x_1,x_2,\ldots)$ becomes

$$W(x_1,x_2,\ldots,p_1,p_2,\ldots) = \frac{1}{h^n}\int\int\cdots e^{-i(p_1y_1+p_2y_2+\cdots)/\hbar} \times\psi(x_1+y_1/2,x_2+y_2/2,\ldots) \times\psi^*(x_1-y_1/2,x_2-y_2/2,\ldots)dy_1dy_2\cdots , \tag{59}$$

where n is the dimension of the system.

The Wigner function is not the only candidate that gives a distribution in x,p space and a representation of expectation values for quantum mechanics in the form of Eq. (11). The other candidates represent trade-offs between the distribution function and the transformed operators, some making the distribution look tamer at the expense of the transform of the operator.[3] All are capable of giving all of the quantum details. It is not surprising that this ambiguity exists and that there is no unique choice. As pointed out in Sec. I, finding a proper probability distribution in phase space to represent quantum mechanics is impossible. Thus it is not surprising that there are many ways of approximately performing this task, each falling short of the goal.

VII. CLASSICAL LIMIT

At this point it might seem that we could take the limit $\hbar\to 0$ and obtain classical physics. We might insist that we begin with a positive distribution in phase space at $t=0$ either by the classical nature of the preparation or by using some smoothing scheme based on the inability to observe details in the distribution in phase space (coarse graining). The equation of evolution of $W(x,p,t)$, Eqs. (41), (44a), and (44b), reduces to the classical case when $\hbar\to 0$. The difference between the Weyl transform, $\tilde{A}(x,p)$, of the operator $\hat{A}=A(\hat{x},\hat{p})$ and the function $A(x,p)$ disappears when $\hbar\to 0$. This difference is due to the fact that $\hat{x}$ and $\hat{p}$ do not commute ($[\hat{x},\hat{p}]=i\hbar$), which led to the extra term in Eq. (37). Thus in this limit we can calculate expectation values in the usual way as an integral of $W(x,p)A(x,p)$ over x and p. We might try to give such an argument but we *cannot*.

The problem with these naive assumptions can be seen easily. Dropping the higher order terms in $\hbar$ in Eq. (44b) is suspect. Note that from the definition of the Wigner function Eq. (10), $(\partial/\partial p)^{2s+1}$ will bring a factor of $1/\hbar^{2s+1}$, which will more than offset the $\hbar^{2s}$ factor unless some help can be found in the density operator. This issue has been considered by Heller,[15] who reached similar conclusions to those expressed here. As an example, consider the ground state of the harmonic oscillator given in Eq. (31). Although we are using states of the harmonic oscillator, we are not assuming that the Hamiltonian dictating the motion is that of the harmonic oscillator. This construction is simply a way of getting a proper Wigner function. If we take $(\partial/\partial p)^{2s+1}$ of this Wigner function and the limit $\hbar \to 0$, we obtain $(-2a^2 p/\hbar^2)^{2s+1} \exp[-a^2 p^2/\hbar^2]$ for the dependence on p and $\hbar$. As $\hbar \to 0$ the exponential becomes narrower with significant values only for $p \sim \hbar/a$. With this constraint $(\partial W_0/\partial p)^{2s+1}$ goes as $1/\hbar^{2s+1}$. Thus the terms in Eq. (44b) that appear to go as $\hbar^{2s}$ actually go as $1/\hbar$ and prevent their neglect in the $\hbar \to 0$ limit. Part of the problem is that as $\hbar \to 0$ the Wigner function of the pure state becomes very narrow in the p direction because for a pure state the width in p is tied to the width in x via $\hbar$. It might be argued that we should have taken the width in p as fixed in the $\hbar \to 0$ limit, allowing the Wigner function to become narrow in the x distribution. It might seem that this limit would avoid the problems with the higher order derivatives in p. In general, such an approach would not be satisfactory. As we saw in Fig. 2 for the harmonic oscillator, initial distributions can become rotated in phase space interchanging the widths of the distributions in x and p.

It is expected that in the classical limit we cannot determine distributions with higher and higher precision. We want to control the widths in x and p independently. Once the width in x is fixed we cannot make the width in p arbitrarily small, but we can construct a mixed state that has an arbitrarily wide distribution in p. This construction is done by forming a mixed state of ground states of the harmonic oscillator in Eq. (31) shifted in the p direction with normalized probability density,

$$P(p_0) = \frac{1}{c\sqrt{\pi}} e^{-p_0^2/c^2}, \tag{60}$$

where c is a positive constant. The Wigner function of the mixed state is

$$\begin{aligned} W(x,p) &= \int W_0(x,p-p_0) P(p_0) dp_0 \\ &= \frac{1}{\pi\sqrt{a^2c^2+\hbar^2}} e^{-x^2/a^2} e^{p^2/(c^2+\hbar^2/a^2)}. \end{aligned} \tag{61}$$

We now have a Wigner function with width a in the x direction and width $\sqrt{c^2+\hbar^2/a^2}$ in p. The $\hbar \to 0$ limit can be taken of this Wigner function and the neglect of the derivatives with respect to p beyond the first in Eq. (44b) can now be justified.

If we apply this same procedure to the double coherent pure state in Eq. (56), we obtain in the limit $\hbar \to 0$,

$$\begin{aligned} W(x,p) = {} & \frac{1}{2\pi ac(1+e^{-(b/a)^2})} e^{-p^2/c^2} [e^{-(x-b)^2/a^2} \\ & + e^{-(x+b)^2/a^2} + 2e^{-x^2/a^2} e^{-b^2/a^2}]. \end{aligned} \tag{62}$$

Again we see that the behavior is considerably smoother than the pure state and closely resembles the expression for the mixed state of two coherent states given in Eq. (57b). All that remains of the nonclassical behavior near (0,0) shown in Fig. 3 is a peak suppressed by a factor of $2e^{-b^2/a^2}$. Again the neglect of terms containing derivatives with respect to p beyond the first order is justified. Can we carry out this program of introducing mixed states and successfully taking the $\hbar \to 0$ for all cases? That is not so clear. Note the concern is not just that W might become negative, although that would be a problem, but the rapid variation of W.

It is well known that many classical nonlinear systems exhibit very complicated behavior which can evolve into distributions that we would expect to have large higher order derivatives.[16] The issue of the incompatibility of classical mechanics and quantum mechanics has been pointed out by Ford[17] based on information theory arguments and is a central question in quantum chaos. This question is still open.[18] A recent paper[19] analyzed the nonlinear Duffing oscillator as a classical system and as a quantum system. Their respective evolutions in phase space are then shown side by side and clearly show a classical system that develops fine structures in phase space, while the quantum system develops negative regions in the corresponding Wigner function.

We may also consider systems that start off classically but evolve into the quantum regime. In the experiments of Arndt and co-workers[20] a beam of C_{60} molecules from an oven passes through a grating with a grating constant of 100 nm. This experiment reveals an interference pattern at a distance of 1.2 m. The interference pattern is clearly a quantum effect. The grating spacing, although fine, is much larger than the de Broglie wavelength of the molecules, which is about 2.8 pm. The reason that the pattern is revealed is due to the growth of transverse coherence with distance from the grating. Thus we have a seemingly classical system that evolves into a quantum system. We could argue that making $\hbar$ very small would reduce the effect, but propagation over a greater length would bring the pattern back.

In the end, what can we say about the classical limit? As we can see the limit is subtle and involves not just the time dependence of the states, but the operators and nature of the states themselves. If we can say that the initial distribution in phase space is positive and smooth everywhere and if the Hamiltonian is such as to leave the distribution sufficiently smooth so as to allow us to neglect the higher order terms in $\hbar$ with their high order derivatives with respect to p, then the opening argument of this section should hold. In the end, we believe that the quantum description correctly describes our world.

We note that the distinction between classical and quantum is not simply the distinction between large and small, but the extent to which we know the distribution. If we pin down the distribution in phase space, either due to the details of preparation, details of evolution, or fineness of measurement, to details approaching $\Delta x \Delta p = \hbar$, the quantum nature will emerge.

VIII. SUMMARY: WIGNER–WEYL VERSUS SCHRÖDINGER

Almost all quantum mechanics texts present the subject based on the Schrödinger equation, wave functions, and operators. The Wigner–Weyl approach presented here is completely equivalent. The question of which approach is to be used depends on the system under consideration and the questions asked. Our initial goal was to find a phase space representation of the quantum state. This representation was given by the Wigner function. It was found to possess some disappointing features due to the quantum character of the system, which is completely described by the formulation.

What was accomplished beyond a visual description of a quantum system? Two were discussed in the paper. For the harmonic oscillator and the free particle the time evolution of the system is simple in this formulation and is identical to that of the classical system. These features are hidden in the standard Schrödinger approach.

The second virtue of the Wigner–Weyl approach is its ability to naturally include mixed states. The Schrödinger equation is written in terms of the wave function, and is limited to a description of pure states. As we saw in Sec. VI the Wigner–Weyl description easily moves from the description of a pure state to that of mixed states. We saw an application of this description in Sec. VII. As an added benefit the time evolution of the Wigner function given in Eqs. (41) and (44) was in a form that helped us understand the classical limit. There are still open questions, but we gained a clearer picture of the problem. Had we started with the Schrödinger equation and taken $\hbar \to 0$ we would conclude that we should drop the kinetic energy.

It is also possible to obtain the Wigner functions corresponding to the energy eigenstates directly from the time evolution of the Wigner function, Eq. (41).[5] Thus for the harmonic oscillator, Eq. (31) could be obtained directly without the use of the result given in Eq. (29).

Should we give up the Schrödinger equation in favor of the Wigner–Weyl approach? Certainly not. The simplicity of the Schrödinger equation makes it easier to solve directly and ideal for finding approximate solutions. However, there is much to be gained by studying the Wigner–Weyl description.

ACKNOWLEDGMENTS

I would like to thank Markus Arndt and Anton Zeilinger for their hospitality during my time in Vienna. I would also like to thank Caslav Brukner and Wolfgang Schleich for several useful conversations.

APPENDIX: DETAILS OF THE DERIVATIONS

In the following we will fill in some details of derivations that were omitted in the main text.

Equation (4). The first task is to express the Weyl transformation in terms of momentum eigenstates. The definition of the Weyl transformation is given in Eq. (3). The identity operator can be expressed as $\hat{1} = \int |p\rangle\langle p| dp$, where the states $|p\rangle$ obey the orthogonality condition $\langle p|p'\rangle = \delta(p-p')$. We substitute this expression on both sides of the operator of the operator $\hat{A}$ on the right-hand side of Eq. (3) giving

$$\widetilde{A} = \int\int\int e^{-ipy/\hbar}\langle x + y/2|p'\rangle\langle p'|\hat{A}|p''\rangle \times\langle p''|x - y/2\rangle dy dp'\, dp''. \tag{A1}$$

Next we note that $\langle x|p\rangle = h^{-1/2}\exp(ixp/\hbar)$ (see, for example, Ref. 21) and use

$$\int \exp(iyp/\hbar)dy = h\delta(p) \tag{A2}$$

to carry out the y integration giving

$$\int\int \delta((p'+p'')/2 - p)\langle p'|\hat{A}|p''\rangle e^{ix(p'-p'')/\hbar}dp'\,dp''. \tag{A3}$$

Next we change variables $u = p' - p''$, $v = p' + p''$, and $du dv = 2dp'\,dp''$. With this change of variables Eq. (A1) becomes

$$\widetilde{A} = \int\int \delta(v - 2p)\langle (v+u)/2|\hat{A}|(v-u)/2\rangle e^{ixu/\hbar}du\,dv, \tag{A4}$$

where we have used the relation $\delta(y/2) = 2\delta(y)$. Carrying out the v integration, we have the desired result

$$\widetilde{A} = \int e^{ixu/\hbar}\langle p + u/2|\hat{A}|p - u/2\rangle du. \tag{A5}$$

Equation (5). We next derive the key relation between the trace of two operators and their respective Weyl transforms. Suppose we have two operators $\hat{A}$ and $\hat{B}$ and their Weyl transforms

$$\widetilde{A}(x,p) = \int e^{-ipy/\hbar}\langle x + y/2|\hat{A}|x - y/2\rangle dy, \tag{A6a}$$

$$\widetilde{B}(x,p) = \int e^{-ipy'/\hbar}\langle x + y'/2|\hat{B}|x - y'/2\rangle dy'. \tag{A6b}$$

We form the product of these two and integrate over all of x,p space and find

$$\int\int \widetilde{A}(x,p)\widetilde{B}(x,p)dx\,dp = \int\int\int\int e^{-ip(y+y')/\hbar}\langle x + y/2|\hat{A}|x - y/2\rangle \times\langle x + y'/2|\hat{B}|x - y'/2\rangle dx\,dp\,dy\,dy'. \tag{A7}$$

The p integration is done using Eq. (A2), giving a delta function which is used to do the y' integration:

$$\int\int \widetilde{A}(x,p)\widetilde{B}(x,p)dx\,dp = h\int\int \langle x + y/2|\hat{A}|x - y/2\rangle \times\langle x - y/2|\hat{B}|x + y/2\rangle dx\,dy. \tag{A8}$$

Then we perform the change of variables $u = x - y/2$, $v = x + y/2$, and $du\,dv = dx\,dy$, giving

$$\int\int \widetilde{A}(x,p)\widetilde{B}(x,p)dx\,dp = h\int\int \langle v|\hat{A}|u\rangle\langle u|\hat{B}|v\rangle du\,dv = h\,\mathrm{Tr}[\hat{A}\hat{B}], \tag{A9}$$

which is Eq. (5), the desired relation between the trace of two operators and their Weyl transforms.

Equation (36). From the definition of the Weyl transform in Eq. (3) we have

$$\widetilde{\hat{p}^2\hat{x}^2} + \widetilde{\hat{x}^2\hat{p}^2} = \int e^{-ipv/\hbar}\langle x + v/2|\hat{p}^2\hat{x}^2 + \hat{x}^2\hat{p}^2|x - v/2\rangle dv \tag{A10a}$$

$$= \int e^{-ipv/\hbar}(2x^2 + v^2/2)\langle x + v/2|\hat{p}^2|x - v/2\rangle dv. \tag{A10b}$$

We insert the identity $\hat{1} = \int |p'\rangle\langle p'| dp'$ just after $\hat{p}^2$ and find

$$\widetilde{\hat{p}^2\hat{x}^2}+\widetilde{\hat{x}^2\hat{p}^2}=\int\int p'^2 e^{-ipv/\hbar}(2x^2+v^2/2)\langle x+v/2|p'\rangle \times\langle p'|x-v/2\rangle dv\,dp' \tag{A11a}$$

$$=-\frac{1}{h}\int\int e^{-ipv/\hbar}(2x^2+v^2/2)\frac{\partial^2}{\partial v^2}e^{ip'v/\hbar}dv\,dp'. \tag{A11b}$$

We next perform two integrations by parts on the v variable[22] and obtain the desired result,

$$\widetilde{\hat{p}^2\hat{x}^2}+\widetilde{\hat{x}^2\hat{p}^2}=-\hbar^2\int\delta(v)\frac{\partial^2}{\partial v^2}[e^{ipv/\hbar}(2x^2+v^2/2)]dv = 2x^2p^2-\hbar^2. \tag{A12}$$

Equation (44a). We note that the integral in the first term of Eq. (42) can be written as

$$\int e^{-ipy/\hbar}\frac{\partial^2\psi^*(x-y/2)}{\partial x^2}\psi(x+y/2)dy = -2\int e^{-ipy/\hbar}\frac{\partial^2\psi^*(x-y/2)}{\partial y\,\partial x}\psi(x+y/2)dy. \tag{A13}$$

Equation (A13) can be integrated by parts to give

$$-\frac{2ip}{\hbar}\int e^{-ipy/\hbar}\frac{\partial\psi^*(x-y/2)}{\partial x}\psi(x+y/2)dy + \int e^{-ipy/\hbar}\frac{\partial\psi^*(x-y/2)}{\partial x}\frac{\partial\psi(x+y/2)}{\partial x}dy. \tag{A14}$$

If combined with the integral in the second term in Eq. (42) rewritten in a similar fashion, we obtain the result in Eq. (44a),

$$\frac{\partial W_T}{\partial t}=-\frac{p}{hm}\frac{\partial}{\partial x}\int e^{-ipy/\hbar}\psi^*(x-y/2)\psi(x+y/2)dy = -\frac{p}{m}\frac{\partial W}{\partial x}. \tag{A15}$$

Equation (44b). For the $\partial W_U/\partial t$ part of $\partial W/\partial t$ we assume that $U(x)$ can be expanded in a power series in x and write

$$U(x+y/2)-U(x-y/2) = \sum_n \frac{1}{n!}\frac{\partial^n U(x)}{\partial x^n}\left[\left(-\frac{1}{2}y\right)^2-\left(\frac{1}{2}y\right)^2\right] \tag{A16a}$$

$$=\sum_{s=0}\frac{1}{(2s+1)!}\left(\frac{1}{2}\right)^{2s}\frac{\partial^{2s+1}U(x)}{\partial x^{2s+1}}y^{2s+1}. \tag{A16b}$$

When Eq. (A16) is incorporated into Eq. (43), we find Eq. (44b).

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