and thereby to the path integral representation of the evolution operator [FeyHib65, Sch81], since

$$
\begin{aligned}
\langle x_{N+1}| U(t) |x_0\rangle &= \langle x_{N+1}| \left[e^{-i\tau K/\hbar} e^{-i\tau V/\hbar} \right]^{N+1} |x_0\rangle \\
&= \int \left[\prod_{i=1}^{N} dx_i \right] \left\{ \prod_{j=0}^{N} \langle x_{j+1}| e^{-i\tau K/\hbar} |x_j\rangle \, e^{-i\tau V(x_j)/\hbar} \right\} \\
&= \int \left[\prod_{i=1}^{N} dx_i \right] \left[\prod_{i=1}^{N+1} \frac{dp_i}{2\pi\hbar} \right] \\
&\quad \times \left\{ \prod_{j=0}^{N} e^{ip_{j+1}(x_{j+1}-x_j)/\hbar} e^{-i\tau p_{j+1}^2/2M\hbar} e^{-i\tau V(x_j)/\hbar} \right\} \\
&= \int \left[\prod_{i=1}^{N} \sqrt{\frac{-iM}{2\pi\hbar\tau}} dx_i \right] \left\{ \prod_{j=0}^{N} e^{iM(x_{j+1}-x_j)^2/2\tau\hbar} e^{-i\tau V(x_j)/\hbar} \right\}
\end{aligned}
\tag{3.10}
$$

which as $N \to \infty$ yields

$$
\langle x_t| U(t) |x_0\rangle = \int_{x(t)=x_t, x(0)=x_0} Dx \, e^{iS/\hbar} \tag{3.11}
$$

The converse is also true, namely, if we take equation (3.11) as the definition of the evolution operator, we may derive the Schrödinger equation. We have

$$
\langle x_t| U(t+\tau) |x_0\rangle = \int \sqrt{\frac{-iM}{2\pi\hbar\tau}} dx' \, e^{iM\left(x_t - x'\right)^2/2\tau\hbar} e^{-i\tau V\left(x'\right)/\hbar} \langle x'| U(t) |x_0\rangle \tag{3.12}
$$

The Gaussian factor makes sure that only values $y \approx x_t$ contribute, so we may expand everything else in powers of $(y - x_t)$ and integrate term by term, whereby

$$
\begin{aligned}
\langle x_t| U(t+\tau) |x_0\rangle &= \left[1 - \frac{i\tau}{\hbar} V(x_t) \right] \langle x_t| U(t) |x_0\rangle \\
&\quad + \frac{i\hbar\tau}{2M} \frac{\partial^2}{\partial x_t^2} \langle x_t| U(t) |x_0\rangle + O\left(\tau^2\right)
\end{aligned}
\tag{3.13}
$$

QED

3.1.1 Wigner functions

So far, we have described states of a quantum system in terms of kets $|\alpha\rangle$ in a Hilbert space. Considering the position and momentum states $|x\rangle$ and $|p\rangle$, we may introduce the wavefunctions in position and momentum representations $\psi(x) = \langle x \mid \alpha\rangle$ and $\psi(p) = \langle p \mid \alpha\rangle$, which are related to each other through a Fourier transform

$$
\psi(p) = \int \frac{dx}{\sqrt{2\pi\hbar}} \, e^{-ipx/\hbar} \psi(x) \tag{3.14}
$$

$|\psi(x)|^2$ and $|\psi(p)|^2$ represent the probability distribution functions for position and momentum, respectively. The question arises on whether these distributions may be obtained as marginal distributions from a joint probability for position and momentum. The answer is of course not, at least in general, since the existence of such a joint probability density would be almost conjured as saying that position and momentum may be simultaneously well defined. Nevertheless, in 1932 Wigner found an object which comes remarkably close [Wig32, HOSW84]. This object is the Wigner function

$$f^W(x,p) = \int \frac{du}{2\pi\hbar}\, e^{-ipu/\hbar}\psi^*\left(x-\frac{u}{2}\right)\psi\left(x+\frac{u}{2}\right) \tag{3.15}$$

Indeed, if we integrate over p we get the probability distribution for x

$$\int dp\; f^W(x,p) = |\psi(x)|^2 \tag{3.16}$$

while integrating over x and switching variables to $x \pm u/2$ we get

$$\int dx\; f^W(x,p) = |\psi(p)|^2 \tag{3.17}$$

The reason why f^W cannot be directly identified as a probability distribution function is that f^W, although real, is not necessarily nonnegative. We shall see examples below.

The dynamics of the Wigner function is also quite remarkable. If the wavefunction obeys the Schrödinger equation (equation (3.1) in the coordinate representation)

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2M}\frac{\partial^2\psi}{\partial x^2} + V(x)\,\psi(x) \tag{3.18}$$

then

$$\begin{aligned}\frac{\partial f^W}{\partial t} = &\frac{1}{i\hbar}\int\frac{du}{2\pi\hbar}\,e^{-ipu/\hbar}\\ &\times\left\{\left(-\frac{\hbar^2}{2M}\right)\left[\psi^*\left(x-\frac{u}{2}\right)\frac{\partial^2\psi}{\partial x^2}\left(x+\frac{u}{2}\right)-\psi\left(x+\frac{u}{2}\right)\frac{\partial^2\psi^*}{\partial x^2}\left(x-\frac{u}{2}\right)\right]\right.\\ &\left.+\left[V\left(x+\frac{u}{2}\right)-V\left(x-\frac{u}{2}\right)\right]\psi^*\left(x-\frac{u}{2}\right)\psi\left(x+\frac{u}{2}\right)\right\}\end{aligned} \tag{3.19}$$

In the first line, we observe that

$$\begin{aligned}&\psi^*\left(x-\frac{u}{2}\right)\frac{\partial^2\psi}{\partial x^2}\left(x+\frac{u}{2}\right)-\psi\left(x+\frac{u}{2}\right)\frac{\partial^2\psi^*}{\partial x^2}\left(x-\frac{u}{2}\right)\\ &= 2\frac{\partial^2}{\partial u\partial x}\left[\psi^*\left(x-\frac{u}{2}\right)\psi\left(x+\frac{u}{2}\right)\right]\end{aligned}$$

After integration by parts, this term contributes

$$\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2M}\right)\left(\frac{2ip}{\hbar}\right)\frac{\partial f^W}{\partial x} \equiv \frac{-p}{M}\frac{\partial f^W}{\partial x} \tag{3.20}$$

The second term is much harder to handle. If the potential is smooth, one can try a Kramers–Moyal expansion [Kra40, Moy49, Kam81]

$$V\left(x+\frac{u}{2}\right)-V\left(x-\frac{u}{2}\right)=2\sum_{k=0}^{\infty}\frac{V^{(2k+1)}(x)}{(2k+1)!}\left(\frac{u}{2}\right)^{2k+1} \tag{3.21}$$

Commuting the integral and the sum, we obtain the second term as

$$\frac{2}{i\hbar}\sum_{k=0}^{\infty}\frac{V^{(2k+1)}(x)}{(2k+1)!}\left[\frac{i\hbar}{2}\frac{\partial}{\partial p}\right]^{2k+1}f^W \tag{3.22}$$

In terms of the classical Hamiltonian $H = p^2/2m + V$, our result reads

$$\frac{\partial f^W}{\partial t}=-\left\{H,f^W\right\}+O\left(\hbar^2\right) \tag{3.23}$$

where the Poisson bracket $\left\{H, f^W\right\}$ was introduced in Chapter 2, equation (2.48). In other words, the dynamics of the Wigner function follows remarkably closely the classical transport equation with external potential $V(x)$. If V is harmonic, there are no higher order terms, and the dynamics followed by the Wigner function is exactly the classical dynamics of a distribution function [Hab04, CDHR98]. However, as we have already remarked, that does not mean that f is classical, as it may be negative in some regions of phase space.

It is clear that we may compute the Wigner function f^W associated with any wavefunction ψ, but the converse is not true: it is easy to imagine phase space functions f^W which cannot be obtained as Wigner functions from *any* ψ. Indeed, it is enough to imagine a distribution function violating Heisenberg's uncertainty principle to exclude such an identification. To the best of our knowledge, there is no simple sufficient condition to see whether a given f^W is a Wigner function, although there are many necessary conditions (such as positivity of the marginal distributions).

To summarize, although f^W itself cannot be understood as a probability density, conveniently smeared versions of f^W are nonnegative and may be used to assign probabilities to different events. This restricted interpretation of the Wigner function will be enough for our requirements below.

Some examples

The simplest possible example of a Wigner function is a momentum state

$$\psi(x)=\frac{e^{i\mathbf{p}x/\hbar}}{\sqrt{2\pi\hbar}} \tag{3.24}$$

Then

$$f^W=\frac{1}{2\pi\hbar}\delta\left(p-\mathbf{p}\right) \tag{3.25}$$

Now consider a stationary wave

$$\psi(x)=\frac{1}{\sqrt{\pi\hbar}}\cos\left(\frac{\mathbf{p}x}{\hbar}\right) \tag{3.26}$$

representing a coherent superposition of two states of opposite momentum. Then

$$f^W(x,p) = \frac{1}{4\pi\hbar}\left[\delta(p-\mathbf{p}) + \delta(p+\mathbf{p})\right] + \cos\left(\frac{2\mathbf{p}x}{\hbar}\right)\delta(p) \tag{3.27}$$

We see that f^W is not nonnegative. The oscillatory terms are related to the interference between the two components of the wave packet [PaHaZu93].

As a second example, let us consider a Gaussian wave packet

$$\psi(x) = \frac{e^{-x^2/4\sigma^2}}{(2\pi\sigma^2)^{1/4}} \tag{3.28}$$

Then

$$f^W(x,p) = \frac{1}{\pi\hbar} e^{-x^2/2\sigma^2} e^{-2\sigma^2(p/\hbar)^2} \tag{3.29}$$

In this case f^W is positive definite, and the dispersions in x and p are what may be expected for a minimum uncertainty state.

In particular, suppose our state is the ground state for a harmonic oscillator. Then $\sigma^2 = \hbar/2M\Omega$, and

$$f^W(x,p) = \frac{1}{\pi\hbar}\exp\left\{-\frac{E}{\varepsilon}\right\}; \qquad \varepsilon = \frac{1}{2}\hbar\Omega,\ E = \frac{p^2}{2M} + \frac{M\Omega^2 x^2}{2} \tag{3.30}$$

As a final example, let us consider a superposition of two Gaussian wave packets

$$\psi(x) = \frac{1}{(2\pi\sigma^2)^{1/4}}\left\{Ae^{-(x-a)^2/4\sigma^2} + Be^{-(x+a)^2/4\sigma^2}\right\} \tag{3.31}$$

leading to

$$\begin{aligned} f^W(x,p) = \frac{e^{-2\sigma^2(p/\hbar)^2}}{\pi\hbar} & \left\{|A|^2 e^{-(x-a)^2/2\sigma^2} + |B|^2 e^{-(x+a)^2/2\sigma^2}\right. \\ & \left. + e^{-x^2/2\sigma^2}\left[AB^* e^{-2ipa/\hbar} + A^* B e^{2ipa/\hbar}\right]\right\} \end{aligned} \tag{3.32}$$

Again, we see nonpositive terms arising from the interference between the different components. If A and B had random phases, f^W would be nonnegative.

Wigner functions and probabilities

We know that if the system is in the state $\psi(x)$, the probability of observing it in the state $\phi(x)$ is

$$P = \left|\int dx\, \phi^*(x)\,\psi(x)\right|^2 \tag{3.33}$$

If we call f_ψ^W and f_ϕ^W the corresponding Wigner functions, and call

$$Q = 2\pi\hbar\int dx dp\, f_\psi^W(x,p)\, f_\phi^W(x,p) \tag{3.34}$$

then $P = Q$. Indeed

$$\begin{aligned} Q &= \int dxdp \int \frac{dudu'}{2\pi\hbar}\, e^{-ip\left(u+u'\right)/\hbar} \psi^* \left(x - \frac{u}{2}\right) \\ &\quad \times \psi\left(x + \frac{u}{2}\right) \phi^* \left(x - \frac{u'}{2}\right) \phi\left(x + \frac{u'}{2}\right) \\ &= \int dxdu\, \psi^* \left(x - \frac{u}{2}\right) \psi\left(x + \frac{u}{2}\right) \phi^* \left(x + \frac{u}{2}\right) \phi\left(x - \frac{u}{2}\right) = P \end{aligned} \tag{3.35}$$

This implies in particular that the inner product (3.34) of two Wigner functions must be positive. Since Gaussian distributions consistent with Heisenberg's principle are allowed Wigner functions, this implies that Gaussian smearings of a Wigner function are positive definite.

3.1.2 Closed time path (CTP) integrals

Recall that states evolve according to equation (3.2). Using the matrix elements (3.11) for the evolution operator, we obtain

$$\psi\left(x, t\right) = \int dx\left(0\right)\; U\left(x, x\left(0\right), t\right) \psi\left(x\left(0\right), 0\right) = \int_{x(t)=x} Dx\; e^{iS/\hbar} \psi\left(x\left(0\right), 0\right) \tag{3.36}$$

in the coordinate representation, where $U\left(x, x\left(0\right), t\right) = \langle x| \,U\left(t\right) |x\left(0\right)\rangle$. By linearity, we infer that the density matrix evolves according to

$$\begin{aligned} \rho\left(x, x', t\right) &= \langle x| \,U\left(t\right) \rho U^\dagger\left(t\right) |x'\rangle \\ &= \int_{x(t)=x, x'(t)=x'} DxDx'\; e^{i\left(S[x]-S\left[x'\right]\right)/\hbar} \rho\left(x\left(0\right), x'\left(0\right), 0\right) \end{aligned} \tag{3.37}$$

The possibility of cyclic permutations under a trace shows that $\mathrm{Tr}\,\rho\left(t\right) = \mathrm{Tr}\,\rho\left(0\right) = 1$, as it should.

We see that the path integral representation involves *two* histories, rather than a single history of the system as in equation (3.11). This observation is the departure point of the so-called closed time path formalism, which we shall develop at length in this book, especially in Chapters 5 and 6; for source references see [Sch60, Sch61, BakMah63, Kel64, ChoSuHa80, CSHY85, SCYC88, DeW86, Jor86, CalHu87, CalHu88, CalHu89]. To investigate further the meaning of these two-time-path integrals, let us consider the expression

$$G^{11}\left(\tau, \tau'\right) = \int_{x(t)=x'(t)} DxDx'\; e^{i\left(S[x]-S\left[x'\right]\right)/\hbar} \rho\left(x\left(0\right), x'\left(0\right), 0\right)\; x\left(\tau\right) x\left(\tau'\right) \tag{3.38}$$

The upper limit is free, provided it is the same for both histories. We may describe this as an integral over single histories defined on a *closed time path* (CTP). This time path has a first branch from 0 to t, where the history takes the values $x\left(t\right)$,