# 2

# Quantum Mechanics and the Path Integral

## 2.1 Schrödinger Equation and Probability

Our starting point will be single-particle quantum mechanics as defined by the Schrödinger equation

$$i\hbar\frac{d}{dt}\Psi(x,t)=\hat{h}\left(x,-i\hbar\frac{d}{dx}\right)\Psi(x,t). \tag{2.1}$$

Here $\hat{h}(x,-i\hbar\frac{d}{dx})$ is a self-adjoint operator, the Hamiltonian on the space of wave-functions $\Psi(x,t)$, where $x$ stands for any number of spatial degrees of freedom. The connection to physics of $\Psi(x,t)$ comes from the interpretation of $\Psi(x,t)$ as the amplitude of the probability to find the particle between $x$ and $x+dx$ at time $t$; hence, the probability density is given by

$$\mathcal{P}[x,x+dx]=\Psi^*(x,t)\Psi(x,t). \tag{2.2}$$

Correspondingly, the probability of finding the particle in a volume $V$ is given by

$$\mathcal{P}[V]=\int_V dx\Psi^*(x,t)\Psi(x,t). \tag{2.3}$$

The state of the system is completely described by the wave function $\Psi(x,t)$. It is the content of a standard course on quantum mechanics to find $\Psi(x,t)$ for a given $\hat{h}(x,-i\hbar\frac{d}{dx})$.

## 2.2 Position and Momentum Eigenstates

For our purposes, we introduce the set of (improper) states $|x\rangle$ which diagonalize the position operator $\hat{X}$, with

$$\hat{X}|x\rangle=x|x\rangle \tag{2.4}$$

and

$$\int dx|x\rangle\langle x|=\mathbb{I}. \tag{2.5}$$

https://doi.org/10.1017/9781009291248.003 Published online by Cambridge University Press

We are in principle working in $d$ dimensions, but we suppress the explicit dependence on the number of coordinates. The states are improper in the sense that the normalization is

$$\langle x|y\rangle = \delta(x-y), \tag{2.6}$$

where $\delta(x-y)$ is the Dirac delta function. We also introduce the set of (improper) states $|p\rangle$ which diagonalize the momentum operator $\hat{P}$

$$\hat{P}|p\rangle = p|p\rangle \tag{2.7}$$

with

$$\int dp|p\rangle\langle p| = 1 \tag{2.8}$$

but as with the position eigenstates

$$\langle p|p'\rangle = \delta(p-p'), \tag{2.9}$$

where $\delta(p-p')$ is the Dirac delta function in momentum space. The improper states $|x\rangle$ and $|p\rangle$ are not vectors in the Hilbert space of states, they have infinite norm. They actually define vector-valued distributions, linear maps from the space of the square integrable functions of $x$ or $p$ or some suitable set of test functions usually taken to be of compact support, to actual vectors in the Hilbert space,

$$|x\rangle : \quad f(x) \to |f\rangle \sim \int dx f(x)|x\rangle, \tag{2.10}$$

where the $\sim$ should be interpreted as "loosely defined by". For a more rigorous definition, see the book by Reed and Simon [107] or Glimm and Jaffe [55].

The operators $\hat{X}$ and $\hat{P}$ must satisfy the canonical commutation relation

$$[\hat{X}, \hat{P}] = i\hbar. \tag{2.11}$$

The algebraic relation Equation (2.11) is not adequate to determine $\hat{P}$ completely; there are infinitely many representations of the commutator Equation (2.11) in which $\hat{X}$ is diagonal. Taking the matrix element of Equation (2.11) between position eigenstates gives

$$(x-y)\langle x|\hat{P}|y\rangle = \langle x|[\hat{X}, \hat{P}]|y\rangle = i\hbar\langle x|y\rangle = i\hbar\delta(x-y). \tag{2.12}$$

For the more mathematically inclined, this expression does not make good sense, since the position and momentum operators are unbounded, though self-adjoint operators. They may only act on their respective domains and, correspondingly, the product of two unbounded operators requires proper analysis of the domains and ranges of the operators concerned and similar other difficulties can exist. We leave these subtleties out in what follows, and refer the interested reader to the

https://doi.org/10.1017/9781009291248.003 Published online by Cambridge University Press

book on functional analysis by Reed and Simon [107]. We find the solution for $\langle x|\hat{P}|y\rangle$ as

$$\begin{aligned}\langle x|\hat{P}|y\rangle &= -i\hbar\frac{d}{dx}\delta(x-y) + c\delta(x-y) \\ &= -i\hbar\frac{d}{dx}\langle x|y\rangle + c\delta(x-y),\end{aligned} \tag{2.13}$$

where $c$ is an arbitrary constant, using the property of the $\delta$ function that $(x-y)\delta(x-y) \equiv 0$. We will call the $x$ representation the one in which the momentum operator is represented by a simple derivative, *i.e.* $c = 0$,

$$\langle x|\hat{P}|y\rangle = -i\hbar\frac{d}{dx}\langle x|y\rangle. \tag{2.14}$$

In this representation,

$$\begin{aligned}\langle x|\hat{P}|p\rangle &= \int dy \langle x|\hat{P}|y\rangle\langle y|p\rangle = \int dy \left(-i\hbar\frac{d}{dx}\langle x|y\rangle\right)\langle y|p\rangle \\ &= -i\hbar\frac{d}{dx}\langle x|p\rangle.\end{aligned} \tag{2.15}$$

Acting to the right directly in the left-hand side of Equation (2.15) gives

$$\langle x|\hat{P}|p\rangle = p\langle x|p\rangle = -i\hbar\frac{d}{dx}\langle x|p\rangle. \tag{2.16}$$

The appropriately normalized solution of the resulting differential equation is

$$\langle x|p\rangle = \frac{1}{(2\pi\hbar)^{\frac{d}{2}}} e^{i\frac{p\cdot x}{\hbar}}, \tag{2.17}$$

where $d$ is the number of spatial dimensions.

### 2.3 Energy Eigenstates and Semi-Classical States

We can write the eigenstate of the Hamiltonian in the form $|\Psi_E\rangle$,

$$\hat{h}(\hat{X},\hat{P})|\Psi_E\rangle = E|\Psi_E\rangle, \tag{2.18}$$

where $\hat{h}(\hat{X},\hat{P})$ is defined such that

$$\langle x|\hat{h}(\hat{X},\hat{P})|f\rangle = \hat{h}\left(x, -i\hbar\frac{d}{dx}\right)\langle x|f\rangle \tag{2.19}$$

for any vector $|f\rangle$ in the Hilbert space. Then

$$\langle x|\hat{h}(\hat{X},\hat{P})|\Psi_E\rangle = \hat{h}\left(x, -i\hbar\frac{d}{dx}\right)\langle x|\Psi_E\rangle = E\langle x|\Psi_E\rangle, \tag{2.20}$$

which implies the energy eigenfunctions are given by

$$\Psi_E(x) = \langle x|\Psi_E\rangle. \tag{2.21}$$

https://doi.org/10.1017/9781009291248.003 Published online by Cambridge University Press

Correspondingly,

$$|\Psi_E\rangle = \int dx|x\rangle\langle x|\Psi_E\rangle = \int dx\Psi_E(x)|x\rangle \tag{2.22}$$

and

$$\hat{h}(x,-i\hbar\frac{d}{dx})\Psi_E(x) = E\Psi_E(x). \tag{2.23}$$

A particle described by $\Psi_E(x)$ is most likely to be found in the region where $\Psi_E(x)$ is peaked. The time-dependent solution of the Schrödinger equation for static Hamiltonians is given by $\Psi_E(x,t) = \Psi_E(x)e^{-\frac{i}{\hbar}Et}$, and the most general state of the system is a linear superposition

$$\Psi(x,t) = \sum_E A_E\Psi_E(x)e^{-\frac{i}{\hbar}Et} \tag{2.24}$$

with

$$\sum_E A_E^* A_E = 1. \tag{2.25}$$

Suppose the Hamiltonian can be modified by adjusting the potential, say, such that $\Psi_E(x)$ approaches a delta function:

$$\Psi_E(x) \to \delta(x - x_0). \tag{2.26}$$

We would then say that a particle in the energy level $E$ is localized at the point $x_0$. But in the limit of Equation (2.26) we clearly have

$$|\Psi_E\rangle \to |x_0\rangle \tag{2.27}$$

from Equation (2.22). Thus the states $|x\rangle$ describe particles localized at the spatial point $x$. This is conceptually important for the semi-classical limit. Semi-classically we think of particles as localized at points in the configuration space. Thus the states $|x\rangle$ and their generalizations are useful in the description of quantum systems in the semi-classical limit.

## 2.4 Time Evolution and Transition Amplitudes

Given a particle in a state $|\Psi;0\rangle = |\Psi\rangle$ at $t = 0$, the Schrödinger equation, Equation (2.1), governs the time evolution of the state. The state at $t = T$ is given by

$$|\Psi;T\rangle = e^{-i\frac{T}{\hbar}\hat{h}(\hat{X},\hat{P})}|\Psi\rangle, \tag{2.28}$$

which satisfies the Schrödinger equation. The exponential of a self-adjoint operator, which accurs on the right-hand side of Equation (2.28), is rigorously defined via the spectral representation [107]. The probability amplitude for finding the particle in a state $|\Phi\rangle$ at $t = T$ is then given by

$$\langle\Phi|\Psi;T\rangle = \langle\Phi|e^{-i\frac{T\hat{h}(\hat{X},\hat{P})}{\hbar}}|\Psi\rangle. \tag{2.29}$$

https://doi.org/10.1017/9781009291248.003 Published online by Cambridge University Press

We could derive an expression for this matrix element in terms of a "path integral". Such an integral would be defined as an integral over the space of all classical paths starting from the initial state and ending at the final state, and we would find that the function that we would integrate is the exponential of $-i$ times the classical action for each path. This is the standard Feynman path integral [45, 46], which was actually suggested by Dirac [40].

### 2.5 The Euclidean Path Integral

Rather than the matrix element Equation (2.29), we are more interested in a path-integral representation of the matrix element

$$\langle \Phi | e^{-\frac{\beta \hat{h}(\hat{X},\hat{P})}{\hbar}} | \Psi \rangle, \tag{2.30}$$

where $\beta$ can be thought of as imaginary time

$$T \to -i\beta. \tag{2.31}$$

The derivation of the path-integral representation of Equation (2.30) is more rigorous than that for Equation (2.29); however, the derivation which follows can be almost identically taken over to the case of real time. This can be completed by the reader. It is the matrix element of Equation (2.30) that will interest us in future chapters.

First of all, due to the linearity of quantum mechanics, it is sufficient to consider the matrix element

$$\langle y | e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})} | x \rangle. \tag{2.32}$$

To obtain Equation (2.30) we just integrate over $x$ and $y$ with appropriate smearing functions as in Equation (2.10). Now we write

$$e^{-\frac{\beta \hat{h}(\hat{X},\hat{P})}{\hbar}} = \underbrace{e^{-\frac{\epsilon \hat{h}(\hat{X},\hat{P})}{\hbar}} \cdot e^{-\frac{\epsilon \hat{h}(\hat{X},\hat{P})}{\hbar}} \cdots e^{-\frac{\epsilon \hat{h}(\hat{X},\hat{P})}{\hbar}}}_{N+1 \text{ factors}}, \tag{2.33}$$

where we mean $N+1$ factors on the right-hand side and $(N+1)\epsilon = \beta$. Next we insert complete sets of position eigenstates

$$\int dz_i |z_i\rangle\langle z_i| = \mathbb{I}, \tag{2.34}$$

where $\mathbb{I}$ is the identity operator. Between the evolution operators appearing on the right-hand side of Equation (2.33), there will be $N$ such insertions, *i.e.* $i : 1 \to N$. Consider one of the matrix elements

$$\langle z_i | e^{-\frac{\epsilon \hat{h}(\hat{X},\hat{P})}{\hbar}} | z_{i-1} \rangle \tag{2.35}$$

between position eigenstates $|z_i\rangle$and $|z_{i-1}\rangle$ for Hamiltonians of the form

$$\hat{h}(\hat{X},\hat{P}) = \frac{\hat{P}^2}{2} + V(\hat{X}). \tag{2.36}$$

https://doi.org/10.1017/9781009291248.003 Published online by Cambridge University Press

Then

$$\begin{aligned}
\langle z_i|e^{-\frac{\epsilon\hat{h}(\hat{X},\hat{P})}{\hbar}}|z_{i-1}\rangle &= \langle z_i|1-\frac{\epsilon}{\hbar}\left(\hat{P}^2/2+V(\hat{X})\right)|z_{i-1}\rangle+\mathrm{o}(\epsilon^2)\\
&= \int dp_i\langle z_i|1-\frac{\epsilon}{\hbar}\left(p_i^2/2+V(z_{i-1})\right)|p_i\rangle\langle p_i|z_{i-1}\rangle+\mathrm{o}(\epsilon^2)\\
&= \int dp_i\left(1-\frac{\epsilon}{\hbar}\left(p_i^2/2+V(z_{i-1})\right)\right)\langle z_i|p_i\rangle\langle p_i|z_{i-1}\rangle+\mathrm{o}(\epsilon^2)\\
&= \int \frac{dp_i}{(2\pi\hbar)^d}e^{-\frac{\epsilon}{\hbar}\left(\frac{p_i^2}{2}+V(z_{i-1})-ip_i\frac{(z_i-z_{i-1})}{\epsilon}\right)+\mathrm{o}(\epsilon^2)}\\
&= \left(\int \frac{dp_i}{(2\pi\hbar)^d}e^{-\frac{\epsilon}{\hbar}\left(\frac{p_i^2}{2}-i\frac{p_i(z_i-z_{i-1})}{\epsilon}-\frac{1}{2}\left(\frac{z_i-z_{i-1}}{\epsilon}\right)^2\right)}\right)\times\\
&\quad\times e^{-\frac{\epsilon}{\hbar}\left(\frac{1}{2}\left(\frac{z_i-z_{i-1}}{\epsilon}\right)^2+V(z_{i-1})\right)+\mathrm{o}(\epsilon^2)},
\end{aligned}\tag{2.37}$$

where in the second step, we have inserted a complete set of momentum eigenstates after letting $V(\hat{X})$ act on the position eigenstate $|z_{i-1}\rangle$. The first factor in the last equality is just a (shifted) Gaussian integral, and can be easily evaluated to give

$$\mathcal{N}_\epsilon = \int \frac{dp_i}{(2\pi\hbar)^d}e^{\frac{-\epsilon}{2\hbar}(p_i-i\frac{(z_i-z_{i-1})}{\epsilon})^2} = \left(\frac{1}{\sqrt{2\pi\hbar\epsilon}}\right)^d. \tag{2.38}$$

Now we use Equations (2.37) and (2.38) in Equation (2.33), inserting an independent complete set of position eigenstates between each of the factors to yield

$$\begin{aligned}
\langle y|e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})}|x\rangle &= \int \frac{dz_1\cdots dz_N}{(2\pi\hbar\epsilon)^{\frac{Nd}{2}}}\prod_{i=1}^{N+1}e^{-\frac{\epsilon}{\hbar}\left(\frac{1}{2}\left(\frac{z_i-z_{i-1}}{\epsilon}\right)^2+V(z_{i-1})\right)+\mathrm{o}(\epsilon^2)}\\
&= \int \frac{dz_1\cdots dz_N}{(2\pi\hbar\epsilon)^{\frac{Nd}{2}}}e^{-\frac{\epsilon}{\hbar}\sum_{i=1}^{N+1}\left(\frac{1}{2}\left(\frac{z_i-z_{i-1}}{\epsilon}\right)^2+V(z_{i-1})\right)+\mathrm{o}(\epsilon^2)},
\end{aligned}\tag{2.39}$$

where we define $z_0 = x$ and $z_{N+1} = y$. Equation (2.39) is actually as far as one can go rigorously. It expresses the matrix element as a path integral over piecewise straight ($N$ pieces), continuous paths weighted by the exponential of a discretized approximation to the negative Euclidean action. In the limit $N\to\infty$, the $\mathrm{o}(\epsilon^2)$ terms are expected to be negligible. Additionally, in the limit that the path becomes differentiable, which is actually almost never the case,

$$\epsilon\sum_{i=1}^{N}\left(\frac{1}{2}\left(\frac{z_i-z_{i-1}}{\epsilon}\right)^2+V(z_{i-1})\right)\to\int d\tau\left(V(z(\tau))+\frac{1}{2}\dot{z}(\tau))^2\right), \tag{2.40}$$

where $\tau\in[0,\beta]$ parametrizes the path such that $z(0)=x$ and $z(\beta)=y$. Hence the matrix element Equation (2.32) can be formally written as the integral over

https://doi.org/10.1017/9781009291248.003 Published online by Cambridge University Press

classical paths,

$$\begin{aligned}\langle y|e^{-\frac{\beta}{\hbar}\hat{h}(\hat{X},\hat{P})}|x\rangle &= \mathcal{N}\int \mathcal{D}z(\tau)e^{-\frac{1}{\hbar}\int_0^\beta d\tau\left(\frac{1}{2}(\dot{z}(\tau))^2+V(z(\tau))\right)} \\ &= \mathcal{N}\int \mathcal{D}z(\tau)e^{-\frac{S_E[z(\tau)]}{\hbar}},\end{aligned} \tag{2.41}$$

where $S_E[z(\tau)]$ is the classical Euclidean action for each path $z(\tau)$, which starts at $x$ and ends at $y$. $\mathcal{D}z(\tau)$ is the formal integration measure over the space of all such paths and $\mathcal{N}$ is a formally infinite or ill-defined normalization constant, the limit of $\frac{1}{(2\pi\hbar\epsilon)^{\frac{Nd}{2}}}$ as $N\to\infty$.

There exists a celebrated measure defined on the space of paths, the so-called Wiener measure [121], which was defined in the rigorous study of Brownian motion. One can use it to define the Euclidean path integral rigorously and unambiguously, certainly for quantum mechanics, but also in many instances for quantum field theory. We are not interested in these mathematical details, and we will use and manipulate the path integral as if it were an ordinary integral. We will have to define what we mean by this measure and normalization more carefully, later. The measure actually only makes sense, in any rigorous way, for the discretized version Equation (2.39) including the limit $N\to\infty$; however, strictly speaking the path integral for smooth paths, Equation (2.41), is just a formal expression.

We will record here the corresponding formula in Minkowski time:

$$\begin{aligned}\langle y|e^{-\frac{iT}{\hbar}\hat{h}(\hat{X},\hat{P})}|x\rangle &= \mathcal{N}\int \mathcal{D}z(t)e^{\frac{i}{\hbar}\int_0^T dt\left(\frac{1}{2}(\dot{z}(t))^2-V(z(t))\right)} \\ &= \mathcal{N}\int \mathcal{D}z(t)e^{\frac{i}{\hbar}S_M[z(t)]}.\end{aligned} \tag{2.42}$$

This formula can be proved formally by following each of the steps that we have done for the case of the Euclidean path integral; we leave the details to the reader. However, the Gaussian integral that we encountered at Equation (2.38) becomes

$$\mathcal{N}_\epsilon = \int \frac{dp_i}{(2\pi\hbar)^d} e^{\frac{-i\epsilon}{2\hbar}\left(p_i - i\frac{(z_i-z_{i-1})}{\epsilon}\right)^2}. \tag{2.43}$$

This expression is ill-defined, but it only contributes to an irrelevant normalization constant. We can make it well-defined by adding a small negative imaginary part to the Hamiltonian, which then yields

$$\mathcal{N}_\epsilon = \left(\sqrt{\frac{i}{2\pi\hbar\epsilon}}\right)^d. \tag{2.44}$$

https://doi.org/10.1017/9781009291248.003 Published online by Cambridge University Press

Adding the imaginary part to the Hamiltonian is known in other words as the "$i$-epsilon" prescription (note this "epsilon" has nothing to do with the $\epsilon$ appearing in our formulas above). Such a deformation can be effected in the case at hand by changing the $p_i \to (1 - i\xi)p_i$ in the exponent of Equation (2.43) with infinitesimal $\xi$ (instead of using the usual "epsilon"). It is tantamount to defining the Minkowski path integral by starting with the Euclidean path integral and continuing this back to Minkowski space.

For the remainder of this book, we will be interested in the path-integral representation, Equation (2.39), of the matrix element Equation (2.32). We will apply methods that are standard for ordinary integrals to obtain approximations for the matrix element. We will use the saddle point method for evaluation of the path integral. This involves finding the critical points of the Euclidean action and then expanding about the critical point in a (functional) Taylor expansion. The value of the action at the critical point is a constant as far as the integration is concerned and just comes out of the integral. This term alone already gives much novel information about the matrix element. It is usually non-perturbative in the coupling constant. The first variation of the action vanishes by definition at the critical point. The first non-trivial term, the second-order term in the Taylor expansion, yields a Gaussian path integral. The remaining higher-order terms in the Taylor expansion give perturbative corrections to the Gaussian integral. The Gaussian integral can sometimes be done explicitly, although this too can be prohibitively complicated.

We will work with the formal path integral, Equation (2.41), rather than the exact discretized version, Equation (2.39). First of all it is much easier to find the critical points of the classical Euclidean action rather than its discretized analogue. Secondly, in the limit that $N \to \infty$, the critical points for the discrete action should approach those of the classical action. The actual path integral to be done always remains defined by the discretized version. The critical point of the classical action is only to be used as a centre point about which to perform the path integral Equation (2.39) in the Gaussian approximation and in further perturbative expansion. As stressed by Coleman [31], the set of smooth paths is a negligible fraction of the set of all paths. However, this does not dissuade us from using a particular smooth path, that which is a solution of the classical equations of motion, as a centre point about which to perform the functional integration in a Gaussian approximation. The Gaussian path integral corresponds to integration over all paths, especially including those which are arbitrarily non-smooth, but which are centred on the particular smooth path corresponding to the solution of the equations of motion, with a quadratic approximation to the action (or what is called Gaussian since it leads to an (infinite) product of Gaussian integrals). It actually receives most of its contribution from extremely non-smooth paths. However, the Gaussian path integral can be evaluated in some cases exactly,

and in other cases in a perturbative approximation. In this way the exact definition of the formal path integral, Equation (2.41), is not absolutely essential for our further considerations. We will, however, continue to frame our analysis in terms of it, content with the understanding that underlying it a more rigorous expression always exists.

https://doi.org/10.1017/9781009291248.003 Published online by Cambridge University Press