Learning outcomes

You'll be able to:

- Distinguish three formulations of quantum mechanics
- Categorise questions each formulation is best placed to answer
- Relate the Hamiltonian and time evolution operator
- Define the conditions for time-translation invariance
- Relate time-translation invariance and energy conservation
- Outline motivation for path integral formulation
- State path integral representation of the propagator
- Apply path integral representation to the propagator of the free particle
- Demonstrate equivalence of the Schrödinger equation and the path integral representation.

Formulations of Quantum Mechanics

Usually, when we think about "solving" a quantum system, we have in mind something like solving the Schrödinger equation to find the time dependence of the wavefunction of the system.

But this is not the only wave to think about quantum mechanics. It turns out there (at least) four "pictures" or formulations of quantum systems, three of which we will study in this course.

1. Schrödinger picture – the one you're probably used to.
2. Heisenberg picture – operators carry time dependence!
3. Path integral – represent quantum amplitudes through "sums over all paths/histories"
4. Interaction picture – a blend of Schrödinger and Heisenberg pictures, relevant for quantum field theory (that is, <u>not</u> this course).

These formulations end up all being equivalent, but they have different advantages and disadvantages and you can think of them as just "changes of variables" for how we understand quantum mechanical systems.

Time translations

Even though in this course we consider only nonrelativistic systems, we can still treat time as somewhat analogous to space and we can investigate time translations.

Suppose that $\Psi(x,t)$ is a solution of the time-dependent Schrödinger equation, so

$$\hat{H}\,\Psi(x,t) = i\hbar \frac{\partial}{\partial t} \Psi(x,t)$$

We can introduce a time evolution operator

$$\hat{U}(t,t_0)\,\Psi(x,t_0) = \Psi(x,t)$$

$\uparrow$ evolves $\Psi(x,t_0)$ to $\Psi(x,t)$

As long as $\frac{\partial}{\partial t}\hat{H} = 0$ (i.e. the Hamiltonian is not explicitly a function of time) then we can write down an expression for $U(t,t_0)$ by Taylor-expanding $\Psi(x,t)$ around t_0

$$\hat{U}(t,t_0)\,\Psi(x,t_0) = \Psi(x,t) \qquad \} \; t = t_0 + \delta t \text{ with } \delta t \text{ infinitesimal}$$

$$= \Psi(x, t_0 + \delta t)$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} (\delta t)^n \frac{\partial^n}{\partial t^n} \Psi(x,t)\Big|_{t=t_0} \qquad \} \text{ since } \frac{\partial}{\partial t}\Psi(x,t) = -\frac{i}{\hbar}\hat{H}\Psi(x,t)$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} (\delta t)^n \left(-\frac{i}{\hbar}\hat{H}\right)^n \Psi(x,t_0)$$

$$= \exp\left[-\frac{i\,\delta t}{\hbar}\hat{H}\right] \Psi(x,t_0)$$

So we deduce

$$\boxed{\hat{U}(t,t_0) = \exp\left[\frac{-i}{\hbar}(t-t_0)\hat{H}\right]}$$

The Hamiltonian is the "generator" of time translation

The time-evolution operator, $U(t,t_0)$, is closely tied to the solution of the Schrödinger equation, which makes sense, because the Schrödinger equation is precisely the equation that governs time evolution!

Let's take $t_0 = 0$ for simplicity. Then we can write

$$\Psi(x,0) = \sum_n c_n \varphi_n(x)$$

no time-dependent phase factor because $e^{-iE_nt/\hbar}\Big|_{t=0} = 1$

stationary energy eigenstates

So the general solution is

$$\begin{aligned}
\Psi(x,t) &= \hat{U}(t)\,\Psi(x,0) \\
&= \sum_n c_n \hat{U}(t)\,\varphi_n(x) \\
&= \sum_n c_n e^{-i\hat{H}t/\hbar}\varphi_n(x) \\
&= \sum_n c_n e^{-iE_nt/\hbar}\varphi_n(x)
\end{aligned}$$

So the time-evolution operator plays the role of the time-dependent phase factors!

This discussion (and all of this course) has been framed in terms of the <u>time-dependent</u> wavefunction. This is known as the "Schrödinger picture" of quantum mechanics. In this picture, the operators have no time dependence themselves (for example $\hat{p} = -i\hbar \frac{\partial}{\partial x}$ does not have "t" in it) and all time dependence is carried by the wavefunction (or the state of the system). The time dependence of measurements comes from the time dependence of the wavefunction, so, for example,

$$\underbrace{\langle \hat{p} \rangle}_{\substack{\text{depends on} \\ \text{time because of} \\ \Psi(x,t)}} = \langle \Psi(x,t) | \underbrace{\hat{p}}_{\substack{\text{no time} \\ \text{dependence}}} | \underbrace{\Psi(x,t)}_{\text{time dependent}} \rangle$$

But this is not the only "picture" of quantum mechanics - there is also the "Heisenberg picture" (and in interacting quantum field theory, we regularly use the "interaction picture", which is a mix of the Schrödinger and Heisenberg pictures).

In the Heisenberg picture, which is entirely equivalent to the Schrödinger picture, the <u>operators</u> have time dependence and the states (or wavefunctions) are time independent.

$$\underbrace{\langle \hat{p} \rangle}_{\substack{\text{still time} \\ \text{dependent, but} \\ \text{now because of} \\ \text{the operator}}} = \langle \varphi_H | \underbrace{\hat{p}_H(t)}_{\substack{\text{time-dependent} \\ \text{operator}}} | \underbrace{\varphi_H}_{\text{no time dependence!}} \rangle$$

The "H" subscript indicates a "Heisenberg picture" operator or wavefunction.

We can think of this operator time dependence as a change of reference frame (in time), just like we could apply a spatial translation to an operator.

$$\boxed{\hat{Q}_H(t) = \hat{U}^+(t)\,\hat{Q}\,\hat{U}(t)}$$

To see the two pictures are equivalent, we can write

$$\langle \Psi(x,t) | \hat{Q} | \Psi(x,t) \rangle = \langle \Psi(x,0)\, \hat{U}^+(t) | \hat{Q} | \hat{U}(t)\, \Psi(x,0) \rangle$$
$$= \langle \Psi(x,0) | \hat{U}^+(t)\, \hat{Q}\, \hat{U}(t) | \Psi(x,0) \rangle$$
$$= \langle \Psi_H(x) | \hat{Q}_H(t) | \Psi_H(x) \rangle$$

This discussion considered only time-independent Hamiltonians, but we can still consider the more general case (this is done in Problems 6.28 and 11.23) for an infinitesimal time interval

$$\hat{U}(t, t_0) = \hat{U}(t_0 + \delta t, t_0) \simeq 1 - \frac{i}{\hbar} \hat{H}(t_0)\, \delta t$$

For a system to be <u>time-translation invariant</u>, then we require

$$\hat{U}(t_1 + \delta t, t_1) = \hat{U}(t_2 + \delta t, t_2) \quad \text{for } t_1 \neq t_2$$

In other words, the time evolution of the system does not depend on the "origin" of time (that is, what time we start counting from)

This is only true if

$$\hat{U}(t_1 + \delta t, t_1) \simeq 1 - \frac{i}{\hbar}\hat{H}(t_1)\,\delta t = \hat{U}(t_2 + \delta t, t_2) \simeq 1 - \frac{i}{\hbar}\hat{H}(t_2)\,\delta t$$

In other words, if

$$\hat{H}(t_1) = \hat{H}(t_2)$$

Thus, for our system to be time-translation invariant, we must have a time-independent Hamiltonian!

$$\uparrow \frac{\partial}{\partial t}\hat{H} = 0$$

From this we learn that energy is <u>conserved</u> (that is, independent of time, as a whole)

$$\frac{d}{dt}\langle E\rangle = \frac{d}{dt}\langle \hat{H}\rangle = \frac{i}{\hbar}\langle [\hat{H},\hat{H}]\rangle + \left\langle \frac{\partial \hat{H}}{\partial t}\right\rangle = 0$$

This is our first example of a symmetry giving rise to a conserved quantity. In this case

$$\boxed{\text{time translation invariance} \Rightarrow \text{energy is conserved.}}$$

We will study this phenomenon in much more detail in later sections of the course.

Path integrals

The path integral formulation is rather different from the two formulations we've seen so far, and it can be hard to see how it could possibly relate to the more standard process of solving the Schrödinger equation. In fact, we will see that one can obtain the Schrödinger equation directly from the path integral, and that there is at least one way of understanding why the path integral is quite natural.

The Schrödinger and Heisenberg pictures are primarily focussed on solving the time evolution of the system through the Hamiltonian of the system. They are the quantum analogues of Hamiltonian mechanics for classical systems.

Path integrals, in contrast, are the analogues of Lagrangian mechanics, because they are based on the action (or Lagrangian) of the system.

Recall $S = \int dt\, L = \int dt\, [T - V]$

Path integrals are the natural formulation for quantum field theory and make explicit the connection between quantum systems and statistical systems.

For our purposes, the central question that the path integral formalism is equipped to answer is

> "What is the probability of finding a particle at point x_b, at a time t_b, given that it started at point x_a at an earlier time t_a?"

The answer to this is given by the propagator

$$P(x_b, t_b | x_a, t_a) = \langle \Psi(x_b, t_b) | \Psi(x_a, t_a) \rangle$$

We've seen that if the Hamiltonian is independent of time, so $\frac{\partial H}{\partial t} = 0$, then the system is translation invariant in time, so the starting time is arbitrary and our propagator obeys

propagator depends only on positions and time elapsed.

$$P(x_b, t_b | x_a, t_a) \equiv P(x_a, x_b ; t_b - t_a)$$

The path integral representation of the propagator is

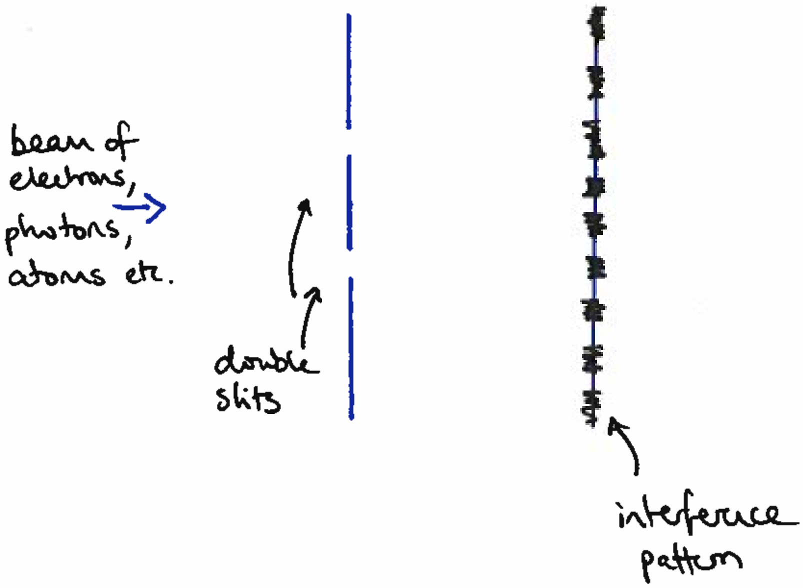
$$\boxed{P(x_a, x_b ; t_b - t_a) = N(t) \int D[x(t)] \exp\left(\frac{i}{\hbar} S[x(t)]\right)}$$

Here:

- $N(t)$ is a normalisation that depends only on $t = t_b - t_a$
- $\int D[x(t)]$ is the path integral measure, which corresponds to an integral over all possible paths $x(t)$

So where does this prescription come from?

One way to motivate this is to go back to our old friend – the double slit experiment.



In the double slit experiment, beams (of electrons, photons, atoms or molecules or...) are fired at two slits and an interference pattern is observed on a screen far from the slits.

This was used by Young to demonstrate the wave-nature of light, but it is just the same with electrons. Most remarkably, the interference pattern is still observed even when individual electrons are fired at the screen – they <u>interfere with themselves</u>!

This is typically taken to demonstrate <u>wave-particle duality</u> for quantum objects, but we can also interpret this as evidence that the electron takes all possible paths to the screen, and that these paths can interfere with each other.

and letting $z_i = y_i - \left(\frac{y_{i-1} + y_{i+1}}{2}\right)^2$

so that

$$(y_2 - y_1)^2 + (y_1 - y_0)^2 = 2\left\{ z_1^2 + \underbrace{\frac{y_0^2 + y_2^2}{2} - \frac{(y_0 + y_2)^2}{4}}_{= \frac{1}{4}(y_0 - y_2)^2} \right\}$$

Now we plug this back into I_1

$$I_1 = \frac{2\hbar\delta}{m} \underbrace{\int_{-\infty}^{\infty} dz_1 \, e^{2iz_1^2}}\cdot e^{\frac{i}{2}(y_0 - y_2)^2}$$

$$= \frac{2\hbar\delta}{m}\sqrt{\frac{\pi i}{2}}\, e^{\frac{i}{2}(y_0 - y_2)^2}$$

Next we move on to the x_2 integral (don't worry, we won't keep this up for much longer). We again change variables $x_2 \to y_2 = \frac{m}{2\hbar\delta} x_2$ and we have

$$I_2 = \frac{2\hbar\delta}{m}\int_{-\infty}^{\infty} dy_2 \, e^{i\left[(y_3 - y_2)^2 + \frac{1}{2}(y_2 - y_0)^2\right]}$$

We can apply the same logic to this one and we'll end up with

$$I_2 = \frac{2\hbar\delta}{m}\sqrt{\frac{(i\pi)^2}{2}}\, e^{\frac{i}{3}(y_3 - y_0)^2}$$

assuming we've done all the $n-1$ to $n=1$ integrals beforehand

Hopefully you're starting to see the pattern! The n^{th} integral is

$$I_n = \frac{2\hbar\delta}{m}\sqrt{\frac{(i\pi)^n}{n+1}}\, e^{\frac{i}{n+1}(y_{n+1} - y_0)^2}$$

Plugging this into the action

$$S_i = \int_{t_i}^{t_{i+1}} dt \ \frac{m}{2}\left[\dot{x}(t)\right]^2 = \frac{m}{2}\int_{t_i}^{t_{i+1}} dt \ \frac{(x_{i+1}-x_i)^2}{\delta^2}$$

$$= \frac{m}{2}\frac{(x_{i+1}-x_i)^2}{\delta^2}\cdot\underbrace{(t_{i+1}-t_i)}_{=\delta} = \frac{m}{2\delta}(x_{i+1}-x_i)^2$$

The path integral prescription tells us to integrate/sum over all possible paths, which means integrating over all possible intermediate positions x_i:

$$P(x_a,x_b;t) = N(t)\int_{-\infty}^{\infty}dx_1\int_{-\infty}^{\infty}dx_2\cdots\int_{-\infty}^{\infty}dx_{N-1}\,\exp\left\{\frac{i}{\hbar}\frac{m}{2\delta}\sum_{i=0}^{N-1}(x_{i+1}-x_i)^2\right\}$$

This doesn't look great, but we can figure out the integrals one-by-one to find the general result. Starting with x_1, we have

$$\int_{-\infty}^{\infty}dx_1\,\exp\left\{\frac{i}{\hbar}\frac{m}{2\delta}\left[(x_2-x_1)^2+(x_1-x_0)^2\right]\right\} \longleftarrow \text{call this } I_1$$

We can simplify I_1 by defining $y_i = \frac{m}{2\hbar\delta}x_i$ so that

$$I_1 = \frac{2\hbar\delta}{m}\int_{-\infty}^{\infty}dy_1\,e^{i\left[(y_2-y_1)^2+(y_1-y_0)^2\right]}$$

and then completing the square

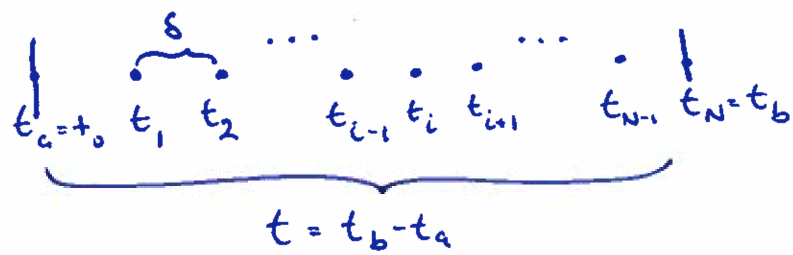
$$(y_2-y_1)^2+(y_1-y_0)^2 = 2y_1^2-2(y_0+y_2)y_1+y_0^2+y_2^2$$
$$= 2\left\{\left[y_1-\frac{(y_0+y_2)}{2}\right]^2+\frac{y_0^2+y_2^2}{2}-\frac{(y_0+y_2)^2}{4}\right\}$$

Free particle

Let's use the free particle as an example to see how this actually works, and how the path integral measure can be defined in practice. We'll restrict our attention to the one-dimensional free particle.

Let $x(t)$ be one possible path (or trajectory) from the point x_a at time t_a to point x_b at time t_b. We will discretise time, that is, divide it into small chunks of time $\delta = \dfrac{(t_b - t_a)}{N}$.

We define $t_a = t_0$ and $t_b = t_N$ so that our timeline can be represented as



Now we label the position at time point t_i as $x_i(t_i)$, where i runs from 1 to $(N-1)$.

Let's consider one particular time chunk. For a free particle $V(x) = 0$ so $\mathcal{L} = T$ and the action depends only on the kinetic energy (the velocity) and not the position.

If δ is small enough, then the velocity will be constant in that time chunk: $\dot{x}_i(t_i) = \dfrac{x_{i+1} - x_i}{\delta}$

This means our propagator takes the form

$$P(x_a, x_b; t) = \underbrace{N(t)\left(\frac{(\pi i)^{N-1}}{N}\right)^{1/2}}_{} e^{i/N (y_N - y_0)^2}$$

It turns out this is $\sqrt{\frac{m}{2\pi i \hbar t}}$

We will not calculate this here

In other words, the propagator for the free particle is

$$\boxed{P(x_a, x_b; t) = \sqrt{\frac{m}{2\pi i \hbar t}} \exp\left[\frac{im}{2\hbar t}(x_b - x_a)^2\right]}$$

This probably seems like a lot of work (it is). Isn't there a better way? Yes! We can actually calculate this propagator directly, using more familiar techniques

time evolution operator

$$P(x_a, x_b; t) = \langle x_b | e^{-\frac{iHt}{\hbar}} | x_a \rangle$$

identity operator (compare 3.106)

$$= \langle x_b | e^{-\frac{it}{\hbar}\hat{p}^2/2m} | x_a \rangle$$

insert complete set of momentum states

$$= \langle x_b | e^{-i\frac{t}{\hbar}\hat{p}^2/2m} \int \frac{dp}{(2\pi)} |p\rangle\langle p | x_a \rangle$$

$e^{\hat{p}}|p\rangle = e^{p}|p\rangle$

$$= \int \frac{dp}{2\pi} e^{-i\frac{t}{\hbar}p^2/2m} \langle x_b | p \rangle \langle p | x_a \rangle$$

see discussion in example 3.9 but note different normalisation

$$= \int \frac{dp}{2\pi\hbar} e^{-\frac{it}{\hbar}p^2/2m} e^{ix_b p/\hbar} e^{-ipx_a/\hbar}$$

$$= \sqrt{\frac{m}{2\pi i \hbar t}} e^{\frac{im}{2t\hbar}(x_b - x_a)^2}$$

the same!

That last derivation was a lot shorter than the path integral one, although of course they gave the same result.

This might make you wonder: what is the point of the path integral?

The answers are:

1. The path integral is the natural language of quantum field theory, which brings together quantum mechanics and special relativity and underpins all of particle and nuclear physics.
2. The path integral relates quantum phenomena to statistical ones and shows us the deep relation between particle and nuclear physics and condensed matter systems.
3. The path integral can be used to solve things numerically when analytic treatments fail.

It might not be obvious here, but, trust me, the path integral is awesome.