Quantum Mechanics II: PHYS 314 (Spring 2021)
Problem Set 2–Solutions.

Overview

In this Problem Set you will demonstrate the equivalence of the path integral formulation and the Schrödinger picture, by deriving the Schrödinger equation from the path integral. You will also write a short summary of the different formulations, aimed at a general science audience, to help you bring together your understanding of the various pictures of quantum mechanics and frame them in a way that makes sense to you. There are two questions.

Question 1 — 40pts

Introduction The Schrödinger equation tells us how to determine the state of a quantum system as a function of time, given an initial state at an earlier time. We can write the Schrödinger equation for a quantum state, $|\Psi(t)\rangle$, as

$$\widehat{H}|\Psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle,$$

which has general solution

$$|\Psi(t)\rangle = e^{-i\widehat{H}(t-t_0)/\hbar}|\Psi(t_0)\rangle$$

for a time-independent Hamiltonian

$$\widehat{H} = \frac{\widehat{p}^2}{2m} + V(\widehat{x}).$$

The corresponding wavefunction is given by the projection of the state $|\Psi(t)\rangle$ onto the spatial eigenstates $|x\rangle$, which we can decompose in terms of the energy eigenfunctions $\psi_n(x)$ as

$$\Psi(x,t) = \langle x|\Psi(t)\rangle = \sum_n c_n e^{-iE_n(t-t_0)/\hbar}\psi_n(x),$$

where the coefficients are given by

$$c_n = \int \mathrm{d}x\, \psi_n^*(x)\Psi(x,t_0).$$

(a) Show that the wavefunction can be written as

$$\Psi(x,t) = \int \mathrm{d}x_0 \langle x,t|x_0,t_0\rangle \Psi(x_0,t_0), \tag{1}$$

where $|x_0, t_0\rangle$ is a position eigenstate, evaluated at position x_0 and time t_0. We will use this expression for the wavefunction to derive the Schrödinger equation from the path integral representation of the propagator.

(b) Consider the wavefunction, $\Psi(x, t_0 + \delta)$, of the system an infinitesimal time δ after the system is prepared in an initial state $\Psi(x_0, t_0)$. These states can be related by an equation of the form in part (a), which is

$$\Psi(x,t_0+\delta) = \int \mathrm{d}x_0 \, \langle x,t_0+\delta|x_0,t_0\rangle \Psi(x_0,t_0). \tag{2}$$

Use the path integral representation to show that the propagator can be approximated by

$$\langle x,t_0+\delta|x_0,t_0\rangle \approx N(\delta) \exp\left(\frac{im}{2\hbar\delta}(x-x_0)^2\right)\left[1-\frac{i\delta}{\hbar}V\left(\frac{x+x_0}{2}\right)\right]. \tag{3}$$

List and justify the approximations you make to reach this result.

(c) Substitute your result from equation (3) into equation (2) and carry out the integrals via a change of variables, $\eta = x - x_0$, to show that the equation (2) can be written as

$$\Psi(x,t_0+\delta) = N(\delta)\sqrt{\frac{2\pi i\hbar\delta}{m}}\left[\Psi(x,t_0) - \frac{i\delta}{\hbar}V\left(x\right)\Psi(x,t_0) - \frac{\hbar\delta}{2im}\frac{\partial^2}{\partial x^2}\Psi(x,t_0)\right]. \tag{4}$$

(d) Consider the case $\delta = 0$ to show that

$$N(\delta) = \sqrt{\frac{m}{2\pi i\hbar\delta}}. \tag{5}$$

(e) Rearrange equation (4) and consider the limit $\delta \to 0$ to derive the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x,t).$$

You have just derived the Schrödinger equation from the path integral representation of the propagator!

Solution 1

(a) The wavefunction can be written as

$$\begin{aligned}\Psi(x,t) &= \langle x|\Psi(t)\rangle \\ &= \langle x|e^{-i\widehat{H}(t-t_0)}|\Psi(t_0)\rangle \\ &= \langle x|e^{-i\widehat{H}(t-t_0)}\int \mathrm{d}x_0|x_0\rangle\langle x_0|\Psi(t_0)\rangle \\ &= \int \mathrm{d}x_0\,\langle x,t|x_0,t_0\rangle\Psi(x_0,t_0),\end{aligned}$$

as required.

(b) We start from the path integral representation of the relevant propagator

$$\langle x, t_0+\delta|x_0,t_0\rangle = N(\delta)\exp\left[\frac{i}{\hbar}S(\dot{x}_0,x_0)\right], \tag{6}$$

which represents just one possible path (we're integrating over the paths separately).

We're considering an infinitesimal time interval, so we can approximate the speed as

$$\dot{x} = \frac{x-x_0}{\delta},$$

and we can assume that the potential is well-represented by the average value, evaluated at the midpoint $(x+x_0)/2$.

The action in this case is then

$$\begin{aligned}S(\dot{x}_0,x_0) &= \int_{t_0}^{t_0+\delta}\mathrm{d}t\left[\frac{m\dot{x}_0^2}{2} - V\left(\frac{x+x_0}{2}\right)\right] \\ &= \left[\frac{m}{2}\left(\frac{x-x_0}{\delta}\right)^2 - V\left(\frac{x+x_0}{2}\right)\right]\int_{t_0}^{t_0+\delta}\mathrm{d}t \\ &= \frac{m}{2\delta}(x-x_0)^2 - \delta\,V\left(\frac{x+x_0}{2}\right).\end{aligned}$$

We now substitute this into or expression for the propagator, and expand the exponential, to obtain

$$\langle x,t_0+\delta|x_0,t_0\rangle \approx N(\delta)\exp\left(\frac{im}{2\hbar\delta}(x-x_0)^2\right)\left[1-\frac{i\delta}{\hbar}\,V\left(\frac{x+x_0}{2}\right)\right],$$

as required.

The approximations we've made are

- We need only a single path in our propagator.
- We assume the position and speed don't depend on time over the infinitesimal time interval δ.
- We approximate the speed as $\dot{x} = (x - x_0)/\delta$.
- We approximate the potential by its average value at the midpoint $V((x+x_0)/2)$.

(c) We plug in our result from part (b) into our initial equation to find

$$\begin{aligned}
\Psi(x, t_0 + \delta) &= \int \mathrm{d}x_0\, N(\delta) \exp\left(\frac{im}{2\hbar\delta}(x - x_0)^2\right) \left[1 - \frac{i\delta}{\hbar} V\left(\frac{x + x_0}{2}\right)\right] \Psi(x_0, t_0) \\
&= N(\delta) \int \mathrm{d}\eta\, \exp\left(\frac{im}{2\hbar\delta}\eta^2\right) \left[1 - \frac{i\delta}{\hbar} V\left(x - \frac{\eta}{2}\right)\right] \Psi(x - \eta, t_0) \\
&= N(\delta) \Bigg[\int \mathrm{d}\eta\, \exp\left(\frac{im}{2\hbar\delta}\eta^2\right) \Psi(x - \eta, t_0) \\
&\qquad - \frac{i\delta}{\hbar} \int \mathrm{d}\eta\, \exp\left(\frac{im}{2\hbar\delta}\eta^2\right) V\left(x - \frac{\eta}{2}\right) \Psi(x - \eta, t_0) \Bigg].
\end{aligned}$$

Now we can expand everything

$$\begin{aligned}
V\left(x - \frac{\eta}{2}\right) &\approx V(x) - \frac{\eta}{2} \frac{\mathrm{d}}{\mathrm{d}x} V(x) \\
\Psi(x - \eta, t_0) &\approx \Psi(x, t_0) - \eta \frac{\mathrm{d}}{\mathrm{d}x} \Psi(x, t_0) + \frac{\eta^2}{2} \frac{\mathrm{d}^2}{\mathrm{d}x^2} \Psi(x, t_0),
\end{aligned}$$

and substitute this into our expression above to obtain

$$\begin{aligned}
\Psi(x, t_0 + \delta) = N(\delta) \Bigg[&\int \mathrm{d}\eta\, \exp\left(\frac{im}{2\hbar\delta}\eta^2\right) \left[\Psi(x, t_0) - \eta \frac{\mathrm{d}}{\mathrm{d}x} \Psi(x, t_0) + \frac{\eta^2}{2} \frac{\mathrm{d}^2}{\mathrm{d}x^2} \Psi(x, t_0)\right] \\
&- \frac{i\delta}{\hbar} \int \mathrm{d}\eta\, \exp\left(\frac{im}{2\hbar\delta}\eta^2\right) \left[V(x) - \frac{\eta}{2} \frac{\mathrm{d}}{\mathrm{d}x} V(x)\right] \\
&\quad \times \left[\Psi(x, t_0) - \eta \frac{\mathrm{d}}{\mathrm{d}x} \Psi(x, t_0) + \frac{\eta^2}{2} \frac{\mathrm{d}^2}{\mathrm{d}x^2} \Psi(x, t_0)\right] \Bigg].
\end{aligned}$$

Any terms that are odd in η will vanish when integrated, and we will drop terms of $\delta\eta^2$, so that we end up with

$$\begin{aligned}
\Psi(x, t_0 + \delta) \approx N(\delta) \Bigg[&\left[1 - \frac{i\delta}{\hbar} V(x)\right] \Psi(x, t_0) \int \mathrm{d}\eta\, \exp\left(\frac{im}{2\hbar\delta}\eta^2\right) \\
&+ \frac{1}{2} \frac{\mathrm{d}^2}{\mathrm{d}x^2} \Psi(x, t_0) \int \mathrm{d}\eta\, \eta^2 \exp\left(\frac{im}{2\hbar\delta}\eta^2\right) \Bigg].
\end{aligned}$$

Carrying out the Gaussian integrals, using the general formula[1]

$$\int_{\infty}^{\infty} \mathrm{d}z \, \exp\left(iaz^2\right) = \sqrt{\frac{i\pi}{a}},$$

we obtain the result

$$\Psi(x, t_0 + \delta) = N(\delta)\sqrt{\frac{2\pi i\hbar\delta}{m}} \left[\Psi(x, t_0) - \frac{i\delta}{\hbar} V(x) \Psi(x, t_0) - \frac{\hbar\delta}{2im} \frac{\partial^2}{\partial x^2} \Psi(x, t_0)\right],$$

as required.

(d) For $\delta = 0$ the left hand side is

$$\Psi(x, t_0 + \delta)_{\delta=0} = \Psi(x, t_0)$$

and the right hand side is

$$N(\delta)\sqrt{\frac{2\pi\hbar\delta}{im}} \Psi(x, t_0).$$

Equating these two, we immediately deduce that

$$N(\delta) = \sqrt{\frac{im}{2\pi\hbar\delta}},$$

as required.

(e) Using this result, we have

$$\Psi(x, t_0 + \delta) = \Psi(x, t_0) - \frac{i\delta}{\hbar} V(x) \Psi(x, t_0) - \frac{\hbar\delta}{2im} \frac{\partial^2}{\partial x^2} \Psi(x, t_0),$$

which we rearrange as

$$\Psi(x, t_0 + \delta) - \Psi(x, t_0) = -\frac{i\delta}{\hbar} V(x) \Psi(x, t_0) - \frac{\hbar\delta}{2im} \frac{\partial^2}{\partial x^2} \Psi(x, t_0).$$

Now we multiply by $i\hbar/\delta$, and we have

$$i\hbar \left(\frac{\Psi(x, t_0 + \delta) - \Psi(x, t_0)}{\delta}\right) = V(x) \Psi(x, t_0) - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x, t_0).$$

The left hand side is just the time derivative of the wavefunction, and so we see that this is exactly the Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)\right] \Psi(x, t),$$

as required.

[1] This formula is good enough for many physicists, but is too vague to satisfy mathematicians, as we're implicitly assuming that the complex square root is defined by its principal value on the first Riemann sheet, so that $\sqrt{i} = e^{i\pi/4}$. A fuller discussion is available in Desbrow, Am. Math. Monthly 105 (1998) 726, and probably many mathematical textbooks on complex analysis and measure theory.

Question 2 **10pts**

Write 250 to 300 words[2] comparing and contrasting the three formulations of quantum mechanics. You should illustrate this with two examples for each formulation, one drawn from the textbook or mentioned in the course materials, and one from beyond the course materials. Your response should be written in full sentences and addressed to a broad, but interested-in-science, audience (so think: a popular science blog post, or article in a popular science magazine, like Scientific American). You will be graded using the following rubric:

Aspect	Points	If you:
Physics	4	Correctly describe the three formulations, including similarities and differences
	2	Correctly characterise two of the three formulations; or describe all three, but miss key information; or fail to describe both similarities and differences
	0	Completely misconstrue the three formulations
Examples	4	Provide two examples for each formulation, one from the course and one not mentioned in the course or textbook
	2	Provide one example for each; or two examples, but not for all formulations; or include only examples mentioned in the course material
	0	Give no examples
Audience	2	Correctly gauge the understanding of the audience, including defining and illustrating unfamiliar terms
	1	Give a too-technical or too-simplistic explanation.

Solution 2

The solution is the rubric above.

[2] I will count.