Lecture 7

Path Integral in Quantum Mechanics

The central problem of quantum mechanics can be solved once we obtain the following object

$$U(x_f, t_f; x_i, t_i) = \langle x_f, t_f | x_i, t_i \rangle \;, \tag{7.1}$$

called the propagator. Knowing U we can evolve the wavefunction in time

$$\begin{aligned} \psi(x_f, t_f) = \langle x_f, t_f | \psi \rangle &= \int dx_i \, \langle x_f, t_f | x_i, t_i \rangle \, \langle x_i, t_i | \psi \rangle \;, \\ &= \int dx_i \, U(x_f, t_f; x_i, t_i) \, \psi(x_i, t_i) \;. \end{aligned} \tag{7.2}$$

Which means that $U(x_f, t_f; x_i, t_i)$ is the *Green function* of the equation of motion for the wavefunction, i.e. of the Schrödinger equation.

We can alternatively write the propagator in terms of the eigenvalues and eigenfunctions of the hamiltonian H:

$$\begin{aligned} U(x_f, t_f; x_i, t_i) &= \langle x_f | e^{-iH(t_f - t_i)/\hbar} | x_i \rangle \;, \\ &= \sum_n \langle x_f | x_n \rangle \langle x_n | x_i \rangle \, e^{-iE_n(t_f - t_i)/\hbar} \;, \\ &= \sum_n e^{-iE_n(t_f - t_i)/\hbar} \, \psi_n^*(x_f) \, \psi_n(x_i) \;. \end{aligned} \tag{7.3}$$

So we see from (7.3) that the propagator contains the information of all the eigenvalues and eigenfunctions of H, which is all the dynamical information of the quantum system. What is typically done is to obtain the E_n's and the $\psi_n(x)$'s and then the propagator $U(x_f, t_f; x_i, t_i)$. The path inetgral allows us to get the propagator directly.

7.1 The Conceptual Idea

Let us start from a well known quantum mechanical situation: the two-slit experiment. The two trajectories, 1 and 2, have different phases (different lengths) and this results in an interference pattern at the screen where we observe.

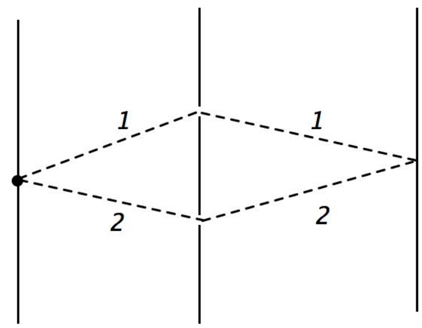

Figure 7.1: Double slit experiment. Different paths lead to different phases at the screen, which results in an interference pattern.

We can imagine that there are (infinitely) many screens with (infinitely) many slits each between the source and the observation screen. The result is that the are (infinitely) many trajectories with different phases interfering. In general, we can think of the amplitude for a particle to go from x_i to x_f as a sum over (infinitely) many trajectories. Only one of them is the classical trajectory.

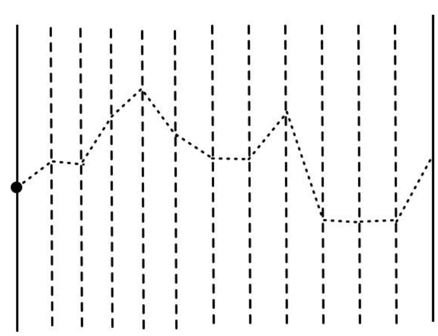

Figure 7.2: Many screens with many slits each. In the limit of infinitely many screens and infinitely many slits, the amplitude is the sum over all possible trajectories between the source and the observation point.

We can try to translate this into the propagator. Intuitively, we can write

$$U(x_f, t_f; x_i, t_i) = \sum_{\text{all trajectories}} A\, e^{i\,\text{phase}} \equiv \int \mathcal{D}x(t)\, e^{i\,\text{phase}} . \tag{7.4}$$

Here, the sum over all the trajectories is signified as an integral where the measure is accounting for all the possible $x(t)$'s. The next question is: what should be the phase ? We know that not all trajectories are equal. The classical trajectory should emerge as the only possible one in the $\hbar \longrightarrow 0$ limit, the classical limit. We will see bellow that this happens if

$$\text{phase} \simeq \frac{S[x(t)]}{\hbar} , \tag{7.5}$$

that is, if the phase is given by the action in units of $\hbar$. In this case we would have

$$U(x_f, t_f; x_i, t_i) = \int \mathcal{D}x(t)\, e^{iS[x(t)]/\hbar} . \tag{7.6}$$

This choice is clearly consistent with the emergence of the classical trajectory in the $\hbar \longrightarrow 0$ limit. To see this, we notice that in this limit the phase oscillates very rapidly, giving rise to cancellations (rapidly oscillating sines and cosines). This is the case for generic trajectories $x(t)$. However, the classical trajectory is special in that it is stationary. This means that because

$$\delta\, S[x_{\text{cl.}}(t)] = 0 , \tag{7.7}$$

the classical trajectory is a saddle point solution not affected by these cancellations. In other words, very close to the classical trajectory the contributions to the phase are *coherent* , i.e. they have the same sign on both sides.

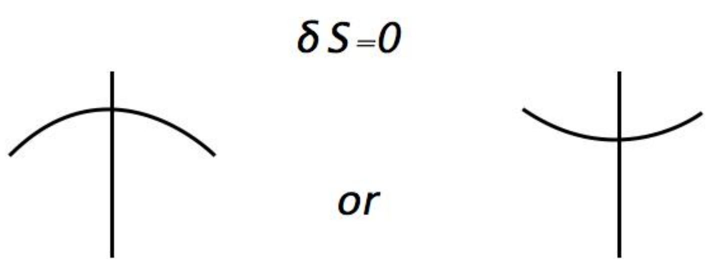

Figure 7.3: The pases add coherently on both sides close to the stationary action corresponding to the classical trajectory.

The question is how far can we go on each side of the stationary point before we loose coherence and cancelations become efficient. If we call $S_{\rm cl.}$ the action associated with the classical trajectory, it is clear that the sign of the contributions would start changing for trajectories outside the interval

$$\frac{S_{\rm cl.}}{\hbar} \pm \pi \ . \tag{7.8}$$

So trajectories that result in actions with $S[x(t)]/\hbar$ inside this interval should have important contributions to the amplitude. It is interesting to illustrate this point with a concrete example.

Example: Let us consider a free particle of mass m. Its classical trajectory is

$$x_{\rm cl}(t) = v\,t \ , \tag{7.9}$$

with a constant velocity we will take to be $v = 1\ cm/s$. We will also consider the alternative trajectory

$$x(t) = a\,t^2 \ , . \tag{7.10}$$

We want the boundaries of both trajectories to be the same. That is, we have the particle start and finish in the same point, say start at $x(0) = 0$, and finish at $x(1\ s) = 1\ cm$.

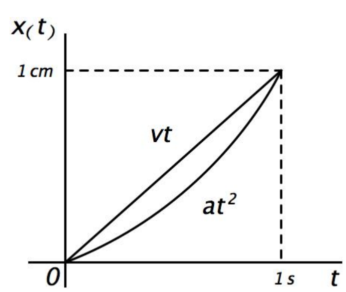

Figure 7.4: Classical trajectory for a free particle and an alternative non-classical one.

With these boundaries, we have that $a = 1cm/s^2$. We compute now the action for the classical trajectory. We have

$$S[x_{\rm cl.}(t)] = \int_0^1 \frac{1}{2}\, m\, \dot{x}_{\rm cl.}^2\, dt = \frac{1}{2}\, m\, v^2 (1\ s) \ . \tag{7.11}$$

On the other hand, the alternative trajectory gives

$$S[x(t)] = \int_0^1 \frac{1}{2}\, m\, \dot{x}(t)^2\, dt = 2ma^2 \int_0^1 t^2\, dt = \frac{2}{3}\, m\, a^2 (1\ s^3)\ . \tag{7.12}$$

The difference between the two actions then is

$$\begin{aligned} \Delta S &= (\frac{2}{3} - \frac{1}{2})\, m\ \ cm^2/s\ , \\ \Delta S &= \frac{1}{6}\, m\, \frac{cm^2}{s^2}\, s\ . \end{aligned} \tag{7.13}$$

We want to see under what circumstances $|\Delta S/\hbar| \leq \pi$. So let us take two values for the mass m.

1. $\underline{m = 1\ g}$:
   Given that $\hbar = 1.05 \times 10^{-34}\, J\, s = 1.05 \times 10^{-27}\, erg.s$ we have

   $$\Delta S = \frac{1}{6}\, erg.s = \frac{1}{6}\ \times 10^{27}\, \hbar \tag{7.14}$$

   or

   $$\frac{\Delta S}{\hbar} \simeq 10^{26} \gg \pi\ . \tag{7.15}$$

   So we see that a particle with $m = 1\ g$ cannot go through this alternative trajectory, and we can actually conclude that it would be forced to stay in trajectories incredibly close to the classical one.

2. $\underline{m_e = 9 \times 10^{-28}\, g}$: The electron mass. Repeating the calculation we see that here we get

   $$\frac{\Delta S}{\hbar} \simeq \frac{1}{6} < \pi\ , \tag{7.16}$$

   so the electron has a lot of room to go into trajectories completely different from the classical given its small mass. In general, if the action is of the order of $\hbar$ or smaller the system will present quantum behavior. If, on the contrary, the action is large in units of $\hbar$ then de-coherence effects set quickly in and only the classical trajectory emerges.

7.2 Derivation of the Path Integral

Starting with the propagator associated with an infinitesimal time difference Δt, we would like to prove the following identity

$$\langle x_1, t+\Delta t | x_0, t\rangle = c\, e^{i\left(L(t)\,\Delta t + O((\Delta t)^2)\right)/\hbar} \ . \tag{7.17}$$

In the above expression c is a constant we will compute, $L(t)$ is the lagrangian at time t, and we will be working at first order in Δt. We consider the hamiltonian

$$H = \frac{p^2}{2m} + V(x) \ , \tag{7.18}$$

which then we can use to write

$$\langle x_1, t+\Delta t | x_0, t\rangle = \langle x_1 | e^{-i\,H\,\Delta t/\hbar} | x_0\rangle \tag{7.19}$$

Going to momentum space, we insert a complete set of momentum states as in

$$\langle x_1, t+\Delta t | x_0, t\rangle = \int dp\, \langle x_1 | p\rangle \langle p | e^{-i\,H\,\Delta t/\hbar} | x_0\rangle \ . \tag{7.20}$$

The first factor in the integral above is the momentum space representation of the wave function

$$\langle x_1 | p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{ip\,x_1/\hbar} \ . \tag{7.21}$$

The second factor can be expanded for small values of Δt as

$$\begin{aligned} \langle p | e^{i\,H\,\Delta t/\hbar} | x_0\rangle &= \langle p| \left(1 - \frac{i}{\hbar}\,H\,\Delta t + O((\Delta t)^2)\right) |x_0\rangle \ , \\ &= \left(1 - \frac{i}{\hbar}\,\frac{p^2}{2m}\Delta t - \frac{i}{\hbar}\,V(x_0)\Delta t + O((\Delta t)^2)\right) \langle p | x_0\rangle \ . \end{aligned} \tag{7.22}$$

The last factor in (7.22) is just the complex conjugate of the momentum representation of the wave-function at x_0, i.e.

$$\langle p | x_0\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{-i\,p\,x_0/\hbar} \ . \tag{7.23}$$

Putting (7.21) and (7.22) back into (7.20) we obtain

$$\begin{aligned} \langle x_1, t+\Delta t | x_0, t\rangle &= \int \frac{dp}{2\pi\hbar}\, e^{ip(x_1-x_0)/\hbar}\, e^{-i(p^2/2m+V(x_0))\Delta t/\hbar} \;, \\ &= \int \frac{dp}{2\pi\hbar}\, e^{i(p(x_1-x_0)-(p^2/2m)\Delta t - V(x_0)\Delta t)/\hbar} \;, \end{aligned} \tag{7.24}$$

where in the first line we have re-exponentiated the last factor which is valid for infinitesimal Δt. In order to do the momentum integral we complete the square. For this we see that we can write

$$\frac{i}{\hbar}\frac{\Delta t}{2m}\left(\frac{2m}{\Delta t}\,p(x_1-x_0)-p^2\right) = -\frac{i\Delta t}{\hbar 2m}\left(p-\frac{m}{\Delta t}\,(x_1-x_0)\right)^2 + \frac{i}{\hbar}\frac{m}{2\Delta t}\,(x_1-x_0)^2 \;, \tag{7.25}$$

which means we can rewrite (7.24) as

$$\langle x_1, t+\Delta t | x_0, t\rangle = e^{\frac{i}{\hbar}\,[\frac{m}{2\Delta t}\,(x_1-x_0)^2 - V(x_0)\Delta t]} \int \frac{dp}{2\pi\hbar}\, e^{-\frac{i}{\hbar}\frac{\Delta t}{2m}[p-\frac{m}{\Delta t}\,(x_1-x_0)]^2} \;. \tag{7.26}$$

The integral in (7.26) can be done using

$$\int_{-\infty}^{+\infty} dp\, e^{-a\,[p-b]^2} = \sqrt{\frac{\pi}{a}} \;, \tag{7.27}$$

which results in

$$\langle x_1, t+\Delta t | x_0, t\rangle = \sqrt{\frac{m}{2\pi\hbar i\Delta t}}\; e^{\frac{i}{\hbar}\,[\frac{1}{2}\,m\frac{(x_1-x_0)^2}{(\Delta t)^2} - V(x_0)]\,\Delta t} \;. \tag{7.28}$$

Noticing that

$$\frac{(x_1-x_0)}{\Delta t} = \dot{x}(t) + O((\Delta t)^2) \;, \tag{7.29}$$

we finally obtain

$$\boxed{\langle x_1, t+\Delta t | x_0, t\rangle = \sqrt{\frac{m}{2\pi\hbar i\Delta t}}\; e^{\frac{i}{\hbar}\,L(t)\,\Delta t + O((\Delta t)^2)} \;,} \tag{7.30}$$

which is (7.17), which we wanted to prove. We can now apply this result for the propagator for an infinitesimal time shift to build the propagator for finite time differences $t_f - t_i$. For this we first consider a discretized interval such that

$$t_f - t_i = N \times \Delta t \; , \tag{7.31}$$

such that we have N differential time intervals.

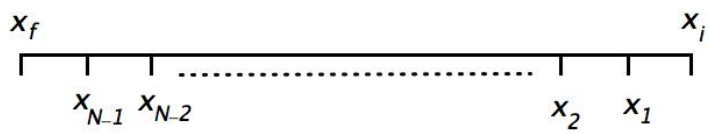

Figure 7.5: Finite interval discretized into N infinitesimal intervals of Δt.

The amplitude can then be written as

$$\begin{aligned}
&\langle x_f, t_f | x_i, t_i \rangle = \\
&\int \langle x_f, t_f | x_{N-1}, t_{N-1} \rangle \, dx_{N-1} \, \langle x_{N-1}, t_{N-1} | x_{N-2}, t_{N-2} \rangle \, dx_{N-2} \, \langle x_{N-2}, t_{N-2} | \ldots \\
&\qquad \ldots \, dx_2 \, \langle x_2, t_2 | x_1, t_1 \rangle \, dx_1 \, \langle x_1, t_1 | x_i, t_i \rangle \; ,
\end{aligned} \tag{7.32}$$

which each of the matrix elements for each infinitesimal interval of the form of (7.30). Then we can write

$$\langle x_f, t_f | x_i, t_i \rangle = \left(\frac{m}{2\pi\hbar i \Delta t} \right)^{N/2} \int \left(\prod_{j=1}^{N-1} dx_j \right) e^{\dfrac{i}{\hbar} \displaystyle\sum_{j=1}^{N} L(t_j) \, \Delta t} \; , \tag{7.33}$$

which when taking the $N \longrightarrow \infty$ and $\Delta t \longrightarrow 0$ limits, can be written in the compact form

$$\boxed{\langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}x(t) \; e^{\frac{iS[x(t)]}{\hbar}} \; ,} \tag{7.34}$$

where we defined

$$\int_{x_i}^{x_f} \mathcal{D}x(t) \equiv \lim_{N\to\infty,\Delta t\to 0} \left(\frac{m}{2\pi\hbar i\Delta t}\right)^{N/2} \int dx_{N-1} \int dx_{N-2} \cdots \int dx_2 \int dx_1 \ . \tag{7.35}$$

7.3 Matrix Elements of Operators

We start with the following example

$$\langle x_f, t_f|\mathbf{x}(\mathbf{t_0})|x_i, t_i\rangle = \int dx(t_0)\, \langle x_f, t_f|x(t_0), t_0\rangle\, x(t_0)\, \langle x(t_0), t_0|x_i, t_i\rangle \ , \tag{7.36}$$

where we have inserted the identity in the form of the integral over $x(t_0)$, and we have acted with the operator on the ket such that

$$\mathbf{x}(\mathbf{t_0})|x(t_0), t_0\rangle = x(t_0)|x(t_0), t_0\rangle \ , \tag{7.37}$$

so that we are integrating over the eigenvalues. Assuming that $t_i < t_0 < t_f$, we can write

$$\begin{aligned} \langle x_f, t_f|\mathbf{x}(\mathbf{t_0})|x_i, t_i\rangle &= \int dx(t_0) \int_{t_0}^{t_f} \mathcal{D}x(t)\, e^{iS[x(t)]/\hbar}\, x(t_0) \int_{t_i}^{t_0} \mathcal{D}x(t)\, e^{iS[x(t)]/\hbar} \\ &= \int_{t_i}^{t_f} \mathcal{D}x(t)\, x(t_0)\, e^{iS[x(t)]/\hbar} \ . \end{aligned} \tag{7.38}$$

We see from (7.38) that the expectation value of the operator looks like an average being weighted by the exponential of the action, integrated over a functional measure. With the appropriate normalization this "statistical" interpretation will play an important role in the applications of the path integral to statistical mechanics and condensed matter systems.

We can generalize this for the product of operators. We start with the product of two operators, assuming that $t_1 < t_2$ and following the steps that lead to (7.38)

$$\langle x_f, t_f|\mathbf{x}(\mathbf{t_2})\, \mathbf{x}(\mathbf{t_1})|x_i, t_i\rangle = \int dx(t_2)\, \langle x_f, t_f|x_2, t_2\rangle\, x(t_2)\, \langle x_2, t_2|x_1, t_1\rangle\, x(t_1)\, \langle x_1, t_1|x_i, t_i\rangle\, dx(t_1) \ . \tag{7.39}$$

This can be written as

$$\langle x_f, t_f | T(\mathbf{x}(\mathbf{t_2})\,\mathbf{x}(\mathbf{t_1})) | x_i, t_i\rangle \;=\int \mathcal{D}x(t)\, x(t_2)\, x(t_1)\, e^{iS[x(t)]/\hbar}\;, \tag{7.40}$$

where we defined the time ordering operator T as

$$T(\mathbf{O}(\mathbf{t_1})\,\mathbf{O}(\mathbf{t_2})) = \begin{cases} \mathbf{O}(\mathbf{t_1})\,\mathbf{O}(\mathbf{t_2}), & \text{for} \;\; t_1 > t_2\;, \\ \\ \mathbf{O}(\mathbf{t_2})\,\mathbf{O}(\mathbf{t_1}), & \text{for} \;\; t_2 > t_1\;, \end{cases} \tag{7.41}$$

Finally, we can generalize this results for the time ordered product of many operators by

$$\boxed{\langle x_f, t_f | T(\mathbf{x}(\mathbf{t_1})\ldots\mathbf{x}(\mathbf{t_n})) | x_i, t_i\rangle \;=\int \mathcal{D}x(t)\, x(t_1)\ldots x(t_n)\, e^{iS[x(t)]/\hbar}\;,} \tag{7.42}$$

It is interesting to note that in both (7.40) and (7.42) the path integral on the right hand side contains the products of *eigenvalues* and not operators. So the products inside the path integrals in these expressions are not time-ordered, even when we are calculating the matrix elements of time-ordered products.

Additional suggested readings

- *An Introduction to Quantum Field Theory*, M. Peskin and D. Schroeder, Chapter 9.1.
- *Quantum Field Theory*, by C. Itzykson and J. Zuber, Chapter 9.1.1.
- *Modern Quantum Mechanics*, by J. J. Sakurai, Chapter 2.5.