Lecture 9

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0.1 Double well potential

One final example we would like to discuss is that of a double well potential shown in Fig. 1. Although this potential does not have a simple analytical solution, it helps illustrate several important concepts. First, we note that if we are interested in energies smaller than the barrier V_0, we can expand the potential around one of the minima $V_{L/R}(x) = \frac{1}{2}V''(\mp a)(x \pm a)^2$. This yields a harmonic oscillator whose center is shifted to $x = \pm a$ with $V''(a) = V''(-a) = m\omega^2$ (which provides the definition for ω). As a result, we expect the low energy eigenstates of a harmonic oscillator centered at $x = \pm a$ to provide a good approximation for the low energy eigenstates of the square well potential. Although these solutions will approach the actual eigenstates of the system as the two wells get more separated, for any finite separation these cannot be exact eigenstates. Otherwise, we will get a double degeneracy of the eigenstates which we have shown is impossible. Furthermore, the eigenstates localized within the left/right well are not invariant under parity although the potential is parity symmetric $V(-x) = V(x)$. Thus a natural ansatz for the approximate eigenstates of the double well is to take the $\pm$ linear combinations of states localized in either well. In particular, the lowest two energy eigenfunctions can be approximated as $\psi_{0,\pm}(x) = \psi_{0,L}(x) \pm \psi_{0,R}(x)$. Since $\psi_{0,L}(0) = \psi_{0,R}(0)$, $\psi_{0,-}$ has a zero at $x = 0$ so it cannot be the ground state. Thus, $\psi_{0,+}$ is a good approximation for the ground state. The energy splitting between the two states is proportional to the matrix elements $\Delta E \sim \langle \psi_{0,L}|\mathcal{H}|\psi_{0,R}\rangle$ can be estimated as $\Delta E \sim \hbar\omega e^{-\frac{a^2}{l^2}}$. This can be seen from the fact that the overlap of $\psi_{0,L}$ and $\psi_{0,R}$ is exponentially small in a [1].

This leads to a very interesting consequence. If we start with a particle localized in one of the wells, whose energy is significantly lower that the barrier, there is a finite probability of finding the particle in the other well after some time. This is because $\psi_{0,L}$ and $\psi_{0,R}$ are not stationary states. For a particle whose initial state $|\psi(t=0)\rangle = |\psi_{0,L}\rangle = \frac{1}{2}(|\psi_+\rangle + |\psi_-\rangle)$ with $E_\pm = E_0 \pm \Delta E$, the time evolution gives

$$|\psi(t)\rangle = e^{\frac{i}{\hbar}\mathcal{H}t}|\psi(0)\rangle = \frac{1}{2}e^{\frac{i}{\hbar}\mathcal{H}t}(|\psi_+\rangle + |\psi_-\rangle) = \frac{e^{\frac{i}{\hbar}E_0 t}}{2}(e^{\frac{i}{\hbar}\Delta E t}|\psi_+\rangle + e^{-\frac{i}{\hbar}\Delta E t}|\psi_-\rangle) \tag{1}$$

[1] To see this, notice that the shifted ground states of the harmonic oscillator are just the coherent states we discussed earlier. The overlap between the left and right eigenfunctions is $\langle \frac{a}{\sqrt{2}l}| - \frac{a}{\sqrt{2}l}\rangle = e^{-a^2/l^2}$

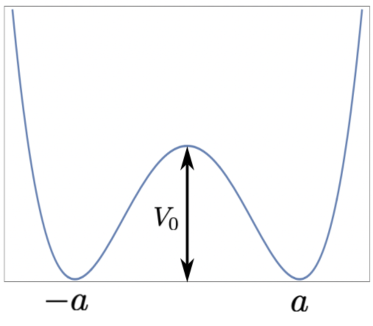

Figure 1: Schematic illustration of the double well potential with minima at $x = \pm a$

Thus, after time $t \sim \frac{\hbar}{\Delta E} \sim \omega^{-1} e^{a^2/l^2}$ an initial particle at $\psi_{0,L}$ will have a sizable overlap with $\psi_{0,R}$ i.e. will have a high probability of being in the right well. The time it takes for the particle to tunnel is exponentially large in the well-separation. It is useful to phrase it in terms of the barrier height instead. If we approximate the double well but two parabolas centered at $\pm a$ by writing $V(x) = \frac{1}{2} m\omega^2 \min((x-a)^2, (x+a)^2)$, then the barrier height $V_0 = \frac{1}{2} m\omega^2 a^2$. Recall that $l^2 = \frac{\hbar}{m\omega}$ leading to $\frac{V_0}{\hbar\omega} = \frac{a^2}{2l^2}$. This means that the tunneling time is exponentially large in the barrier height measured in units of $\hbar\omega$, $t \sim \frac{\hbar}{\Delta E} \sim \omega^{-1} e^{\frac{2V_0}{\hbar\omega}}$ or alternatively the tunneling rate exponentially small. This indicates that while a quantum mechanical particle can tunnel through a classically impossible barrier, the tunneling probability is exponentially suppressed in the barrier height.

1 Path integrals

Let me briefly review what we have discussed in the course so far. In the first two weeks, we discussed the structure of the quantum theory in terms of kets and operators. We motivated this formalism through the Stern-Gerlach experiment which naturally lead us to describing the quantum states in terms of vectors in a finite dimensional Hilbert space and to describing the different operations and observables as operators on this space. We have also seen how we can generalize these notions to continuous variables described by kets and operators in an infinite-dimensional Hilbert space. In the following lectures, we added dynamics to the theory by introducing the time-evolution operator which lead to the time dependent Schrödinger equation for states in the Schrödinger picture and the Heisenberg equation of motion in the Heisenberg picture. We have also seen how to solve the Schrödinger equation in the position basis for several cases, including the free particle and the harmonic oscillator.

One feature of the operator formalism of the quantum theory, which you can see either as a feature or as a bug, is that it is in some sense maximally different from the classical theory and it is generally hard to take the classical limit. In problem set 3, we have discussed Ehrenfest theory which showed that the expectation values of quantum operators satisfy the classical equations of motion, but there was no simple way to take the classical limit by taking some parameter (this parameter turns out to be $\hbar$) to zero and reproducing classical mechanics [2]

I would also like to emphasize that although we tried to motivate several elements of the formalism we introduced, we have not really 'derived' any of the fundamental laws. Instead, we used some minimal experimentally motivated assumptions to postulate the formalism and derive its consequences. Today I will discuss another formulation of the quantum theory that can be similarly motivated using some minimal experimentally motivated assumptions. Although this formulation is equivalent to the operator formalism, it connects more naturally to the classical limit and is thus very convenient for semiclassical approximations.

Similar to how we used the Stern-Gerlach experiment to motivate the Hilbert space or operator formulation of the quantum theory, I will now use a simple experiment to motivate the path integral formulation. I would like to think again of having a 19th century physicist teleported to the present day and showing them this one experiment and trying to use it to deduce the formalism of the quantum theory. That experiment is the double slit experiment we considered earlier. In the double slit experiment (see Fig. 2a), we found that the wave-like interference pattern on the wall can only be understood by summing together two wave-like contributions coming from the two slits. The intensity measured on the screen is itself independent on the overall phase of the wave but it depends strongly on the **relative** phase of the waves coming from the two slits leading to constructive (destructive) interference when the waves are in-phase (out-of-phase). To describe this interference phenomenon, it is known from classical waves that it is very convenient to use complex numbers. So we assign a complex number to each of the two paths the electron can go through. This complex number is nothing but the probability amplitude we discussed earlier. The final intensity on the screen, or the probability of a particle hitting the screen, is given by summing these complex number from the two different parths then taking the absolute value squared. Now since the probability is the square

[2] Compare this to special relativity which reproduces Newtonian mechanics in the limit $c \to \infty$.

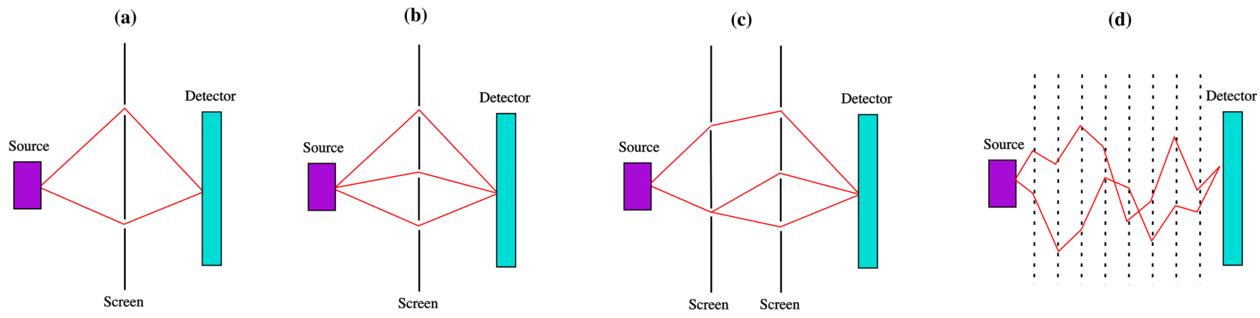

Figure 2: Schematic illustration of the (a) double slit experiment, (b) a similar setup where the screen has three holes allowing for three distinct trajectories, (c) a cascaded setup with two screens with different number of holes (d) the path integral limit of infinite number of screens with infinite number of holes

of the amplitude, it follows that the amplitude for the composition of two events, e.g. a particle travelling from A to B and then B to C is the product of the amplitudes of the two events. We will see now how using these two assumption plus a third assumption motivated from the correspondence to classical physics will be all we need to write the path integral formulation.

Let us first see what these assumptions lead us when we consider more complicated variants of the double slit experiment (similar to what we did with the Stern-Gerlach device). First, let us consider adding a third hole to the screen, then clearly we are adding three amplitudes for the particle to go through any of the three holes as shown in Fig. 2b. Generization to n-holes is straightforward, we have to add the ampltiudes from all the holes. Next let us consider adding another screen with a bunch of holes. Then the rules above tell us that the total amplitude is obtained by summing the amplitude of the electron going through every pair of holes from the first and second screens with every amplitude formed as the product of the amplitude of going from the screen to the first hole, from the first hole to the second hole, then from the second hold to the detector. This is pictorially illustrated in Fig. 2c. Since a screen with infinitely many holes is just equivalent to removing the screen altogether, in the limit of infinitely many screens with infinitely many holes, we basically end up with a sum over all possible paths/trajectories to go from the source to the detector (See Fig. 2d). The amplitude for every path is obtained by breaking up the path into small pieces and taking the product of these pieces.

Let us introduce some notation to facilitate discussing these amplitudes. We denote the probability amplitude of a particle to travel from a point x_i at time $t_i = 0$ to a point x_f at time $t_f = T$ by $\langle x_f, t_f | x_i, t_i \rangle$. Our discussion above is equivalent to the statement that we break up the time interval $T = t_f - t_i$ into $N \to \infty$ intervals with width $\Delta t = \frac{T}{N}$. Denoting $t_n = t_i + n\Delta t$ such that $t_0 = t_i$ and $t_N = t_f$ we can write the probability amplitude $\langle x_f, t_f | x_i, t_i \rangle$ as

$$\langle x_f, T | x_i, 0 \rangle = \int dx_1 \dots dx_{N-1} \langle x_f, t_f | x_{N-1}, t_{N-1} \rangle \langle x_{N-1}, t_{N-1} | x_{N-2}, t_{N-2} \rangle \dots \\ \times \langle x_2, t_2 | x_1, t_1 \rangle \langle x_1, t_1 | x_i, t_i \rangle \quad (2)$$

We have now reduced the problem of calculating the probability amplitude over a finite time interval T to that of an infinitesmal time-interval $\langle x', t + \Delta t | x, t \rangle$.If we are deriving the path integral from the operator formalism, we can simply write $\langle x', t + \Delta t | x, t \rangle = \langle x' | e^{-\frac{i}{\hbar}\mathcal{H}\Delta t} | x \rangle$ and evaluate this expression. We will discuss this later. Instead, we will now try to guess the answer based on some physical assumptions similar to what a 19th century physicist not exposed to quantum mechanics will do. First, we can write $x' = x + \frac{x'-x}{\Delta t}\Delta t$ and define $\dot{x} := \frac{x'-x}{\Delta t}$. At the moment, this is just a definition of a new symbol $\dot{x}$, but we will see later that the paths that yield the main contributions to the path integral are those smooth paths where x and x' approach each other as δt approaches zero, so $\dot{x}$ will reproduce the time derivative of that path $x(t)$ parametrized by t. The path integral is intended to capture interference effects between different paths which suggests writing $\langle x', t + \Delta t | x, t \rangle \propto e^{i\varphi(x, \dot{x}, t, \Delta t)}$. Furthermore, we expect that the phase associated with infinitesmal time evolution is infinitesmal, thus we write $\varphi(x, \dot{x}, t, \Delta t) = f(x, \dot{x}, t)\Delta t + O((\Delta t)^2)$, leading to $\langle x', t + \Delta t | x, t\rangle \propto e^{i f(x,\dot{x},t)\Delta t}$. Substituting in (2) leading to

$$\langle x_f, T | x_i, 0\rangle = \int \mathcal{D}x(t) e^{i \int_0^T dt f(x,\dot{x},t)}, \qquad \mathcal{D}x(t) \propto \prod_{l=1}^{N-1} dx_l \tag{3}$$

The integral over all possible intermediate values x_l can thus be phrased as an integral over all paths $x(t)$ satisfying $x(0) = x_i$ and $x(T) = x_f$ with the amplitude associated with each path given by integrating some functional $f(x, \dot{x}, t)$ that depends on the path. We would now like to determine what this functional is.

To proceed further, we make the requirement that our theory reduces to classical mechanics in the limit $\hbar \to 0$. Here, let me digress a bit to review some basic concepts in classical mechanics. When we are introduced to classical mechanics in high school, we are introduced to Newton's laws whose central concept is that of force and how it causes acceleration. Newton's second law $F = m\ddot{x}$ relates the force to the second derivative of position so we need to specify both position and velocity (its first derivative) at an initial time to solve for a particles motion. In the 19th century, new formulations of classical mechanics that center the concepts of momentum and energy were introduced. In Hamilton's formulation, we define a Hamiltonian function of coordinate x and momentum p given by the sum of kinetic and potential energies $H(p, x) = \frac{p^2}{2m} + V(x)$. The relation between p and x as well as Newton's second law are derived from Hamilton's equations of motion

$$\dot{p} = -\frac{\partial H}{\partial x}, \qquad \dot{x} = \frac{\partial H}{\partial p} \tag{4}$$

Several elements of Hamiltonian mechanics carry over to the operator formalism of the quantum theory where the Hamiltonian, p and x are promoted to operators. Here we also consider time evolution given some initial values of x and p.

Another formulation of classical mechanics is centered on the concept of Lagrangian which depends on position x and velocity $\dot{x}$. It can be obtained from the Hamiltonian through a so-called Legendre transformation that gets rid of the momentum in favor of the velocity $\dot{x}$

$$L(x, \dot{x}) = p\dot{x} - H(x, p) = \frac{1}{2}m\dot{x}^2 - V(x) \tag{5}$$

The Lagrangian is the difference between the kinetic and potential energies. The time integral of the Lagrangian along some classical path is called the action

$$S = \int_0^T dt L(x(t), \dot{x}(t)) \tag{6}$$

A central concept in the Lagrangian formulation of classical mechanics is the stationary action principle. This means that the system will take the trajectory $x_0(t)$ for which the variation of the action δS vanishes. This means that if we write $x(t) = x_0(t) + \delta x(t)$ and expand the action above in $\delta x(t)$, the leading term vanishes. This is equivalent to the Euler-Lagrange equations

$$\frac{\partial}{\partial x}L - \frac{d}{dt}\frac{\partial}{\partial \dot{x}}L = 0 \tag{7}$$

The least action principle is an unusual way to formulate classical mechanics in terms of a global or integral condition rather than a local (differential) condition. One of its intuitive applications is Fermat's principle in optics which states that light chooses the path of least time to travel between a pair of points A and B. This for example explains snell's law of diffraction where light chooses to travel longer in the medium where its speed is faster. It is also related to a popular riddle asking for the path you should take to save a drowning person if your speed on land v_{land} is higher than your speed in water v_{water}.

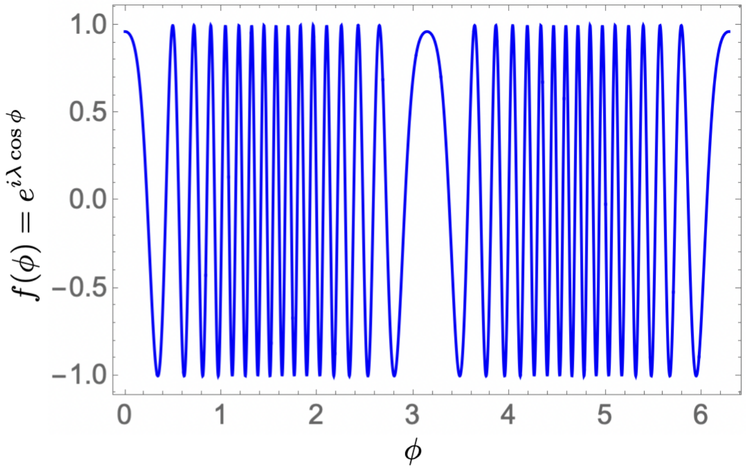

Figure 3: Plot of the function $f(\phi) = e^{i\lambda\cos\phi}$ for $\lambda = 50$.

One final fact we need to review is the saddle point approximation. This is the statement that the integral

$$\int dx\, e^{i\lambda f(x)} \tag{8}$$

for large λ is dominated by the stationary points or extrema of $f(x)$, where $f'(x) = 0$, in the limit of large λ. The reason is that for large λ, any interval of width Δx will contain several terms with different phases differing by $\lambda f'(x)\Delta x$ which generally cancel out whenever $\lambda f'(x)\Delta x \sim 1$. Around stationary points, however, the phase oscillates much slowly and there is no cancellation. This is illustrated in Fig. 3 which plots the real part of $e^{i\lambda\cos\phi}$ for $\lambda = 50$. We see that the function changes slowly at the minimum and the maximum of the cosine function at π and 0, respectively.

With this background in mind, we see that the path integral in (3) will be dominated by the paths where the quantity $\int_0^T dt f(x, \dot{x}, t)$ in the exponential is stationary. Comparing to the stationary action principle of classical mechanics leads to the identification $f(x, \dot{x}, t) = \lambda L(x, \dot{x})$, where λ has units of inverse action and taking $\lambda \to \infty$ corresponds to the classical limit. This leads to the identification $\lambda = \frac{1}{\hbar}$ which yields [3]

$$\langle x_f, T | x_i, 0\rangle = \int_{x(0)=x_i}^{x(T)=x_f} \mathcal{D}x(t)\, e^{\frac{i}{\hbar}\int_0^T dt L[x,\dot{x}]} = \int_{x(0)=x_i}^{x(T)=x_f} \mathcal{D}x(t)\, e^{\frac{i}{\hbar}S} \tag{9}$$

The path integral formalism allows us to formulate the quantum theory in terms of purely classical variables; $x(t)$ here is a classical trajectory not an operator. The price we have to pay is that we have to sum over all possible classical trajectories with some complex phases. It also gives us a measure of how quantum mechanical a problem is by comparing the magnitude of the action to $\hbar$. Interestingly, path integral provides some intuition for the classical stationary action principle. One can ask: how does the system know which path leads to stationary action? the answer in the path integral formalism is that the system really probes all possible trajectories and that is how it can decide which one gives the stationary action.

[3]note that this does not completely fix the numerical prefactor; we could have $\lambda = \frac{c}{\hbar}$ with c being an $O(1)$ number. However, this amounts to a redefinition of $\hbar$. The question then becomes how $\hbar$ defined here is related to $\hbar$ defined in the operator formalism e.g. using $[x, p] = i\hbar$. As we will see by relating path integral to the operator formalism that the two definitions of $\hbar$ are the same. Alternatively, we can take $\hbar$ as a parameter that we can determine by comparing to experiments; for example by comparing the period of the double slit interference pattern in experiment with a simple path integral calculation