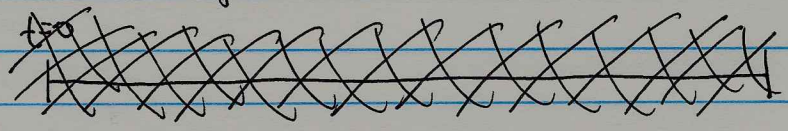
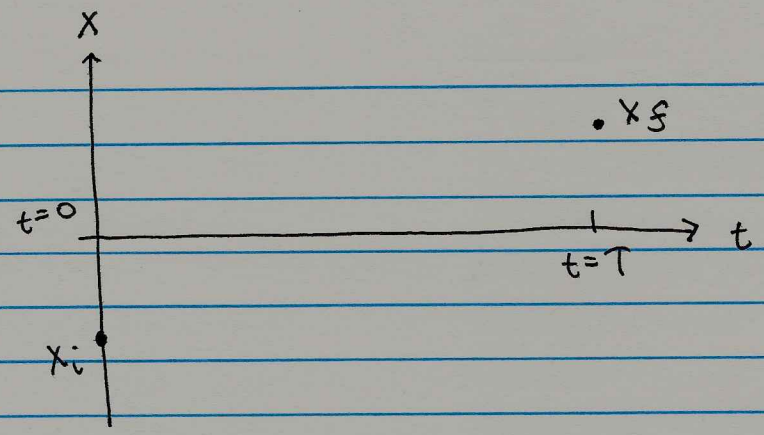
Phys 342 Lecture 34

I hope you're doing well, circumstances notwithstanding, and welcome to some more quantum mechanics. As mentioned earlier, the content that we will cover from now to the end of the semester (a total of six lectures) will not have a corresponding homework set. So, especially because we are far apart, this material is completely supplemental, but I hope you can read it and find it useful. Correspondingly, the material I will cover in these lectures is not covered at all in Griffiths and Schroeter, so I hope this is also is novel and exposes you to a very different way of thinking about quantum mechanics.

This week, we will introduce the path integral, which I don't think I exaggerate when I say is the most powerful and general formulation of quantum mechanics. Further, the path integral is very easily extended to incorporate special relativity, which we had mentioned is very challenging and inconvenient within the context of the Schrödinger equation. So, what is the idea of this path integral? Our goal will be to calculate the amplitude for a quantum mechanical particle that starts at position x_i at time $t=0$ and ends at position x_f at some later time $t=T>0$. In some sense, this question is analogous to what you ask in an introduction to kinematics in Physics 101; however, its analysis in quantum mechanics will prove to be a bit more complicated than in the first week of physics.

Let's draw a picture of what we are working with:





In this picture, we have drawn time on the abcissa and space on the ordinate axes. I have placed the initial and final positions, x_i and x_f, appropriately. We want to find the probability amplitude for ending up ~~at~~ at x_f at $t=T$ given that we start at x_i at $t=0$. So, here's what we will do. We can just write down the answer first, then we will work to unpack it. Let's express the state of the particle at $t=0$ as:

$|x_i, t=0\rangle$, which is an eigenstate of the position operator

$\hat{x}\,|x_i, t=0\rangle = x_i|x_i, t=0\rangle$, with eigenvalue of that ~~state~~ initial position.

Next, we can write down the final state of the particle at $t=T$ as:

$|x_f, t=T\rangle$, which is also an eigenstate of the position operator:

$\hat{x}\,|x_f, t=T\rangle = x_f|x_f, t=T\rangle$, but evaluated at time $t=T$.

We know how to move from $t=0$ to $t=T$: we just translate in time with the unitary time translation operator, the exponentiated Hamiltonian:

$$|x_f, t=T\rangle = e^{+i\hat{H}T/\hbar}\,|x_f, t=0\rangle.$$

Using the time translation operator, we can then express

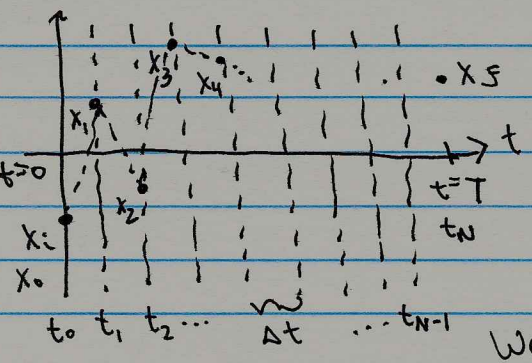
all eigenstates of position in terms of states evaluated at time $t=0$, say. Then, the transition amplitude from position x_i at $t=0$ to x_f at $t=T$ is:

$$\langle x_f, t=T | x_i, t=0\rangle = \left(e^{+i\frac{\hat{H}t}{\hbar}} |x_f, t=0\rangle\right)^\dagger |x_i, t=0\rangle$$

$$\equiv \langle x_f | e^{-i\frac{\hat{H}T}{\hbar}} |x_i\rangle,$$

where in the final line, we suppress all time dependence of the states because it is explicitly included in the exponentiated Hamiltonian operator. So, this is one answer: we just act the Hamiltonian on our position eigenstates and evaluate the inner product.

However, let's see if we can express it in another, ultimately much more useful and powerful, way. The idea will be the following. Going back to our picture of the initial and final states:



we will divide the total time T into N steps with small time intervals of

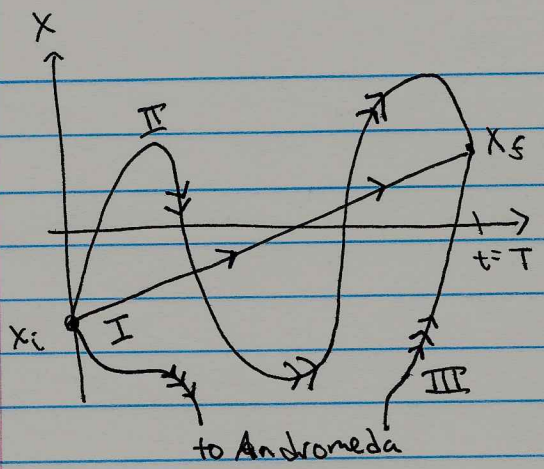
$$\Delta t = \frac{T}{N}.$$

We will denote the corresponding n^{th} time step as $t_n = n\Delta t$, so that $t=0$ is $n=0$, and $t=T$ is the N^{th} step. Further, at each of these time steps, the particle can have <u>any</u> position $x_n \in (-\infty, \infty)$ at the n^{th} step. I have drawn the first four possible positions x_1, x_2, x_3, x_4 at times t_1, t_2, t_3, and t_4 in the figure for illustration.

Now, I want to emphasize something: given this set up, all we require of the particle is that it is at $x_i = x_0$ at $t=0$ and $x_f = x_N$ at $t=T$. That's it. We only measure its initial and final positions and perform no measurements in the range $0<t<T$, exclusive of its endpoints. Because time evolution is a probabilistic process in quantum mechanics, anything that does not expressly have 0 probability to occur in that intermediate time will happen, according to its probability. Also, because we make no measurements in the intermediate times, we have to sum together the probability amplitudes for anything in the intermediate times to occur. This is familiar from expanding a wavefunction in a complete sum of energy eigenstates, given an initial wavefunction at $t=0$. We write the wavefunction at time t as:

$\psi(x,t) = \sum_{n=0}^{\infty} \beta_n e^{\frac{-iE_n t}{\hbar}} |\psi_n\rangle$, where $|\psi_n\rangle$ are energy eigenstates and the β_n are properly the probability amplitudes for the wavefunction to be in any energy eigenstate at $t=0$. The exponential phase factors of energy just control how the probability amplitudes evolve in time.

Now, with these observations, anything with non-zero probability can occur and that we make no measurements in the intermediate time, means that to calculate the transition amplitude $\langle x_f, t=T | x_i, t=0\rangle$, we have to sum over all possible (i.e., non-zero probability) trajectories that the particle can take between these points, weighted by their probability amplitudes. For example, let's draw just three possible trajectories:



Path I (→) is just a straight line and what we expect for a classical particle experiencing no external forces. That would be the answer classically, but there are other paths that have non-zero probability. Path II (↗↘↗) travels from x_i to x_f in a curvy trajectory in this (t,x) plane. In space its trajectory would actually consist of several loops; can you tell how many? Finally example path III (↗↘↗↘↗) is really wild, and the particle goes all the way out to the Andromeda galaxy before coming back to point x_f. Again, unless something expressly forbids a trajectory from happening, it has a non-zero probability and must be included in the sum.

This construction of "sum over paths" or "sum over histories" will produce the path integral, another way to express a quantum system distinct from the Schrödinger equation, yet completely equivalent as one can derive the path integral from the schrödinger equation (as we will do), and vice-versa. The path integral was introduced by Richard Feynman and Albert Hibbs in a textbook "Quantum Mechanics and the Path Integral" in 1965. Feynman actually credits Paul Dirac for the idea from a cryptic comment Dirac made in the 1930s. Before deriving it, I want to make one more comment about the path of a quantum mechanical particle. These example paths I drew were

both continuous and smooth (continuous derivatives). The path of a quantum mechanical particle had better be continuous; otherwise a particle could travel from anywhere to anywhere instantaneously (i.e. "teleport"). Another way to express continuity is that if you made measurements of the position of a particle in rapid succession, the particle had better not move far from one measurement to the next. However, there is no such logical requirement of smoothness; that is purely aesthetics. In the space of continuous functions, those functions that are also smooth is measure-zero: if you were just drawing continuous functions out of a hat you would never pull out a smooth function. That is to say that the trajectory of a quantum mechanical particle is continuous but not smooth. Perhaps a familiar example of a continuous, non-smooth function is the value of the Stock market as a function of time.

Okay, with those comments out of the way, let's derive the path integral. Back on page 3, we had divided up the time from $t=0$ to $t=T$ into N steps. At each of those time steps, we can insert a complete set of position eigenstates. For instance, at time $t_n = n\Delta t$, we have the completeness relation:

$$1 = \int dx_n \, |x_n, t_n\rangle\langle x_n, t_n|, \quad \text{where the integral}$$

over positions x_n represents the continuous sum over eigenstates. Inserting this "1" at every time in our transition amplitude, we have:

$$\langle x_f, T | x_i, t=0 \rangle = \langle x_N, t_N | x_{N-1}, t_{N-1} \rangle \langle x_{N-1}$$

$$\langle x_f, t=T | x_i, t=0\rangle \equiv \langle x_N, t_N | x_0, t_0\rangle$$

$$= \int dx_1 dx_2 \cdots dx_{N-1} \langle x_N, t_N | x_{N-1}, t_{N-1}\rangle \langle x_{N-1}, t_{N-1} | x_{N-2}, t_{N-2}\rangle$$

$$\times \cdots \langle x_2, t_2 | x_1, t_1\rangle \langle x_1, t_1 | x_0, t_0\rangle$$

$$= \int dx_1 dx_2 \cdots dx_{N-1} \prod_{i=0}^{N-1} \langle x_{i+1}, t_{i+1} | x_i, t_i\rangle.$$

Note that the inner products in the integrand are still evaluated between states separated in time by Δt. We can evaluate them at the same time by introduction of the time translation operator:

$U(\Delta t) = e^{+i\frac{\hat{H}\Delta t}{\hbar}}$. That is, for the inner product between states at time t_n and $t_n + \Delta t$, we can write:

$$\langle x_{n+1}, t_{n+1} | x_n, t_n\rangle = \langle x_{n+1}, t_n | e^{-i\frac{\hat{H}\Delta t}{\hbar}} | x_n, t_n\rangle$$

$$\equiv \langle x_{n+1} | e^{-i\frac{\hat{H}\Delta t}{\hbar}} | x_n\rangle,$$ where we can drop the time in the states as the inner product involves states evaluated at the same time. Additionally, we will sandwich a complete set of momentum eigenstates in this inner product, where we note that

$$1 = \int dp_n |p_n\rangle\langle p_n| \quad \text{and we have}$$

$$\langle x_{n+1} | e^{-i\frac{\hat{H}\Delta t}{\hbar}} | x_n\rangle = \int dp_n \langle x_{n+1} | p_n\rangle \langle p_n | e^{-i\frac{\hat{H}\Delta t}{\hbar}} | x_n\rangle.$$

Now, it's straightforward to interpret the Hamiltonian sandwiched between the position and momentum eigenstates. These eigenstates just force a particular basis in which to

express the Hamiltonian: the mixed position/momentum basis (as we typically do). We are always free to reorder operators using their commutation relation, so if we push all position operators right and momentum operators left, then:

$\langle p_n | \hat{H}(\hat{P}, \hat{X}) | x_n \rangle = H(p_n, x_n) \langle p_n | x_n \rangle$, where now

$H(p_n, x_n)$ is just a function of momentum p_n and position x_n, and not an operator.

With these manipulations, our inner product of position states becomes:

$$\langle x_{n+1} | e^{-i\frac{\hat{H}\Delta t}{\hbar}} | x_n \rangle = \int dp_n \langle x_{n+1} | p_n \rangle \langle p_n | e^{-i\frac{\hat{H}\Delta t}{\hbar}} | x_n \rangle$$

$$= \int dp_n e^{-i\frac{H(p_n, x_n)\Delta t}{\hbar}} \langle x_{n+1} | p_n \rangle \langle p_n | x_n \rangle.$$

Continuing, we can evaluate these inner products of position and momentum eigenstates. Let's focus on $\langle x_{n+1} | p_n \rangle$ for a second. Reading from right to left, this is a momentum eigenstate $|p_n\rangle$ expressed in the position basis with coordinate x_{n+1}. We know what this is: it's just an imaginary exponential:

$\langle x_{n+1} | p_n \rangle \propto e^{\frac{i p_n x_{n+1}}{\hbar}}$. Correspondingly, $\langle p_n | x_n \rangle \propto e^{-\frac{i p_n x_n}{\hbar}}$,

so that: $\langle x_{n+1} | p_n \rangle \langle p_n | x_n \rangle = e^{+\frac{i}{\hbar} p_n (x_{n+1} - x_n)}$

Now, I had only written that these inner products are proportional to the imaginary exponentials, not equal to. We fix the proportionality constant by demanding a normalization

of the integral over p_n:

$$\int_{-\infty}^{\infty} dp_n \langle x_{n+1}|p_n\rangle\langle p_n|x_n\rangle \propto \int_{-\infty}^{\infty} dp_n\, e^{-\frac{i}{\hbar}p_n(x_n - x_{n+1})} = 2\pi\hbar\,\delta(x_n - x_{n+1}),$$

where the final equality follows from identities of Fourier transforms. If we want the result to exclusively be a δ-function, with coefficient 1, then,

$$\langle x_{n+1}|p_n\rangle\langle p_n|x_n\rangle = \frac{e^{-\frac{i}{\hbar}p_n(x_n - x_{n+1})}}{2\pi\hbar}.$$

We'll end this lecture by just putting all of the pieces together thus far. We have shown that:

$$\langle x_{n+1}, t_{n+1}\,|\,x_n, t_n\rangle = \langle x_{n+1}|e^{\frac{-i\hat{H}\Delta t}{\hbar}}|x_n\rangle$$

$$= \int dp_n \langle x_{n+1}|p_n\rangle\langle p_n|e^{\frac{-i\hat{H}\Delta t}{\hbar}}|x_n\rangle$$

$$= \int dp_n\, e^{\frac{-iH(p_n,x_n)\Delta t}{\hbar}} \langle x_{n+1}|p_n\rangle\langle p_n|x_n\rangle$$

$$= \int \frac{dp_n}{2\pi\hbar} \exp\left[-\frac{i}{\hbar}\left(H(p_n,x_n)\Delta t - p_n(x_{n+1}-x_n)\right)\right],$$

for $\Delta t \to 0$.

Plugging this into our transition amplitude, we have:

$$\langle x_f, t=T\,|\,x_i, t=0\rangle = \int \frac{dp_1}{2\pi\hbar}dx_1 \frac{dp_2}{2\pi\hbar}dx_2 \cdots \frac{dp_{N-1}}{2\pi\hbar}dx_{N-1}$$

$$\times \exp\left[+\frac{i}{\hbar}\sum_{n=1}^{N-1}\left(p_n(x_{n+1}-x_n) - H(p_n,x_n)\Delta t\right)\right]$$

We'll take the $N\to\infty$ limit and understand what the integrals in this expression mean next time.