Ph 1b Recitation Notes

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1 Time-Independent Solutions to the Schrödinger Equation

Unlike classical mechanics, quantum mechanics has a somewhat finite number of problems to solve. The way in which we define a problem is by the potential function $V(x)$. Remember that the Schrödinger Equation tells us how a particle moves, so the way to see these potential functions is as a force on the particle.

1.1 Infinite Square Well

The potential function for the infinite square well problem is

$$V(x) = \begin{cases} 0 & \text{if } 0 \leq x \leq a \\ \infty & \text{otherwise} \end{cases} \tag{1}$$

The idea behind this potential is that there is a free particle surrounded by two infinitely rigid walls that restrict the particle between $x = 0$ and $x = a$.

Since the particle will be inside the walls, we have the boundary conditions $\psi(x \leq 0) = 0$, $\psi(x \geq a) = 0$, where $V(x) = 0$. If we substitute this in the time-independent Schrödinger Equation, we get

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = E\psi(x) \tag{2}$$

This can be easily solve assuming that $E > 0$ (you will show in the homework that there are no normalizable solutions where $E \leq 0$). We can find (see lecture notes) that the solutions to the infinite square well are

$$\Psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) e^{-i\left(n^2\pi^2\hbar/2ma^2\right)t} \tag{3}$$

where the energy is $E_n = n^2\pi^2/2ma^2$, for positive integers n. Linear combinations of these states give you the full wavefunction.

Note that these states are orthonormal, which means that they satisfy

$$\int_0^a \mathrm{d}x \psi_m(x)^* \psi_n(x) = \delta_{mn} \tag{4}$$

where δ_{mn} is the Kronecker delta (which is 1 if $m = n$ and 0 otherwise).

These states also form a complete set, meaning any function $f(x)$ can be formed from a linear combination of them.

If we want the full solution given an initial condition $\Psi(x, 0)$, we can set the coefficients as

$$c_n = \int_0^a \mathrm{d}x \psi_n(x)^* \Psi(x,0) \tag{5}$$

Note that the lowest energy state is called the *ground* state (here, $n = 1$).

1.2 Simple Harmonic Oscillator

You know the simple harmonic oscillator from classical mechanics has potential $V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2$. What happens if we use this potential? The equation to solve becomes

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \psi(x) = E\psi(x) \tag{6}$$

There are two standard ways to solve this: 1) the brute-force way, and 2) the nice algebraic way. Both require some computation, so see the lecture notes or textbook for the details.

I will point out a couple things about the algebraic way. The key to this method is to use these "ladder" operators $\hat{a}_+$ and $\hat{a}_-$. These are defined as

$$\hat{a}_\pm = \frac{1}{\sqrt{2\hbar m\omega}}(\pm i\hat{p} + m\omega\hat{x}) \tag{7}$$

You can show that for the simple harmonic oscillator the Hamiltonian is $\hat{H} \equiv \frac{\hat{p}^2}{2m} + V(x) = \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)$, so these operators act to raise or lower the energy levels (since the eigenvalues of the Hamiltonian are the energy levels). We can specifically find (see lecture notes) that the energy levels are $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$. Once we have the ground state solution ψ_0, we can use this ladder operators to find the rest (namely, $\psi_n = \frac{1}{\sqrt{n!}}(\hat{a}_+)^n\psi_0$). To find the ground state, we simply need to set $0 = \hat{a}_-\psi_0$ (since the minimum energy state is $n = 0$ since we require $E > 0$ for bound state solutions to this potential, see lecture notes for derivation) to find that

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) \tag{8}$$

It's a good exercise to find the next few stationary states. The general form for any n requires the use of Hermite polynomials $H_n(\xi)$, which satisfy Rodrigues formula $H_n(\xi) = (-1)^n e^{\xi^2}\frac{\mathrm{d}^n}{\mathrm{d}\xi^n}\left(e^{-\xi^2}\right)$. And the general simple harmonic oscillator solution can be given using Hermite polynomials by

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n(\xi) \exp\left(-\frac{1}{2}\xi^2\right) \tag{9}$$

where $\xi = x\sqrt{\frac{m\omega}{\hbar}}$.

Something interesting to note about the harmonic oscillator is that there is no non-zero energy state. This is very different from the classical case, where it is possible to have a spring that has zero kinetic and potential energy (at the equilibrium configuration). This is not true at the quantum scale, when you get to small enough energies. However, this is not inconsistent with classical mechanics because you can converge on the classical probability distribution if you increase n enough (see Griffiths Figure 2.7 for example).

1.3 Free Particle

Now, we consider $V(x) = 0$ everywhere (not just inside a square well). The key conceptual difference here is that the particle is not bound like it was in the square well. Since we have the same equation to solve as the square well case though, we get the same general solution, but different boundary conditions. In general, we have

$$\Psi(x,t) = Ae^{ik(x - \frac{\hbar k}{2m}t)} + Be^{-ik(x + \frac{\hbar k}{2m}t)} \tag{10}$$

where $k \equiv \frac{\sqrt{2mE}}{\hbar}$. This is the solution for the wavefunction with a given energy E (note that now, the energy is not discrete!).
The general solution is a wave packet. That is to say, some linear combination of different energy solutions (which we can represent by integrating over k),

$$\Psi(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k\psi_k(k)e^{i(kx-\omega(k)t)} \tag{11}$$

where $\psi_k(k)$ are the coefficients. These coefficients are determined from the initial conditions $\Phi(x,0)$ with

$$\psi_k(k) = \int_{-\infty}^{\infty} \mathrm{d}x e^{-ikx}\Psi(x,0) \tag{12}$$

This can easily be obtained by using Plancherel's Theorem, namely,

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k e^{ikx} f_k(x) \iff f_k(x) = \int_{-\infty}^{\infty} \mathrm{d}x e^{-ikx} f(x) \tag{13}$$

Also relevant here is Parseval's Theorem, which is

$$\int_{-\infty}^{\infty} \mathrm{d}x |f(x)|^2 = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k |f_k(k)|^2 \tag{14}$$

Fourier analysis like this will come up often when solving these initial value problems in QM. For an example, see how an initially Gaussian wave packet is setup in the lecture notes and it may be a good exercise to find out how it evolves in time. Broadly, the wave packet spreads out in position over time.

1.4 Bound vs Scattering States

For the next set of potentials, it's worth quickly understanding the difference between bound and free/scattering states. In classical mechanics, a particle is "bound" if its energy level low enough so that it has two turning points. In quantum mechanics, particles can tunnel through barriers (as you will see with the dirac function potential). This means that it is what happens at infinity that matters for determining if the particle is bound or free. Generally for a 1D particle, this means that

$$\begin{cases} E < V(-\infty) \text{ and } V(+\infty) & \implies \text{bound state} \\ E > V(-\infty) \text{ or } V(+\infty) & \implies \text{scattering state} \end{cases} \tag{15}$$

But if the potential function goes to 0 at $\pm\infty$, then a bound state is when $E > 0$ and a scattering state when $E < 0$.

1.5 Dirac Function Potential

The Dirac delta function potential is

$$V(x) = \alpha\delta(x) \tag{16}$$

where $\delta(x)$ is the Dirac delta. This is an interesting object that follows a few rules. Namely, it follows

$$\delta(x) = \begin{cases} \infty & \text{if } x = 0 \\ 0 & \text{otherwise} \end{cases} \tag{17}$$

But it is normalized such that the integral is finite

$$\int_a^b \delta(x-c)f(x) = \begin{cases} f(c) & \text{if } a \le x \le b \\ 0 & \text{otherwise} \end{cases} \tag{18}$$

You can see the lecture notes or the textbook for a derivation, but I'll reiterate a few points. Once again, we have zero ponential wherever the particle is (i.e. where there is no infinite potential), we can thus solve for a free particle on each side of the Dirac delta. For the bound states, we can find that

$$\psi(x) = Ae^{\kappa x} + Be^{-\kappa x} \tag{19}$$

with $\kappa = \frac{\sqrt{-2mE}}{\hbar}$.

The tricky part is getting the boundary conditions. We already know that $\psi(\pm\infty) = 0$, so we can solve the function on each side but we will need another condition to connect these solutions together. The trick is to force $\psi(x)$ to be continuous and for $\frac{\mathrm{d}\psi}{\mathrm{d}x}$ to be continuous except at points where the potential function is infinite. You can do this and show that there is one bound solution ($E < 0$) where

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2} \tag{20}$$

with energy $E = -\frac{m\alpha^2}{2\hbar^2}$.

For the scattering states, we can find general solutions

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \tag{21}$$

with $k = \frac{\sqrt{2mE}}{\hbar}$. An impose the same continuity conditions, yielding two solutions

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \tag{22}$$

$$\psi(x) = Fe^{ikx} + Ge^{-ikx} \tag{23}$$

where

$$F + G = A + B \tag{24}$$

$$F - G = A(1 + 2i\beta) - B(1 - 2i\beta) \tag{25}$$

where $\beta \equiv \frac{m\alpha}{\hbar^2 k}$. This gives reflection (R) and transmission coefficients (T)

$$R \equiv \frac{|B|^2}{|A|^2} = \left[1 + \left(\frac{2\hbar^2 E}{m\alpha^2}\right)\right]^{-1} \tag{26}$$

$$T \equiv \frac{|F|^2}{|A|^2} = \left[1 + \left(\frac{m\alpha^2}{2\hbar^2 E}\right)\right]^{-1} \tag{27}$$

2 Recitation Problems

2.1 Griffiths Problem 2.4

2.2 Griffiths Example 2.5

2.3 Custom Problem (adapted from one by Rohan Shenoy)

You are playing a game with your friend, who invites you into their laboratory. They have prepared a 1000, identical harmonic oscillator experiments. The potential is $V(x) = \frac{1}{2}m\omega^2 x^2$.

Every experiment begins in the same initial state $\Psi(x, 0)$. They measure the energy of each of the experiments and tell you the average $\bar{E}_{\text{measured}} = 3\hbar\omega$ at $t = 0$. They also let you know that Ψ is configured such that

$$\Psi(x, 0) = \frac{1}{\sqrt{3}}\psi_0 + \frac{1}{\sqrt{2}}\psi_2 + c_m\psi_m$$

for some integer m.

Part 1: Your friend asks you to guess the value of m.

Solution: We know $\sum_n |c_n|^2 = 1 \implies |c_m|^2 = \frac{1}{6}$ and that $\langle \hat{H} \rangle = \sum_n |c_n|^2 E_n$. Doing some math, and plugging in values for $E_n = \hbar\omega(n + \frac{1}{2})$ gives $m = 9$.

Part 2: Your friend now asks for the average of the energy measurements if they were measured at times $t_1 = \frac{3\pi}{\omega}$ and $t_2 = \frac{5\pi}{\omega}$ instead.

Solution: The coefficients will change in time as $c_n(t) = c_n e^{-iE_n t/\hbar} = c_n e^{-i(n+\frac{1}{2})\omega t}$. So, each will evolve as $c_0(t) = \frac{1}{\sqrt{3}} e^{-i(\frac{1}{2}\omega t)}$, $c_2(t) = \frac{1}{\sqrt{2}} e^{-i(\frac{5}{2}\omega t)}$, and $c_9(t) = \frac{1}{\sqrt{6}} e^{-i(\frac{19}{2}\omega t)}$. However, the probabilities of each stationary state will remain constant since we are taking their magnitude squared and phase information is lost. Thus, the expectation value of the energy will remain $3\hbar\omega$ at each time.

Part 3: Your friend wants to be sure that you know the conceptual framework behind QM, so he asks one more question: Why did they need to set up many different experiments? In other words, why could they not have just gone with measuring one experiment repeated multiple times?

Solution: Measuring the particle would collapse it to one state of the states in the initial superposition (ψ_0, ψ_2 or ψ_m), which would then continue to yield the same solution repeatedly, so long as the experiments where done in quick enough succession.

2.4 Griffiths Problem 2.21

2.5 Griffiths Problem 2.43