Midterm I Recap

Lecture 17

Physics 342
Quantum Mechanics I

Monday, March 10th, 2008

17.1 Introduction

In the context of the first midterm, there are a few points I'd like to make about solving and interpreting Schrödinger's equation. I'll go in order of the problems, and use the midterm itself as a venue for review.

17.2 Problem 1

17.2.1 Part a.

We are asked to sketch wave functions for two different potentials. In the first figure, we are told that: The energy of the state is larger than the potential, so that $E - V_0 > 0$. In the region where the wave function is already drawn, then, we have a solution to:

$$-\frac{\hbar^2}{2\,m}\,\psi''(x) + V_0\,\psi(x) = E\,\psi(x) \longrightarrow \boxed{\psi''(x) = -\underbrace{\frac{2\,m}{\hbar^2}\,(E - V_0)}_{\equiv \bar{k}^2 > 0}\,\psi(x)}. \tag{17.1}$$

The real part is drawn, with some amplitude, so we are looking at a function: $\sin(\bar{k}\,x)$. An oscillation like this has wavelength defined to be the length of one full cycle,

$$\sin(2\,\pi) = \sin(\bar{k}\,\bar{\lambda}) \longrightarrow \boxed{\bar{\lambda} = \frac{2\,\pi}{\bar{k}}}. \tag{17.2}$$

Now we are to continue the sketch in a region where there is no potential, so

$$\psi''(x) = -\underbrace{\frac{2\,m\,E}{\hbar^2}}_{\equiv k^2 > 0}\,\psi(x). \tag{17.3}$$

Our sketch must respect the continuity and derivative continuity of the wave function. In addition, it will be oscillatory, and it has wavelength $\lambda = \frac{2\,\pi}{k}$. What is the relation between λ and $\bar{\lambda}$? From their definition, we know that

$$\bar{k}^2 = k^2 - \frac{\hbar^2}{2\,m}\,V_0, \tag{17.4}$$

where we have used the fact that *the energy of a state is fixed.* We are drawing a wave function that has definite energy, an eigenfunction of the Hamiltonian for a potential with a mild discontinuity in it. Given the above, we conclude that $\bar{k} < k$, and therefore that

$$\frac{1}{\bar{k}} > \frac{1}{k} \longrightarrow \boxed{\bar{\lambda} > \lambda}, \tag{17.5}$$

so we should draw: A sinusoidal function that connects continuously and derivative-continuously to the existing sketch and has a shorter wavelength.

For the second potential, we are told that the energy of our state is greater than zero, and less than V_0. Think about what Schrödinger's equation will tell us about the solution when $V(x) = V_0$:

$$-\frac{\hbar^2}{2\,m}\,\psi''(x) + V_0\,\psi(x) = E\,\psi(x) \longrightarrow \boxed{\psi''(x) = -\underbrace{\frac{2\,m}{\hbar^2}\,(E - V_0)}_{<0}\,\psi(x)}, \tag{17.6}$$

so that the right-hand side has a constant that can be written as $\frac{2\,m}{\hbar^2}\,(V_0 - E)$ which is positive – the solutions to $\psi''(x) = K^2\,\psi(x)$ for positive K^2 are growing and decaying exponentials, and we should draw: A decaying exponential that connects continuously and derivative-continuously to the existing sketch.

17.2.2 Part b.

Here we are inverting the "usual" physical setup. Typically, we are given a potential and want to find the associated stationary states. But in this case, we are given a stationary state, and asked to find the potential (and energy) for which this *is* a stationary state. We assume that Schrödinger's equation is satisfied:

$$-\frac{\hbar^2}{2\,m}\,\psi''(x) + V(x)\,\psi(x) = E\,\psi(x), \tag{17.7}$$

and all we need to do in this case is "solve for $V(x)$"

$$V(x) = \frac{E\,\psi(x) + \frac{\hbar^2}{2\,m}\,\psi''(x)}{\psi(x)} \tag{17.8}$$

and impose the condition that $V(0) = 0$. To do this, we must insert the $\psi(x) = A\,x\,e^{-\alpha\,x^2}$ and its second derivative. Before proceeding, notice that the normalization constant A in this case *cannot matter* – look at the right-hand-side of (17.8). Now, the derivative and second derivative of $\psi(x)$ can be written as:

$$\begin{aligned}
\psi'(x) &= \frac{1}{x}\,\psi(x) - 2\,\alpha\,x\,\psi(x) \\
\psi''(x) &= -\frac{1}{x^2}\,\psi(x) + \frac{1}{x}\,\psi'(x) - 2\,\alpha\,\psi(x) - 2\,\alpha\,x\,\psi'(x) \\
&= \left(4\,\alpha^2\,x^2 - 6\,\alpha\right)\,\psi(x),
\end{aligned} \tag{17.9}$$

and we see, with a wave of relief, that the second derivative is itself proportional to $\psi(x)$, so the right-hand-side of (17.8) is going to work out nicely:

$$V(x) = E + \frac{\hbar^2}{2\,m}\left(4\,\alpha^2\,x^2 - 6\,\alpha\right). \tag{17.10}$$

We know that $V(0) = 0$, and this can be used to solve for E:

$$E = \frac{3\,\alpha\,\hbar^2}{m}, \tag{17.11}$$

whereupon

$$V(x) = \frac{2\,\alpha^2\,\hbar^2}{m}\,x^2 \tag{17.12}$$

and we see that the potential here is that of a harmonic oscillator. From the wavefunction itself, we can get the units for α – an exponential has *arguments that are unitless*, so $|\alpha| = L^{-2}$ to get $\alpha\,x^2$ unitless. From here, we can check the units for our E and $V(x)$.

17.2.3 Part c.

This question has an interesting loop-hole in it. We are told that there are four possible energy measurements, and the state with lowest energy (the ground state) has energy 5 J. Now the first quantum mechanical observation is that the wave function of this system $\Psi(x,t)$ must be a linear combination of four stationary states, i.e. ones satisfying:

$$-\frac{\hbar^2}{2\,m}\,\psi_i''(x) + V(x)\,\psi_i(x) = E_i\,\psi_i(x) \qquad i = 1,2,3,4, \tag{17.13}$$

since possible energy measurements are drawn from the eigenvalues E_i. Our second quantum mechanical observation is that *when a measurement is made, the state of the system becomes that of the eigenvector associated with the measurement.* I have intentionally left out any reference to energy in the italicized comment: A measurement is associated with a Hermitian operator – position measurements are associated with $\hat{x}$, momentum measurements are associated with $\hat{p}$, and energy measurements are associated with $\hat{H}$. The eigenstate that the system collapses into is an eigenstate of the associated operator. For example, in our case, we are measuring energy, so we expect the system to be in an eigenstate of $\hat{H}$ after an energy measurement. If we measured position, we expect the system to be (subsequent to the measurement) in an eigenstate of $\hat{x}$ (delta function). If we measured momentum, we expect the system to be in an eigenstate of momentum ($e^{i\,\frac{p}{\hbar}\,x}$).

Since we are measuring energy, we are interested in the eigenstates of the Hamiltonian – we are told that our measurement returned the first excited state. Here is the loophole: The problem does not specify *what type of probability density to draw.* Suppose we wanted to draw the *position* probability density associated with an eigenvector of the Hamiltonian, what we would call $\rho(x) = \psi_2^*(x)\,\psi_2(x)$ where $\psi_2(x)$ represents the first excited state (in position basis). What do we know about such states from our experience? Think of the infinite square well, that has first excited state given by $\sin(2\,\pi\,x/a)$, and hence has one node in its graph for $x \in [0,a]$. For the harmonic oscillator, the first excited state is $\sim x\,e^{-\alpha\,x^2}$, and this also has one node in its graph[1]. So we had better sketch a probability density $(\psi_2(x)^*\,\psi_2(x))$ that has a zero.

But, the problem is open to interpretation – one could sketch the probability density for energy – we know that the state of the system is ψ_2 – what,

[1] In fact, the spectrum that is given in this problem corresponds precisely to the harmonic oscillator, with $\hbar\,\omega = 10$ J.

then, is the probability a subsequent measurement returns E_2? Answer: $\rho(E_n) = \delta_{n2}$ – we will, with probability 1, make a measurement of E_2. So, one could draw a valid probability density for energy that looked like a spike at E_2, but then the axis of your probability density had better read: E_n.

17.3 Problem 2

This problem is a piecewise-patching-together nightmare. The setup is the only interesting element here. The potential naturally partitions space into three sections: $x < -a$, $-a < x < 0$ and $x > 0$, and energy into three sections: $E < -V_0$, $-V_0 < E < 0$ and $E > 0$ as shown in Figure 17.1.

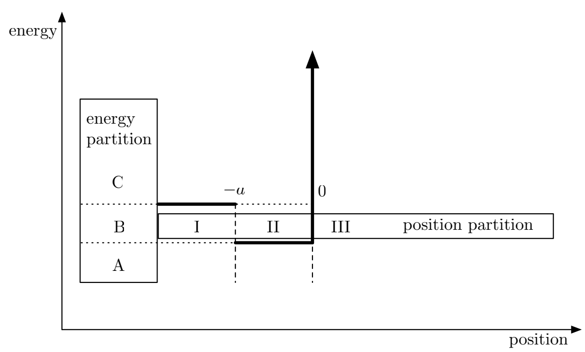


Figure 17.1: The potential splits space up into three regimes: I, II, and III. In addition, it suggests three separate energy regimes: A, B, and C.

We know immediately that no states with energy in region A exist (they are not normalizable since these states would have energy less than the minimum of the potential). In addition, the wavefunction in spatial region III, $x > 0$ must be zero (think of the infinite square well): $\psi_{III}(x) = 0$.

17.3.1 Part a.

We are asked to find the scattering states – this corresponds to states with energy in region C: $E > 0$. Then in regions I and II, we have

$$\begin{aligned} \psi_I'' &= -\underbrace{\frac{2\,m}{\hbar^2}\,E}_{\equiv k^2>0}\,\psi_I \\ \psi_{II}'' &= -\underbrace{\frac{2\,m}{\hbar^2}\,(E+V_0)}_{\equiv \bar{k}^2>0}\,\psi_{II} \end{aligned} \tag{17.14}$$

from Schrödinger's equation. In addition, we know that $\psi_{III}(x) = 0$. The solutions read:

$$\begin{aligned} \psi_I(x) &= A\,e^{i\,k\,x} + B\,e^{-i\,k\,x} \\ \psi_{II}(x) &= F\,e^{i\,\bar{k}\,x} + G\,e^{-i\,\bar{k}\,x} \\ \psi_{III}(x) &= 0. \end{aligned} \tag{17.15}$$

What we have, then, are oscillatory solutions with different wavelengths in regions I and II, and a constant (zero) solution in region III. We expect to be able to solve for B, F and G in terms of A, and A will be the single left-over constant available for normalization of the wave function.

The boundary conditions consist of continuity at $x = -a$ and $x = 0$, and derivative continuity at $x = -a$ (remember that, for the square well, we only needed continuity at the ends of the well in order to get a complete solution up to normalization). From

$$\psi_I(-a) = \psi_{II}(-a) \qquad \psi_I'(-a) = \psi_{II}'(-a) \qquad \psi_{II}(0) = \psi_{III}(0) = 0 \tag{17.16}$$

we can find the desired relations.

17.3.2 Part b.

Here, we are talking about bound states – these are stationary states with energy in regime B: $-V_0 < E < 0$. In regions I and II of space, we will now have

$$\begin{aligned} \psi_I''(x) &= -\underbrace{\frac{2\,m\,E}{\hbar^2}}_{<0}\,\psi_I(x) \\ \psi_{II}''(x) &= -\underbrace{\frac{2\,m}{\hbar^2}\,(E+V_0)}_{>0}\,\psi_{II}(x) \end{aligned} \tag{17.17}$$

and the solution in I becomes growing and decaying exponentials, and in II, oscillation. We throw out the growing exponential in I, ensure that we match at $x = -a$ in a continuous and derivative-continuous way, then have oscillation inside the well, but we must have $\psi_{II}(0) = 0$ to ensure continuity at $x = 0$.

17.4 Problem 3

What we are given here is an initial state that consists of an equal linear combination of stationary states for the infinite square well. Remember that:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\Bigl(\frac{n\,\pi\,x}{a}\Bigr) \tag{17.18}$$

solves $-\frac{\hbar^2}{2\,m}\,\psi_n''(x) + V(x)\,\psi_n(x) = E_n\,\psi_n(x)$ for this potential, with the requirements: $\psi_n(0) = \psi_n(a) = 0$. So our initial state is:

$$\bar{\psi}(x) = \frac{1}{\sqrt{2}}\left(\psi_1(x) + \psi_2(x)\right). \tag{17.19}$$

17.4.1 Part a.

From our statistical interpretation of the wave function, we know that:

$$P\Bigl(x \in [0, \frac{1}{2}\,a]\Bigr) = \int_0^{\frac{1}{2}\,a} \bar{\psi}^*(x)\,\bar{\psi}(x)\,dx. \tag{17.20}$$

The initial wavefunction is clearly normalized already, since we can write it as:

$$\begin{aligned}\int_0^a \bar{\psi}(x)^*\,\psi(x)\,dx &= \frac{1}{2}\Biggl\{\underbrace{\int_0^a \psi_1^*(x)\,\psi_1(x)\,dx}_{=1} + \underbrace{\int_0^a \psi_1^*(x)\,\psi_2(x)\,dx}_{=0} \\ &\quad + \underbrace{\int_0^a \psi_2^*(x)\,\psi_1(x)\,dx}_{=0} + \underbrace{\int_0^a \psi_2^*(x)\,\psi_2(x)\,dx}_{=1}\Biggr\} \\ &= 1,\end{aligned} \tag{17.21}$$

using orthonormality.

Now, while it is true that:

$$\psi_1 \cdot \psi_2 \equiv \int_0^a \psi_1^*(x)\, \psi_2(x)\, dx = 0 \tag{17.22}$$

it is *not the case that restricting the integration region preserves this*, i.e.

$$\int_0^{\frac{1}{2}\,a} \psi_1^*(x)\, \psi_2(x)\, dx \neq 0. \tag{17.23}$$

There are a variety of ways to calculate this integral, we can do integration by parts, or rewrite the trigonometric sine function in terms of the easy-to-integrate exponentials. However you like, you will not get zero.

17.4.2 Part b.

Here, one can either hit the initial wave function with $\hat{H}$ and integrate (from the definition):

$$\langle H \rangle = \int_0^a \bar{\psi}^*(x) \left(-\frac{\hbar^2}{2\,m} \frac{d^2}{dx^2} \right) \bar{\psi}(x)\, dx, \tag{17.24}$$

or use the fact that the stationary states are eigenfunctions of the Hamiltonian: $\hat{H}\, |\psi_n\rangle = E_n\, |\psi_n\rangle$:

$$\begin{aligned} \langle H \rangle &= \frac{1}{2} \Big(\langle \psi_1 |\, \hat{H}\, | \psi_1 \rangle + \langle \psi_2 |\, \hat{H}\, | \psi_1 \rangle + \langle \psi_1 |\, \hat{H}\, | \psi_2 \rangle + \langle \psi_2 |\, \hat{H}\, | \psi_2 \rangle \Big) \\ &= \frac{1}{2} \left(E_1 + E_2 \right). \end{aligned} \tag{17.25}$$

17.4.3 Part c.

Since we know the stationary states that make up the initial wave function, the time-dependent wave-function is just the superposition of the time-dependent wave function for each of the stationary states:

$$\begin{aligned} \Psi(x,t) &= \frac{1}{\sqrt{a}} \left(\sin\!\left(\frac{\pi\, x}{a} \right) e^{-i\, \frac{E_1}{\hbar}\, t} + \sin\!\left(\frac{2\, \pi\, x}{a} \right) e^{-i\, \frac{E_2}{\hbar}\, t} \right) \\ &= \frac{1}{\sqrt{2}} \left(\psi_1(x)\, e^{-i\, \frac{E_1}{\hbar}\, t} + \psi_2(x)\, e^{-i\, \frac{E_2}{\hbar}\, t} \right). \end{aligned} \tag{17.26}$$

The probability, as a function of time now, is (as in the first part):

$$
\begin{aligned}
P\left(x \in [0, \frac{1}{2}\,a]\right) &= \int_0^{\frac{1}{2}\,a} \Psi(x,t)^*\,\Psi(x,t)\,dx \\
&= \frac{1}{2}\int_0^{\frac{1}{2}} \left(\psi_1(x)^2 + 2\,\cos\!\left(\frac{(E_1 - E_2)\,t}{\hbar}\right)\psi_1(x)\,\psi_2(x) + \psi_2(x)^2\right)\,dx
\end{aligned}
\tag{17.27}
$$

(where we have used the fact that the $\{\psi_n(x)\}_{n=1}^{\infty}$ are real). Note that this probability is now a function of time, and that at time $t = 0$, reproduces the result from part a. We know the integrals from the first part:

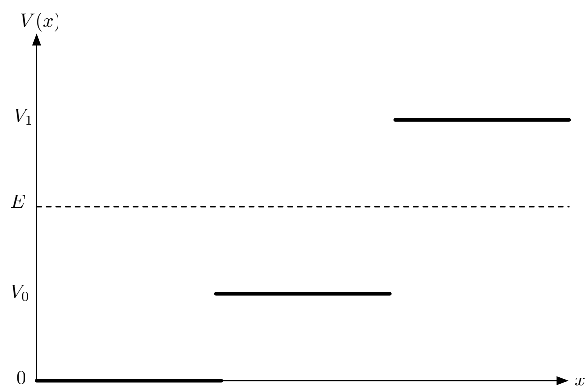
$$
P(x \in [0, \frac{1}{2}\,a]) = \frac{1}{2} + 2\,\cos\!\left(\frac{(E_1 - E_2)\,t}{\hbar}\right)\int_0^{\frac{1}{2}\,a} \psi_1(x)\,\psi_2(x)\,dx. \tag{17.28}
$$

Homework

Reading: Griffiths, pp. 1–130.

Problem 17.1

For the potential shown below, sketch a plausible stationary state with energy E – use the line at E as the x-axis of your sketch. Don't worry about amplitude, but make sure that all boundary conditions and relative wavelengths are clearly satisfied.



Problem 17.2

We find a free particle at location x_0 (ignore experimental error, and suppose that we know it is *exactly* at x_0).

a. Write down the position probability density immediately after the measurement in the position basis – i.e. What is $\psi(x)$?

b. Find the momentum wave function (useful in calculating the momentum probability density) immediately after the measurement – i.e. What is $\psi(p) = \langle p|\psi\rangle$? Comment on the momentum probability density in this case (can it represent a usable probability density?)

Problem 17.3

Using Euler's formula $e^{i\,\theta} = \cos\theta + i\,\sin\theta$, evaluate the integral:

$$I = \int_0^{\frac{1}{2}\,a} \sin\!\left(\frac{\pi\,x}{a}\right)\,\sin\!\left(\frac{2\,\pi\,x}{a}\right)\,dx. \tag{17.29}$$

Problem 17.4

Write the most general 2×2 matrix:

$$\mathbb{A} \doteq \begin{pmatrix} a & b \\ c & d \end{pmatrix} \tag{17.30}$$

with a, b, c, d $\in \mathbb{C}$, write the constraints you must place on the coefficients for $\mathbb{A}$ to be Hermitian: $\mathbb{A} = \mathbb{A}^\dagger$. Express this most general Hermitian $\mathbb{A}$ in terms of its real and imaginary parts – how many real numbers do you get to choose?