Physics 326: Quantum Mechanics I
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Problem Set 2 Solutions

Problem 1

Griffiths 2.2

Show that the energy E must exceed the minimum value of the potential $V(x)$ for every normalizable solution to the time-independent Schrödinger equation. What is the classical analog to this statement? Hint: Rewrite eq. 2.5 in the form

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}[V(x) - E]\psi$$

If $E < V_{\min}$, then ψ and its second derivative always have the same sign. Argue that such a function cannot be normalized.

For ψ to be normalizable, we require $\lim_{x\to\pm\infty} = 0$. Suppose $\psi > 0$ as $x \to \infty$. Then $d^2\psi/dx^2 > 0$, which means that ψ is turning up away from zero. Likewise, if $\psi < 0$, then $d^2\psi/dx^2 < 0$, which means that ψ is turning down away from zero. In both cases $|\psi|^2$ would be increasing in the limits $x \to \pm\infty$ and the wave function would not be normalizable.

Classically, it is not possible for a particle to have total energy E lower than the minimum of the potential $V_{\min}$.

Problem 2

Griffiths 2.5

Suppose a particle in an infinite square well potential is in an even mixture of the first two stationary states:

$$\Psi(x, 0) = A[\psi_1(x) + \psi_2(x)]$$

(a) Normalize $\Psi(x, 0)$ (Easy, if you exploit the orthonormality of ψ_1 and ψ_2.)

$$1 = \int |\Psi|^2 dx = |A|^2 \int (|\psi_1|^2 + \psi_1^*\psi_2 + \psi_2\psi_1^* + |\psi_2|^2)dx = 2|A|^2$$

because the cross-terms vanish by orthonormality of the stationary states. Thus, $A = 1/\sqrt{2}$.

(b) Find $\Psi(x,t)$ and $|\Psi(x,t)|^2$. Express the latter as a sinusoidal function of time (to simplify, let $\omega \equiv \pi^2\hbar/2ma^2$).

Just plug in the properly-normalized stationary states and include the time-dependent phase factors:

$$\begin{aligned}
\Psi(x,t) &= \frac{1}{\sqrt{2}}\left[\psi_1 e^{-iE_1t/\hbar} + \psi_2 e^{-iE_2t/\hbar}\right] \\
&= \sqrt{\frac{1}{a}}\left[\sin\left(\frac{\pi x}{a}\right)e^{-i\omega t} + \sin\left(\frac{2\pi x}{a}\right)e^{-i4\omega t}\right] \\
&= \sqrt{\frac{1}{a}}e^{-i\omega t}\left[\sin\left(\frac{\pi x}{a}\right) + \sin\left(\frac{2\pi x}{a}\right)e^{-3i\omega t}\right]
\end{aligned}$$

where we used $E_n = n^2\hbar\omega$.

$$\begin{aligned}
|\Psi|^2 &= \frac{1}{a}\left[\sin^2\left(\frac{\pi x}{a}\right) + \sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\left(e^{-i\omega t} + e^{3i\omega t}\right) + \sin^2\left(\frac{2\pi x}{a}\right)\right] \\
&= \frac{1}{a}\left[\sin^2\left(\frac{\pi x}{a}\right) + \sin^2\left(\frac{2\pi x}{a}\right) + 2\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\cos(3\omega t)\right]
\end{aligned}$$

Note how the probability density has a time-dependent oscillation, at frequency 3ω.

(c) Compute $\langle x\rangle$. Note that it oscillates in time. What is the angular frequency of the oscillation? What is the *amplitude* of the oscillation?

$$\begin{aligned}
\langle x\rangle &= \int x|\Psi(x,t)|^2 dx \\
&= \frac{1}{a}\int_0^a x\left[\sin^2\left(\frac{\pi x}{a}\right) + \sin^2\left(\frac{2\pi x}{a}\right) + 2\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\cos(3\omega t)\right]dx
\end{aligned}$$

Do the integral term by term:

$$\int_0^a x\sin^2\left(\frac{\pi x}{a}\right)dx = \frac{a^2}{4}$$

$$\int_0^a x\sin^2\left(\frac{2\pi x}{a}\right)dx = \frac{a^2}{4}$$

The last term we can make easier by a trig substitution,

$$\begin{aligned}
\int_0^a x\left[2\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\right]dx &= \frac{1}{2}\int_0^a x\left[\cos\left(\frac{\pi x}{a}\right) - \cos\left(\frac{3\pi x}{a}\right)\right]dx \\
&= -\frac{16a^2}{9\pi^2}
\end{aligned}$$

Putting it all back together,

$$\langle x\rangle = \frac{1}{a}\left[\frac{a^2}{4}+\frac{a^2}{4}-\frac{16a^2}{9\pi^2}\cos 3\omega t\right] = \frac{a}{2}\left[1-\frac{32}{9\pi^2}\cos 3\omega t\right]$$

So, the angular frequency is obviously $3\omega = 3\pi^2\hbar/2ma^2$ and the amplitude is $(a/2)(32/9\pi^2) = 0.36(a/2)$. Note that the amplitude had better be less than $a/2$: otherwise the particle is going outside the box!

(d) Compute $\langle p\rangle$.

Doing it the easy way,

$$\langle p\rangle = m\frac{d\langle x\rangle}{dt} = m\frac{a}{2}\left(\frac{-32}{9\pi^2}\right)(-3\omega)\sin 3\omega t = \frac{8\hbar}{3a}\sin 3\omega t$$

(e) What energies might you measure for this particle and what is the probability of measuring each energy? Compute the expectation value of H. How does it compare with E_1 and E_2?

The two possible energies are $E_1 = \pi^2\hbar^2/2ma^2$ and $E_2 = 2\pi^2\hbar^2/ma^2$. They have equal probability $P_1 = P_2 = 1/2$.

$$\langle H\rangle = \frac{1}{2}(E_1+E_2) = \frac{5\pi^2\hbar^2}{4ma^2}$$

Thus, the expectation value of H is the average of the energies. You will not, of course, ever measure this value (why not?).

Problem 3

Griffiths 2.7

A particle in the infinite square well has initial wave function

$$\Psi(x,0) = \begin{cases} Ax, & 0 \le x \le a/2 \\ A(a-x), & a/2 \le x \le a \end{cases}$$

(a) Sketch $\Psi(x,0)$. Determine the normalization constant A.

$$1 = A^2\int_0^{a/2} x^2 dx + A^2\int_0^{a/2}(a-x)^2 dx = \frac{A^2a^3}{12}$$

Thus, $A = 2\sqrt{3}a^{-3/2}$.

(b) Find $\Psi(x,t)$.

Recall that the method for finding the future time evolution of the wave function is to expand the initial state as a linear combination of stationary states, with coefficients c_n determined by integrating the product of the stationary state with the initial state (this is the inner product of those functions),

$$c_n = \int_{\infty}^{\infty} \psi_n^*(x)\Psi(x,0)dx$$

For this case,

$$c_n = \int_0^{a/2} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \frac{2\sqrt{3}}{a^{3/2}} x dx + \int_{a/2}^{a} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \frac{2\sqrt{3}}{a^{3/2}} (a-x) dx$$

Rewrite this in terms of simple integrals over the trig functions and simplify to

$$c_n = \frac{4\sqrt{6}}{(n\pi)^2} \sin\left(\frac{n\pi}{2}\right) = \begin{cases} 0, & n \text{ even} \\ (-1)^{(n-1)/2} \frac{4\sqrt{6}}{(n\pi)^2}, & n \text{ odd} \end{cases}$$

Thus, the complete wave function is

$$\Psi(x,t) = \frac{4\sqrt{6}}{\pi^2} \sqrt{\frac{2}{a}} \sum_{n=1,3,5...} (-1)^{(n-1)/2} \frac{1}{n^2} \sin\left(\frac{n\pi x}{a}\right) e^{-iE_n t/\hbar}$$

with $E_n = n^2\pi^2\hbar^2/2ma^2$

(c) What is the probability of measuring E_1?

$P_1 = |c_1|^2 = \frac{16\times 6}{\pi^4} = 0.9855$.

(d) Compute the expectation value of the energy.

$$\langle H \rangle = \sum |c_n|^2 E_n = \frac{96}{\pi^4} \frac{\pi^2\hbar^2}{2ma^2} \sum_{1,3,5,...} \frac{1}{n^2} = \frac{6\hbar^2}{ma^2}$$

where we used the fact that the infinite series sums to $\pi^2/8$ (look this up in a book of tables of integrals, products, and series).

Problem 4

Griffiths 2.38

A particle of mass m is in the ground state ($n = 1$) of the infinite square well. Suddenly, the well expands to twice its original size – the right wall moves from $x = a$ to $x = 2a$ – leaving the wave function (momentarily) undisturbed. We immediately measure the energy of the particle.

(a) What is the most probable result of this energy measurement? What is the probability of getting that result?

The new energies are

$$E_n = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$$

The probability of measuring E_n is $P_n = |c_n|^2$, where c_n is the coefficient of ψ_n in the expansion of $\Psi(x, 0)$, similar to problem 3(b) above. The original ground state wave function is $\Psi(x, 0) = \sqrt{2/a}\sin \pi x/a$. The new stationary states are

$$\psi_n(x) = \sqrt{2/2a}\sin\left(\frac{n\pi}{2a}x\right)$$

Thus, the coefficients are (note the integral is only over $(0, a)$ because the initial wave function is zero at $x > a$!),

$$\begin{aligned} c_n &= \frac{\sqrt{2}}{a}\int_0^a \sin\left(\frac{\pi}{a}x\right)\sin\left(\frac{n\pi}{2a}x\right)dx \\ &= \frac{\sqrt{2}}{2a}\int_0^a \cos\left[\left(\frac{n}{2}-1\right)\frac{\pi x}{a}\right] - \cos\left[\left(\frac{n}{2}+1\right)\frac{\pi x}{a}\right]dx \\ &= \frac{1}{\sqrt{2}a}\left\{\frac{\sin\left[\left(\frac{n}{2}-1\right)\frac{\pi x}{a}\right]}{(n/2-1)\pi/a} - \frac{\sin\left[\left(\frac{n}{2}+1\right)\frac{\pi x}{a}\right]}{(n/2+1)\pi/a}\right\}\Bigg|_0^a \\ &= \frac{4\sqrt{2}}{\pi}\frac{\sin(n/2+1)\pi}{(n^2-4)} \end{aligned}$$

but, of course, that only works if $n \neq 2$. Fortunately, the case $n = 2$ is easy to do analytically,

$$c_2 = \frac{\sqrt{2}}{a}\int_0^a \sin^2(\pi x/a)dx = \frac{1}{\sqrt{2}}$$

Simplify the result for $n \neq 2$ above and square our results and we find

$$P_n = |c_n|^2 = \begin{cases} 1/2, & n = 2 \\ \frac{32}{\pi^2(n^2-4)^2}, & n\,\text{odd} \\ 0, & n\,\text{otherwise} \end{cases}$$

Try the new ground state, $n = 1$. It has probability $|c_1|^2 = 32/9\pi^2 = 0.36$. This is smaller than $|c_2|^2$, as are all the other probabilities. Thus, as we might have guessed by inspection, the most probably energy is $E_2 = \pi^2\hbar^2/2ma^2$, which is the same as the energy of its initial state. It has probability $|c_2|^2 = 1/2$.

(b) What is the *next* most probably result, and what is its probability?

$E_1 = \pi^2\hbar^2/8ma^2$, with probability 0.36 as computed above.

(c) What is the *expectation value* of the energy? (Hint: If you find yourself confronted with an infinite series, try another method.)

Don't sum the infinite series $\sum |c_n|^2 E_n$. Instead, compute the expectation value of the Hamiltonian, *acting on the initial wave function*,

$$\langle H \rangle = \int \Psi^* H \Psi dx = \frac{2}{a}\int_0^a \sin\left(\frac{\pi x}{a}\right)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\sin\left(\frac{\pi x}{a}\right)dx = \frac{\pi^2\hbar^2}{2ma^2}$$

which is the same as the energy of the initial state.