Phys 3810, Spring 2011
Exam #1

1. What is the physical meaning of the *expectation value* of a particular physical quantity Q?

The expectation value is the average value of Q that one would get for a large number of measurements of the particle (at time t) for the quantum state in question.

2. Why must a *legal* wave function (for a quantum state) be normalized?

To be normalized the wave function must integrate to 1 over all the relevant space: $\int |\psi|^2 \, d\tau = 1$. This is required because this integral give the probably to find a particle $anywhere$ and the total probability must be 1... if particles are not allowed to disappear!

3. A stationary state is one where the space and time dependences are separated. Identify another property of a stationary state relevant to physics.

The energy uncertainty is zero for such a state, that is, every measurement of energy would return the same value. Also, the expectation value of any observable is constant.

4. For an electron confined to a one-dimensional box of length 1.5×10^{-10} m what is the difference of energies for the first and second stationary states? Express the answer in eV. Use $m_{\rm e} = 9.11 \times 10^{-31}$ kg.

Using the result of the energies of a 1-D box, $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ for $n = 1, 2, \ldots$ we get

$$\begin{aligned} E_2 - E_1 &= \frac{\pi^2\hbar^2}{2ma^2}(4-1) = \frac{3}{2}\frac{\pi^2(1.055\times 10^{-34}\ \mathrm{J\ \cdot s})^2}{(9.11\times 10^{-31}\ \mathrm{kg})(1.5\times 10^{-10}\ \mathrm{m})^2} \\ &= 8.04 \times 10^{-18}\ \mathrm{J} = 50.2\ \mathrm{eV} \end{aligned}$$

5. A particle of mass is confined to a 1–D box of length a with $0 < x < a$. At $t = 0$ its wave function is given by

$$\Psi(x,0) = A\left[4\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) - 3\sqrt{\frac{2}{a}}\sin\left(\frac{3\pi x}{a}\right)\right]$$

Note the explicit 1–D box wave functions!

a) Find A.

Using $\psi_n(x)$ to shorten the notation, the initial quantum state (wave function) is

$$\Psi(x,0) = A[4\psi_1(x) - 3\psi_3(x)]$$

and since the $\psi_n(x)$'s are orthonormal, the integral $\int \Psi^*\Psi\, dx$ gives

$$\int_0^a \Psi^*\Psi\, dx = A^2[16+9] = 25A^2 = 1$$

where the last comes from normalization. This gives

$$A = \tfrac{1}{5}$$

b) Write down the full wave function $\Psi(x,t)$.

As $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ for these states, the full time dependence is restored by attaching $e^{-iE_nt/\hbar}$ to each term in the expansion in stationary states. This gives:

$$\begin{aligned}
\Psi(x,t) &= \sum_i^\infty c_n\psi_n(x)e^{-iE_nt/\hbar} = \tfrac{4}{5}\psi_1(x)e^{-iE_1t/\hbar} - \tfrac{3}{5}\psi_3(x)e^{-iE_3t/\hbar} \\
&= \frac{4}{5}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)\exp\left(-\frac{i\pi^2\hbar^2}{2ma^2}t\right) - \frac{3}{5}\sqrt{\frac{2}{a}}\sin\left(\frac{3\pi x}{a}\right)\exp\left(-\frac{9i\pi^2\hbar^2}{2ma^2}t\right)
\end{aligned}$$

c) What is the expectation value of the energy E for this state?

$$\begin{aligned}
\langle E\rangle &= \sum_n |c_n|^2 E_n = \tfrac{16}{25}E_1 + \tfrac{9}{25}E_3 \\
&= [\tfrac{16}{25}\cdot 1 + \tfrac{9}{25}\cdot 9]\frac{\pi^2\hbar^2}{2ma^2} = \frac{97}{50}\frac{\pi^2\hbar^2}{2ma^2}
\end{aligned}$$

d) Find $\langle x\rangle$, or at least *show how* it is found.

Hint: It may save some writing to denote the 1–D box stationary states (space part) by $\psi_n(x)$ and use their properties.

Use

$$\Psi(x,t) = \frac{4}{5}\psi_1(x)e^{-iE_1t/\hbar} - \frac{3}{5}\psi_3(x)e^{-iE_3t/\hbar}$$

to get

$$\begin{aligned}
\langle x\rangle &= \int_{-\infty}^{\infty} \Psi^*(x,t)x\Psi(x,t) \\
&= \int_{-\infty}^{\infty}\left[\frac{4}{5}\psi_1(x)e^{iE_1t/\hbar} - \frac{3}{5}\psi_3(x)e^{iE_3t/\hbar}\right] x \left[\frac{4}{5}\psi_1(x)e^{-iE_1t/\hbar} - \frac{3}{5}\psi_3(x)e^{-iE_3t/\hbar}\right] dx \\
&= \frac{16}{25}\langle\psi_1|x\psi_1\rangle + \frac{9}{25}\langle\psi_3|x\psi_3\rangle - \frac{12}{25}\left(\langle\psi_1|x\psi_3\rangle e^{-i(E_3-E_1)t/\hbar} + \langle\psi_3|x\psi_1\rangle e^{i(E_1-E_3)t/\hbar}\right) \\
&= \frac{16}{25}\langle\psi_1|x\psi_1\rangle + \frac{9}{25}\langle\psi_3|x\psi_3\rangle - \frac{12}{25}\cdot 2\cos\left(\frac{(E_3-E_1)t}{\hbar}\right)\langle\psi_3|x\psi_1\rangle
\end{aligned}$$

where we used

$$\langle\psi_1|x\psi_3\rangle = \langle\psi_3|x\psi_1\rangle$$

and some other math.

At this point there are just a couple boring integrals to do. Leaving out the tedious steps, one finds

$$\langle\psi_1|x\psi_1\rangle = \langle\psi_3|x\psi_3\rangle = \frac{a}{2}$$

and it turns out that

$$\langle\psi_3|x\psi_1\rangle = 0$$

so that we get

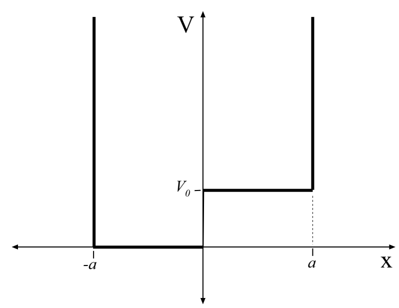
$$\langle x\rangle = (\tfrac{16}{25} + \tfrac{9}{25})\frac{a}{2} = \frac{a}{2}$$

all of which is similar to one of the homework problems. Anyways, here there *happens to be* no time dependence to $\langle x\rangle$.

6. *Big New Problem:*

A particle of mass m moves in one dimension in a potential given by:

$$V(x)\begin{cases} \infty & x < -a \\ 0 & -a < x < 0 \\ V_0 & 0 < x < a \\ \infty & x > a \end{cases}$$



as graphed at the right; this is a 1–D box with a step. We want to solve the TISE for this potential.

We will assume that $E > V_0$ (we can be sure there are such solutions). Give an outline for how one would solve the Schrödinger equation for this potential.

a) Obviously the wave function is zero for $|x| > a$. Write down the general solution for $\psi(x)$ in the regions $-a < x < 0$ and $0 < x < a$. You can (and should) define some symbols to shorten the notation but make clear what they are.

For $x < -a$ and $x > a$ we clearly have $\psi = 0$. For the region $-a < x < 0$ we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

and the usual definition $k \equiv \frac{\sqrt{2mE}}{\hbar}$ gives

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

so that here the general solution is

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

For $0 < x < a$ we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi$$

and with the definition $\ell \equiv \frac{\sqrt{2m(E-V_0)}}{\hbar}$ (which is real from the assumption on E) we have

$$\frac{d^2\psi}{dx^2} = -\ell^2\psi$$

so that here the general solution is

$$\psi(x) = C\sin(\ell x) + D\cos(\ell x)$$

b) Write down the boundary conditions that the solution must satisfy and give a summary of *how* you would solve for the energies E. The complete answer would involve a lot of algebra. Just demonstrate how you would do things.

The boundary condition (continuity of ψ), $\psi = 0$ at $x = -a$ gives

$$-A\sin(ka) + B\cos(ka) = 0$$

and the one at $x = a$ gives

$$C\sin(\ell a) + D\cos(\ell a) = 0$$

As noted in class, for this pathological case, we don't need to have the derivative of ψ continuous there. But we do need continuity of ψ and its derivative at $x = 0$. The condition on ψ gives

$$A \cdot 0 + B \cdot 1 = C \cdot 0 + D \cdot 1 \qquad \Longrightarrow \qquad B = D$$

and the one on $d\psi/dt$ gives

$$kA\cos(0) - kB\sin(0) = \ell C\cos(0) - \ell D\sin(0) \qquad \Longrightarrow \qquad kA = \ell C \qquad \Longrightarrow \qquad C = \frac{k}{\ell}A$$

Which can eliminate C and D in the first two equations. The first two equations can be rearranged to give

$$A\sin(ka) = B\cos(ka)$$

$$C\sin(\ell a) = -D\cos(\ell a) \qquad \Longrightarrow \qquad \frac{k}{\ell}A\sin(\ell a) = -B\cos(\ell a)$$

Dividing one equation by the other gives

$$\frac{k}{\ell}\frac{\sin(\ell a)}{\sin(ka)} = -\frac{\cos(\ell a)}{\cos(ka)} \qquad \Longrightarrow \qquad k\tan(\ell a) = -\ell\tan(ka)$$

This will allow one solve for E; these equations can also give the ratio A/B. We can get A and B separately from the normalization condition. That's as far as I want to take it here.

7. Show how the kinetic energy operator $\hat{p}^2/2m$ can be expressed in terms of the raising and lowering operators a_+ and a_-.

Using the definitions of a_+ and a_-, we have

$$a_- - a_+ = \frac{1}{\sqrt{2\hbar m\omega}}(2i\hat{p}) \qquad \Longrightarrow \qquad \hat{p} = \frac{1}{2i}\sqrt{2\hbar m\omega}(a_- - a_+) = i\sqrt{\frac{\hbar m\omega}{2}}(a_+ - a_-)$$

Use this to construct the kinetic energy operator:

$$\frac{1}{2m}\hat{p}^2 = \frac{1}{2m}(-1)\frac{\hbar m\omega}{2}(a_+ - a_-)^2 = -\frac{\hbar\omega}{4}(a_+ - a_-)^2$$

Expand the square and get

$$\hat{T} = -\tfrac{1}{4}\hbar\omega(a_+^2 + a_-^2 - a_-a_+ - a_+a_-) = \frac{\hbar\omega}{4}(a_-a_+ + a_+a_- - a_+^2 - a_-^2)$$

8. From one of homework problem, if you were to evaluate $\langle T\rangle$ and $\langle V\rangle$ for the $n = 2$ state of the HO, what would you expect to get for each? (There is a theorem which says that the reasonable guess is correct.)

It is clear that we must get

$$\langle T\rangle + \langle V\rangle = \langle E\rangle_2 = \hbar\omega(2 + \tfrac{1}{2}) = \tfrac{5}{2}\hbar\omega$$

In the homework problem we found that for both the $n = 0$ and $n = 1$ states the total energy was *equally divided* between kinetic and potential energies, that is,

$$\langle T\rangle = \langle V\rangle = \tfrac{1}{2}\langle H\rangle = \tfrac{1}{2}E_n$$

And this turns out to be the case because of one application of a result generally (and confusingly) known as the **virial theorem**

9. Suppose the wave packet function $\phi(k)$ is a simple step function:

$$\phi(k) = \begin{cases} 0 & k < b \\ A & -b < k < b \\ 0 & k > b \end{cases}$$

What (full) wave function $\Psi(x,t)$ results from this? What condition must A satisfy?

Use this step-type function in

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \phi(k)e^{i(kx - \frac{\hbar k^2}{2m}t)}\,dk$$

and get

$$\Psi(x,t) = \frac{A}{\sqrt{2\pi}}\int_{-b}^{b} e^{i(kx - \frac{\hbar k^2}{2m}t)}\,dk$$

at which point one really has to stop because this doesn't have a closed form.

As to the second question, the value of A must give a normalized $\Psi(x,0)$. Note

$$\begin{aligned}\Psi(x,0) &= \frac{A}{\sqrt{2\pi}}\int_{-b}^{b} e^{ikx}\,dk \\ &= \frac{A}{\sqrt{2\pi}}\frac{1}{ix}e^{ikx}\Big|_{-b}^{b} = \frac{A}{\sqrt{2\pi}}\frac{1}{ix}(2i)\sin(bx) = A\sqrt{\frac{2}{\pi}}\frac{\sin(bx)}{x}\end{aligned}$$

and so the condition that $\Psi(x,0)$ be normalized is

$$\frac{2A^2}{\pi}\int_{-\infty}^{\infty}\frac{\sin^2(bx)}{x^2}\,dx = 1$$

In fact, the integral can be done, giving

$$\frac{2A^2}{\pi}\pi b = 2A^2 b = 1 \qquad \Longrightarrow \qquad A = \frac{1}{\sqrt{2b}}$$

but you didn't need to go that far.

10. For the scattering states of a 1–D potential which is zero at large x, we used the "bad" solutions to get the coefficients T and R. Summarize the physical content of these quantities.

These coefficients are the (squared) ratio of coefficients for the outgoing wave to the wave for a solution with incoming and outgoing "plane waves". The physical interpretation is that T gives the probability that a particle coming in from the left will pass through the potential and travel onward to the right, with a similar interpretation for R for the reflected wave.

Useful Equations

Math

$$\int_0^\infty x^n e^{-x/a} = n!\, a^{n+1}$$

$$\int_0^\infty x^{2n} e^{-x^2/a^2}\, dx = \sqrt{\pi}\frac{(2n)!}{n!}\left(\frac{a}{2}\right)^{2n+1} \qquad \int_0^\infty x^{2n+1} e^{-x^2/a^2}\, dx = \frac{n!}{2}a^{2n+2}$$

$$\int_a^b f\,\frac{dg}{dx}\,dx = -\int_a^b \frac{df}{dx}\,g\,dx + fg\Big|_a^b$$

Numbers

$$\hbar = 1.05457\times 10^{-34}\ \mathrm{J\cdot s} \qquad m_{\mathrm{e}} = 9.10938\times 10^{-31}\ \mathrm{kg} \qquad m_{\mathrm{p}} = 1.67262\times 10^{-27}\ \mathrm{kg}$$

$$e = 1.60218\times 10^{-19}\ \mathrm{C} \qquad c = 2.99792\times 10^{8}\ \tfrac{\mathrm{m}}{\mathrm{s}} \qquad 1\ \mathrm{eV} = 1.602\times 10^{-19}\ \mathrm{J}$$

Physics

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi \qquad P_{ab} = \int_a^b |\Psi(x,t)|^2\,dx \qquad p \to \frac{\hbar}{i}\frac{d}{dx}$$

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2\,dx = 1 \qquad \langle x\rangle = \int_{-\infty}^{\infty} x|\Psi(x,t)|^2\,dx \qquad \langle p\rangle = \int_{-\infty}^{\infty} \Psi^*\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi\,dx$$

$$\sigma = \sqrt{\langle j^2\rangle - \langle j\rangle^2} \qquad \sigma_x\sigma_p \geq \frac{\hbar}{2}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi \qquad \phi(t) = e^{-iEt/\hbar} \qquad \Psi(x,t) = \sum_{n=1}^{\infty} c_n\psi_n(x)e^{-iE_nt/\hbar} = \sum_{n=1}^{\infty}\Psi_n(x,t)$$

∞ Square Well: $$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \qquad \psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$$

$$\int \psi_m(x)^*\psi_n(x)\,dx = \delta_{mn} \qquad c_n = \int \psi_n(x)^* f(x)\,dx \qquad \sum_{n=1}^{\infty}|c_n|^2 = 1 \qquad \langle H\rangle = \sum_{n=1}^{\infty}|c_n|^2E_n$$

Harmonic Oscillator: $$V(x) = \tfrac{1}{2}m\omega^2x^2 \qquad \frac{1}{2m}[p^2 + (m\omega x)^2]\psi = E\psi$$

$$a_\pm \equiv \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x) \qquad [A,B] = AB - BA \qquad [x,p] = i\hbar$$

$$H(a_+\psi) = (E+\hbar\omega)(a_+\psi) \qquad H(a_-\psi) = (E-\hbar\omega)(a_+\psi) \qquad a_-\psi_0 = 0$$

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \qquad \psi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sqrt{\frac{2m\omega}{\hbar}}\,xe^{-\frac{m\omega}{2\hbar}x^2}$$

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2} \qquad H_0 = 1 \qquad H_1 = 2\xi \qquad H_2 = 4\xi^2 - 2 \qquad H_3 = 8\xi^3 - 12\xi$$

Free particle: $\qquad \Psi_k(x) = Ae^{i(kx - \frac{\hbar k^2}{2m})t} \qquad v_{\text{phase}} = \dfrac{\omega}{k} \qquad v_{\text{group}} = \dfrac{d\omega}{dk}$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m}t)}\, dk \qquad \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx}\, dx$$

Delta Fn Potl: $\qquad \psi(x) = \dfrac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2} \qquad E = -\dfrac{m\alpha^2}{2\hbar^2}$

$$R = \frac{1}{1 + (2\hbar^2 E/m\alpha^2)} \qquad T = \frac{1}{1 + (m\alpha^2/2\hbar^2 E)}$$