Phys 3810, Spring 2009
Exam #1

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

The expectation value of Q (for a particular quantum state Ψ) is the result one gets if one makes many repeated measurements of Q (at the same time t) and then takes the average.

2. Show that the operator for p is Hermitian. Explain all the steps!

When the $\hat{p}$ operator sits in an integral between two wave functions, using integration by parts we can do the steps:

$$\int_{-\infty}^{\infty} \phi^* \hat{p} \psi \, dx \;=\; \int_{-\infty}^{\infty} \phi^* \frac{\hbar}{i} \frac{\partial}{\partial x} \psi \, dx \;=\; \frac{\hbar}{i} \int_{-\infty}^{\infty} \left(-\frac{\partial \phi^*}{\partial x} \right) \psi \, dx$$

But now the factors in front can be brought inside

$$= \int_{-\infty}^{\infty} \left(\frac{\hbar}{(-i)} \right) \left(\frac{\partial \phi^*}{\partial x} \right) \psi \, dx = \int_{-\infty}^{\infty} \left(\frac{\hbar}{i} \frac{\partial \phi}{\partial x} \right)^* \psi \, dx$$

But the last is the inner product of $(\hat{p}\phi)$ with ψ, whereas we started with the inner product of ϕ with $(\hat{p}\psi)$. The fact that we can switch the position of the $\hat{p}$ operator in this way shows that $\hat{p}$ is Hermitian.

3. What is a stationary state?

A stationary state is a state $\Psi(x,t)$ which can be expressed as a separated function of of x and t. With this condition, the Schrødinger equation requires the wave function to be of the form

$$\Psi(x,t) = \psi(x) e^{-iEt/\hbar}$$

Such a state has the nice property that expectation values don't depend on time.

A general solution to the Schrødinger equation can be built up from all of the stationary state solutions.

4. A particle in the infinite square well has the initial wave function

$$\Psi(x,0) = A \sin(\pi x/a)(1 + \cos(\pi x/a)) \qquad (0 \le x \le a)$$

Determine A, find $\Psi(x,t)$. What is the expectation value of the energy? *Hint: The decomposition into the stationary states can be done by inspection!*

As the stationary states are given by

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

the given state can be decomposed easily:

$$\begin{aligned}\Psi(x,0) &= A(\sin(\pi x/a) + \sin(\pi x/a)\cos(\pi x/a)) = A(\sin(\pi x/a) + \tfrac{1}{2}\sin(2\pi x/a)) \\ &= A\sqrt{\frac{a}{2}}\left(\sqrt{\frac{2}{a}}\sin(\pi x/a) + \tfrac{1}{2}\sqrt{\frac{2}{a}}\sin(2\pi x/a)\right) = A\sqrt{\frac{a}{2}}(\psi_1(x) + \tfrac{1}{2}\psi_2(x))\end{aligned}$$

and in this form we can use the orthonormality of the $\psi_n(x)$'s.

Normalizing $\Psi(x,0)$ gives

$$\int_{-\infty}^{\infty} |\Psi(x,0)|^2\, dx = A^2\frac{a}{2}(1 + \tfrac{1}{4}) = \frac{5A^2 a}{8} = 1$$

This gives

$$A^2 = \frac{8}{5a} \qquad \Longrightarrow \qquad A = 2\sqrt{\frac{2}{5a}}$$

Then the decomposition is

$$\Psi(x,0) = \frac{2}{\sqrt{5}}(\psi_1(x) + \tfrac{1}{2}\psi_2(x))$$

With

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2} \qquad E_2 = \frac{4\pi^2\hbar^2}{2ma^2}$$

then putting in the time dependence gives

$$\Psi(t) = \frac{2}{\sqrt{5}}(\psi_1(x)e^{-iE_1t/\hbar} + \tfrac{1}{2}\psi_2(x)e^{-iE_2t/\hbar})$$

The expectation of value of the energy at $t = 0$ is (using orthonormality)

$$\langle E\rangle = \int \Psi(x,0)\hat{H}\Psi(x,0)\, dx = \frac{4}{5}(E_1 + \tfrac{1}{4}E_2) = \tfrac{4}{5}E_1 + \tfrac{1}{5}E_2$$

which is, pulling out the common factor,

$$\frac{\pi^2\hbar^2}{2ma^2}(1\cdot\frac{4}{5} + 4\cdot\frac{1}{5}) = \frac{8}{5}\frac{\pi^2\hbar^2}{2ma^2} = \frac{8\pi^2\hbar^2}{10ma^2}$$

This is same as the $\langle E\rangle$ at all other times, from the orthogonality of the stationary states.

5. An electron is confined to a one–dimensional box of length 2.0×10^{-10} m. Find the difference in energies between ground state and first excited state.

As the energy levels of the confined particle are given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}\ ,$$

the energy of the ground state (above the bottom of the well) is

$$E_1 = \frac{\pi^2(1.055\times 10^{-34}\ \mathrm{J\cdot s})^2}{2(9.11\times 10^{-31}\ \mathrm{kg})(2.0\times 10^{-10}\ \mathrm{m})^2} = 1.51\times 10^{-18}\ \mathrm{J}$$

As the energies are proportional to n^2, the energy of the second state is

$$E_2 = 4E_1 = 6.03 \times 10^{-18} \text{ J}$$

The difference in energies is

$$\Delta E = E_2 - E_1 = 4.52 \times 10^{-18} \text{ J} = 28.2 \text{ eV}$$

6. Show how one can apply the lowering operator a_- to the first excited state of the harmonic oscillator $\psi_1(x)$, to get $\psi_0(x)$.

Use

$$\psi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sqrt{\frac{2m\omega}{\hbar}}xe^{-\frac{m\omega}{2\hbar}x^2} \qquad \text{and} \qquad a_- = \frac{1}{\sqrt{2\pi\hbar\omega}}(ip+m\omega x) = \frac{1}{\sqrt{2\pi\hbar\omega}}(\hbar\frac{d}{dx}+m\omega x)$$

to get

$$\begin{aligned} a_-\psi_1(x) &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sqrt{\frac{2m\omega}{\hbar}}\frac{1}{\sqrt{2\pi\hbar\omega}}\left(\hbar\frac{d}{dx}+m\omega x\right)xe^{-\frac{m\omega}{2\hbar}x^2} \\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\hbar}\left(\hbar(1-\frac{m\omega}{\hbar}x^2)+m\omega x^2\right)e^{-\frac{m\omega}{2\hbar}x^2} \\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}e^{-\frac{m\omega}{2\hbar}x^2} \end{aligned}$$

and since we are supposed to get

$$a_-\psi_1(x) = \sqrt{1}\,\psi_0(x) = \psi_0(x)$$

then we conclude

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

which is correct!

7. The wave function for a free particle was found to be

$$\Psi_k(x) = Ae^{i(kx-\frac{\hbar k^2}{2m}t)}$$

Why did we declare this to be a "bad" wave function and thus conclude that there was no such thing as a free particle with definite energy?

Such a wave function is not normalizeable and as such, cannot represent the probability distribution for the location of a particle and thus not a valid physical (quantum) state. A free particle with definite energy does has have this sort of wave function for a solution, and so there is strictly speaking no such thing as a free particle with definite energy (or definite momentum).

8. Give your definition of *bound* and *scattering* states.

A bound (stationary) state is one for which the wave function is normalizeable, so that the wave function dies off at $x \to \pm\infty$. It represents a particle which because of a negative potential, can't move out to infinity where $V = 0$.

A scattering state is not normalizeable and does not die off as x gets large. It represents a particle with enough energy that it can "escape" a negative potential function which might be present.

9. A free particle has the initial wave function

$$\Psi(x,0) = Axe^{-a|x|}$$

where A and a are positive real constants.

a) Normalize $\Psi(x,0)$.

We have

$$\int_{-\infty}^{\infty} |\Psi(x,0)|^2\, dx = |A|^2 \int_{-\infty}^{\infty} x^2 e^{-2a|x|}\, dx = 2|A|^2 \int_0^{\infty} x^2 e^{-2ax}\, dx$$

Use the gaussian integral results, get:

$$= 2|A|^2(2)\frac{1}{(2a)^3} = \frac{|A|^2}{2a^3} = 1$$

which gives

$$A = \sqrt{2}a^{3/2}$$

b) Find the wave packet function $\phi(k)$.

The wave packet function is given by

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0)e^{-ikx}\, dx$$

so using our result (with the normalization),

$$\phi(k) = \frac{1}{\sqrt{2\pi}}\sqrt{2}a^{3/2} \int_{-\infty}^{\infty} xe^{-a|x|}e^{ikx}\, dx = \frac{a^{3/2}}{\sqrt{\pi}} \int_{-\infty}^{\infty} xe^{-a|x|}(\cos(kx) + i\sin(kx))\, dx$$

That's really good enough, but if we want to go further, we note that as $e^{-a|x|}$ and $\cos(kx)$ are both even functions and x is odd, the cosine term gives a zero integral and we're left with

$$\phi(k) = \frac{ia^{3/2}}{\sqrt{\pi}} \int_{-\infty}^{\infty} xe^{-a|x|}\sin(kx)\, dx = \frac{2ia^{3/2}}{\sqrt{\pi}} \int_0^{\infty} xe^{-ax}\sin(kx)\, dx$$

The integral needed here exists in tables; we don't want to re-derive it right now! One gets

$$\phi(k) = \frac{2ia^{3/2}}{\sqrt{\pi}} \frac{2ak}{(a^2+k^2)^2} = \frac{4ia^{5/2}k}{\sqrt{\pi}(a^2+k^2)^2}$$

At least I think I did that right. Anyway, it could be worked out.

c) Construct $\Psi(x,t)$ in the form of an integral (which you don't need to evaluate).

Having $\phi(k)$, the full time--dependent $\Psi(x,t)$ is constructed via

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

using the $\phi(k)$ that we got in (b); but since this integral will be very hard to work we'll leave it at that.

10. The finite square well was a potential given by:

$$V(x) = \begin{cases} -V_0 & \text{for } \; -a < x < a \\ 0 & \text{for } \; |x| > a \end{cases}$$

What boundary conditions were imposed upon ψ for a proper solution?

At the boundaries of the well ($x = \pm a$) we required that the wavefunction $\psi(x)$ be continuous and that its derivative, $\frac{d\psi}{dx}$ be continuous. (We require the derivative condition because the potential only makes a finite jump at the boundary.)

11. What was the physical meaning of the transmission coefficient T derived for the finite square well potential?

T represents the probability that an incident particle with *nearly* definite energy E will keep moving freely past the well, rather than being reflected backwards in the direction from whence it came.

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

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

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

Physics

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

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

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

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

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

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

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

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

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

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

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

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

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