Phys 3810, Spring 2010
Exam #1

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

This refers to a particle (or, later, system of particles) prepared in a particular "quantum state". Repeated measurements of the physical quantity in question will give an average which is the expectation value of the quantity for that state.

2. The operator for $p = \frac{\hbar}{i}\frac{d}{dx}$ is Hermitian, but the operator $\frac{d}{dx}$ is not. Explain the difference.

The problem is that for wave functions ψ and ϕ which die off at infinity, when we take integral of the operator sandwiched between two states, we can do an integration by parts:

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

but this is not equal to the integral that we get when the operator is applied to the first element, namely

$$\int_{-\infty}^{\infty}\left(\frac{d\phi^(x)}{dx}\right)^*\psi(x)\,dx$$

because of the minus sign. The additional factor of i sitting inside the complex conjugation) takes care of that.

3. What is a stationary state?

A stationary state is (described by) a wave function which is a product of space and time parts and solves the Schrödinger equation. It thus has the form $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$ with $\psi(x)$ satisfying the TISE.

For such states, the expectation value of any observable is $constant$.

4. A particle in the harmonic oscillator potential starts in the state

$$\Psi(x,0) = A[2\psi_0(x) + 5\psi_1(x)]\ .$$

where ψ_0 and ψ_1 represent (normalized) HO wave functions.

a) Find A (i.e. normalize).

Using orthonormality of the HO wave functions, we get

$$\begin{aligned}\int \Psi^*(x,0)\Psi(x,0)\,dx &= A^2\int[2\psi_0(x)+5\psi_1(x)]^2\,dx \\ &= A^2\int[4\psi_0(x)^2+25\psi_1(x)^2]\,dx = 29A^2 = 1\end{aligned}$$

and this gives

$$A = \frac{1}{\sqrt{29}}$$

b) Construct $\Psi(x,t)$ and $|\Psi(x,t)|^2$.

To get $\Psi(x,t)$, include the oscillating exponential factor with each spatial part of a stationary state in the linear combination. Note,

$$E_0 = \tfrac{1}{2}\hbar\omega \qquad \text{and} \qquad E_1 = \tfrac{3}{2}\hbar\omega$$

so including the factors of $e^{\frac{-iEt}{\hbar}}$ gives

$$\Psi(x,t) = \frac{1}{\sqrt{29}}\left[2\psi_0(x)e^{-i\omega t/2} + 5\psi_1(x)e^{-i3\omega t/2}\right]$$

and $|\Psi(x,t)|^2$ is this expression times its complex conjugate. Note that in the squared terms the time dependence cancels. We get:

$$|\Psi(x,t)|^2 = \frac{1}{29}\left[4|\psi_0(x)|^2 + 25|\psi_1(x)|^2 + 10\psi_0(x)\psi_1(x)[e^{i\omega t(-1+3)/2} + e^{i\omega t(1-3)/2}\right]$$

The two exponentials combine to give a cosine term, so (recalling that the ψ's are real):

$$\Longrightarrow \qquad = \frac{1}{29}\left[4|\psi_0(x)|^2 + 25|\psi_1(x)|^2 + 20\psi_0(x)\psi_1(x)\cos(2\omega t/2)\right]$$

so

$$|\Psi(x,t)|^2 = \frac{1}{29}\left[4|\psi_0(x)|^2 + 25|\psi_1(x)|^2 + 20\psi_0(x)\psi_1(x)\cos(\omega t)\right]$$

c) Find $\langle x\rangle$.

Recall that $\langle x\rangle = \int x|\Psi(x,t)|^2 dx$ so using the answer from the last part we get

$$\langle x\rangle = \frac{1}{29}\int_{-\infty}^{\infty}\left[4x|\psi_0(x)|^2 + 25x|\psi_1(x)|^2 + 20x\psi_0(x)\psi_1(x)\cos(\omega t)\right]\,dx$$

which we notice gives zero for the first two terms by the symmetry of the functions. For the last term, the factors without an x go outside and we need only evaluate

$$\begin{aligned}
\int_{-\infty}^{\infty} x\psi_0(x)\psi_1(x)\,dx &= \int_{-\infty}^{\infty}\left(\frac{m\omega}{\pi\hbar}\right)^{1/2} x\sqrt{\frac{2m\omega}{\hbar}}xe^{-m\omega x^2/\hbar}\,dx \\
&= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\sqrt{\frac{2m\omega}{\hbar}}\int_{-\infty}^{\infty} x^2 e^{-m\omega x^2/\hbar} \\
&= \sqrt{2}\frac{m\omega}{\hbar}\frac{1}{\sqrt{\pi}}2\sqrt{\pi}\cdot 2\left(\tfrac{1}{2}\sqrt{\frac{\hbar}{m\omega}}\right)^3 \\
&= \frac{1}{\sqrt{2}}\sqrt{\frac{\hbar}{m\omega}}
\end{aligned}$$

Putting this back into the previous equation gives

$$\langle x \rangle = \frac{20}{29\sqrt{2}}\sqrt{\frac{\hbar}{m\omega}}\cos(\omega t)$$

We note that here $\langle x \rangle$ does depend on time, and that's because the state $|\Psi(x,t)|^2$ is *not* a stationary state.

d) If you made measurements of the energy of this particle, what average value would you get?

The coefficients of the stationary states, when squared, give the probabilities of getting the corresponding energy value in a measurement. This gives

$$\langle E \rangle = \frac{4}{29}E_0 + \frac{25}{29}E_1 = \frac{1}{29}\hbar\omega(4 \cdot \tfrac{1}{2} + 25 \cdot \tfrac{3}{2}) = 1.36\hbar\omega$$

5. A HCl molecule can be modeled as a single mass (the H atom, with an effective mass of 1.63×10^{-27} kg) oscillating harmonically.

The difference between the energies of the first and second levels is 0.358 eV. Find the angular frequency of the motion ω and the effective force constant k of the oscillator. (Recall that $\omega = \sqrt{\frac{k}{m}}$ for the HO.)

As the energy levels of the HO are given by $\hbar\omega(n + \frac{1}{2})$, the spacing between adjacent levels is $\hbar\omega$. Solve for ω:

$$\Delta E \hbar\omega = 0.358 \text{ eV} = 5.74{\times}10^{-20} \text{ J} \qquad \Longrightarrow \qquad \omega = \frac{\Delta E}{\hbar} = \frac{(5.74 \times 10^{-20} \text{ J})}{(1.055 \times 10^{-34} \text{ J}\cdot\text{s})} = 5.43{\times}10^{14} \text{ s}^{-1}$$

From $\omega^2 = k/m$, from the given value of the (effective) mass, get

$$k = m\omega^2 = (1.63 \times 10^{-27} \text{ kg})(5.43 \times 10^{14} \text{ s}^{-1})^2 = 481\tfrac{\text{N}}{\text{m}}$$

6. Show explicitly that the lowering operator a_- applied to the ground state of the harmonic oscillator $\psi_0(x)$ does indeed give zero.

The lowering operator is

$$a_- \equiv \frac{1}{\sqrt{2\hbar m\omega}}(+ip + m\omega x) = \frac{1}{\sqrt{2\hbar m\omega}}(+\hbar\frac{d}{dx} + m\omega x)$$

Applied to the HO ground state, this gives

$$\begin{aligned}
\frac{1}{\sqrt{2\hbar m\omega}}(+\hbar\frac{d}{dx} + m\omega x)\psi_0(x) &= \frac{1}{\sqrt{2\hbar m\omega}}(+\hbar\frac{d}{dx} + m\omega x)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \\
&= \frac{1}{\sqrt{2\hbar m\omega}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}(+\hbar\frac{d}{dx} + m\omega x)e^{-\frac{m\omega}{2\hbar}x^2} \\
&= \frac{1}{\sqrt{2\hbar m\omega}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(+\hbar\frac{(-m\omega)x}{\hbar} + m\omega x\right)e^{-\frac{m\omega}{2\hbar}x^2} \\
&= 0
\end{aligned}$$

(Recall that in the operator approach the wave function $\psi_0(x)$ was found by solving the DE that came from $a_-\psi_0 = 0$, so this is no news!

7. a) 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?

The solution which gives a definite energy and satisfies the boundary conditions cannot be normalized, i.e. it has probability everywhere. It can't represent a physical state of the system, though it can be *useful* in the calculation of certain physical quantities.

b) How does one (mathematically) construct a possible *physical* wave function for a free particle?

One obtains an appropriate "envelope function" $\phi(k)$ from somewhere (this function must be normalizable in the variable k), and then makes the full wave function $\Psi(x,t)$ via

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

8. A free particle has the initial wave function

$$\Psi(x,0) = \begin{cases} -A & -a < x < 0 \\ +A & 0 < x < a \end{cases}$$

where A and a are positive real constants.
a) Normalize $\Psi(x,0)$.

We need to have

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2\, dx = 2aA^2 = 1$$

so that $A = \frac{1}{\sqrt{2a}}$.

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

Use the ..uh.. $\phi(k)$ formula,

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

It saves a little time to note that $\Psi(x,0)$ is an odd function, while the $\cos kx$ part of e^{-ikx} is even. This gives:

$$\begin{aligned} \phi(k) &= \frac{2}{\sqrt{2a}} \frac{1}{\sqrt{2\pi}} \int_0^a (-i) \sin kx\, dx = -\frac{1}{\sqrt{\pi a}} \frac{i}{k} \cos(kx)\Big|_0^a \\ &= -\frac{i}{k}\frac{1}{\sqrt{\pi a}}(\cos ka - 1) = \frac{2i}{k}\frac{1}{\sqrt{\pi a}} \sin^2(ka/2) \end{aligned}$$

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

We get $\Psi(x,t)$ back from $\phi(k)$ by attaching a stationary state for each k and then summing over all k's:

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

This gives

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

and at this point we realize that this integral probably *can* be worked with clever algebra but will probably take way too long.

9. Give a definition of *bound* and *scattering* states for a (potential $V(x)$ which could give rise to both).

A bound state has an energy value less than the (minimal) asymptotic value of the potential (normally taken to be zero). It is normalizable.

As used in our text, a scattering state satisfies the time-independent Schrödinger equation for the given potential (and so has a definite energy), but cannot be normalized. While we can make well-behaved wave packets out of them it is useful to deal with the original (bad) states and deal with their normalization problem somehow.

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

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

and its general solution for a symmetric bound state was found to be

$$\psi(x) = \begin{cases} Fe^{-\kappa x} \, , & \text{for } \ x > a \\ D\cos(lx) \, , & \text{for } \ -a < x < a \\ Fe^{\kappa x} \, , & \text{for } \ x < -a \end{cases}$$

where

$$\kappa = \frac{\sqrt{-2mE}}{\hbar} \qquad \text{and} \qquad l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

a) Derive the boundary condition that results from the continuity of ψ.

The value of the wave function at $x = a$ has the same value for the $-a < x < a$ expression as for the $a < x$ expression. This gives

$$Fe^{-\kappa a} = D\cos(la)$$

b) Derive the boundary condition that results from continuity of of $d\psi/dx$.

The value of the *derivative of* ψ evaluated at $x = a$ is the same when done for the $-a < x < a$ expression as for the $a < x$ expression. This gives

$$-F\kappa e^{-\kappa x}\Big|_{x=a} = -Dl\sin(la)\Big|_{x=a} \qquad \Longrightarrow \qquad F\kappa e^{-\kappa a} = Dl\sin(la)$$

Dividing this result by the previous one gives

$$\kappa = l\tan(la)$$

which we note is a (messy) equation *only* involving the energy E.

c) There are three constants to be found: F, D and the energy E. What is the *third* condition which determines all of their values?

The third condition is that of normalization of the (whole) wave function. However, we only need the boundary conditions to solve for the energy.

11. The continuum solutions for the delta function potential (or the finite square well) by definition have arbitrary (positive) values for the energy and have non-zero probability densities all over space! Nevertheless we were able to extract some "physical" information from the solutions.

Summarize what that information was.

The information was the behavior of particles interacting with the potential in a one--dimensional collision. Particle incident from one direction will have a probability to go forward or bounce backward and these probabilities were computed with the transmission and reflection coefficients T and R.

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

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

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

Physics

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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