Phys 3810, Spring 2012
Exam #1

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

For a set of quantum systems prepared in the *same* "state" $\psi(x)$ the *average* value of the measurement of Q is the expectation value $\langle Q \rangle$.

2. In problem 1.18 we used the formula for the de Broglie wavelength corresponding to temperature T:

$$\lambda = \frac{h}{\sqrt{3mk_BT}}$$

How did we use this formula to conclude that electrons in a typical solid must be treated quantum mechanically?

To answer the question of whether quantum mechanics is important, we took the de Broglie wavelength λ to be the interparticle spacing and found the corresponding temperature T. If it is *higher* than the known temperature of the system then the actual wavelength must be *larger* than the particle spacing, and then quantum effects are important.

For electrons in a typical solid we found the "quantum temperature" to be much higher than any earthly conditions so quantum effects are important here.

3. A stationary state is one where the space and time dependences are separated.

a) How do they differ from general quantum states in terms of the results of energy measurements?

For a (particular) stationary state a measurement of the energy always returns the same value.

b) Show that for such a state the expectation value of any observable $Q(x,p)$ is constant.

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

$$\begin{aligned}\langle \hat{Q} \rangle &= \int_{-\infty}^{\infty} \Psi^*(x,t)\hat{Q}(x,p)\Psi(x,t)dx \\ &= \int_{-\infty}^{\infty} \psi^*(x)e^{+iEt/\hbar}\hat{Q}(x,p)\psi(x)e^{-iEt/\hbar}dx = \int_{-\infty}^{\infty} \psi^*(x)\hat{Q}(x,p)\psi(x)dx\end{aligned}$$

The last expression does not depend on time.

4. For an electron confined to a one-dimensional box the difference of energies for the first and second stationary states is 4.50 eV. What is the length of the box? Use $m_e = 9.11 \times 10^{-31}$ kg.

As the energies of the stationary states of the box are given by $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ with $n = 1, 2, \ldots$, the difference in energies of the first and second states is

$$\Delta E = \frac{\pi^2\hbar^2}{2ma^2}(2^2 - 1^2) = \frac{3\pi^2\hbar^2}{2ma^2} = 4.5 \text{ eV} = 7.2 \times 10^{-19} \text{ J}$$

This gives

$$a^2 = \frac{3\pi^2\hbar^2}{2m(7.2 \times 10^{-19} \text{ J})} = 2.5 \times 10^{-19} \text{ m}^2$$

So then

$$a = 5.0 \times 10^{-10} \text{ m}$$

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

$$\Psi(x, 0) = A[2\psi_2(x) - \psi_3(x)]$$

where the ψ_n's are the (normalized!) box wave functions.

For all of these parts you can use the basic properties of the box wave functions shown on the problem sets.

a) Find A. This shouldn't take much time.

Normalization gives

$$\begin{aligned} 1 &= |A|^2 \int_{-\infty}^{\infty} \Psi^*(x,0)\Psi(x,0)\, dx \\ &= |A|^2 \int_{-\infty}^{\infty} (2\psi_2(x) - \psi_3(x))^2 \, dx = |A|^2(4+1) \end{aligned}$$

In the last step we have used the orthonormality of the solutions, wherein the integral of the square of the $\psi(x)'s$ give 1 and the integral of a product of different ψ_n's gives zero. Then:

$$1 = 5|A|^2 \qquad \Longrightarrow \qquad A = \frac{1}{\sqrt{5}}$$

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

Attach a wiggly exponential factor to each term in the expansion of $\Psi(x, 0)$. Thus:

$$\Psi(x,t) = \frac{2}{\sqrt{5}}\psi_2(x)e^{-iE_2t/\hbar} - \frac{1}{\sqrt{5}}\psi_1(x)e^{-iE_3t/\hbar}$$

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

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

The fact that the ψ_n's satisfy the Schrödinger equation give $\langle E \rangle$ as a weighted average of the energies of the states:

$$\begin{aligned} \langle E \rangle &= \sum_n |c_n|^2 E_n = \frac{4}{5}E_2 + \frac{1}{5}E_3 \\ &= \left(\frac{4}{5} \cdot 4 + \frac{1}{5} \cdot 9\right) \frac{\pi^2\hbar^2}{2ma^2} = \frac{5\pi^2\hbar^2}{2ma^2} \end{aligned}$$

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

$\langle x\rangle$ may be time-dependent so we have to average x over the *full* wave function:

$$
\begin{aligned}
\langle x\rangle &= \int \Psi^*(x,t)x\Psi(x,t) \\
&= \int_{-\infty}^{\infty}\left(\tfrac{2}{\sqrt{5}}\psi_2(x)e^{+iE_2t/\hbar} - \tfrac{1}{\sqrt{5}}\psi_3(x)e^{+iE_3t/\hbar}\right)x\left(\tfrac{2}{\sqrt{5}}\psi_2(x)e^{-iE_2t/\hbar} - \tfrac{1}{\sqrt{5}}\psi_3(x)e^{-iE_3t/\hbar}\right)dx \\
&= \tfrac{4}{5}\langle\psi_2|x\psi_2\rangle + \tfrac{1}{5}\langle\psi_3|x\psi_3\rangle - \tfrac{2}{5}\langle\psi_2|x\psi_3\rangle\left(e^{i(E_2-E_3)t/\hbar} + e^{-i(E_2-E_3)t/\hbar}\right) \\
&= \tfrac{4}{5}\langle\psi_2|x\psi_2\rangle + \tfrac{1}{5}\langle\psi_3|x\psi_3\rangle - \tfrac{4}{5}\cos((E_2-E_3)t/\hbar)\langle\psi_2|x\psi_3\rangle
\end{aligned}
$$

Note the possible dependence on time. If we choose to spend the time to evaluate the integrals we get

$$\langle\psi_2|x\psi_2\rangle = \frac{2}{a}\int_0^a x\sin^2(2\pi x/a)\,dx = \frac{a}{2}$$

and

$$\langle\psi_3|x\psi_3\rangle = \frac{2}{a}\int_0^a x\sin^2(3\pi x/a)\,dx = \frac{a}{2}$$

But we also get

$$\langle\psi_2|x\psi_3\rangle = \frac{2}{a}\int_0^a x\sin(2\pi x/a)\sin(3\pi x/a)\,dx = -\frac{48}{25}\frac{a}{\pi^2}$$

When these are put into the last equation we have

$$
\begin{aligned}
\langle x\rangle &= \frac{4}{5}\frac{a}{2} + \frac{1}{5}\frac{a}{2} - \frac{4}{5}\left(\frac{-48a}{25\pi^2}\right)\cos((E_2-E_3)t/\hbar) \\
&= \frac{a}{2} + \frac{192a}{125\pi^2}\cos((E_2-E_3)t/\hbar)
\end{aligned}
$$

6. a) Show how the factor (operator) $\hat{x}^2$ can be expressed in terms of the raising and lowering operators a_+ and a_-.

Using the definition of the $a_\pm$ operators, we find that the sum is

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

Then

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a_+ + a_-)$$

and this gives

$$x^2 = \frac{\hbar}{2m\omega}(a_+^2 + a_+a_- + a_-a_+ + a_-^2)$$

b) Use this expression to find $\langle V \rangle$ for the $n = 3$ state of the HO. (Did you get what you expected, from a HW problem?)

Since $V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2$, the expectation value of V for the $n = 3$ state is

$$\begin{aligned} \langle V \rangle_3 &= \tfrac{1}{2}m\omega^2 \int \psi_3^* x^2 \psi \, dx \\ &= \tfrac{1}{2}m\omega^2 \frac{\hbar}{2m\omega} \int \psi_3^* (a_+^2 + a_+ a_- + a_- a_+ + a_-^2) \psi_3 \, dx \end{aligned}$$

Now the operators a_+^2 or a_-^2 operating on the ψ_3 gives a wave function proportional to ψ_5 or ψ_1 and then orthogonality of the HO wave functions gives zero in the integral. But using the formulae for the action of $a_\pm$ on ψ_n, the middle terms give:

$$a_+ a_- \psi_3 = \sqrt{3 \cdot 3}\psi_3 \qquad \text{and} \qquad a_- a_+ \psi_3 = \sqrt{4 \cdot 4}\psi_3$$

and the using the fact the wave functions are normalized, the previous expression gives

$$\langle V \rangle_3 = \frac{\hbar\omega}{4}(3 + 4) = \tfrac{7}{4}\hbar\omega$$

Now the total energy of the $n = 3$ state is

$$E_3 = \hbar\omega(3 + \tfrac{1}{2}) = \tfrac{7}{2}\hbar\omega$$

so $\langle V \rangle$ is half of this. This is what we got on a HW set.

7. From one of homework problem, if you were to evaluate $\langle T \rangle$ and $\langle V \rangle$ for the $n = 4$ state of the HO, what would you expect to get for each? (There is a theorem which says that the reasonable guess is correct.)

Oops. Some overlap with the previous problem. Anyways, on the homework we found that for a couple particular cases the expectation values of the kinetic and potential energies were each half of the energy value forthe state. Since for the $n = 4$ state the energy is

$$E_4 = \hbar\omega(4 + \tfrac{1}{2}) = \tfrac{9}{2}\hbar\omega$$

we thus expect

$$\langle T \rangle_4 = \tfrac{9}{4}\hbar\omega \qquad \text{and} \qquad \langle V \rangle_4 = \tfrac{9}{4}\hbar\omega$$

8. Analytic solution for the Harmonic Oscillator

a) How did we deduce (from the Schrödinger equations) that we should pull out a common exponential factor $e^{-\xi^2/2}$ in the HO wave functions?

We considered the form of the Schrödinger equation at very large distance, wherein the potential terms overwhelms the energy ($E\psi$) term. The approximate solution for *this* had the form $e^{-\xi/2}$ so it was reasonable to pull off this factor and solve for the remaining part of $\psi(x)$.

b) What was the logical connection between recursion formula for the coefficients of the polynomial $v(\xi)$ and the allowed values of in HO and the allowed values of the energy. (How did one give the other?)

If a term arising from the recursion formula is zero, then the succeeding terms will also be zero; but if this does not occur then the infinite series which results will dominate over the decaying exponential already pulled off and give a wave function which cannot be normalized. The recursion formula $must$ give a zero term and the possibilities for this give the permitted values of the energy.

c) What behavior is shown by the graph of $|\psi_n(x)|^2$ for the HO stationary states when n is large?

9. A free particle is initially described by the the function

$$\Psi(x,0) = \frac{A}{x^2 + a^2}$$

a) Find A or at least show how one would go about finding it.

The wave function must be normalized at $t = 0$, thus

$$1 = \int \Psi^*(x,0)\Psi(x,0)\,dx = |A|^2 \int_{-\infty}^{\infty} \frac{dx}{(x^2+a^2)^2}$$

then do the integral to find A. It's an easy integral for Maple (not really available during exam) but we get:

$$1 = |A|^2 \frac{\pi}{2a^3} \qquad \Longrightarrow \qquad |A|^2 = \frac{2a^3}{\pi} \qquad \Longrightarrow \qquad A = \sqrt{\frac{2a^3}{\pi}}$$

b) Show how one would find the "envelope function" $\phi(k)$.

The envelope function $\phi(k)$ is the Fourier transform of $\Psi(x,0)$, specifically,

$$\begin{aligned}\phi(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx}\,dx \\ &= \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{e^{-ikx}}{(x^2+a^2)^2}\,dx\end{aligned}$$

This integral would be a nice exercise in contour integration but let's just leave it at this.

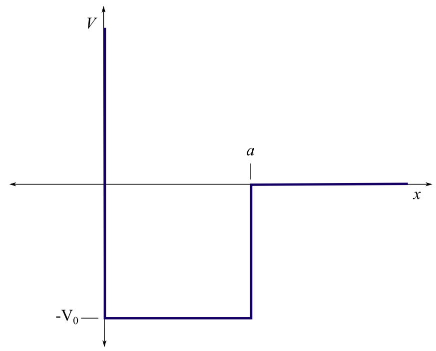
10. For the scattering states of a 1–D potential which is zero at large x, we used the "bad" solutions to get the coefficients T and R. What is the physical content of these quantities?

For a hypothetical one-dimensional scattering experiment, T is the ratio of the number of particle which go forward (to large positive values of x) to the number that came in from $-\infty$. R is the ration of the number that bounce back to the number that came in.

11. Consider the one-dimensional potential

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

a) Make a simple graph (picture) of $V(x)$.



b) Consider a (possible) bound state in this potential. Find the general form of $\psi(x)$ for the regions $0 < x < a$ and $a < x$. Convenient parameters may be our usual

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

For $0 < x < a$, the Schrödinger equation is

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

which can be rewritten as

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

and has general solution

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

but the boundary condition $\psi(0) = 0$ (see part (c)) demands that $B = 0$ so that the general solution now is $\psi = A\sin lx$.

For $a < x$ the Schrödinger equation is

$$-\frac{\hbar^s}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad \Longrightarrow \qquad \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \equiv \kappa^2\psi$$

since E is negative for a bound state. The general solution here must be a decaying exponential so that it is $\psi = Ce^{-\kappa x}$.

c) What are the boundary conditions that $\psi(x)$ must satisfy?

As $x = 0$ is a hard wall, the wave function must equal zero there; as the behavior of the potential is crazy we don't need to have continuity of $d\psi/dx$ here. We have already implemented this in part (b).

At $x = a$ both ψ and $d\psi/dx$ must be continuous.

At $x = \infty$ the wave function ψ must approach zero; we've already implemented this in (b).

The boundary condition at $x = a$ gives

$$A \sin la = Ce^{-\kappa a} \qquad lA \sin la = -\kappa Ce^{-\kappa a}$$

and dividing these gives

$$l \cot la = -\kappa$$

which is a transcendental equation for the E that is hiding inside the κ and l. In fact this is the same equation you got for the $antisymmetric\ states$ of the box potential for a box $-a < x < a$. The solutions for the energy values are the same!

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

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

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

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

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

$$a_+\psi_n = \sqrt{n+1}\,\psi_{n+1} \qquad a_-\psi_n = \sqrt{n}\,\psi_{n-1} \qquad \psi_n = \frac{1}{\sqrt{n!}}(a_+)^n\psi_0$$

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

$$\psi_2(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2}} \left(\frac{2m\omega}{\hbar}x^2 - 1\right) e^{-\frac{m\omega}{2\hbar}x^2}$$

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

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

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