Physics 130– Problem Set # 5

(due Wednesday, Feb. 20)

1. This problem revisits two of the bound state problems that we solved earlier in the course. We now know that the expectation value of the energy for a particle in one dimension in an arbitrary normalized state $|\psi\rangle$ can be written

$$\langle H\rangle = \langle\psi|\, H\,|\psi\rangle = \int dx\psi^*(x)\Big[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\Big]\psi(x)$$

and that the lowest-energy eigenstate minimizes this expression.

(a) Show that the expression for $\langle H\rangle$ can be rewritten as a sum of kinetic and potential energies

$$\langle H\rangle = T + V = \int dx\ \frac{\hbar^2}{2m}\Big|\frac{d\psi}{dx}\Big|^2 + \int dx V(x)|\psi(x)|^2$$

(b) Set $V = \frac{1}{2}m\Omega^2x^2$, appropriate to the harmonic oscillator problem. Let $a = (\hbar/m\Omega)^{\frac{1}{2}}$. Consider states $\psi(x,b)$ of the form

$$\psi(x) = \Big[\frac{b}{\pi a^2}\Big]^{1/4}\exp[-\frac{1}{2}bx^2/a^2]$$

Check that these wavefunctions are normalized.

(c) Evaluate T and V for these wavefunctions. Show that T increases as $b\to\infty$ and that V increases as $b\to 0$.

(d) Find the value of b that minimizes $\langle H\rangle$. Compare the resulting wavefunction to the known exact solution.

(e) Show that, at the minimum, $T = V$.

(f) Generalize the conclusions of part (a) to a potential problem in 3 dimensions.

(g) For the Hydrogen atom problem

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$$

consider states $\psi(x,b)$ of the form

$$\psi(x,b) = \Big[\frac{b^3}{\pi a_0^3}\Big]^{1/2}\exp[-br/a_0]$$

where a_0 is the Bohr radius. Show that these wavefunctions are normalized.

(h) Compute T and V for these wavefunctions. Show that conclusions similar to those of part (c) hold, and that the minimum of $\langle H\rangle$ with respect to b gives the exact solution for the lowest eigenfunction.

(i) Show that $T = -\frac{1}{2}V$ at the minimum.

2. This problem discusses some further features of the operator solution of the harmonic oscillator problem. Use the notation for this problem presented in the lecture notes. (Griffiths' notation is slightly different.) Parts (a) through (e) should be done using the operator algebra, without any explicit use of Schrödinger wavefunctions.

   (a) Assuming that the state $|0\rangle$ is normalized, $\langle 0|0\rangle = 1$, show that

   $$\left\langle 0|aa^\dagger|0\right\rangle = 1$$

   Show that the result implies that

   $$|1\rangle = a^\dagger |0\rangle$$

   is normalized: $\langle 1|1\rangle = 1$. In a similar way, find the normalization constants N_n for the higher states

   $$|n\rangle = N_n (a^\dagger)^n |0\rangle$$

   (b) Write the operators X and P in terms of a and $a^\dagger$. Check that these combinations are Hermitian.

   (c) Consider the matrix elements

   $$\langle m| X |n\rangle \qquad \text{and} \qquad \langle m| P |n\rangle$$

   for all $m, n = 0, 1, \ldots,$. It is not so hard to compute these matrix elements, because they vanish unless $m = n \pm 1$. Show this, and then compute the nonzero cases.

   (d) Evaluate the expectation values of kinetic and potential energy in the ground state $|0\rangle$. Use the resolution of the identity

   $$\mathbf{1} = \sum_n |n\rangle \langle n|$$

   to evaluate the matrix elements of X^2 and P^2. Compare to your result in part (e) of problem 1.

   (e) Compute T, V, and $\langle H\rangle$ in each excited state.

   (f) Using the representation

   $$X\psi(x) = x\psi(x) \qquad P\psi(x) = -i\hbar\frac{d}{dx}\psi(x)$$

write the equation

$$a\,|0\rangle = 0$$

as a differential equation for the wavefunction $\psi_0(x) = \langle x|0\rangle$, and solve this equation. Compare to the exact solution derived earlier.

(g) Compute the wavefunction for the state $|1\rangle$ by computing

$$\langle x|1\rangle = \left\langle x|a^\dagger|0\right\rangle$$

and compare to the known solution.

3. In class, we saw that the momentum space version of a Schrödinger wavefunction is obtained from the position space wavefunction by

$$\widetilde{\psi}(\vec{p}) = \int d^3x e^{-i\vec{p}\cdot\vec{x}/\hbar}\ \psi(\vec{x})$$

(a) Show that, if $\psi(\vec{x})$ is normalized to

$$\int d^3x|\psi(\vec{x})|^2 = 1$$

then $\widetilde{\psi}(\vec{p})$ is normalized to

$$\int \frac{d^3p}{(2\pi\hbar)^3}|\psi(\vec{p})|^2 = 1$$

(b) For a spherically symmetric wavefunction $\psi(r)$, write $\psi(p)$ as a 1-dimensional integral over r.

(c) Perform this integral for the wavefunctions given in problem 1, part (g). Sketch the real-space and momentum-space wavefunctions for different values of b.

(d) Compute the momentum-space wavefunction for the 2P, $m = 0$ wavefunction of the Hydrogen atom. [The angular integral in this case is trickier than that in the spherically symmetric case. Here is a method that is not so difficult: For any set of three axes $\hat{1}$, $\hat{2}$, $\hat{3}$, the following relation holds: If θ_{12} is the angle between $\hat{1}$ and $\hat{2}$, etc., then

$$\cos\theta_{23} = \cos\theta_{12}\cos\theta_{13} + \sin\theta_{12}\sin\theta_{13}\cos(\phi_{12} - \phi_{13})$$

To prove this, take the $\hat{1}$ axis as the $\hat{z}$ axis and consider the computation of $\cos\theta_{23}$ in (x, y, z) coordinates. A very nice way to use this formulae is to take the direction of $\vec{p}$ as $\hat{1}$, the direction of $\vec{x}$ as $\hat{2}$, and the direction of the real $\hat{z}$ axis as $\hat{3}$. And, remember that we are integrating over the orientation of $\vec{x}$ holding the orientation of $\vec{p}$ – and that of the $\hat{z}$ axis – fixed.]

(e) Compute the momentum-space wavefunction of the 2P, $m = 1$ wavefunction of the Hydrogen atom. This should be trivial if you use the result of part (d) appropriately.