PHY521; Quantum Mechanics, Problem Set 3

Due Wednesday 13 Sep 2006 at the beginning of class.

1. Commutators and the uncertainty principle.

In class we noted that the way to determine whether two quantities can be known ("diagonalized") simultaneously in quantum mechanics is to calculate the commutator of the two operators A and B that measure those quantities. Both quantities can be known simultaneously iff the operator commutator $[A, B] \equiv AB - BA$ vanishes identically. Thus for example the fact that $[x, p_x] = +i\hbar \neq 0$ tells you that the coordinate x and its conjugate momentum p_x cannot be known simultaneously. The commutator is easily evaluated by operating on a test function f with x and $p_x = -i\hbar\partial/\partial x$.

Calculate the commutator of the following pairs of operators using this procedure, and thereby determine which pairs can be simultaneously diagonalized. (Assume you are in 3D, so vectors have three orthogonal spatial components.)

a) (*2 pts*) z and p_z

b) (*2 pts*) x_i and p_j (The indices i and j are 1,2,3).

c) (*2 pts*) p_x and $\vec{p}^2$

d) (*2 pts*) $\vec{r}^2$ and $\vec{p}^2$

e) (*2 pts*) p_x and L_z

In part e, L_z is the z-component of the angular momentum operator, $\vec{L} = \vec{r} \times \vec{p}$, so $L_z = xp_y - yp_x = -i\hbar(x\partial/\partial y - y\partial/\partial x)$. Much of the work in parts c-e can be simplified through the use of the identity $[A, BC] = B[A, C] + [A, B]C$, which is true by inspection.

2. 1D Square Well.

The even bound-state wavefunctions of a 1D square well of depth $V_0 < 0$ and width d satisfy the eigenvalue equation

$$\chi \tan(\chi) = \sqrt{\xi^2 - \chi^2}, \tag{1}$$

where $\chi = kd/2$. Here $\xi > 0$ is a dimensionless well depth parameter, defined by $\xi^2 = \frac{1}{2}|V_0|/(\hbar^2/md^2)$.

a) (*5 pts*) Solve this eigenvalue equation numerically, and plot the dimensionless binding energy $e = E/(\hbar^2/md^2) < 0$ (y-axis) of the even bound states versus the dimensionless well depth $v = |V_0|/(\hbar^2/md^2) > 0$ (x-axis) over the range $0 < v < 200$. Be careful to show *all* even bound states.

b) (*5 pts*) The odd bound states satisfy a similar eigenvalue equation,

$$-\chi \cot(\chi) = \sqrt{\xi^2 - \chi^2}. \tag{2}$$

Use a graphical construction to establish the (negative) values of V_0 at which the 1st, 2nd, 3rd, *etc.* odd bound states appear as $|V_0|$ is increased (as the well deepens). Note that new bound states appear in an alternating sequence of even and odd states.

3. Excited 1D SHO.

The general result for the 1D SHO energy eigenstate wavefunction $\psi_n(x)$ is

$$\psi_n(x) = \eta_n H_n(s)\, e^{-s^2/2} \tag{3}$$

where s is the dimensionless length variable

$$s = \frac{(km)^{1/4}}{\hbar^{1/2}}\, x \ , \tag{4}$$

H_n is the n^{th} Hermite polynomial, and η_n is the normalization constant.

a) (*2 pts*) Use the orthonormality relation for Hermite polynomials to show that the normalization is

$$\eta_n = \frac{1}{\pi^{1/4}} \frac{1}{(2^n n!)^{1/2}} \frac{(km)^{1/8}}{\hbar^{1/4}} \ . \tag{5}$$

b) (*3 pts*) Evaluate the matrix elements of x and x^2 in the nth excited state,

$$\langle n|x|n\rangle = \int_{-\infty}^{\infty} \psi_n^*(x) x \psi_n(x)\, dx \tag{6}$$

and

$$\langle n|x^2|n\rangle = \int_{-\infty}^{\infty} \psi_n^*(x) x^2 \psi_n(x)\, dx \ . \tag{7}$$

Use these results to evaluate the variance Δx (the rms distance from the origin at which the particle will be found) in the nth excited state.

c) (*3 pts*) Repeat this exercise in momentum space; evaluate $\langle n|p_x|n\rangle$, $\langle n|p_x^2|n\rangle$ and Δp_x.

d) (*2 pts*) From your results above, show that the classical SHO virial theorem $\langle KE\rangle = \langle PE\rangle$ holds for these quantum mechanical expected values in all energy eigenstates.