Homework 6

Due in class Sept. 30

1. A particle traveling through a double slit apparatus is described by the wave function

$$\psi(x) \propto e^{-(\frac{x}{\Delta})^2}$$

an infinitesimal time before t = 0 (before it hits the slits). You should assume that $\Delta \gg 2l$. The coordinate x is transverse to the

particle's direction of travel through the apparatus, and we will ignore the behavior in the direction of travel (so v_0 doesn't matter, right?). At t = 0 the particle passes through the slits, so you know that the position of the particle is $x = \pm l$ with some uncertainty. In effect, the slits have measured the position of the particle!

- (a) What do you expect to happen as the system evolves in time? For instance, what do you expect $|\psi(x,t)|^2$ to look like as the particle travels past the slits? Sketches would be good.
- (b) Assuming that the uncertainty in the particle's position at each slit can be represented by a Gaussian distribution with standard deviation a, write down the wave function immediately after the particle leaves the slits. You may assume $a \ll l$.
- (c) Find the time-dependent wave function for any positive time t.
- (d) Calculate the probability density $|\psi(x,t)|^2$ and discuss it physically.
- (e) Plot $|\psi(x,t)|^2$ for several times t, from being small compared to $\tau = \frac{ma^2}{\hbar}$, to being comparable to τ , to being large compared to τ . Were your expectations in (a) above correct? Discuss the why's and why not's.

2. Consider a square well of width a and depth $-V_0$ such that there is only a single bound state. Now add a second, identical well at a distance l (center to center) away. Such a potential is qualitatively very much like what an electron might see in a diatomic molecule (like H_2^+). The electron moves much faster than the heavy protons, so they appear essentially fixed in space. The approximation that uses this fact is called the Born-Oppenheimer approximation and is widely used in studies of molecules.

- (a) What symmetries does this system possess?
- (b) Calculate the bound state wave functions and energies as a function of l. Plot the energies as a function of l— these turn out to be effective potential curves for the motion of the protons (once the proton-proton repulsion is added). Explain the behavior of the curves as a function of l, especially the limits $l \to 0$ and $l \to \infty$. You may want to plot the wave function at a couple of representative values.
- (c) Using the eigenstates of a single square well, you can build approximate solutions to the double well problem by superposing them in the appropriate way. Do so, and calculate the energies (as a function of l) of these approximate solutions. Does this approach help you explain the difference in energy between the two bound state solutions?

- (d) Add one more potential well a distance *l* from its neighbor. What symmetries does the system have now? Follow your approach in (c) and construct approximate bound state wave functions using the single well eigenstates. How do the energies of these states behave with *l*?
- (e) By looking at the pattern of bound state energies for one well, two wells, and three wells, can you speculate what the bound state energies of the system will look like for N wells? This progression captures the essential physics of going from the structure of an atom (one well), to the structure of a molecule (two and three wells), to the structure of a solid (N wells).

3. Let us now consider a more realistic model for a molecular potential:

$$V(x) = V_0 \left[\left(\frac{x}{\alpha}\right)^2 - 1 \right]^2$$

where α and V_0 are constants. A potential of this form is a good model for the position x of the nitrogen atom in ammonia, NH₃. The shape of ammonia can be pictured as a pyramid with a triangular base — the H's lie at the corners of the base, and the N at the top. There is no reason, however, for the nitrogen to stay above the H's, and it can tunnel through the base to be on bottom.

- (a) Sketch or plot the potential. What symmetries does it possess? Sketch your guess for the ground and first excited state wave functions.
- (b) For a particle localized on one side of the barrier, the potential appears nearly harmonic near the minimum. Find the effective harmonic potential for such a particle.
- (c) Construct an approximate ground and first excited state wave function as a linear combination of the ground states of the right- and left-side simple harmonic oscillator (SHO) potentials from (b). [Just like you did in 2(c) above for the square wells.] Calculate the energies of your approximate states from the expectation value of the Hamiltonian with the full potential. Use $V_0 = \frac{6\hbar^2}{m\alpha^2}$ and $V_0 = \frac{8\hbar^2}{m\alpha^2}$. Explain the change in energies between these two values of V_0 . The energies of the SHO states were the same — why are the energies of your approximate states different?
- (d) Estimate the time it takes for a particle localized to the left of the barrier to appear on the right side [use the values of V_0 from (c)]. [HINT: Your approximate eigenstates will evolve approximately in time with a phase $e^{-iEt/\hbar}$ where E is the energy you calculated in (c)].
- 4. For the potential

$$V(x) = -V_0 a \left(\delta(x-a) + \delta(x+a)\right)$$

with a and V_0 positive, real constants.

- (a) What do you expect the transmission coefficient to look like? Make a sketch.
- (b) Calculate the reflection and transmission coefficients for scattering from this potential. Plot R and T and discuss them.

