Physical Chemistry 1410
Exam #1
February 7, 2006
You may use your text and notes from class.
Other materials are not allowed, Good Luck!

1. (18 pts) Indicate (by circling the T or F) which of the following statements is true or false

(a) Radioactive decay is the result of tunneling. T F

(b) The problem of a particle in a rectangular 2D box necessarily displays degenerate levels. $E = \frac{h^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2}\right)$ T F

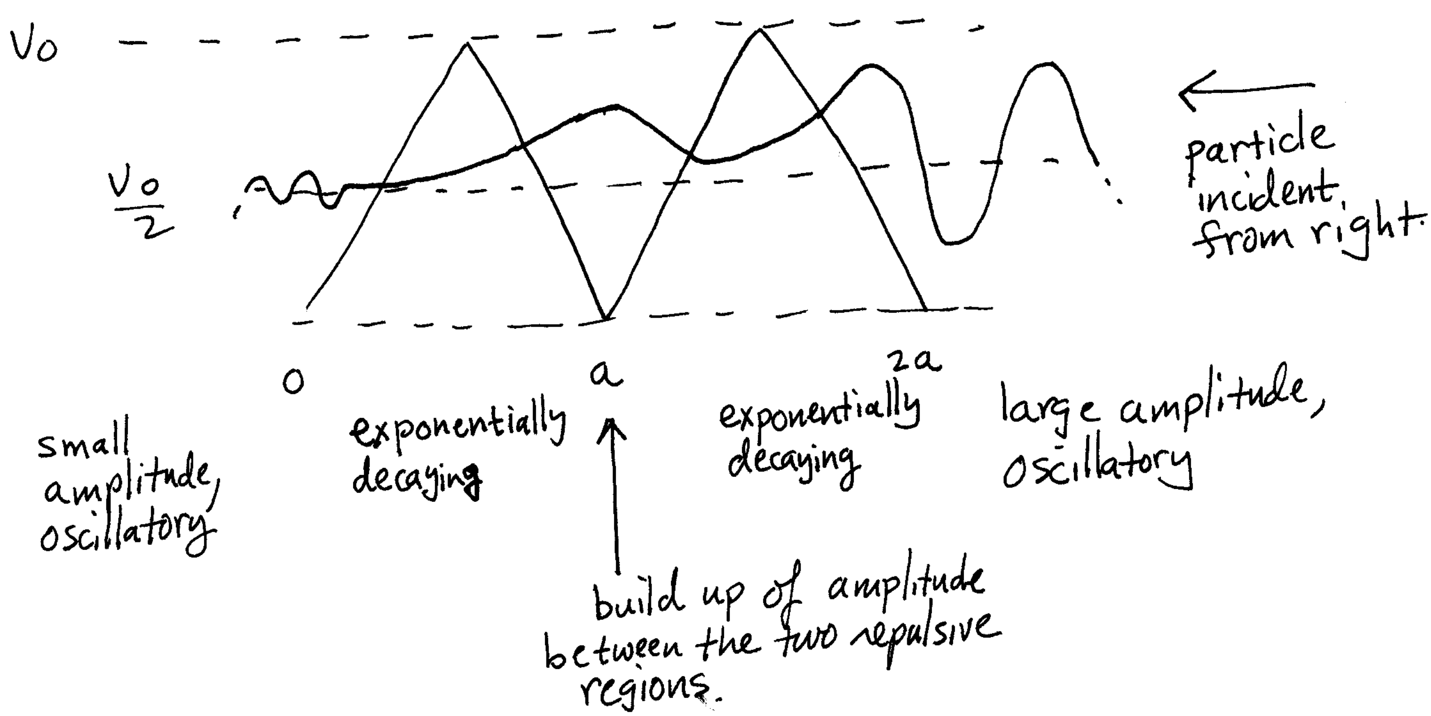
(c) If one measures the momentum of several identical particle-in-the-box systems all in their ground states, one will find only three different values of the momentum. There are only 2 values T F

(d) $x \sin\left(\frac{n\pi x}{a}\right)$ is an acceptable wavefunction for the particle-in-the-box problem. This is an acceptable wavefunction. T F

(e) Tunneling is more important for D (deuterium) than normal hydrogen (H). T F

(f) The average of x^3 for the ground state of the harmonic oscillator problem is zero. Can show using properties of even/odd functions T F

2. (12 pts) Consider the situation of an electron with energy $E = V_o/2$ incident from the right on the potential shown in below. Sketch on the figure a possible wavefunction for the electron. The key here is to correctly depict the qualitative form of the wavefunction.



3. (14 pts) Is $[\cos(bx)]e^{-\alpha x^2}$ an acceptable wavefunction for the ground state of the harmonic oscillator? Why or why not?

It is an acceptable wavefunction for the harmonic oscillator. However, because there could be some confusion due to the reference to "ground state", full credit was also given if you said "No because of the nodes".

Is it an eigenfunction of the Hamiltonian? Why or why not?

It is not an eigenfunction of H (unless $b=0$) since it is a linear combination of eigenfunctions.

4. (14 pts) Consider the problem of a particle in the 2-dimensional harmonic potential $\frac{1}{2}k(x^2+y^2)$. What is the general expression for the energy levels?

$E = h\nu(n_x+n_y+1)$, $n_x, n_y = 0, 1, 2, \ldots$

What is the form of the ground state wavefunction?

$\psi \sim e^{-\frac{\alpha}{2}x^2} e^{-\frac{\alpha}{2}y^2}$

5. (18 pts) Which of the following operators commute? (Circle the letters in the cases the operators commute.)

(a) $(x+\frac{2d}{dx})$ and $(2x-\frac{d}{dx})$

(b) H and x for a free particle

(c) H and p_x^2 for the harmonic oscillator

(d) p_x and p_x^2

(e) H and t, where t is the operator for time

(f) p_x and p_y

In class I stated that H is independent of time. In that case H and t commute. However credit was given for either answer, as some students recalled the uncertainty relation between energy and time.

6. (10 pts) If quantum mechanical observables are real, why is $\frac{h}{i}\frac{d}{dx}$ an acceptable quantum mechanical operator? If ψ is an eigenfunction of $h/i\ d/dx$, then it contains "i" in such a way that the "i's" cancel out when the operator operates on ψ. Otherwise we have to use $\langle\psi|\frac{\hbar}{i}\frac{d}{dx}|\psi\rangle$, which will turn out to be independent of i.

7. (14 pts) What is the average energy associated with the wavefunction

$$\psi = \begin{cases} 0, & x < -\frac{a}{2} \\ (x-\frac{a}{2})(x+\frac{a}{2}), & -\frac{a}{2} \le x \le \frac{a}{2} \\ 0, & x > \frac{a}{2} \end{cases}$$

for the particle in the finite box problem. Where V = V_o for $x < -\frac{a}{2}$ and $x > \frac{a}{2}$ and V = 0 for $-\frac{a}{2} \le x \le \frac{a}{2}$? $\langle E\rangle = \dfrac{\langle\psi|-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}|\psi\rangle}{\langle\psi|\psi\rangle} = \dfrac{-\frac{\hbar^2}{2m}\langle\psi|\frac{d^2}{dx^2}|\psi\rangle}{\langle\psi|\psi\rangle}$

Is this energy above or below that of the ground state of this system? Explain.

$$\langle\psi|\frac{d^2}{dx^2}|\psi\rangle = \int_{-a/2}^{a/2}(x^2-\frac{a^2}{4})\,2\,dx = \left(\frac{2x^3}{3}-\frac{a^2x}{2}\right)\Big|_{-a/2}^{a/2} = -\frac{a^3}{3}$$

$$\langle\psi|\psi\rangle = \int_{-a/2}^{a/2}\left(x^4-\frac{x^2a^2}{2}+\frac{a^4}{16}\right)dx = \left(\frac{x^5}{5}-\frac{a^2x^3}{6}+\frac{a^4x}{16}\right)\Big|_{-a/2}^{a/2} = \frac{a^5}{30}$$

$$\langle E\rangle = \frac{\frac{\hbar^2}{2m}\left(\frac{a^3}{3}\right)}{(a^5/30)} = \frac{10\hbar^2}{2ma^2} = \frac{10h^2}{8\pi^2ma^2}$$

which is only slightly higher than the exact ground state energy of the finite particle-in-the box problem.

The energy for our "guess" function is above the true energy because the guess function is a linear combination of eigenfunctions of the system.