**Chemistry 120A Midterm 1 Solutions, Fall 2014**

1. (a) (6 points) To find the wave vector $k$ we use the equation:

$$p = \hbar k$$

Plugging in for the values given in the problem:

$$k = p/\hbar = m * v/\hbar = \frac{10^{-30}kg * 1.3 * 10^{7}m/s}{6 * 10^{-34}m^2kg/s} \approx 2 * 10^{10}m^{-1}$$

(b) (6 points) The condition for diffraction for a particle on a slit is (i.e. interference occurs when):

$$n\lambda = dsin(\theta)$$

While the maximum value of $sin(\theta)$ is 1, to observe diffraction $d$ must be on the order of $\lambda$. For the particle:

$$\lambda = 2\pi/k \approx \frac{6}{2 * 10^{10}m^{-1}} \approx 3 * 10^{-10}m$$

(c) (8 points) In the Bohr model of the atom, momentum is quantized, which for a particle in a perfectly circular orbits gives the following condition:

$$l = r \times p = rmv = n\hbar$$

$$n = rmv/\hbar = \frac{10^{-10}m * 10^{-30}kg * 1.3 * 10^{7}m/s}{6 * 10^{-34}m^2kg/s} \approx 2$$

2. See picture below. Each item is worth five points each.

3. (a) (7 points) The probability of measuring a certain value of energy is given by $P = |a_n|^2$. We thus have: $P(E_0) = |\sqrt{2/3}|^2 = 2/3$ and $P(E_1) = |-\sqrt{1/3}|^2 = 1/3$ .

(b) (7 points) One can either calculate $\langle\psi|\hat{H}|\psi\rangle$ or recognize that

$$\langle\psi|\hat{H}|\psi\rangle = \langle E\rangle = \sum_n |a_n|^2 E_n = (2/3)\Big(\frac{\hbar\omega}{2}\Big) + (1/3)\Big(\frac{3\hbar\omega}{2}\Big) = \frac{5\hbar\omega}{6}$$

(c) (13 points) Integral runs from $-\infty$ to $\infty$

$$\langle\psi|\hat{x}|\psi\rangle = \int \left(\sqrt{\frac{2}{3}}\phi_0 e^{iE_0 t/\hbar} - \sqrt{\frac{1}{3}}\phi_1 e^{iE_1 t/\hbar}\right) x \left(\sqrt{\frac{2}{3}}\phi_0 e^{-iE_0 t/\hbar} - \sqrt{\frac{1}{3}}\phi_1 e^{-iE_1 t/\hbar}\right)$$

$$= \frac{2}{3}\int \phi_0\ x\ \phi_0 + \frac{1}{3}\int \phi_1\ x\ \phi_1 - \frac{\sqrt{2}}{3}\int \phi_0 x \phi_1 e^{i(E_0-E_1)t/\hbar} - \frac{\sqrt{2}}{3}\int \phi_1 x \phi_0 e^{-i(E_0-E_1)t/\hbar}$$

$$= 0 + 0 - \frac{\sqrt{2}}{3}\int \phi_1 x \phi_0 (2\cos\omega t) \qquad \text{with } (E_1 - E_0)/\hbar = \omega$$

$$= -\frac{2\sqrt{2}}{3}(\cos\omega t)\left(\frac{\alpha}{\pi}\right)^{1/4}\left(\frac{4\alpha^3}{\pi}\right)^{1/4}\int x e^{-\alpha x^2}$$

$$= -\frac{2\sqrt{2}}{3}(\cos\omega t)\left(\frac{\alpha}{\pi}\right)^{1/4}\left(\frac{4\alpha^3}{\pi}\right)^{1/4}\left(\frac{\pi}{4\alpha^3}\right)^{1/2}$$

$$= -\frac{2\sqrt{2}}{3}(\cos\omega t)\left(\frac{1}{4}\right)^{1/4}\left(\frac{\alpha}{\alpha\sqrt{\alpha}}\right)$$

$$= -\frac{2}{3}(\cos\omega t)\left(\frac{1}{\sqrt{\alpha}}\right)$$

(d) (13 points) We use the sudden approximation. $\psi_{new} = \psi_{old} = \phi_0$

i. (short way) for HO we have $\langle T\rangle = \langle V\rangle = \langle E\rangle/2 = \frac{\hbar\omega}{4}$ when we use the HO ground state wavefunction. The only difference between the old potential and the new potential is that $V_{new} = 2V_{old}$. Thus:

$$\langle E\rangle = \langle T\rangle + \langle V_{new}\rangle = \frac{\hbar\omega}{4} + 2\left(\frac{\hbar\omega}{4}\right) = \frac{3\hbar\omega}{4}$$

ii. (longer way)

$$\langle E\rangle = \int \phi_0 \hat{H}\phi_0 = \int \phi_0\left(\hat{T} + \hat{V}_{new}\right)\phi_0$$

$$= \langle T\rangle + \int \phi_0\left(\hat{V}_{new}\right)\phi_0$$

$$= \frac{\hbar\omega}{4} + \left(\frac{\alpha}{\pi}\right)^{1/2}\kappa\int x^2 e^{-\alpha x^2}$$

$$= \frac{\hbar\omega}{4} + \left(\frac{\alpha}{\pi}\right)^{1/2}\kappa\left(\frac{\pi}{4\alpha^3}\right)^{1/2}$$

$$= \frac{\hbar\omega}{4} + \frac{\kappa}{2\alpha}$$

$$= \frac{\hbar\omega}{4} + \frac{\hbar^2\alpha}{2m}$$

$$= \frac{\hbar\omega}{4} + \frac{\hbar\omega}{2}$$

$$= \frac{3\hbar\omega}{4}$$

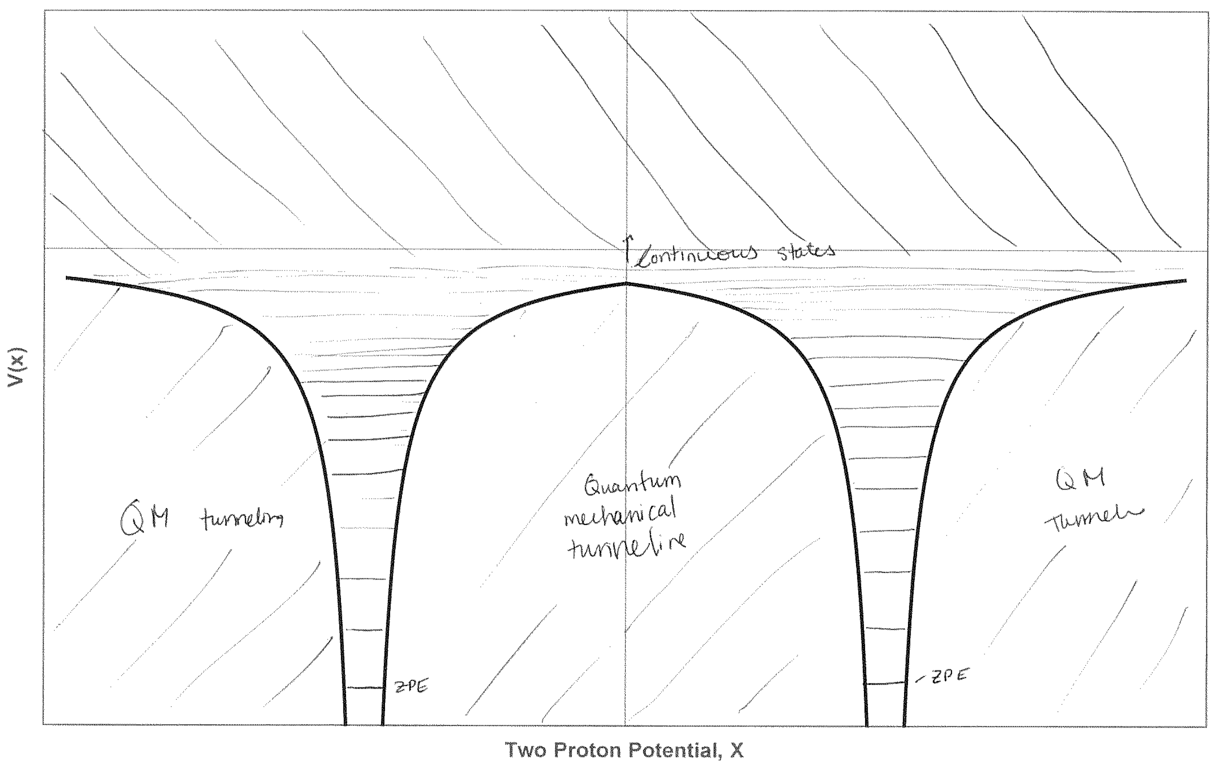


Figure 1: Particle in Coulomb potential of 2 protons for Problem 2