Nov. 12, 2007

Chemistry 1410, Hour Exam 2: Problem 2 (take home **).

<u>Due</u>: Nov. 14, 2007 ,in class.

** N.B.: You may use any written materials you wish, but you may <u>*not*</u> talk to *anybody* about this exam problem until after it has been handed in.

2) [35%] The atoms of diatomic molecule, masses m_1, m_2 [hence with reduced mass $\mu = m_1 m_2 /(m_1 + m_2)$], are bound by the central potential $v(r) = \frac{1}{2}kr^2$. Thus, if the molecule is in angular momentum state l (with possible values $l = 0,1,2,...$), the relative motion of the atoms in the molecule is determined by the effective radial potential:

$$v^{eff}(r) = \frac{1}{2}kr^2 + \frac{\hbar^2 l(l+1)}{2\mu r^2}$$

a) Show that the minimum value of $v^{eff}(r)$ occurs precisely at the radius $r_m = \left[\frac{\hbar^2 l(l+1)}{\mu k}\right]^{1/4}$.

b) For nonzero values of l, compute $d^2 v^{eff}(r)/dr^2$ at the value $r = r_m$. [Hint: the answer turns out to be *in*dependent of the value of *l*.]

c) Using the quadratic approximation to $v^{eff}(r)$ obtained by expanding it in a 2nd order Taylor Series about $r = r_m$, calculate the difference between the lowest two quantum mechanical energy eigenvalues corresponding to a given non-zero value of l. [Hints: i) Think "harmonic oscillator": consult Fig. 1; ii) Again, the answer turns out to be *in*dependent of the value of *l*.]

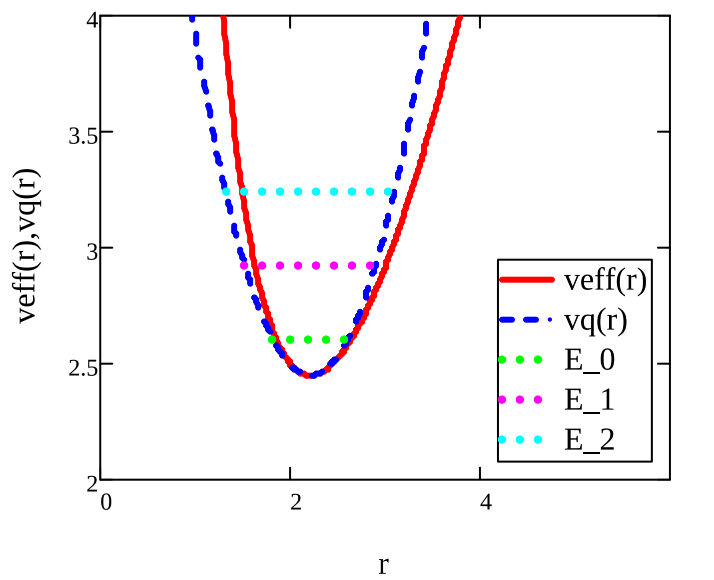

Fig. 1 Sketch of $v^{eff}(r)$ vs. $vq(r) = v^{quad}(r)$ = quadratic expansion of $v^{eff}(r)$ about the minimum of the latter. Also shown are the 3 lowest energy levels of (harmonic oscillator!) $v^{quad}(r)$.