Oct. 31, 2007

Chem. 1410

Practice Problem for Hour Exam 2, solution

1) Starting from

$$v^{eff}(r) = \frac{1}{2}k(r - r_e)^2 + \hbar^2 l(l+1)/2\mu r^2 \quad , \qquad [A1]$$

The minimum occurs at the position r_m such that $dv^{eff}(r_m)/dr = 0$. Thus the equation we need to solve is:

$$0 = k(r_m - r_e) - \frac{\hbar^2 l(l+1)}{\mu r_m^3} \qquad [A2]$$

Making the substitution $r_m = r_e + x$ and using the small x expansion of $1/r_m^4$ provided in the statement of the problem, Eq. A2 becomes:

$$0 = kx - \frac{\hbar^2 l(l+1)}{\mu r_e^3}(1 - \frac{3x}{r_e}) \quad ,$$

which solves to

$$x = \frac{r_e}{\left(3 + \frac{k\mu r_e^4}{\hbar^2 l(l+1)}\right)} \quad , \qquad [A3]$$

QED.

Note: we expect x>0 (i.e., $r_m > r_e$) because of centrifugal distortion (pulling the masses on the spring farther apart as they spin about their common center of mass).

b) For the specified numerical parameters [$\hbar^2 l(l+1) = 9$, $\mu = 5, k = 1, r_e = 2$], we evaluate $x = 0.168$, an thus $x/r_e = 0.084 \ll 1$. Thus, we expect a quadratic expansion of $v^{eff}(r)$ expanded around the (approximate) minimum $r_m = r_e + x$ (with x given by Eq. A3) to represent the full $v^{eff}(r)$ accurately in the region near the potential minimum. This is shown graphically in Fig. A1.

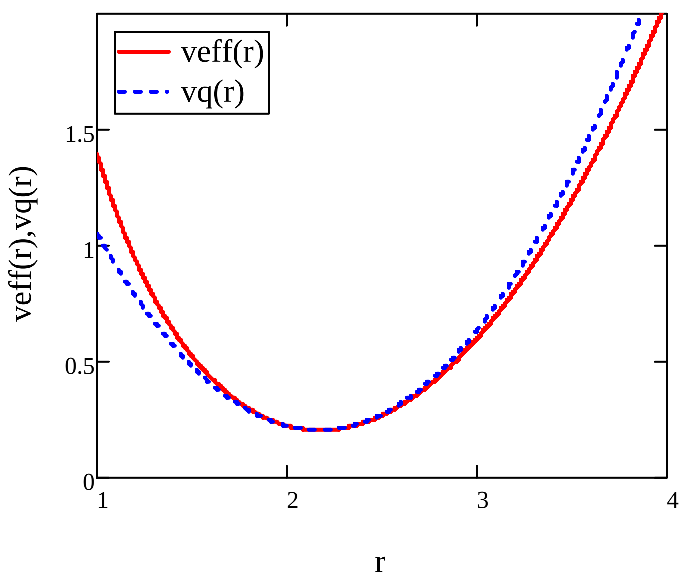

Fig. A1. Comparison of exact (anharmonic) $v^{eff}(r)$ with quadratic expansion $vq(r)$ about the approximate minimum of the potential determined here.

Note: A print-out of the Mathcad module used to generate Fig. A1 is appended, FYI.