

Problem Set 7 (due 02.12.2010)

(7.1) Morse potential

(3 points)

The Morse potential introduced in the lecture reads

$$V_M(R) = D_e \left[e^{-2\alpha(R-R_0)} - 2e^{-\alpha(R-R_0)} \right].$$

- (i) Plot $V_M(R)$ for the H_2 -values $D_e = 4.75 \text{ eV}$, $R_0 = 0.742 \text{ \AA}$, and $\alpha R_0 = 1.44$.
(ii) How is α related to D_e and k_s , where k_s is the force constant which appeared in the Taylor expansion of $E_s(R)$, i.e.,

$$E_s(R) \simeq E_s(R_0) + \frac{1}{2}k_s(R - R_0)^2.$$

(7.2) Centrifugal distortion

(3 points)

In the lecture we decoupled rotational and vibrational motion by substituting R_0 for R in the centrifugal term. Instead, consider

$$\left(-\frac{\hbar^2}{2\mu} \frac{d^2}{dR^2} + V_{\text{eff}}(R) - \bar{E}_{s\nu K} \right) \mathcal{F}_{\nu K}^s(R) = 0$$

where $\bar{E}_{s\nu K} = E_{s\nu K} - E_s(\infty)$ and

$$V_{\text{eff}}(R) = V_M(R) + \frac{\hbar^2}{2\mu} \frac{K(K+1)}{R^2}$$

with $V_M(R)$ as given in problem (7.1). Show that the equilibrium internuclear separation is then stretched approximatively to

$$R_1 \simeq R_0 + \frac{\hbar^2}{2\mu} \frac{K(K+1)}{\alpha^2 R_0^3 D_e}.$$

(7.3) Repetition: Bosonic creation and annihilation operators

(4 points)

Let \hat{b} and \hat{b}^\dagger be Bosonic annihilation and creation operators,

$$[\hat{b}, \hat{b}^\dagger] = \hat{1}$$

and

$$\hat{n} = \hat{b}^\dagger \hat{b}$$

the occupation number operator, $\hat{n}|n\rangle = n|n\rangle$. Show that

- (i) $[\hat{b}^q, \hat{n}] = q\hat{b}^q$ and $[\hat{b}^{\dagger q}, \hat{n}] = -q\hat{b}^{\dagger q}$, with q a positive integer, and
(ii) $\hat{b}|n\rangle = \sqrt{n}|n-1\rangle$ and $\hat{b}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$.