Chemistry 483

Practice Second Examination

11 October 2009

- 1. (40 points) Define and/or characterize
- a) Secular Determinant

b) Trial function

c) Rigid Rotor

d) Hamiltonian for He

e) Morse Potential

f) Radial Distribution Function

g) Force constant

h) Parity

2. (15 points) Show that the most probable value of r in the 1s state of H is a_0

3. (15 points)

If one selects $\psi = e^{-\alpha r^2}$ as the trial function for the H atom and applies the variation method one finds the energy (in atomic units) has the form

$$E(\alpha) = \frac{3\alpha}{2} - Z\sqrt{\frac{8\alpha}{\pi}}$$

Determine the optimal value of α and the associated energy. Compare with the exact energy.

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4. (15 points) Use perturbation theory and calculate the first order correction to the energy of the ground state of a harmonic oscillator when it is subjected to the perturbation

$$V_{pert} = \frac{\gamma}{6} x^3$$

Recall that

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2}$$

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5. (15 points) The force constant of ${}^{79}Br{}^{79}Br$ is 240 Nm⁻¹. Calculate the fundamental vibrational frequency and the zero-point energy of ${}^{79}Br{}^{79}Br$.