

Problem Set 6 (due 25.11.2010)

(6.1) Rotator

(3 points)

Consider a point particle of mass m whose motion is constraint to a fixed distance r_0 from the origin. Write down the Hamiltonian \hat{H} and solve the Schrödinger equation $\hat{H}\Psi(\theta, \phi) = E\Psi(\theta, \phi)$, i.e., determine eigenenergies and eigenstates.

(6.2) Rotational energy

(2 points)

Use simple arguments based on the results of (6.1) in order to estimate the ratio of electronic to rotational energy in a homonuclear diatomic molecule,

$$\frac{E_e}{E_r} = \frac{M}{m}.$$

(6.3) Overlap integral

(5 points)

Calculate the integrals

$$I(R) = \int \psi_{1s}(r_A)\psi_{1s}(r_B) d^3r,$$
$$H_{AA}(R) = \int \psi_{1s}(r_A)\hat{H}_e\psi_{1s}(r_A) d^3r,$$

which occurred during the lecture in the treatment of H_2^+ .

$$\psi_{1s}(r) = \pi^{-1/2} e^{-r}$$

is the hydrogenic ground state wave function in atomic units, and $r_{A,B}$ are the distances to the locations of the nuclei A, B , respectively. The electronic Hamiltonian in atomic units is given by

$$\hat{H}_e = -\frac{1}{2}\nabla_{\mathbf{r}}^2 - \frac{1}{r_A} - \frac{1}{r_B} + \frac{1}{R}.$$

Hint: Use the confocal elliptic coordinates introduced in the lecture.