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- 1. For the configuration of a diatomic molecule, in the rest frame of the two nuclei, write down the full system Hamiltonian. Make the Born-Oppenheimer approximation of the electrons moving much faster than the two nuclei and obtain the separation of nuclear and electronic wavefunctions. Write down the separate Schrodinger equations for the nuclear and the electronic part.
- 2. The Schroedinger equation for one electron in an attractive 1D deltafunction potential  $V(x) = -e^2\delta(x)$  is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} - e^2\delta(x)\psi(x) = E\psi(x)$$

In atomic units ( $\hbar = m = e^2 = 1$ ), the normalized ground state wave function is  $\psi_1(x) = e^{-|x|}$  and the corresponding energy is  $E_1 = -1/2$ . Consider a 1D  $H_2$  molecule with a  $\delta$ -like both ion-electron attraction and electron-electron repulsion. Ions are fixed a distance R apart and ignore ion-ion repulsion. Write down the Schroedinger equation for this 1D  $H_2$  molecule. Construct a gerade molecular orbital for this molecule with the proper normalization. Calculate the ground state energy for the molecule using this molecular orbital.

- 3. Given that the equivalent force constant C of a vibrating HCl molecule is about 470 nt/m, estimate the energy difference (in eV) between the lowest and the first vibrational state of HCl. Given that the rotational inertia of HCl has the value  $I = 2.66 \times 10^{-47}$  kg-m<sup>2</sup>, estimate the energy difference between the lowest and first excited rotational state of HCl.
- 4. Consider a harmonic oscillator with a slightly increased spring constant  $k' = (1 + \epsilon)k$ . Calculate the first order perturbation in the energy.