Exercise 09

1 Hydrogen atom in a magnetic field

Show that the Hamiltonian operator for a hydrogen atom in an external field, where the field is in the z direction is given by

$$\hat{H} = \hat{H}_0 + \frac{\mu_B B_z}{\hbar}\hat{L}_z$$

where $\hat{H}_0$ is the Hamiltonian operator of a hydrogen atom in the absence of the magnetic field and μ_B is the Bohr magneton $\frac{\hbar e}{2m_e}$.

Show that the wave functions of the Schrödinger equation for a hydrogen atom in a magnetic field are the same as those for the hydrogen atom in the absence of the field.

Finally, show that the energy associated with the wave function ψ_{nlm} is

$$E = E_n^{(0)} + \mu_B B_z m$$

where $E_n^{(0)}$ is the energy in the absence of the magnetic field and m is the magnetic quantum number.

2 Perturbation theory

We introduce the Morse potential

$$V(x) = D\left(1 - e^{-\beta x}\right)^2$$

as a description of the intramolecular potential energy of a diatomic molecule. The constants D and β are different for each molecule (for H_2: $D = 7.61 \times 10^{-19}$ J and $\beta = 0.0193$ pm$^-1$).

First expand the Morse potential in a power series about x (hint: Use the expansion $e^x = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + ...$).

What is the Hamiltonian operator for the Morse potential? Show that the Hamiltonian operator can be written in the form

$$\hat{H} = -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + ax^2 + bx^3 + cx^4 + ...$$

How are the constants a, b, c, related to the constants D and β? What part of the Hamiltonian operator would you associate with $\hat{H}^{(0)}$, and what are the functions $\psi_n^{(0)}$ and energies $E_n^{(0)}$?

Use the perturbation theory to evaluate the first-order corrections to the energy of the first three states that arise from the cubic and quartic terms. Using these results, how different are the first two energy levels of H_2 if its intramolecular potential is described by a harmonic oscillator potential or the quartic expansion of the Morse potential?

Solve with pen and paper and report all important intermediate steps of your calculations. Hand in the report at the office 35.17 before next Wednesday at noon.