Hydrogen Molecule

In this problem, we will solve a toy model for the quantum mechanics of the hydrogen molecule, H_2.

To begin, let us first think of a toy model for a covalent bond. To this end, let us consider an electron of mass m placed in the following double-well potential:

$$V(x) = -\alpha \left[\delta\left(x + \frac{L}{2}\right) + \delta\left(x - \frac{L}{2}\right)\right].$$

The kinetic part of the Hamiltonian is simply a 1D kinetic term. Our first goal will be to model the energy of the covalent bond, E_{cov}, to be twice the energy of the lowest energy bound state of a single electron placed in the above potential.

(a) Verify that the Hamiltonian commutes with the parity operator, which sends $x \to -x$.

(b) Using the previous part to simplify your calculation, explain why there are exactly two bound states in this model, with energy given by

$$E = -\frac{\hbar^2\lambda^2}{2m}$$

with λ one of the two solutions to the equation

$$1 \pm \mathrm{e}^{-\lambda L} = \frac{\hbar^2\lambda}{m\alpha}.$$

(c) Discuss what happens to the bound state energies in the limit $L \to 0$.

(d) Discuss what happens to the bound state energies in the limit $L \to \infty$, and give a physical interpretation for what happens.

(e) Next, find the leading correction to to the energies at large, but finite L. What is the length scale over which the covalent bond becomes relevant?

(f) Using that the typical distance of the electron from the hydrogen atom is about 10^{-10} m, and the energy of the electron in its ground state is about -2×10^{-18} J, what is a reasonable value for α?

Now, what repels the atoms apart is the electrostatic repulsion between the two protons, which have charge $e = 1.6 \times 10^{-19}$ C. We can define the total energy of this system as

$$E(L) = E_{\text{cov}}(L) + \frac{e^2}{4\pi\epsilon_0 L}.$$

(g) Plot this function numerically for various values of α, relative to $e^2/4\pi\epsilon_0$. Comment on what you see.

(h) Now, use the value of α you estimated in part (f). Does this value predict that the hydrogen molecule is stable? If so, estimate the bond length of this molecule.