Ex6551: Two charged particles in a 3D harmonic well with Coulomb interaction

Submitted by: Rotem Serphos and Uri Zamir

The problem:

Two particles with charge e are placed in a 3D harmonic well $V(r) = \frac{1}{2}m\omega^2 r^2$ the Coulomb interaction is $U(r_1, r_2) = \frac{e^2}{|r_1 - r_2|}$. Assume that they both occupy the same Gaussian orbitals e^{-r^2/a^2}.

Note: You can assume that the two particles are identical but distinguishable, or that they are bosons, or that they are electrons in a singlet state. The calculation is the same in all 3 cases.

(1) Determine the exact a for non-interacting particles in the ground state. Calculate the correction to the energy using 1st order perturbation theory. Specify what is the small dimensionless parameter.

(2) Determine the optimal values of a using the variational scheme. Compare the result that is obtained for the ground state energy using this scheme, with the result of the previous item. Are they consistent?

The solution:

(1) Finding a when there is no interaction between the particles:
While the two particles are not interacting, we can break the Hamiltonian into two, $\mathcal{H}_1 + \mathcal{H}_2$, each can be described as an independent isotropic 3D harmonic oscillator.

$$\psi_i(x, y, z) = C H_{n_x} H_{n_y} H_{n_z} e^{-\frac{m\omega}{2}(x^2+y^2+z^2)}$$

Where C is a constant, and H_{n_i} are Hermite polynomials.
It is given that the particles occupy the Gaussian orbitals, so the Hermite polynomials must be constant (H_0). This leaves us with Gaussian function of the form $Ce^{-\frac{r^2}{a^2}}$ for each particle, where $r^2 = x^2 + y^2 + z^2$ and $a^{-2} = \frac{m\omega}{2}$. so we can conclude that the parameter a must be:

$$a = \sqrt{\frac{2}{m\omega}}$$

for both of the particles.

The wavefunction of identical particles must have the following symmetry:

$$|\psi\rangle = C|\psi_1\rangle|\psi_2\rangle$$

Where $C^2 = \frac{8}{\pi^3 a^6}$ is the normalization constant.
The natural coordinates for the problem:

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$$

$$\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$$

The first order perturbation calculation yields:

$$E^{[1]} = \langle\psi|V|\psi\rangle = C^2 \int \frac{e^2}{r} e^{-2(\frac{\frac{1}{2}r^2+2R^2}{a^2})} r^2 R^2 dr dR (d\Omega)^2 = \frac{2\pi^{3/2}e^2}{a}$$

Using dimensional analysis we can find λ:

$$\lambda = \frac{e^2}{a\omega}$$

(2) Using the information from the previous item, we can obtain variation with Gaussian wave function:

$$< \mathcal{H} >= \frac{4}{ma^2} + m\omega^2 a^2 + \frac{2\pi^{3/2}e^4}{a^2\omega}$$

And it's easy to check that the Hamiltonian agrees with the non interacting Hamiltonian for $\lambda = 0$. After minimization of the Hamiltonian with respect to a, one gets:

$$a^4 = \frac{4}{m^2\omega^2} + \frac{\pi^{3/2}e^4}{2m\omega^3} = a_0^4 + \frac{\pi^{3/2}e^4}{2m\omega^3}$$

Where $a_0 = \sqrt{\frac{2}{m\omega}}$. We can see that for $\frac{e^2}{\omega a_0} << 1$ the value of a is consistent with the one calculated in last section. The results therefor are consistent. In the first section, the result was taken from the quantum harmonic oscillator, completely neglecting the interaction between the particles. On the other hand, the last was derivated including the interaction.