Project 2

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Introduction

Theory

Electrons in a confined, two dimensional harmonic oscillator potnetial with the given (idealized) Hamiltionian below is in quantum mechanics called quantum dots.

$$\hat{H} = \sum_{i=1}^{N}\left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2\right) + \sum_{i<j}\frac{1}{r_{ij}}$$

,

where $r_{ij} = |r_1 - r_2|$, the distance between the electrons. Natural units ($\hbar = c = e = m_e = 1$) are used and energies are in atomic units (a.u). The first term/sum of the hamiltonian is the harmonic oscillator part, well known from quantum mechanic. It is whats called the unpertubated part. Because electrons repels each other, a repulsion term(the second sum) is added. This term is whats called the pertubation of the system. The modulus of the positions of the electrons (for a given electron i) as

$$r_i = \sqrt{r_{i_x}^2 + r_{i_y}^2}$$

.

The system will be utilized for closed shells, ie. N = 2, 6, 12 and 20 electrons.

Wavefunction

The wavefunction for a two dimentional system with the Harmonic Osccilator potential is given by

$$\Phi_{n_x,n_y}(x,y) = AH_{n_x}(\sqrt{\omega}x)H_{n_y}(\sqrt{\omega}y \exp\left[-\frac{\omega}{2}(x^2+y^2)\right]$$

where H_{n_x} are Hermite polynomials, and A is the normaliation constant. For the lowest lying state $n_x = n_y = 0$ and hence the energy is $\epsilon_{n_x,n_y} = \omega(n_x+n_y+1 = \omega$.

The energy of the ground state for two electrons without interaction, is simply the sum of the energies: $\epsilon_{n_x,n_y} = 2 \times (0+0+1) = 2\omega$.

The wavefunction for the unpartubated stystem is given by

$$\Phi(\mathbf{r_1}, \mathbf{r_2}) = C \exp\left[-\frac{\omega}{2}(\mathbf{r_1}^2 + \mathbf{r_2}^2)\right]$$

where $\mathbf{r_i} = \sqrt{ri_x{}^2 + r_{i_y}^2}$. The total spin in the ground state is simply zero as the two electrons living in the state is pared with opposite spins (eg. $\pm 1/2$).

The ground state energy is given by the unpartubated system. Adding a pertubation/interaction will rise the energy. For the simplest system with two electrons, this pertubation can be found through partubation theory, whilst for a higher number of particles, other measurments/actions must be taken to find the energy(??)

Method

Results

Discussion

Conclusion

Appendix