

FYS4150: Project 5

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1 Physical background

1.1 Quantum dots

Consider a system of electrons confined in a pure three-dimensional isotropic harmonic oscillator potential, with an idealized Hamiltonian given by

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

where we have used natural units $\hbar = c = e = m_e = 1$, and all energies are in atomic units a.u. Our system consists of $N = 2$ particles, and the hamiltonian describes a harmonic oscillator and the repulsive interaction between two electrons

$$\hat{H}_1 = \sum_{i<j} \frac{1}{r_{ij}}, \quad (2)$$

where the distance between electrons is given by $r_{ij} = \sqrt{\mathbf{r}_1 - \mathbf{r}_2}$. The modulus for the position of a single electron is given as $r_i = \sqrt{x_i^2 + y_i^2 + z_i^2}$.

1.2 The non-interacting case

For the unperturbed system the Hamiltonian is

$$\hat{H}_0 = \sum_{i=1}^N \left(-\frac{1}{2} \nabla_i^2 + \frac{1}{2} \omega^2 r_i^2 \right). \quad (3)$$

If we set $\hbar\omega = 1$ the exact energy for 2 electrons is 3 a.u. The *wavefunction* for an electron in an oscillator potential in 3D is

$$\phi_{n_x, n_y, n_z}(x, y, z) = A H_{n_x}(\sqrt{\omega}x) H_{n_y}(\sqrt{\omega}y) H_{n_z}(\sqrt{\omega}z) \exp(-\omega(x^2 + y^2 + z^2)/2), \quad (4)$$

where the functions $H_{n_x}(\sqrt{\omega}x)$ are the hermite polynomials, and A is a normalization constant. For the ground state $n_i = 0$ and the energy of a single electron is $\epsilon_{n_x, n_y, n_z} = \omega(n_x + n_y + n_z + 3/2) = 3/2\omega$. In this case the electrons don't interact, so the total energy is just the sum of energies

$$E_0 = \frac{3\omega}{2} + \frac{3\omega}{2} = 3\omega$$

The total spin should be 0. Electrons are fermions, so they must have antisymmetric wavefunctions. If their quantum numbers are all the same $n_i = 0$, they must have different spin, so $S_{total} = \frac{1}{2} - \frac{1}{2} = 0$.

1.3 Trial wave functions

The trial wavefunctions we want to use are

$$\Psi_{T1}(\mathbf{r}_1, \mathbf{r}_2) = C \exp(-\alpha\omega(r_1^2 + r_2^2)/2), \quad (5)$$

$$\Psi_{T2}(\mathbf{r}_1, \mathbf{r}_2) = C \exp(-\alpha\omega(r_1^2 + r_2^2)/2) \exp\left(\frac{r_{12}}{2(1 + \beta r_{12})}\right), \quad (6)$$

where α, β are variational parameters. To find the energy of the first trial state, we use the hamiltonian operator on the state

$$\begin{aligned} \hat{H}_0 \Psi_{T1} &= \frac{1}{2} \left(-(\nabla_1^2 + \nabla_2^2) + \omega^2 r_1^2 + \omega^2 r_2^2 \right) C \exp(-\alpha\omega(r_1^2 + r_2^2)/2) \\ &= \frac{1}{2} (\alpha\omega(\nabla_1 + \nabla_2)(x_1 + y_1 + z_1 + x_2 + y_2 + z_2) + \omega^2(r_1^2 + r_2^2)) C \exp(-\alpha\omega(r_1^2 + r_2^2)/2) \\ &= \frac{1}{2} (6\alpha\omega - \alpha^2\omega^2(r_1^2 + r_2^2)) + \omega^2(r_1^2 + r_2^2) C \exp(-\alpha\omega(r_1^2 + r_2^2)/2) \\ &= 3\alpha\omega - \frac{\omega^2}{2} (1 - \alpha^2) C \exp(-\alpha\omega(r_1^2 + r_2^2)/2) \\ &= E_{T1} \Psi_{T1} \end{aligned}$$

where we have used that $\nabla x_1 e^{-\alpha\omega(r_1^2 + r_2^2)/2} = (1 - \alpha\omega x_1^2) e^{-\alpha\omega(r_1^2 + r_2^2)/2}$. So the energy of the first test function is

$$E_{T1} = 3\alpha\omega + \frac{\omega^2}{2} (1 - \alpha^2) (r_1^2 + r_2^2) + 3\alpha\omega. \quad (7)$$

1.4 Hydrogen atom

We can view the hydrogen atom as a harmonic oscillator.

2 Implementation

2.1 Variational Monte Carlo

energy_alpha_T1.pdf