

Homework4

1. The exchange energy of a uniform electron gas

Consider a uniform gas of electrons of density ρ neutralized by a uniform background of opposite charge. Hence the system is neutral. Suppose it is a closed shell system, so the number of spin up electrons is equal to that of spin down. Using the Hartree-Fock approximation, derive an expression of the exchange energy, which should be negative, as a function of the gas density. Explain your derivation step by step.

Hint: $\rho = \sum_i^N |\phi_i(\vec{r})|^2$, where $\phi_i(\vec{r})$ is a single particle wavefunction entering the Slater determinant that defines the Hartree-Fock many body wavefunction. Try plane waves as possible eigenfunctions of the Hartree-Fock equation.

Include all your references. Write your own words. If there are five consecutive words the same as other writings, it may be word-for-word plagiarism, which is the so called “five (consecutive) words” rule.

2. Correlated quantum chemistry methods

Choose a paper in the literature describing calculations of the properties of a given molecule, carried out utilizing *correlated* quantum chemistry methods (not DFT ones). Describe in detail how the calculations of that paper are performed, including level of theory, level of numerical accuracy, verification and validation of the results, which experiments were chosen to compare with. Justify why you were interested in choosing that specific paper.

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