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Problem Set 6 (due 22.11.2011)

Questions

(Q1) What is meant by *mean field*-method? What is the simplification as compared to the many-body Schrödinger equation?

(Q2) What is the difference between Hartree theory and Hartree-Fock theory?

(Q3) Assume you wrote a code that is able to find the ground state of atomic hydrogen within one second total CPU time. Estimate an optimistic, lower limit for the CPU time a corresponding code would consume to determine the ground state of copper by (i) solving the Schrödinger equation, (ii) solving the Hartree-Fock equation.

(Q4) Which atom is bigger, hydrogen or uranium?

(6.1) Two-particle interaction *(6 points)*

As in the lecture, let $|\Psi\rangle$ be a Slater determinant constructed from single-particle states $|\psi_i\rangle$, $|\Psi_{ph}\rangle$ a particle-hole excitation, $|\Psi_{p_1p_2h_1h_2}\rangle$ a two-particle-two-hole excitation, and $\hat{W}$ a two-body operator. Show that

$$\langle\Psi|\sum_{i<j}\hat{W}(i,j)|\Psi\rangle = \frac{1}{2}\sum_{i,j}\Big(\langle\psi_i\psi_j|\hat{W}|\psi_i\psi_j\rangle - \langle\psi_i\psi_j|\hat{W}|\psi_j\psi_i\rangle\Big), \tag{1}$$

$$\langle\Psi_{ph}|\sum_{i<j}W(i,j)|\Psi\rangle = \sum_{i}\Big(\langle\psi_i\psi_p|\hat{W}|\psi_i\psi_h\rangle - \langle\psi_i\psi_p|\hat{W}|\psi_h\psi_i\rangle\Big), \tag{2}$$

and

$$\langle\Psi_{p_1p_2h_1h_2}|\sum_{i<j}\hat{W}(i,j)|\Psi\rangle = \langle\psi_{p_1}\psi_{p_2}|\hat{W}|\psi_{h_1}\psi_{h_2}\rangle - \langle\psi_{p_1}\psi_{p_2}|\hat{W}|\psi_{h_2}\psi_{h_1}\rangle. \tag{3}$$

(6.2) Single-particle density *(2 points)*

Show that the Hartree-Fock single-particle density

$$\rho(\boldsymbol{r}) = \sum_{i=1}^{N}\sum_{m_s}|\psi_i(\boldsymbol{r},m_s)|^2 \tag{4}$$

can be written as

$$\rho(\boldsymbol{r}) = \langle\Psi|\sum_{i=1}^{N}\delta(\boldsymbol{r}\hat{1}-\hat{\boldsymbol{r}}_i)|\Psi\rangle. \tag{5}$$

(6.3) Hartree-Fock for He *(2 points)*

Write down the Hartree-Fock equation for the spatial ground state orbital $\psi_{1s}(r)$ of helium. Does it differ from the corresponding Hartree equation?