Advanced Quantum Theory
WS 15/16

Prof. Dr. Dieter Bauer
Dr. Yaroslav Lutsyshyn
M.Sc. Julius Rapp

Problem Set 5 (due Monday, 16.11.2015 in the lecture)

Questions

(Q1) What is the difference between a Hartree treatment of a many-electron system and a Hartree-Fock treatment?

(Q2) Two smart and sober theoretical physicists both claim that they did Hartree-Fock theory for some atomic system but come up with different ground state energies. What could be the reason?

(Q3) What is the essential assumption on which Thomas-Fermi theory is based?

(5.1) Slater determinants and two-particle interaction *(2 points)*

In the lecture, we calculated expectation values and matrix elements of sums $\sum_i \hat{V}(i)$ (where $\hat{V}$ is a one-body operator) with respect to Slater determinants.

Now, let $\hat{W}(i,j)$ be a two-body operator. As in the lecture, let $|\Psi\rangle$ be a Slater determinant constructed from single-particle states $|\psi_i\rangle$ and $|\Psi_{ph}\rangle$ a one-particle-one-hole excitation.

Show that

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

and

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

(5.2) Hartree-Fock for helium *(3 points)*

For He in spin-singlet configuration the two relevant single-particle states are $|1s+\rangle$ and $|1s-\rangle$. Proceeding strictly formally like for the Be example in the lecture notes, derive the Hartree-Fock equation governing the spatial ground state orbital $\psi_{1s}(r)$.

*Does the Hartree-Fock equation differ from the corresponding Hartree equation in this case?

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(5.3) KOOPMANS THEOREM *(2 points)*

Use the expression for the total Hartree-Fock energy E (see lecture notes, section 3.3.3) to prove Koopmans' theorem

$$E_N - E^*_{N-1} = \varepsilon_{\text{valence orbital}} = -I_{\text{p}}.$$

Give a physical explanation what that means.

(5.4) THOMAS-FERMI *(3 points)*

(a) Starting from $\int \mathrm{d}^3 r\, \rho(\boldsymbol{r}) = N$, show that

$$Z \int_0^{x_0} [\chi(x)]^{3/2} \sqrt{x}\, \mathrm{d}x = N,$$

where $\chi(x)$ is the Thomas-Fermi function introduced in the lecture, Z is the nuclear charge number, N is the number of electrons, and x_0 is the zero of $\chi(x)$.

(b) Show that for $x \to \infty$ the Thomas-Fermi function becomes $\chi(x) = 144/x^3$. Use this result to prove that the asymptotic behavior of the Thomas-Fermi density $\rho(r)$ is $\sim r^{-6}$.

*How should the correct asymptotic behavior be instead?