Prof. Dr. Dieter Bauer
Dr. Yaroslav Lutsyshyn
Dipl.-Phys. Volker Mosert

Advanced Quantum Theory
WS 12/13

Problem Set 5 (due Monday, 19.11.2012 in the lecture)

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 a Hartree treatment of a many-electron system and a Hartree-Fock treatment?

(Q3) What is *correlation*?

(5.1) Antisymmetrization operator *(4 points)*

(i) Let the operator

$$\hat{A}^- = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \hat{P}$$

(notation explained in the lecture) be applied to an arbitrary N-particle state $|\phi\rangle$, i.e.,

$$|\Psi\rangle = \hat{A}^-|\phi\rangle.$$

Subsequently, an arbitrary permutation operator $\hat{Q}$ is applied to $|\Psi\rangle$. Show

$$\hat{Q}|\Psi\rangle = (-1)^Q|\Psi\rangle,$$

which means that $\hat{A}^-$ is indeed the antisymmetrization operator.

(ii) Show that

$$\hat{A}^-\hat{A}^- = \sqrt{N!}\,\hat{A}^-.$$

Hint: Use the fact that permutations form a group.

(iii) Consider the product of three single-particle states

$$|\phi\rangle = |1s+\rangle|1s-\rangle|2s+\rangle$$

(where $+, -$ indicate $m_s = \pm 1/2$). Write down explicitly $|\Psi\rangle = \hat{A}^-|\phi\rangle$.

cont'd overleaf

(5.2) The "exponential wall" *(2 points)*

Assume you wrote a code that is able to find the ground state of atomic hydrogen within one second total CPU time. The wavefunction in your code is represented on a cleverly chosen, discrete grid of only $N_{\mathrm{H}} = 10$ grid points. The run time of your code scales linearly with N_{H}, that is, on a doubled grid it takes two seconds to find the (perhaps more accurate) ground state.

Estimate lower limits for the CPU times and the required storage capacities an extended code based on the same numerical algorithm would consume to determine the ground state of copper by

(i) solving the full many-electron Schrödinger equation,

(ii) solving the corresponding Hartree-Fock equation.

(5.3) Two-particle interaction *(4 points)*

In the lecture we calculated Slater-determinant matrix elements of a one-body operator $\hat{V}(i)$. 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 particle-hole excitation.

Show that

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

and

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