UNIVERSITY OF OSLO

FACULTY OF MATHEMATICS AND NATURAL SCIENCES

Exam in FYS-KJM4480, Quantum mechanics for Many-particle Systems, Fall 2011
Day of exam: Friday December 9, 2.30pm
Exam hours: four (4) hours
This examination paper consists of 3 pages.

Allowed material: Rottmann: Matematische Formelsamlung (In Norwegian, English or German)
Two A4 sheets with own notes (totaling 4 pages).
Approved numerical calculator.

Make sure that your copy of this examination paper is complete before answering, check the number of pages. You can answer in English, German or Norwegian. The final written exam counts 70% of the final mark. The remaining 30% is accounted for by the midterm assignment.

Exam problems a)-i) (Make sure all problems are included in your set)

Let $\hat{H} = \hat{H}_0 + \hat{H}_I$ and $|\Phi_n\rangle$ be the eigenstates of $\hat{H}_0$ and that $|\Psi_n\rangle$ are the corresponding ones for $\hat{H}$. Assume that the ground states $|\Phi_0\rangle$ and $|\Psi_0\rangle$ are not degenerate. We can then write the energy of the ground state as

$$E_0 - \varepsilon_0 = \frac{\langle\Phi_0|\hat{H}_I|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle},$$

with $\hat{H}|\Psi_0\rangle = E_0|\Psi_0\rangle$ and $H_0|\Phi_0\rangle = \varepsilon_0|\Phi_0\rangle$. We define also the projection operators $\hat{P} = |\Phi_0\rangle\langle\Phi_0|$ and $\hat{Q} = 1 - \hat{P}$. These operators satisfy $\hat{P}^2 = \hat{P}$, $\hat{Q}^2 = \hat{Q}$ and $\hat{P}\hat{Q} = 0$.

a) Show that for any ω we have can write the ground state energy as

$$E_0 = \varepsilon_0 + \sum_{n=0}^{\infty} \langle\Phi_0|\hat{H}_I\left(\frac{\hat{Q}}{\omega - \hat{H}_0}(\omega - E_0 + \hat{H}_I)\right)^n|\Phi_0\rangle.$$

b) Discuss these results for $\omega = E_0$ (Brillouin-Wigner perturbation theory) and $\omega = \varepsilon_0$ (Rayleigh-Schrödinger perturbation theory). Compare the first few terms in these expansions and discuss the differences.

c) Show that the onebody part of the Hamiltonian

$$\hat{H}_0 = \sum_{pq}\langle p|\hat{h}_0|q\rangle a_p^\dagger a_q$$

can be written, using standard annihilation and creation operators, in normal-ordered form as

$$\hat{H}_0 = \sum_{pq}\langle p|\hat{h}_0|q\rangle a_p^\dagger a_q = \sum_{pq}\langle p|\hat{h}_0|q\rangle\left\{a_p^\dagger a_q\right\} + \sum_i\langle i|\hat{h}_0|i\rangle,$$

and that the two-body Hamiltonian

$$\hat{H}_I = \frac{1}{4}\sum_{pqrs} \langle pq|\,\hat{v}\,|rs\rangle\, a_p^\dagger a_q^\dagger a_s a_r,$$

can be written

$$\hat{H}_I = \frac{1}{4}\sum_{pqrs} \langle pq|\,\hat{v}\,|rs\rangle \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \sum_{pqi} \langle pi|\,\hat{v}\,|qi\rangle \left\{a_p^\dagger a_q\right\} + \frac{1}{2}\sum_{ij} \langle ij|\,\hat{v}\,|ij\rangle$$

Explain the meaning of the various symbols. Which reference vacuum has been used? Write down the diagrammatic representation of all these terms.

d) Use the diagrammatic representation of the Hamiltonian operator from the previous exercise to set up all diagrams (use either anti-symmetrized Goldstone diagrams or Hugenholz diagrams) to second order (including the reference energy) in Rayleigh Schrödinger perturbation theory that contribute to the expectation value of E_0.

Use the diagram rules to write down their closed-form expressions. If a Hartree-Fock basis is used, which diagrams remain?

We consider now a one-particle system with the following Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_I$ where

$$\hat{H}_0 = \sum_p \varepsilon_p a_p^\dagger a_p,$$

and

$$\hat{H}_I = g\sum_{pq} a_p^\dagger a_q.$$

The strength parameter g is a real constant. The first part of the Hamiltonian plays the role of the unperturbed part, with

$$\langle p|\,\hat{h}_0\,|q\rangle = \delta_{p,q}\varepsilon_p.$$

We have only two one-particle states, with $\varepsilon_1 < \varepsilon_2$, and we will let the first state $p = 1$ correspond to the model space and the other, $p = 2$, correspond to the excluded space. Use labels $ijk\dots$ for hole states (below the Fermi level) and labels $abc\dots$ for particle (virtual) states (above the Fermi level).

e) Use the results from exercise c) to write down the above Hamiltonian in a normal-ordered form and set up all diagrams. Use an X to indicate the interaction part H_I.

f) Define the ground state (which is our model space) as

$$|\Phi_0\rangle = a_i^\dagger\,|0\rangle = a_1^\dagger\,|0\rangle\,,$$

and the excited state as

$$|\Phi_i^a\rangle = a_a^\dagger a_i\,|\Phi_0\rangle\,,$$

where $a = 2$ and $i = 1$. Set up the Hamiltonian matrix (a 2×2 matrix) and find the exact energy and expand the exact result for the ground state in terms of the parameter g.

g) Find the ground state energy to third order in Rayleigh-Schödinger perturbation theory and compare the results with the expansion of the exact energy from the previous exercise. Write down all diagrams which contribute and comment your results.

The final part deals with coupled-cluster theory. Since we have only a one-body problem, coupled-cluster theory truncated at the level of T_1 is exact. The similarity transformed normal-ordered Hamiltonian can then be written out as

$$\bar{H} = \hat{H}_N + \left(\hat{H}_N \hat{T}\right)_c + \frac{1}{2}\left(\hat{H}_N \hat{T}^2\right)_c + \ldots +,$$

where only linked diagrams appear. The expectation value of the ground state energy (beyond the reference energy is)

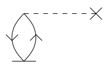
$$\mathrm{E_{CCS}} = \langle \Phi_0 | \bar{H} | \Phi_0 \rangle ,$$

and the amplitudes t_i^a are determined from the equation

$$0 = \langle \Phi_i^a | \bar{H} | \Phi_0 \rangle .$$

For the latter we need to take into account diagrams which lead to a final excitation level of $+1$ only.

h) Set up the definition of the operator $\hat{T} = \hat{T}_1$. We will use a diagrammatic approach only to find the diagrammatic contribution to the ground state beyond the reference energy. Show that the only possibility is

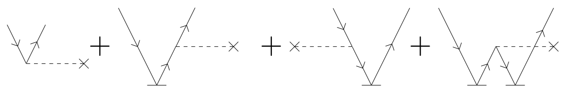
$E_{CCS} =$ 

Find the closed form expression.

i) Show, using a diagrammatic approach and keeping in mind the final excitation level, that the only diagrams that lead to

$$0 = \langle \Phi_i^a | \bar{H} | \Phi_0 \rangle ,$$

are

$0 =$ 

Set up the final closed form expressions and the algorithm for finding the amplitudes t_i^a. Can you solve the problem?