Exercises FYS-KJM4480, Fall semester 2009

Exercises week 46, November 15-19 2010

Exercise 15, perturbation theory

Let $H = H_0 + V$ and $|\phi_n\rangle$ be eigenstates of H_0 and $|\psi_n\rangle$ the corresponding ones for H. Assume that the ground state eigenstates $|\phi_0\rangle$ and $|\psi_0\rangle$ are not degenerate.
2a) Show that

$$E_0 - \varepsilon_0 = \frac{\langle\phi_0| V |\psi_0\rangle}{\langle\phi_0|\psi_0\rangle},$$

with $H|\psi_0\rangle = E_0|\psi_0\rangle$ and $H_0|\phi_0\rangle = \varepsilon_0|\phi_0\rangle$. Define the operators $P = |\phi_0\rangle\langle\phi_0|$ and $Q = 1 - P$. Show that these operators are idempotent. Show also that for any z (a real number) we have

$$|\psi_0\rangle = \langle\phi_0|\psi_0\rangle \sum_{n=0}^{\infty} \left(\frac{Q}{z - H_0}(z - E_0 + V)\right)^n |\phi_0\rangle,$$

and

$$E_0 = \varepsilon_0 + \sum_{n=0}^{\infty} \langle\phi_0| V \left(\frac{Q}{z - H_0}(z - E_0 + V)\right)^n |\phi_0\rangle.$$

Discuss these results for $z = E_0$ (Brillouin-Wigner pert. theory) and $z = \varepsilon_0$ (Rayleigh-Schrödinger pert. theory). Compare the first terms in these expansions (to third order in the interaction)
2b) Consider thereafter a system composed of two fermions in the pair orbitals $|m_0\rangle$ and $|-m_0\rangle$ in one single shell j with $2j + 1 > 2$. The projection of j takes the values $m = -j, -j+1, \dots j-1, j$. Assume that the matrix elements for the interaction between particles takes the shape

$$\langle m, -m| v |m', -m'\rangle = -G.$$

This as an example of the so-called pairing force, which is widely used in nuclear physics and the theory of superconductivity and superfluidity.

How would you define the single-particle part of the Hamiltonian operator? Show that the Brillouin-Wigner expansion from 2a) results in

$$E_0 = -(j + 1/2)G.$$

Show by exact diagonalization that this is the exact eigenvalue of the ground state and find the exact non-degenerate ground state.
2c) Use thereafter Rayleigh-Schrödinger perturbation theory and discuss the differences.

Exercise 16

Show that

$$\int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 H_1(t_1)H_1(t_2) = \frac{1}{2}\int_{t'}^{t} dt_1 \int_{t'}^{t} dt_2 T\left[H_1(t_1)H_1(t_2)\right]$$

Hint: Use the definition of T in order to distinguish between $t_1 > t_2$ and $t_1 < t_2$;

$$\int_{t'}^{t} dt_1 \int_{t'}^{t} dt_2 T\left[H_1(t_1)H_1(t_2)\right] = \int_{t'}^{t} dt_1 \left\{\int_{t'}^{t_1} dt_2 H_1(t_1)H_1(t_2) + \int_{t_1}^{t} dt_2 H_1(t_2)H_1(t_1)\right\}$$

Show that the last term on the right-hand side equals the first term (change the order of the integrations and thereafter integration variables). The area of integration for the first term is shown in the figure below.

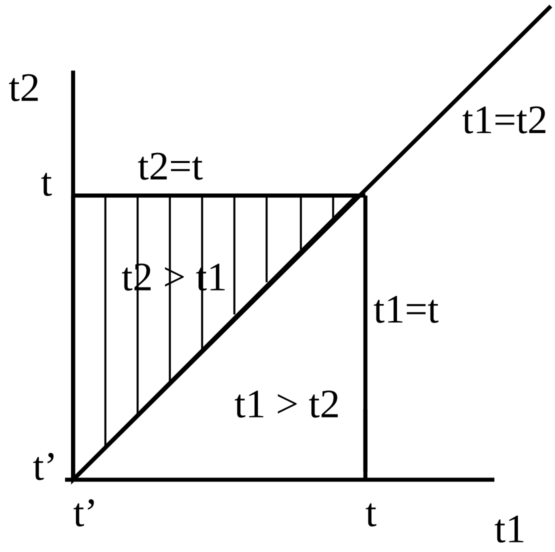

FIG. 1: Integration variables of exercise 16.

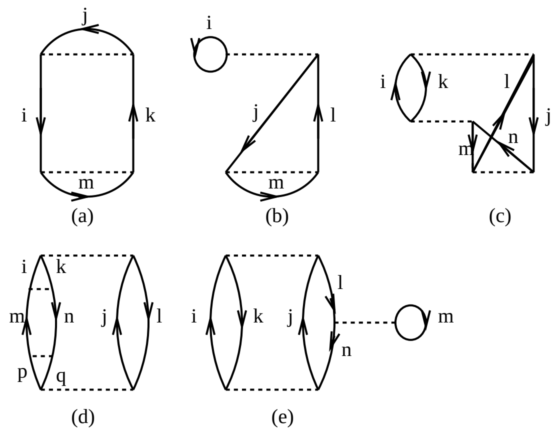

FIG. 2: Diagrams of exercise 17.

Exercise 17

Consider the following diagrams: (i) Set up the expressions for diagrams (a)-(e).
(ii) Diagram (b) does not give a contribution for a uniform and degenerate electron gas (or any uniform degenerate infinite system). Explain why. What about diagram (a)?
(iii) Diagram (c) is a so-called exchange diagram. Can you find the corresponding direct diagram?
(iv) Can you find the exchange diagram of diagram (e) under the assumption that the exchange takes place at the middle vertex?

Exercise 18

Explain how the Hartree-Fock approximation can be used to cancel the diagrams of (a) in the figure. Set up their corresponding expressions. Find thereafter the expression for the diagram in (b).

Exercise 19

Compute the contribution to ΔE_0 for the diagram shown here. Can the crossing hole lines have the same quantum

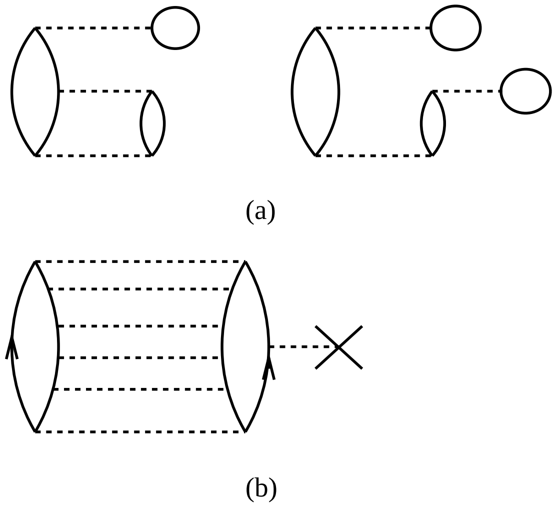

FIG. 3: Diagrams of exercise 18.

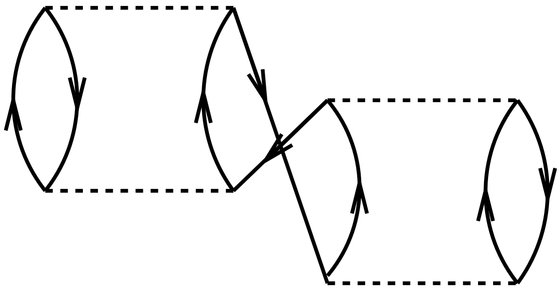

FIG. 4: Diagram of exercise 19.

numbers?

Exercise 20

Write the following diagrams in the particle-hole representation.

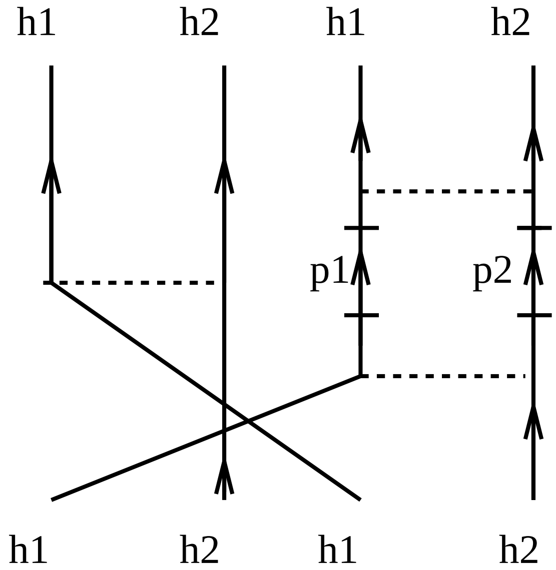

FIG. 5: Diagrams to be transformed to the particle-hole representation of exercise 20