.

NTNU
Faculty of Natural Sciences
Department of Physics

Exam TFY 4210 Quantum theory of many-particle systems, spring 2017

Lecturer: Assistant Professor Pietro Ballone
Department of Physics
Phone: 73593645

Examination support:

Approved calculator
Rottmann: Matematisk Formelsamling
Rottmann: Matematische Formelsammlung
Barnett & Cronin: Mathematical Formulae
The exam has 5 problems, with subproblems (i), (ii), ...
All subproblems have the same weight.
The sum the weights is 125% of the full mark .

There are 7 pages in total. Some useful formulas are given on the last page

Thursday, 1 June, 2017
09.00-13.00h

Problem (1)

(i) Compute the matrix element:

$$\langle 0 \mid \hat{a}_\alpha \hat{a}_\beta \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger \mid 0 \rangle \tag{1}$$

for Fermions and for Bosons.
Distinguish the case $\alpha \neq \beta$ and $\alpha = \beta$.

(ii) Consider a many-electron system.
The number of particles is given by the operator:

$$\hat{N} = \sum_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha \tag{2}$$

where $\hat{a}_\alpha^\dagger$, $\hat{a}_\alpha$ are creation and annihilation operators for the state α.

Show that:

$$[\hat{N}, \hat{a}_\alpha] = -\hat{a}_\alpha \tag{3}$$

$$[\hat{N}, \hat{a}_\alpha^\dagger] = \hat{a}_\alpha^\dagger \tag{4}$$

(iii) Let us consider the Boson operators $a_\lambda^\dagger$ and a_λ, and let $f(a_\lambda^\dagger)$ or $f(a_\lambda)$ be polynomial functions of their argument.
For instance:

$$f(a_\lambda) = c_0 + c_1 a_\lambda + c_2 a_\lambda^2 ... + c_n a_\lambda^n \tag{5}$$

Show that:

$$[a_\lambda, f(a_\lambda^\dagger)] = \frac{\partial f(a_\lambda^\dagger)}{\partial a_\lambda^\dagger} \tag{6}$$

and:

$$[a_\lambda^\dagger, f(a_\lambda)] = -\frac{\partial f(a_\lambda)}{\partial a_\lambda} \tag{7}$$

Problem (2)

The time ordered correlation function of two operators $\hat{A}$ and $\hat{B}$ is defined as:

$$\chi^T_{AB}(t) \equiv -i\langle \Psi_0 \mid T[\hat{A}(t)\hat{B}(0)] \mid \Psi_0\rangle \tag{8}$$

where $\mid \Psi_0\rangle$ is the ground state, the time dependence in the Heisenberg representation is:

$$\hat{A}(t) = e^{i\hat{H}t}\hat{A}e^{-i\hat{H}t} \tag{9}$$

and the time ordering operator is by:

$$T[\hat{A}(t_1)\hat{B}(t_2)] = \begin{cases} \hat{A}(t_1)\hat{B}(t_2) & t_1 > t_2 \\ \hat{B}(t_2)\hat{A}(t_1) & t_2 > t_1 \end{cases} \tag{10}$$

(Notice: there is no (-1) factor associated to the interchange of Fermion operators).

(i) Compute the Fourier transform:

$$\chi^T_{AB}(\omega) = \lim_{\eta\to 0^+}\int_{-\infty}^{+\infty} \chi^T_{AB}(t)e^{i\omega t-\eta|t|}dt \tag{11}$$

and show that it is given by:

$$\chi^T_{AB}(\omega) = -i\sum_n \left(\frac{A_{0n}B_{n0}}{\omega - \omega_{n0} + i\eta} - \frac{B_{0n}A_{n0}}{\omega + \omega_{n0} - i\eta}\right) \tag{12}$$

where $A_{0n} = \langle \Psi_0 \mid \hat{A} \mid \Psi_n\rangle$, $\{\Psi_0, \Psi_1, ...\}$ are eigenstates of the Hamiltonian, and $\hbar\omega_{n0} = E_n - E_0 > 0$.

The causal version of the same correlation function is given by:

$$\chi_{AB}(t) \equiv -i\theta(t)\langle \Psi_0 \mid [\hat{A}(t), \hat{B}(0)] \mid \Psi_0\rangle \tag{13}$$

where [.., ..] is the commutator.

(ii) Compute the Fourier transform of $\chi_{AB}(\omega)$ and compare it to that of χ^T_{AB}.

(iii) Comment on the position of the poles in the complex ω plane for $\chi^T_{AB}(\omega)$ and $\chi_{AB}(\omega)$.

Problem (3)

(i) The exchange-correlation energy functional of a many-electron system in 1D is given by:

$$E_{XC}[\rho] = \int \alpha[\rho(x)]^{4/3} dx + \frac{1}{2} \int K(\rho) \left[\frac{d\rho(x)}{dx} \right]^2 dx \tag{14}$$

where α is a positive numerical coefficient.

Compute the exchange-correlation potential:

$$\mu_{XC}(x) = \frac{\delta E_{XC}}{\delta \rho(x)} \tag{15}$$

(ii) According to Hartree-Fock, the total energy $e(r_s)$ per particle of the spin unpolarised homogeneous electron liquid is:

$$e(r_s) = e_k(r_s) + e_x(r_s) = \frac{2.21}{r_s^2} - \frac{0.916}{r_s} \tag{16}$$

where r_s is the Wigner-Seitz radius ($r_s = [3/(4\pi\rho)]^{(1/3)}$, ρ being the electron density), $e_k(r_s)$ is the kinetic energy per particle and $e_x(r_s)$ is the exchange energy per particle. Numerical coefficients are in Rydberg energy units.
Compute the pressure P as a function of the density, with pressure defined as:

$$P = -\left(\frac{\partial E}{\partial V} \right)_N \tag{17}$$

where E is the system ground state energy, V is the volume, and the derivative is computed at constant number of particles.

Is there an optimal density for the homogeneous electron liquid, and, in such a case, could you estimate this optimal density?

Problem (4)

The order n term in the perturbative expansion of the time ordered correlation function $\chi^T_{AB}(t)$ is:

$$\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \int_{-\infty}^{\infty} dt_1 ... \int_{-\infty}^{\infty} dt_n \langle \Phi_0 \mid T[\hat{A}_I(t)\hat{B}_I\hat{H}_1(t_1)\hat{H}_1(t_2)...\hat{H}_1(t_n)] \mid \Phi_0 \rangle \tag{18}$$

For the sake of definiteness, assume that $\hat{A}$ and $\hat{B}$ are single particle operators:

$$\hat{A} = \sum_{\alpha\beta} A_{\alpha\beta} \hat{a}^\dagger_\alpha \hat{a}_\beta \tag{19}$$

$$\hat{B} = \sum_{\gamma\delta} B_{\gamma\delta} \hat{a}^\dagger_\gamma \hat{a}_\delta \tag{20}$$

and the perturbation Hamiltonian contains a pair interaction term:

$$\hat{H}_{1I} = \frac{1}{2} \sum_{abcd} v_{abcd} \hat{a}^\dagger_a \hat{a}^\dagger_b \hat{a}_c \hat{a}_d \tag{21}$$

(i) List all the pairing schemes of creation and annihilation operator for the order $n = 0$ term of Eq. 18.

(ii) Count all the pairing schemes for the $n = 1$ term (you don't need to write them down) and verify that they are $4! = 24$
Argue that in general the number of all pairing schemes is $(2n + 2)!$ for the order n term of Eq. 18.

(iii) Write down the integral corresponding to the zero order diagram:

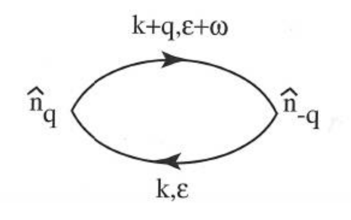

Figure 1: Zero order diagram

Please use the reciprocal space notation (consistent with the labels on the figure).

Problem (5)

Consider a system of Fermions interacting through the pair potential:

$$v(r) = e^2 \frac{e^{-\lambda r}}{r} \tag{22}$$

whose Fourier transform is:

$$v_{\mathbf{q}} = \frac{4\pi e^2}{q^2 + \lambda^2} \tag{23}$$

To first order in the interaction strength, the energy of the state that arises from the non-interacting state with momentum occupation numbers $\mathcal{N}_{\mathbf{k}\sigma}$ is given by:

$$E\left[\mathcal{N}_{\mathbf{k}\sigma}\right] = \sum_{\mathbf{k}\sigma} \frac{\hbar^2 k^2}{2m} \mathcal{N}_{\mathbf{k}\sigma} + \frac{1}{2V} \sum_{\mathbf{k}\sigma\mathbf{k}'\sigma'} \left[v_0 - v_{\mathbf{k}-\mathbf{k}'} \delta_{\sigma\sigma'}\right] \mathcal{N}_{\mathbf{k}\sigma} \mathcal{N}_{\mathbf{k}'\sigma'} \tag{24}$$

(a) Substitute $\mathcal{N}_{\mathbf{k}\sigma} = \mathcal{N}^{(0)}_{\mathbf{k}\sigma} + \delta\mathcal{N}_{\mathbf{k}\sigma}$ (where $\mathcal{N}^{(0)}_{\mathbf{k}\sigma} = \Theta(k_F - k)$ are the ground state occupation numbers) to obtain the Landau energy functional. Give explicit expressions for the quasi-particle energy and for the Landau interaction function.

(b) Calculate the Landau parameter F_1^s and the effective mass of the quasi-particle.

What happens for $\lambda \to 0$?

Some useful relations:

Commutation relations for Bosons:

$$[\hat{a}_\alpha, \hat{a}_\beta] = [\hat{a}^\dagger_\alpha, \hat{a}^\dagger_\beta] = 0 \tag{25}$$

$$[\hat{a}_\alpha, \hat{a}^\dagger_\beta] = \delta_{\alpha\beta} \tag{26}$$

Anti-commutation relations for Fermions:

$$\{\hat{a}_\alpha, \hat{a}_\beta\} = \{\hat{a}^\dagger_\alpha, \hat{a}^\dagger_\beta\} = 0 \tag{27}$$

$$\{\hat{a}_\alpha, \hat{a}^\dagger_\beta\} = \delta_{\alpha\beta} \tag{28}$$

Fourier transform:

$$f(\omega) = \int_{-\infty}^{\infty} f(\tau) e^{i\omega\tau} d\tau \tag{29}$$

$$f(\tau) = \int_{-\infty}^{\infty} f(\omega) e^{-i\omega\tau} \frac{d\omega}{2\pi} \tag{30}$$

Special relation:

$$\frac{1}{x \pm i\eta} = P\left(\frac{1}{x}\right) \mp i\pi\delta(x) \tag{31}$$

Chain-rule for thermodynamic derivatives:

$$V\frac{\partial}{\partial V} = -\rho\frac{\partial}{\partial\rho} = \frac{r_s}{3}\frac{d}{dr_s} \tag{32}$$

In this equation r_s is the Wigner-Seitz radius $r_s = [3/(4\pi\rho)]^{(1/3)}$, ρ being the electron density.

Landau energy functional for the normal electron liquid:

$$E[\mathcal{N}_{\mathbf{k},\sigma}] = E_0 + \sum_{\mathbf{k},\sigma} \mathcal{E}_{\mathbf{k},\sigma}\delta\mathcal{N}_{\mathbf{k},\sigma} + \frac{1}{2}\sum_{\mathbf{k},\sigma,\mathbf{k}',\sigma'} f_{\mathbf{k},\sigma,\mathbf{k}',\sigma'}\delta\mathcal{N}_{\mathbf{k},\sigma}\delta\mathcal{N}_{\mathbf{k}',\sigma'} \tag{33}$$

- $\mathcal{E}_{\mathbf{k},\sigma}$ is the isolated quasi-particle energy;
- $f_{\mathbf{k},\sigma,\mathbf{k}',\sigma'}$ is the Landau interaction function;
- $\delta\mathcal{N}_{\mathbf{k},\sigma}$ is the deviation of the quasi-particle distribution from the ground state one ($T = 0$ K).