

NTNU
Faculty of Natural Sciences
Department of Physics

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

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Examination support:

Approved calculator

Rottmann: Matematisk Formelsamling

Rottmann: Mathematische 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:

$$\langle 0 | \hat{a}_\alpha \hat{a}_\beta \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger | 0 \rangle \quad (1)$$

for Fermions and for Bosons.

Distinguish the case $\alpha \neq \beta$ and $\alpha = \beta$.

Solution:

The definition of Fermion creation and annihilation operators is as follows:

$$\hat{a}_\alpha^\dagger | n_1, n_2, \dots, n_\alpha, \dots \rangle = \delta n_{\alpha,0} (\pm 1)^{S_\alpha} \sqrt{n_\alpha + 1} | n_1, n_2, \dots, n_\alpha + 1, \dots \rangle \quad (2)$$

$$\hat{a}_\alpha | n_1, n_2, \dots, n_\alpha, \dots \rangle = \delta n_{\alpha,1} (\pm 1)^{S_\alpha} \sqrt{n_\alpha} | n_1, n_2, \dots, n_\alpha - 1, \dots \rangle \quad (3)$$

where:

$$S_\alpha = \sum_{\gamma < \alpha} n_\gamma \quad (4)$$

There is no sign factor and no delta-function factor in the case of Bosons:

$$\hat{a}_\alpha^\dagger | n_1, n_2, \dots, n_\alpha, \dots \rangle = \sqrt{n_\alpha + 1} | n_1, n_2, \dots, n_\alpha + 1, \dots \rangle \quad (5)$$

$$\hat{a}_\alpha | n_1, n_2, \dots, n_\alpha, \dots \rangle = \sqrt{n_\alpha} | n_1, n_2, \dots, n_\alpha - 1, \dots \rangle \quad (6)$$

Hence:

(i) $\alpha \neq \beta$, Fermions:

$$\hat{a}_\beta^\dagger | 0 \rangle = | \beta \rangle$$

$$\hat{a}_\alpha^\dagger | \beta \rangle = | \alpha \beta \rangle$$

$$\hat{a}_\beta | \alpha \beta \rangle = - | \alpha \rangle$$

$$\hat{a}_\alpha | \alpha \rangle = | 0 \rangle \rightarrow \langle 0 | \hat{a}_\alpha \hat{a}_\beta \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger | 0 \rangle = -1$$

A different way would be to interchange (once) the operators using the anti-commutation rule, to obtain:

$$\langle 0 | \hat{a}_\alpha \hat{a}_\beta \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger | 0 \rangle = -\langle 0 | (1 - \hat{n}_\alpha)(1 - \hat{n}_\beta) | 0 \rangle \quad (7)$$

giving again $\langle 0 | \hat{a}_\alpha \hat{a}_\beta \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger | 0 \rangle = -1$.

The case $\alpha = \beta$ is trivial for Fermions, since the double application of $\hat{a}_\alpha^\dagger$ to $| 0 \rangle$ annihilates the state.

The Boson case gives (nearly) the same result for the $\alpha \neq \beta$ case, only the sign being different (result = +1), because of the commutation relations replacing anti-commutation.

There is a slight difference for the $\alpha = \beta$ case:

$$\begin{aligned}\hat{a}_\alpha^\dagger | 0 \rangle &= | \alpha \rangle \\ \hat{a}_\alpha^\dagger | \alpha \rangle &= \sqrt{2} | \alpha \alpha \rangle \\ \sqrt{2} \hat{a}_\alpha | \alpha \alpha \rangle &= 2 | \alpha \rangle \\ 2 \hat{a}_\alpha | \alpha \rangle &= 2 | 0 \rangle \rightarrow \langle 0 | \hat{a}_\alpha \hat{a}_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha^\dagger | 0 \rangle = 2\end{aligned}$$

(ii) Consider a many-electron system.

The number of particles is given by the operator:

$$\hat{N} = \sum_{\alpha} \hat{a}_\alpha^\dagger \hat{a}_\alpha \quad (8)$$

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

Show that:

$$[\hat{N}, \hat{a}_\alpha] = -\hat{a}_\alpha \quad (9)$$

$$[\hat{N}, \hat{a}_\alpha^\dagger] = \hat{a}_\alpha^\dagger \quad (10)$$

Solutions:

We need to compute:

$$\begin{aligned}[\hat{N}, \hat{a}_\alpha] &= \left[\sum_{\beta} \hat{a}_\beta^\dagger \hat{a}_\beta, \hat{a}_\alpha \right] = [\hat{a}_\alpha^\dagger \hat{a}_\alpha, \hat{a}_\alpha] = \\ &= \hat{a}_\alpha^\dagger \hat{a}_\alpha \hat{a}_\alpha - \hat{a}_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha\end{aligned} \quad (11)$$

The first term vanishes because $\hat{a}_\alpha^2 = 0$. We consider the second term:

$$-\hat{a}_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha = -\hat{a}_\alpha (1 - \hat{a}_\alpha \hat{a}_\alpha^\dagger) = -\hat{a}_\alpha$$

where the anti-commutation relation of Fermions has been used, and the last term has been neglected for the same $\hat{a}_\alpha^2 = 0$ reason.

The $[\hat{N}, \hat{a}_\alpha^\dagger] = \hat{a}_\alpha^\dagger$ is completely analogous to the previous one.

(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:

$$f(a_\lambda) = c_0 + c_1 a_\lambda + c_2 a_\lambda^2 \dots + c_n a_\lambda^n \quad (12)$$

Show that:

$$[a_\lambda, f(a_\lambda^\dagger)] = \frac{\partial f(a_\lambda^\dagger)}{\partial a_\lambda^\dagger} \quad (13)$$

and:

$$[a_\lambda^\dagger, f(a_\lambda)] = -\frac{\partial f(a_\lambda)}{\partial a_\lambda} \quad (14)$$

Solution:

The starting point is the relation:

$$[A, B^n] = nB^{n-1}[A, B] \quad (15)$$

which is valid provided B commutes with the $[A, B]$ commutator. The relation is easy to verify, using for instance the induction principle. If A, B are creation and annihilation operators, then their commutator is a number (zero or a delta), and this commutes with any remaining product of operators. The relation above, therefore, is valid.

Let us consider the commutator between $a_\lambda^\dagger$ and $f(a_\lambda)$:

$$[a_\lambda^\dagger, f(a_\lambda)] = c_1[a_\lambda^\dagger, a_\lambda] + c_2[a_\lambda^\dagger, a_\lambda^2] \dots + c_n[a_\lambda^\dagger, a_\lambda^n] \quad (16)$$

where I neglected the commutator of $a_\lambda^\dagger$ with the complex number c_0 . The result is:

$$[a_\lambda^\dagger, f(a_\lambda)] = c_1[a_\lambda^\dagger, a_\lambda] + 2c_2 a_\lambda [a_\lambda^\dagger, a_\lambda] \dots + n c_n a_\lambda^{n-1} [a_\lambda^\dagger, a_\lambda] \quad (17)$$

Since $[a_\lambda^\dagger, a_\mu] = -\delta_{\lambda,\mu}$, we obtain:

$$[a_\lambda^\dagger, f(a_\lambda)] = -\{c_1 + 2c_2 a_\lambda + \dots + n c_n a_\lambda^{n-1}\} = -\frac{\partial f(a_\lambda)}{\partial a_\lambda} \quad (18)$$

The derivation for $[a_\lambda, f(a_\lambda^\dagger)]$ is completely analogous.

Problem (2)

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

$$\chi_{AB}^T(t) \equiv -i \langle \Psi_0 | T[\hat{A}(t)\hat{B}(0)] | \Psi_0 \rangle \quad (19)$$

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

$$\hat{A}(t) = e^{i\hat{H}t} \hat{A} e^{-i\hat{H}t} \quad (20)$$

and the time ordering operator is by:

$$T[\hat{A}(t_1)\hat{B}(t_2)] = \begin{cases} \hat{A}(t_1)\hat{B}(t_2) & t_1 > t_2 \\ \hat{B}(t_2)\hat{A}(t_1) & t_2 > t_1 \end{cases} \quad (21)$$

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

(i) Compute the Fourier transform:

$$\chi_{AB}^T(\omega) = \lim_{\eta \rightarrow 0^+} \int_{-\infty}^{+\infty} \chi_{AB}^T(t) e^{i\omega t - \eta|t|} dt \quad (22)$$

and show that it is given by:

$$\chi_{AB}^T(\omega) = -i \sum_n \left(\frac{A_{0n}B_{n0}}{\omega - \omega_{n0} + i\eta} - \frac{B_{0n}A_{n0}}{\omega + \omega_{n0} - i\eta} \right) \quad (23)$$

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

Solution:

There is a slight subtlety in the way to translate the time ordering of t_1 and t_2 into the single time argument of $\chi_{AB}^T(t)$.

According to the definition:

$$T[\hat{A}(t_1)\hat{B}(t_2)] = \begin{cases} \hat{A}(t_1)\hat{B}(t_2) & t_1 > t_2 \\ \hat{B}(t_2)\hat{A}(t_1) & t_2 > t_1 \end{cases} \quad (24)$$

Let us change variables, from t_1 and t_2 to $t = t_1 - t_2$ and t_2 . Then:

$$T[\hat{A}(t+t_2)\hat{B}(t_2)] = \begin{cases} \hat{A}(t+t_2)\hat{B}(t_2) & t > 0 \\ \hat{B}(t_2)\hat{A}(t+t_2) & t < 0 \end{cases} \quad (25)$$

In these relations t_2 plays the role of an irrelevant origin, and we re-write:

$$\chi_{AB}^T(t) = \begin{cases} \hat{A}(t)\hat{B} & t > 0 \\ \hat{B}\hat{A}(t) & t < 0 \end{cases} \quad (26)$$

Let us now compute:

$$\int_{-\infty}^{+\infty} \chi_{AB}^T(t) e^{i\omega t - \eta|t|} dt = \int_{-\infty}^0 \langle \Psi_0 | \hat{B}\hat{A}(t) | \Psi_0 \rangle e^{i\omega t + \eta t} dt + \int_0^{\infty} \langle \Psi_0 | \hat{A}(t)\hat{B} | \Psi_0 \rangle e^{i\omega t - \eta t} dt \quad (27)$$

Inserting the explicit time-dependence:

$$\begin{aligned} &= \int_{-\infty}^0 \langle \Psi_0 | \hat{B} e^{i\hat{H}t} \hat{A} e^{-i\hat{H}t} | \Psi_0 \rangle e^{i\omega t + \eta t} dt + \int_0^{\infty} \langle \Psi_0 | e^{i\hat{H}t} \hat{A} e^{-i\hat{H}t} \hat{B} | \Psi_0 \rangle e^{i\omega t - \eta t} dt \quad (28) \\ &= \int_{-\infty}^0 e^{-iE_0 t} \langle \Psi_0 | \hat{B} e^{i\hat{H}t} \hat{A} | \Psi_0 \rangle e^{i\omega t + \eta t} dt + \int_0^{\infty} e^{iE_0 t} \langle \Psi_0 | \hat{A} e^{-i\hat{H}t} \hat{B} | \Psi_0 \rangle e^{i\omega t - \eta t} dt \end{aligned}$$

Inserting a complete basis of eigenfunctions of the Hamiltonian:

$$= \sum_n \int_{-\infty}^0 e^{i(E_n - E_0)t} \langle \Psi_0 | \hat{B} | \Psi_n \rangle \langle \Psi_n | \hat{A} | \Psi_0 \rangle e^{i\omega t + \eta t} dt \quad (29)$$

$$\begin{aligned} &+ \sum_n \int_0^{\infty} e^{-i(E_n - E_0)t} \langle \Psi_0 | \hat{A} | \Psi_n \rangle \langle \Psi_n | \hat{B} | \Psi_0 \rangle e^{i\omega t - \eta t} dt \\ &= \sum_n B_{0n} A_{n0} \int_{-\infty}^0 e^{i\omega_{n0}t} e^{i\omega t + \eta t} dt \quad (30) \end{aligned}$$

$$\begin{aligned} &+ \sum_n A_{0n} B_{n0} \int_0^{\infty} e^{-i\omega_{n0}t} e^{i\omega t - \eta t} dt \\ &= \sum_n B_{0n} A_{n0} \left. \frac{e^{i\omega_{n0}t} e^{i\omega t + \eta t}}{i\omega_{n0} + i\omega + \eta} \right|_{-\infty}^0 \quad (31) \end{aligned}$$

$$\begin{aligned} &+ \sum_n A_{0n} B_{n0} \left. \frac{e^{-i\omega_{n0}t} e^{i\omega t - \eta t}}{-i\omega_{n0} + i\omega - \eta} \right|_0^{\infty} \\ &= -i \sum_n \frac{B_{0n} A_{n0}}{\omega_{n0} + \omega - i\eta} \quad (32) \end{aligned}$$

$$+i \sum_n \frac{A_{0n}B_{n0}}{\omega - \omega_{n0} + i\eta}$$

Now multiplying times $-i$, we obtain:

$$\chi_{AB}^T(\omega) = \sum_n \left(\frac{A_{0n}B_{n0}}{\omega - \omega_{n0} + i\eta} - \frac{B_{0n}A_{n0}}{\omega + \omega_{n0} - i\eta} \right) \quad (33)$$

where it is understood that η is an infinitesimal positive quantity.

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

$$\chi_{AB}(t) \equiv -i\theta(t)\langle \Psi_0 | [\hat{A}(t), \hat{B}(0)] | \Psi_0 \rangle \quad (34)$$

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

(ii) Compute the Fourier transform of $\chi_{AB}(t)$ and compare it to that of χ_{AB}^T .

Solution:

The Fourier transform of $\chi_{AB}(t)$ is:

$$\chi_{AB}(\omega) = \lim_{\eta \rightarrow 0^+} \int_{-\infty}^{+\infty} \chi_{AB}(t) e^{i\omega t - \eta|t|} dt \quad (35)$$

Let us compute:

$$\begin{aligned} \int_{-\infty}^{\infty} \chi_{AB}(t) e^{i\omega t - \eta|t|} dt &= \int_0^{\infty} \langle \Psi_0 | \hat{A}(t) \hat{B} - \hat{B} \hat{A}(t) | \Psi_0 \rangle e^{i\omega t - \eta t} dt \\ &= \int_0^{\infty} \langle \Psi_0 | e^{i\hat{H}t} \hat{A} e^{-i\hat{H}t} \hat{B} - \hat{B} e^{i\hat{H}t} \hat{A} e^{-i\hat{H}t} | \Psi_0 \rangle e^{i\omega t - \eta t} dt \end{aligned} \quad (36)$$

Inserting a complete set of eigenfunctions of the Hamiltonian:

$$\begin{aligned} &= \sum_n A_{0n} B_{n0} \int_0^{\infty} e^{-i(E_n - E_0)t} e^{i\omega t - \eta t} dt - \sum_n A_{n0} B_{0n} \int_0^{\infty} e^{i(E_n - E_0)t} e^{i\omega t - \eta t} dt \\ &= \sum_n A_{0n} B_{n0} \left. \frac{e^{-i\omega_{n0}t} e^{i\omega t - \eta t}}{-i\omega_{n0} + i\omega - \eta} \right|_0^{\infty} - \sum_n A_{n0} B_{0n} \left. \frac{e^{i\omega_{n0}t} e^{i\omega t - \eta t}}{i\omega_{n0} + i\omega - \eta} \right|_0^{\infty} \\ &= i \sum_n \frac{A_{0n} B_{n0}}{\omega - \omega_{n0} + i\eta} - i \sum_n \frac{A_{n0} B_{0n}}{\omega + \omega_{n0} + i\eta} \end{aligned} \quad (37)$$

Multiplying not times $-i$ we obtain:

(Note: I need to check whether this $-i$ is correct or not!)

$$\chi_{AB}(\omega) = \sum_n \frac{A_{0n} B_{n0}}{\omega - \omega_{n0} + i\eta} - \sum_n \frac{A_{n0} B_{0n}}{\omega + \omega_{n0} + i\eta}$$

where again η is an infinitesimal positive quantity.

This is the same expression of $\chi_{AB}^T(\omega)$ apart from changing the sign of $i\eta$ in the second sum.

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

Solution:

The poles of $\chi_{AB}^T(\omega)$ in the complex ω plane are at $\omega = \omega_{n0} - i\eta$ and at $\omega = -\omega_{n0} + i\eta$. Therefore, $\chi_{AB}^T(\omega)$ has poles both in the upper and in the lower imaginary half-plane.

By contrast, $\chi_{AB}(\omega)$ has poles only in the negative imaginary half-plane.

Problem (3)

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

$$E_{XC}[\rho] = \int \alpha[\rho(x)]^{4/3} dx + \frac{1}{2} \int K(\rho) \left[\frac{d\rho(x)}{dx} \right]^2 dx \quad (38)$$

where α is a positive numerical coefficient.

Compute the exchange-correlation potential:

$$\mu_{XC}(x) = \frac{\delta E_{XC}}{\delta \rho(x)} \quad (39)$$

Solution:

To determine the functional derivative we need to make the change:

$$\rho(x) \rightarrow \rho(x) + \delta\rho(x) \quad (40)$$

$$\frac{d}{dx}\rho(x) \rightarrow \frac{d}{dx}\rho(x) + \frac{d}{dx}\delta\rho(x) \quad (41)$$

into Eq. ??, keeping the linear terms in the integrand.

$$\begin{aligned} E_{XC}[\rho + \delta\rho] &= \int \alpha[\rho(x) + \delta\rho(x)]^{4/3} dx \\ &+ \frac{1}{2} \int K(\rho + \delta\rho) \left(\frac{d\rho(x)}{dx} + \frac{d\delta\rho(x)}{dx} \right)^2 dx \\ &= \int \alpha[\rho^{4/3}(x) + \frac{4}{3}\rho^{1/3}(x)\delta\rho(x) + \dots] dx \\ &+ \frac{1}{2} \int [K(\rho) + \frac{\partial K(\rho)}{\partial \rho} \delta\rho(x)] \left[\left(\frac{d\rho(x)}{dx} \right)^2 + 2 \frac{d\rho(x)}{dx} \frac{d\delta\rho(x)}{dx} \right] dx \end{aligned} \quad (42)$$

Linear terms (in $\delta\rho(x)$) in the integrand are:

$$\frac{4}{3}\alpha\rho^{1/3}(x) + \frac{1}{2} \frac{\partial K(\rho)}{\partial \rho} \left(\frac{d\rho(x)}{dx} \right)^2 \quad (43)$$

These are terms appearing in the XC potential.

We have also:

$$\frac{1}{2} \int K(\rho) \left[2 \frac{d\rho(x)}{dx} \frac{d\delta\rho(x)}{dx} \right] dx \quad (44)$$

that needs to be transformed into a term linear in $\delta\rho$ while now it is linear in $d\delta\rho/dx$. We achieve our aim integrating by parts:

$$\begin{aligned} \frac{1}{2} \int K(\rho) \left[2 \frac{d\rho(x)}{dx} \frac{d\delta\rho(x)}{dx} \right] dx = \\ K(\rho) \frac{d\rho(x)}{dx} \delta\rho(x) \Big|_{-\infty}^{\infty} - \int \frac{d}{dx} \left[K(\rho) \frac{d\rho(x)}{dx} \right] \delta\rho(x) dx \end{aligned} \quad (45)$$

The first term vanishes because the variation $\delta\rho(x)$ vanishes at $\pm\infty$. The full XC potential is:

$$\mu_{XC} = \frac{4}{3} \alpha \rho^{1/3}(x) - \frac{1}{2} \frac{\partial K(\rho)}{\partial \rho} \left(\frac{d\rho(x)}{dx} \right)^2 - K(\rho) \frac{d^2 \rho(x)}{dx^2} \quad (46)$$

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

$$e(r_s) = e_k(r_s) + e_x(r_s) = \frac{2.21}{r_s^2} - \frac{0.916}{r_s} \quad (47)$$

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:

$$P = - \left(\frac{\partial E}{\partial V} \right)_N \quad (48)$$

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?

Solution:

For a homogeneous system:

$$P = - \left(\frac{\partial E}{\partial V} \right)_N = -N \left(\frac{\partial \epsilon}{\partial V} \right)_N \quad (49)$$

where ϵ is the total energy per particle. (One could argue that E is always N times the energy per electron, a fortiori for indistinguishable particles; in any case we need the energy to be a unique function of the average density).

All the partial derivatives are computed at fixed number of particles N .

It is useful to consider:

$$\frac{\partial}{\partial V} = \frac{\partial \rho}{\partial V} \frac{\partial}{\partial \rho} \quad (50)$$

Since $\rho = N/V$, $\partial \rho / \partial V = -N/V^2$. Therefore:

$$P = - \left(\frac{N}{V} \right)^2 \frac{\partial \epsilon}{\partial \rho} = -\rho^2 \frac{\partial \epsilon}{\partial \rho} \quad (51)$$

At point (ii) it has been shown that:

$$\rho \frac{\partial \epsilon}{\partial \rho} = -\frac{r_s}{3} \frac{d\epsilon(r_s)}{dr_s} \quad (52)$$

Hence:

$$\begin{aligned} \frac{P}{\rho} &= -\rho \frac{\partial \epsilon}{\partial \rho} = -\frac{r_s}{3} \frac{d}{dr_s} \left\{ \frac{2.21}{r_s^2} - \frac{0.916}{r_s} \right\} \\ &= -\frac{r_s}{3} \left\{ -2 \frac{2.21}{r_s^3} + \frac{0.916}{r_s^2} \right\} = \frac{2}{3} \frac{2.21}{r_s^2} - \frac{1}{3} \frac{0.916}{r_s} \end{aligned} \quad (53)$$

When this expression vanishes at:

$$2 \frac{2.21}{r_s^2} - \frac{0.916}{r_s} = 0 \quad \rightarrow \quad r_s \sim 5 \quad (54)$$

$P = 0$, implying that at this density the total energy as a function of V is stationary. A quick sketch of $E(r_s)$ shows that the stationary point is a minimum of E versus V (or vs ρ , or vs r_s). In this sense, according to Hartree-Fock, $r_s \sim 5$ is a natural reference state for the homogeneous electron liquid.

Problem (4)

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

$$\frac{1}{n!} \left(-\frac{i}{\hbar} \right)^n \int_{-\infty}^{\infty} dt_1 \dots \int_{-\infty}^{\infty} dt_n \langle \Phi_0 | T[\hat{A}_I(t) \hat{B}_I \hat{H}_1(t_1) \hat{H}_1(t_2) \dots \hat{H}_1(t_n)] | \Phi_0 \rangle \quad (55)$$

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

$$\hat{A} = \sum_{\alpha\beta} A_{\alpha\beta} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\beta} \quad (56)$$

$$\hat{B} = \sum_{\gamma\delta} B_{\gamma\delta} \hat{a}_{\gamma}^{\dagger} \hat{a}_{\delta} \quad (57)$$

and the perturbation Hamiltonian contains a pair interaction term:

$$\hat{H}_{1I} = \frac{1}{2} \sum_{abcd} v_{abcd} \hat{a}_a^{\dagger} \hat{a}_b^{\dagger} \hat{a}_c \hat{a}_d \quad (58)$$

(i) List all the pairing schemes of creation and annihilation operator for the order $n = 0$ term of Eq. 55.

Solution

Pairing schemes for the term of order n , containing $2n + 2$ destruction operators and $2n + 2$ creation operators are obtained by list creation and annihilation operators in two parallel columns;
choose any one of the $(2n + 2)!$ ways of pairing an element from the first column with one of the right column.

Hence, at order $n = 0$ one has:

$$\begin{array}{ccc} \hat{A}(t) & \hat{a}_{\beta}(t) & \hat{a}_{\alpha}^{\dagger}(t) \\ \hat{B} & \hat{a}_{\delta} & \hat{a}_{\gamma}^{\dagger} \end{array} \quad (59)$$

and we have two pairing schemes: $\langle \hat{a}_{\beta}(t) \hat{a}_{\alpha}^{\dagger}(t) \rangle \langle \hat{a}_{\delta} \hat{a}_{\gamma}^{\dagger} \rangle$, and $\langle \hat{a}_{\beta}(t) \hat{a}_{\gamma}^{\dagger} \rangle \langle \hat{a}_{\delta} \hat{a}_{\alpha}^{\dagger}(t) \rangle$. The original sequence in Eq. 55 was: $\hat{a}_{\alpha}^{\dagger}(t) \hat{a}_{\beta}(t) \hat{a}_{\gamma}^{\dagger} \hat{a}_{\delta}$. Therefore, the first pairing has (+) sign (even number of interchanges needed to obtain the ordering in the pairs), while the second pairing has (−) sign, because the number of interchanges (3) to go from the original to the pairing ordering is odd.

(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. 55.

Solution:

At order $n = 1$ one has eight operators, four creation and four annihilation operators. Each term arising from Wick's theorem contains four pairs, each made of an annihilation and a creation operator (otherwise the contribution vanishes).
To be more detailed, each contributing term (or "pairing") is of the form:

$$\langle \hat{a}_\beta \hat{a}_\alpha^\dagger \rangle \langle \hat{a}_\delta \hat{a}_\gamma^\dagger \rangle \langle \hat{a}_c \hat{a}_a^\dagger \rangle \langle \hat{a}_d \hat{a}_b^\dagger \rangle \quad (60)$$

To find all possible terms, we resort again to the two-column scheme:

$$\begin{array}{ccc} \hat{A}(t) & \hat{a}_\beta(t) & \hat{a}_\alpha^\dagger(t) \\ \hat{B} & \hat{a}_\delta & \hat{a}_\gamma^\dagger \\ \hat{H}_1 & \hat{a}_c(t_1) & \hat{a}_a^\dagger(t_1) \\ \hat{H}_1 & \hat{a}_d(t_1) & \hat{a}_b^\dagger(t_1) \end{array} \quad (61)$$

We pick the first operator on the left column, and pair with any of the $(2n + 2)$ operators on the right column. There are $(2n + 2) \times (2n + 2)$ choices to do so ($(2n + 1)$ choices from the first column, times $(2n + 2)$ choices from the second column).

Then, we pick a second operator from the remaining $(2n + 1)$ on the left, and pair it to one of the $(2n + 1)$ operators on the right: $(2n + 1) \times (2n + 1)$ choices.
etc.

At the end, we identified $[(2n + 2)!]^2$ choices. However, many of these are simply permutations of the same pairs. With the construction above, for instance, we pick both:

$$\langle \hat{a}_\beta \hat{a}_\alpha^\dagger \rangle \langle \hat{a}_\delta \hat{a}_\gamma^\dagger \rangle \langle \hat{a}_c \hat{a}_a^\dagger \rangle \langle \hat{a}_d \hat{a}_b^\dagger \rangle \quad (62)$$

and:

$$\langle \hat{a}_\beta \hat{a}_\alpha^\dagger \rangle \langle \hat{a}_c \hat{a}_a^\dagger \rangle \langle \hat{a}_\delta \hat{a}_\gamma^\dagger \rangle \langle \hat{a}_d \hat{a}_b^\dagger \rangle \quad (63)$$

that however are identical.

This however is easy to compensate: one only needs to divide by the number of permutations of pairs in each term, that is $(2n + 2)!$.

Therefore, the number of distinct terms, or "pairings", is $[(2n + 2)!]^2 / (2n + 2)! = (2n + 2)!$.

In the $n = 1$ case, the number of distinct pairings is $4! = 24$.

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

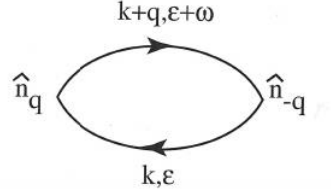


Figure 1: Zero order diagram

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

Solution:

The diagram corresponds to the integral:

$$-i \sum_{\sigma} \int \frac{d\mathbf{k}}{(2\pi)^d} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} G_{\sigma}^{(0)}(\mathbf{k}, \epsilon) G_{\sigma}^{(0)}(\mathbf{k} + \mathbf{q}, \epsilon + \omega) \quad (64)$$

The numerical factor includes a $(i)^{n+1} = i$, and a (-1) for a single Fermionic loop, giving $-i$.

Matrix elements associated to the external vertices are not specified (one could use the $\hat{n}_{\mathbf{q}}$ and $\hat{n}_{-\mathbf{q}}$ operators shown in the figure) since we are not told of the origin of the diagram.

As a complement (not required), one can add that using the expression:

$$G_{\sigma}^{(0)}(\mathbf{k}, \omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}\sigma} + i\eta_{\mathbf{k},\sigma}} \quad (65)$$

(where the definition $\eta_{\mathbf{k}\sigma} \equiv \eta \text{sign}(k - k_F)$ has been introduced), it is possible to compute explicitly:

$$= \sum_{\sigma} \int \frac{d\mathbf{k}}{(2\pi)^d} \frac{n_{\mathbf{k}\sigma} - n_{\mathbf{k}+\mathbf{q}\sigma}}{\omega + \epsilon_{\mathbf{k}\sigma} - \epsilon_{\mathbf{k}+\mathbf{q}\sigma} + i\eta_{\omega}} \quad (66)$$

where now $\eta_{\omega} \equiv \eta \text{sign}(\omega)$.

Problem (5)

Consider a system of Fermions interacting through the pair potential:

$$v(r) = e^2 \frac{e^{-\lambda r}}{r} \quad (67)$$

whose Fourier transform is:

$$v_{\mathbf{q}} = \frac{4\pi e^2}{q^2 + \lambda^2} \quad (68)$$

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:

$$E[\mathcal{N}_{\mathbf{k}\sigma}] = \sum_{\mathbf{k}\sigma} \frac{\hbar^2 k^2}{2m} \mathcal{N}_{\mathbf{k}\sigma} + \frac{1}{2V} \sum_{\mathbf{k}\sigma \mathbf{k}'\sigma'} [v_0 - v_{\mathbf{k}-\mathbf{k}'} \delta_{\sigma\sigma'}] \mathcal{N}_{\mathbf{k}\sigma} \mathcal{N}_{\mathbf{k}'\sigma'} \quad (69)$$

(i) Substitute $\mathcal{N}_{\mathbf{k}\sigma} = \mathcal{N}_{\mathbf{k}\sigma}^{(0)} + \delta\mathcal{N}_{\mathbf{k}\sigma}$ (where $\mathcal{N}_{\mathbf{k}\sigma}^{(0)} = \Theta(k_F - k)$ 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.

Solution:

The energy functional is:

$$E[\delta\mathcal{N}_{\mathbf{k}\sigma}] = \sum_{\mathbf{k}\sigma} \frac{\hbar^2 k^2}{2m} [\mathcal{N}_{\mathbf{k}\sigma}^{(0)} + \delta\mathcal{N}_{\mathbf{k}\sigma}] + \frac{1}{2V} \sum_{\mathbf{k}\sigma \mathbf{k}'\sigma'} [v_0 - v_{\mathbf{k}-\mathbf{k}'} \delta_{\sigma\sigma'}] [\mathcal{N}_{\mathbf{k}\sigma}^{(0)} + \delta\mathcal{N}_{\mathbf{k}\sigma}] [\mathcal{N}_{\mathbf{k}'\sigma'}^{(0)} + \delta\mathcal{N}_{\mathbf{k}'\sigma'}] \quad (70)$$

$$= E_0 + \sum_{\mathbf{k}\sigma} \left[\frac{\hbar^2 k^2}{2m} + 2 \frac{1}{2V} \sum_{\mathbf{k}'\sigma'} [v_0 - v_{\mathbf{k}-\mathbf{k}'} \delta_{\sigma\sigma'}] \mathcal{N}_{\mathbf{k}'\sigma'}^{(0)} \right] \delta\mathcal{N}_{\mathbf{k}\sigma} + \frac{1}{2V} \sum_{\mathbf{k}\sigma \mathbf{k}'\sigma'} [v_0 - v_{\mathbf{k}-\mathbf{k}'} \delta_{\sigma\sigma'}] \delta\mathcal{N}_{\mathbf{k}\sigma} \mathcal{N}_{\mathbf{k}'\sigma'}^{(0)}$$

where:

$$E_0 = \sum_{\mathbf{k}\sigma} \frac{\hbar^2 k^2}{2m} \mathcal{N}_{\mathbf{k}\sigma}^{(0)} + \frac{1}{2V} \sum_{\mathbf{k}\sigma \mathbf{k}'\sigma'} [v_0 - v_{\mathbf{k}-\mathbf{k}'} \delta_{\sigma\sigma'}] \mathcal{N}_{\mathbf{k}'\sigma'}^{(0)} \mathcal{N}_{\mathbf{k}\sigma}^{(0)} \quad (71)$$

The bare quasi-particle energy is:

$$\mathcal{E}_{\mathbf{k}\sigma} = \left[\frac{\hbar^2 k^2}{2m} + \frac{1}{V} \sum_{\mathbf{k}'\sigma'} [v_0 - v_{\mathbf{k}-\mathbf{k}'} \delta_{\sigma\sigma'}] \mathcal{N}_{\mathbf{k}'\sigma'}^{(0)} \right] \quad (72)$$

This could be defined more explicitly by computing the integral. This is not strictly required by the exercise. The Landau interaction function is:

$$f_{\mathbf{k}\sigma; \mathbf{k}'\sigma'} = \frac{1}{V} [v_0 - v_{\mathbf{k}-\mathbf{k}'} \delta_{\sigma\sigma'}] \quad (73)$$

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

What happens for $\lambda \rightarrow 0$?

Solution:

According to the definition:

$$F_1^s = \frac{N(0)^\star}{2} \int [v_{\mathbf{0}} - v_{\mathbf{k}-\mathbf{k}'} + v_{\mathbf{0}}] P_1(\cos \theta) \frac{d\Omega}{\Omega} = -\frac{N(0)^\star}{2} \int v_{\mathbf{k}-\mathbf{k}'} \cos \theta \frac{\sin \theta d\theta d\phi}{4\pi} \quad (74)$$

$$v_{\mathbf{k}-\mathbf{k}'} = \frac{4\pi}{(\mathbf{k} - \mathbf{k}')^2 + \lambda^2} = \frac{4\pi}{k^2 + k'^2 + \lambda^2 - 2kk' \cos \theta} \quad (75)$$

The terms in $v_{\mathbf{0}}$ are neglected because the integral from 0 to π of a constant times $P_1(\cos \theta)$ vanishes.

$\mathbf{k}, \mathbf{k}'$ have nearly the same modulus ($= k_F$) and span all possible relative angles.

$$F_1^s = -\frac{2\pi N(0)^\star}{2} \int_0^\pi \frac{\cos \theta \sin \theta d\theta d\phi}{2k_F^2 + \lambda^2 - 2k_F^2 \cos \theta} \quad (76)$$

Change variable from θ to $u = \cos \theta$, $du = -\sin \theta d\theta$.

$$F_1^s = -\pi N(0)^\star \int_{-1}^1 \frac{u du}{a + bu} = \quad (77)$$

where $a = 2k_F^2 + \lambda^2$, $b = -2k_F^2$.

$$\begin{aligned} F_1^s &= -\frac{\pi N(0)^\star}{b} \int_{-1}^1 \frac{(a + bu - a) du}{a + bu} = -\frac{\pi N(0)^\star}{b} \left\{ 2 - \frac{a}{b} \log \left| \frac{a+b}{a-b} \right| \right\} \\ &= \frac{\pi N(0)^\star}{2k_F^2} \left\{ 2 + \frac{2k_F^2 + \lambda^2}{2k_F^2} \log \left(\frac{\lambda^2}{4k_F^2 + \lambda^2} \right) \right\} \end{aligned} \quad (78)$$

Then it is obvious how to compute the effective mass $m^\star = m(1 + F_1^s)$.

For $\lambda \rightarrow 0$ the F_1^s coefficient diverges.

Some useful relations:

Commutation relations for Bosons:

$$[\hat{a}_\alpha, \hat{a}_\beta] = [\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger] = 0 \quad (79)$$

$$[\hat{a}_\alpha, \hat{a}_\beta^\dagger] = \delta_{\alpha\beta} \quad (80)$$

Anti-commutation relations for Fermions:

$$\{\hat{a}_\alpha, \hat{a}_\beta\} = \{\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger\} = 0 \quad (81)$$

$$\{\hat{a}_\alpha, \hat{a}_\beta^\dagger\} = \delta_{\alpha\beta} \quad (82)$$

Fourier transform:

$$f(\omega) = \int_{-\infty}^{\infty} f(\tau) e^{i\omega\tau} d\tau \quad (83)$$

$$f(\tau) = \int_{-\infty}^{\infty} f(\omega) e^{-i\omega\tau} \frac{d\omega}{2\pi} \quad (84)$$

Special relation:

$$\frac{1}{x \pm i\eta} = P \left(\frac{1}{x} \right) \mp i\pi\delta(x) \quad (85)$$

Chain-rule for thermodynamic derivatives:

$$V \frac{\partial}{\partial V} = -\rho \frac{\partial}{\partial \rho} = \frac{r_s}{3} \frac{d}{dr_s} \quad (86)$$

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:

$$E[\mathcal{N}_{\mathbf{k},\sigma}] = E_0 + \sum_{\mathbf{k},\sigma} \mathcal{E}_{\mathbf{k},\sigma} \delta\mathcal{N}_{\mathbf{k},\sigma} + \frac{1}{2} \sum_{\mathbf{k},\sigma,\mathbf{k}',\sigma'} f_{\mathbf{k},\sigma,\mathbf{k}',\sigma'} \delta\mathcal{N}_{\mathbf{k},\sigma} \delta\mathcal{N}_{\mathbf{k}',\sigma'} \quad (87)$$

- $\mathcal{E}_{\mathbf{k},\sigma}$ 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).