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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: 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 $\alpha = \beta$.

Solution:

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

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

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

where:

$$S_\alpha = \sum_{\gamma<\alpha} n_\gamma \tag{4}$$

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

$$\hat{a}_\alpha^\dagger \mid n_1, n_2, ..., n_\alpha, ...\rangle = \sqrt{n_\alpha + 1} \mid n_1, n_2, ..., n_\alpha + 1, ...\rangle \tag{5}$$

$$\hat{a}_\alpha \mid n_1, n_2, ..., n_\alpha, ...\rangle = \sqrt{n_\alpha} \mid n_1, n_2, ..., n_\alpha - 1, ...\rangle \tag{6}$$

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

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

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

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

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

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

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

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

The case $\alpha = \beta$ is trivial for Fermions, since the double application of $\hat{a}_\alpha^\dagger$ to $\mid 0\rangle$ 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 replacig anti-commutation.

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

$$\hat{a}^\dagger_\alpha \mid 0\rangle = \mid \alpha\rangle$$

$$\hat{a}^\dagger_\alpha \mid \alpha\rangle = \sqrt{2} \mid \alpha\alpha\rangle$$

$$\sqrt{2}\hat{a}_\alpha \mid \alpha\alpha\rangle = 2 \mid \alpha\rangle$$

$$2\hat{a}_\alpha \mid \alpha\rangle = 2 \mid 0\rangle \rightarrow \langle 0 \mid \hat{a}_\alpha \hat{a}_\alpha \hat{a}^\dagger_\alpha \hat{a}^\dagger_\alpha \mid 0\rangle = 2$$

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

$$\hat{N} = \sum_\alpha \hat{a}^\dagger_\alpha \hat{a}_\alpha \tag{8}$$

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

Show that:

$$[\hat{N}, \hat{a}_\alpha] = -\hat{a}_\alpha \tag{9}$$

$$[\hat{N}, \hat{a}^\dagger_\alpha] = \hat{a}^\dagger_\alpha \tag{10}$$

Solutions:
We need to compute:

$$[\hat{N}, \hat{a}_\alpha] = \left[\sum_\beta \hat{a}^\dagger_\beta \hat{a}_\beta, \hat{a}_\alpha\right] = \left[\hat{a}^\dagger_\alpha \hat{a}_\alpha, \hat{a}_\alpha\right] = \tag{11}$$

$$= \hat{a}^\dagger_\alpha \hat{a}_\alpha \hat{a}_\alpha - \hat{a}_\alpha \hat{a}^\dagger_\alpha \hat{a}_\alpha$$

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

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

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

The $[\hat{N}, \hat{a}^\dagger_\alpha] = \hat{a}^\dagger_\alpha$ 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:

$$f(a_\lambda) = c_0 + c_1 a_\lambda + c_2 a_\lambda^2 ... + c_n a_\lambda^n \tag{12}$$

Show that:

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

and:

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

Solution:

The starting point is the relation:

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

which is valid provided B commutes with the $[A, B]$ commutator. The relation is easy to very, 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 $f(a_\lambda)$:

$$[a_\lambda^\dagger, f(a_\lambda)] = c_1[a_\lambda^\dagger, a_\lambda] + c_2[a_\lambda^\dagger, a_\lambda^2] ... + c_n[a_\lambda^\dagger, a_\lambda^n] \tag{16}$$

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

$$[a_\lambda^\dagger, f(a_\lambda)] = c_1[a_\lambda^\dagger, a_\lambda] + 2c_2 a_\lambda [a_\lambda^\dagger, a_\lambda] ... + nc_n a_\lambda^{n-1}[a_\lambda^\dagger, a_\lambda] \tag{17}$$

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

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

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

Problem (2)

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

$$\chi^T_{AB}(t) \equiv -i\langle\Psi_0 \mid T[\hat{A}(t)\hat{B}(0)] \mid \Psi_0\rangle \tag{19}$$

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

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

and the time ordering operator is by:

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

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

(i) Compute the Fourier transform:

$$\chi^T_{AB}(\omega) = \lim_{\eta\to 0^+}\int_{-\infty}^{+\infty} \chi^T_{AB}(t)e^{i\omega t-\eta|t|}dt \tag{22}$$

and show that it is given by:

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

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

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 $\chi^T_{AB}(t)$.
According to the definition:

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

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

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

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

$$\chi^T_{AB}(t) = \begin{cases} \hat{A}(t)\hat{B} & t > 0 \\ \\ \hat{B}\hat{A}(t) & t < 0 \\ \end{cases} \tag{26}$$

Let us now compute:

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

Inserting the explicit time-dependence:

$$= \int_{-\infty}^{0} \langle \Psi_0 \mid \hat{B} e^{i\hat{H}t} \hat{A} e^{-i\hat{H}t} \mid \Psi_0 \rangle e^{i\omega t + \eta t} dt + \int_0^{\infty} \langle \Psi_0 \mid e^{i\hat{H}t} \hat{A} e^{-i\hat{H}t} \hat{B} \mid \Psi_0 \rangle e^{i\omega t - \eta t} dt \tag{28}$$

$$= \int_{-\infty}^{0} e^{-iE_0 t} \langle \Psi_0 \mid \hat{B} e^{i\hat{H}t} \hat{A} \mid \Psi_0 \rangle e^{i\omega t + \eta t} dt + \int_0^{\infty} e^{iE_0 t} \langle \Psi_0 \mid \hat{A} e^{-i\hat{H}t} \hat{B} \mid \Psi_0 \rangle e^{i\omega t - \eta t} dt$$

Inserting a complete basis of eigenfunctions of the Hamiltonian:

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

$$+ \sum_n \int_0^{\infty} e^{-i(E_n - E_0)t} \langle \Psi_0 \mid \hat{A} \mid \Psi_n \rangle \langle \Psi_n \mid \hat{B} \mid \Psi_0 \rangle e^{i\omega t - \eta t} dt$$

$$= \sum_n B_{0n} A_{n0} \int_{-\infty}^{0} e^{i\omega_{n0} t} e^{i\omega t + \eta t} dt \tag{30}$$

$$+ \sum_n A_{0n} B_{n0} \int_0^{\infty} e^{-i\omega_{n0} t} e^{i\omega t - \eta t} dt$$

$$= \sum_n B_{0n} A_{n0} \left. \frac{e^{i\omega_{n0} t} e^{i\omega t + \eta t}}{i\omega_{n0} + i\omega + \eta} \right|_{-\infty}^{0} \tag{31}$$

$$+ \sum_n A_{0n} B_{n0} \left. \frac{e^{-i\omega_{n0} t} e^{i\omega t - \eta t}}{-i\omega_{n0} + i\omega - \eta} \right|_{0}^{\infty}$$

$$= -i \sum_n \frac{B_{0n} A_{n0}}{\omega_{n0} + \omega - i\eta} \tag{32}$$

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

Now multiplying times $-i$, we obtain:

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

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

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

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

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

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

Solution:

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

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

Let us compute:

$$\int_{-\infty}^{\infty}\chi_{AB}(t)e^{i\omega t-\eta|t|}dt=\int_0^{\infty}\langle\Psi_0\mid\hat{A}(t)\hat{B}-\hat{B}\hat{A}(t)\mid\Psi_0\rangle e^{i\omega t-\eta t}dt \tag{36}$$

$$=\int_0^{\infty}\langle\Psi_0\mid e^{i\hat{H}t}\hat{A}e^{-i\hat{H}t}\hat{B}-\hat{B}e^{i\hat{H}t}\hat{A}e^{-i\hat{H}t}\mid\Psi_0\rangle e^{i\omega t-\eta t}dt$$

Inserting a complete set of eigenfunctions of the Hamiltonian:

$$=\sum_n A_{0n}B_{n0}\int_0^{\infty}e^{-i(E_n-E_0)t}e^{i\omega t-\eta t}dt-\sum_n A_{n0}B_{0n}\int_0^{\infty}e^{i(E_n-E_0)t}e^{i\omega t-\eta t}dt \tag{37}$$

$$=\sum_n A_{0n}B_{n0}\left.\frac{e^{-i\omega_{n0}t}e^{i\omega t-\eta t}}{-i\omega_{n0}+i\omega-\eta}\right|_0^{\infty}-\sum_n A_{n0}B_{0n}\left.\frac{e^{i\omega_{n0}t}e^{i\omega t-\eta t}}{i\omega_{n0}+i\omega-\eta}\right|_0^{\infty}$$

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

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 $\chi^T_{AB}(\omega)$ 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 $\chi^T_{AB}(\omega)$ and $\chi_{AB}(\omega)$.

Solution:

The poles of $\chi^T_{AB}(\omega)$ in the complex ω plane are at $\omega = \omega_{n0} - i\eta$ and at $\omega = -\omega_{n0} + i\eta$. Therefore, $\chi^T_{AB}(\omega)$ 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:

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

where α is a positive numerical coefficient.

Compute the exchange-correlation potential:

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

Solution:

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

$$\rho(x) \to \rho(x) + \delta\rho(x) \tag{40}$$

$$\frac{d}{dx}\rho(x) \to \frac{d}{dx}\rho(x) + \frac{d}{dx}\delta\rho(x) \tag{41}$$

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

$$E_{XC}[\rho + \delta\rho] = \int \alpha[\rho(x) + \delta\rho(x)]^{4/3}dx \tag{42}$$

$$+\frac{1}{2}\int K(\rho+\delta\rho)\left(\frac{d\rho(x)}{dx} + \frac{d\delta\rho(x)}{dx}\right)^2 dx$$

$$= \int \alpha[\rho^{4/3}(x) + \frac{4}{3}\rho^{1/3}(x)\delta\rho(x) + ...]dx$$

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

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

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

These are terms appearing in the XC potential.

We have also:

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

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:

$$\frac{1}{2}\int K(\rho)[2\frac{d\rho(x)}{dx}\frac{d\delta\rho(x)}{dx}]dx = \tag{45}$$

$$K(\rho)\frac{d\rho(x)}{dx}\delta\rho(x)\Big|_{-\infty}^{\infty} - \int \frac{d}{dx}\left[K(\rho)\frac{d\rho(x)}{dx}\right]\delta\rho(x)dx$$

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

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

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

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

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:

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

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:

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

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:

$$\frac{\partial}{\partial V} = \frac{\partial \rho}{\partial V}\frac{\partial}{\partial \rho} \tag{50}$$

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

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

At point (ii) it has been shown that:

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

Hence:

$$\frac{P}{\rho} = -\rho\frac{\partial \epsilon}{\partial \rho} = -\frac{r_s}{3}\frac{d}{dr_s}\left\{\frac{2.21}{r_s^2} - \frac{0.916}{r_s}\right\} \tag{53}$$

$$-\frac{r_s}{3}\left\{-2\frac{2.21}{r_s^3} + \frac{0.916}{r_s^2}\right\} = \frac{2}{3}\frac{2.21}{r_s^2} - \frac{1}{3}\frac{0.916}{r_s}$$

When this expression vanishes at:

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

$P = 0$, 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 $\chi^T_{AB}(t)$ is:

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

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

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

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

and the perturbation Hamiltonian contains a pair interaction term:

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

(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:

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

and we have two pairing schemes: $\langle \hat{a}_\beta(t)\hat{a}^\dagger_\alpha(t)\rangle\langle \hat{a}_\delta \hat{a}^\dagger_\gamma\rangle$, and $\langle \hat{a}_\beta(t)\hat{a}^\dagger_\gamma\rangle\langle \hat{a}_\delta \hat{a}^\dagger_\alpha(t)\rangle$. The original sequence in Eq. 55 was: $\hat{a}^\dagger_\alpha(t)\hat{a}_\beta(t)\hat{a}^\dagger_\gamma \hat{a}_\delta$. 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:

$$\langle \hat{a}_\beta \hat{a}^\dagger_\alpha \rangle \langle \hat{a}_\delta \hat{a}^\dagger_\gamma \rangle \langle \hat{a}_c \hat{a}^\dagger_a \rangle \langle \hat{a}_d \hat{a}^\dagger_b \rangle \tag{60}$$

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

$$\begin{array}{ccc} \hat{A}(t) & \hat{a}_\beta(t) & \hat{a}^\dagger_\alpha(t) \\ \hat{B} & \hat{a}_\delta & \hat{a}^\dagger_\gamma \\ \hat{H}_1 & \hat{a}_c(t_1) & \hat{a}^\dagger_a(t_1) \\ \hat{H}_1 & \hat{a}_d(t_1) & \hat{a}^\dagger_b(t_1) \end{array} \tag{61}$$

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:

$$\langle \hat{a}_\beta \hat{a}^\dagger_\alpha \rangle \langle \hat{a}_\delta \hat{a}^\dagger_\gamma \rangle \langle \hat{a}_c \hat{a}^\dagger_a \rangle \langle \hat{a}_d \hat{a}^\dagger_b \rangle \tag{62}$$

and:

$$\langle \hat{a}_\beta \hat{a}^\dagger_\alpha \rangle \langle \hat{a}_c \hat{a}^\dagger_a \rangle \langle \hat{a}_\delta \hat{a}^\dagger_\gamma \rangle \langle \hat{a}_d \hat{a}^\dagger_b \rangle \tag{63}$$

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:

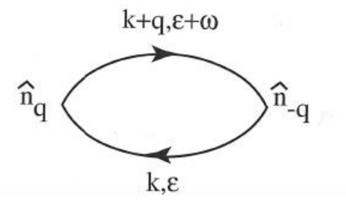

Figure 1: Zero order diagram

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

Solution:

The diagram corresponds to the integral:

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

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:

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

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

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

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

Problem (5)

Consider a system of Fermions interacting through the pair potential:

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

whose Fourier transform is:

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

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:

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

(i) 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.

Solution:

The energy functional is:

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

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

where:

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

The bare quasi-particle energy is:

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

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

$$f_{\mathbf{k}\sigma;\mathbf{k}'\sigma'} = \frac{1}{V} \left[v_0 - v_{\mathbf{k}-\mathbf{k}'}\delta_{\sigma\sigma'}\right] \tag{73}$$

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

What happens for $\lambda \to 0$?

Solution:

According to the definition:

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

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

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.

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

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

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

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

$$F_1^s = -\frac{\pi N(0)^\star}{b} \int_{-1}^{1} \frac{(a + bu - a)du}{a + bu} = -\frac{\pi N(0)^\star}{b} \left\{ 2 - \frac{a}{b} \log\left|\frac{a+b}{a-b}\right| \right\} \tag{78}$$

$$= \frac{\pi N(0)^\star}{2k^F} \left\{ 2 + \frac{2k_F^2 + \lambda^2}{2k_F^2} \log\left(\frac{\lambda^2}{4k_F^2 + \lambda^2}\right) \right\}$$

Then it is obvious how to compute the effective mass $m^\star = m(1 + F_1^s)$.
For $\lambda \to 0$ the F_1^s coefficient diverges.

Some useful relations:

Commutation relations for Bosons:

$$[\hat{a}_\alpha, \hat{a}_\beta] = [\hat{a}^\dagger_\alpha, \hat{a}^\dagger_\beta] = 0 \tag{79}$$

$$[\hat{a}_\alpha, \hat{a}^\dagger_\beta] = \delta_{\alpha\beta} \tag{80}$$

Anti-commutation relations for Fermions:

$$\{\hat{a}_\alpha, \hat{a}_\beta\} = \{\hat{a}^\dagger_\alpha, \hat{a}^\dagger_\beta\} = 0 \tag{81}$$

$$\{\hat{a}_\alpha, \hat{a}^\dagger_\beta\} = \delta_{\alpha\beta} \tag{82}$$

Fourier transform:

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

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

Special relation:

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

Chain-rule for thermodynamic derivatives:

$$V\frac{\partial}{\partial V} = -\rho\frac{\partial}{\partial \rho} = \frac{r_s}{3}\frac{d}{dr_s} \tag{86}$$

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:

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

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