Exercise-sheet 9 (December 21, 2015)

1 In-class exercises

1.1 Dyson's equation

Revisit the ideas (and the diagramatic representation) behind Dyson's equation

$$G(\boldsymbol{x}\tau,\boldsymbol{x}'\tau') = G^{(0)}(\boldsymbol{x}\tau,\boldsymbol{x}'\tau') + \iint_0^\beta d\tau_1 d\tau_1' \iint d^3x_1 d^3x_1' G^{(0)}(\boldsymbol{x}\tau,\boldsymbol{x_1}\tau_1)\Sigma^*(\boldsymbol{x_1}\tau_1,\boldsymbol{x_1'}\tau_1')G(\boldsymbol{x_1'}\tau_1',\boldsymbol{x}'\tau'), \quad (1)$$

where $G(\boldsymbol{x}\tau,\boldsymbol{x}'\tau')$ is the full (interacting) Green's function, $G^{(0)}(\boldsymbol{x}\tau,\boldsymbol{x}'\tau')$ is the free particle Green's function and $\Sigma^*(\boldsymbol{x}\tau,\boldsymbol{x}'\tau')$ is the *proper* self-energy.

1.2 Self-consistent Hartree-Fock approximation

Consider the generic Hamiltonian $H = H_0 + H_1$, where

$$H_0 = \int d^3x\, \psi^\dagger(\boldsymbol{x}) \left(-\frac{\nabla^2}{2m} - \mu + U(\boldsymbol{x}) \right) \psi(\boldsymbol{x}), \quad (2)$$

with $U(\boldsymbol{x})$ a static spin-independent external potential and

$$H_1 = \frac{1}{2} \iint d^3x d^3x' \psi^\dagger(\boldsymbol{x})\psi^\dagger(\boldsymbol{x}')V(\boldsymbol{x}-\boldsymbol{x}')\psi(\boldsymbol{x}')\psi(\boldsymbol{x}), \quad (3)$$

where $V(\boldsymbol{x}-\boldsymbol{x}')$ is a two-body potential.

(a) Draw (the diagrams of) the self-consistent Hartree-Fock approximation for the proper self-energy and the corresponding Dyson's equation, in real space.

(b) Given the following expansion for $\tilde{G}(\boldsymbol{x},\boldsymbol{x}',\omega_n)$ and $\tilde{G}^{(0)}(\boldsymbol{x},\boldsymbol{x}',\omega_n)$

$$\tilde{G}(\boldsymbol{x},\boldsymbol{x}',\omega_n) = \sum_j \frac{\phi_j(\boldsymbol{x})\phi_j^*(\boldsymbol{x}')}{i\omega_n - (\epsilon_j - \mu)} \quad \text{and} \quad \tilde{G}^{(0)}(\boldsymbol{x},\boldsymbol{x}',\omega_n) = \sum_j \frac{\phi_j^{(0)}(\boldsymbol{x})\phi_j^{(0)*}(\boldsymbol{x}')}{i\omega_n - (\epsilon_j^{(0)} - \mu)}, \quad (4)$$

with $H\phi_j(\boldsymbol{x}) = (\epsilon_j - \mu)\phi_j(\boldsymbol{x})$ and $H_0\phi_j^{(0)}(\boldsymbol{x}) = (\epsilon_j^{(0)} - \mu)\phi_j^{(0)}(\boldsymbol{x})$, find the self-consistent Hartree-Fock equations for the set $\{\phi_j(\boldsymbol{x})\}$.

2 Homework - due date: January 11, 2016 (50 points).

2.1 Self-consistent Hartree-Fock in k-space (15 points)

Consider a uniform system where the external potential $U(\boldsymbol{x}) = 0$ (see equation 2) and the proper self-energy $\Sigma^*(\boldsymbol{x}, \boldsymbol{x}') = \Sigma^*(\boldsymbol{x} - \boldsymbol{x}')$.

(a) Draw once again (the diagrams of) the self-consistent Hartree-Fock approximation for the proper self-energy and the corresponding Dyson's equation, just as was done in the exercise class, but this time in momentum space.

(b) Use Feynman rules in momentum space to give an expression for the proper self-energy in terms of the two-body potential V.

(c) Use Dyson's equation to find the self-consistency condition for the energy of the interacting system.

2.2 First-order perturbation theory of the electron gas (35 points)

Consider an interacting electron gas placed in a uniformly distributed positive background, chosen such as to maintain the overall charge neutrality of the system. Assume the system is confined to a large cubical box of length L with periodic boundary conditions, such that the single-particle wave functions are plane-waves

$$\psi_{\boldsymbol{k}}(\boldsymbol{x}) = \frac{1}{\sqrt{V}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}}, \tag{5}$$

with $V = L^3$ the volume of the box and $k_i = 2\pi n_i/L$, $n_i = 0, \pm 1, \pm 2, \ldots$

The total Hamiltonian of the system reads

$$H = H_{el} + H_b + H_{el-b}, \tag{6}$$

where

$$H_{el} = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m} + \frac{e^2}{2} \sum_{i \neq j}^{N} \frac{e^{-\mu|\boldsymbol{r}_i - \boldsymbol{r}_j|}}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}, \tag{7}$$

is the electronic Hamiltonian,

$$H_b = \frac{e^2}{2} \iint d^3x \, d^3x' \, n(\boldsymbol{x}) n(\boldsymbol{x}') \frac{e^{-\mu|\boldsymbol{x} - \boldsymbol{x}'|}}{|\boldsymbol{x} - \boldsymbol{x}'|}, \tag{8}$$

is the energy of the positive background whose particle density is $n(\boldsymbol{x})$ and

$$H_{el-b} = -e^2 \sum_{i=1}^{N} \int d^3x \, n(\boldsymbol{x}) \frac{e^{-\mu|\boldsymbol{x} - \boldsymbol{r}_i|}}{|\boldsymbol{x} - \boldsymbol{r}_i|}, \tag{9}$$

is the interaction energy between the electrons and the positive background.

The exponential convergence factor in equations (7) - (9) is introduced so that the expressions remain well-defined in the thermodynamic limit ($V \to \infty$, $N \to \infty$ but N/V finite). At the end of the calculation we will let μ vanish.

(a) Given that the only dynamical variables of our problem are the electrons of the system, H_b and H_{el-b} are just real numbers. Compute these quantities. (HINT: the integrals are readily evaluated by shifting the origin of integration, e.g. $\boldsymbol{z} \equiv \boldsymbol{x} - \boldsymbol{x}'$ with $\boldsymbol{x}'$ fixed in eq. 8)

(b) The electronic Hamiltonian can be written in a second-quantized form as follows

$$H_{el} = \sum_{\boldsymbol{k},\boldsymbol{k'}} \langle \boldsymbol{k}| \frac{p^2}{2m} |\boldsymbol{k}'\rangle c^\dagger_{\boldsymbol{k}} c_{\boldsymbol{k}'} + \frac{e^2}{2} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} \langle \boldsymbol{k}_1 \boldsymbol{k}_2| \frac{e^{-\mu|\boldsymbol{x}-\boldsymbol{y}|}}{|\boldsymbol{x}-\boldsymbol{y}|} |\boldsymbol{k}_3 \boldsymbol{k}_4\rangle c^\dagger_{\boldsymbol{k}_1} c^\dagger_{\boldsymbol{k}_2} c_{\boldsymbol{k}_4} c_{\boldsymbol{k}_3}, \tag{10}$$

where $c^\dagger_{\boldsymbol{k}}$ ($c_{\boldsymbol{k}}$) creates (annihilates) and electron with momentum $\boldsymbol{k}$.

Evaluate the matrix elements in equation (10) (e.g. by inserting resolutions of the identity as $\mathbb{1} = \int d^3x |\boldsymbol{x}\rangle\langle\boldsymbol{x}|$) and show the Hamiltonian of the full system H can be rewritten as

$$H = \sum_{\boldsymbol{k}} \frac{k^2}{2m} c^\dagger_{\boldsymbol{k}} c_{\boldsymbol{k}} + \frac{1}{V}\frac{e^2}{2} \sum_{\boldsymbol{kpq}} \frac{4\pi}{q^2+\mu^2} c^\dagger_{\boldsymbol{k}+\boldsymbol{p}} c^\dagger_{\boldsymbol{p}-\boldsymbol{q}} c_{\boldsymbol{p}} c_{\boldsymbol{k}} - \frac{e^2}{2}\frac{N^2}{V}\frac{4\pi}{\mu^2}. \tag{11}$$

(c) Show the $\boldsymbol{q} = 0$ term in the second sum of equation (11) simplifies to $\frac{e^2}{2}\frac{4\pi}{\mu^2}\frac{1}{V}(\hat{N}^2 - \hat{N})$, with $\hat{N}$ the total number operator.

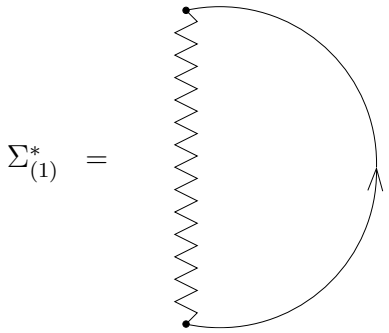
Remark I: Since we are interested in the zero-temperature limit of our problem, we shall deal with states of fixed number of particles and we may replace $\hat{N}$ by its eigenvalue N. Thus we see the $\boldsymbol{q} = 0$ component of $V(\boldsymbol{q})$ cancels the uniform positive background. The remaining term yields and energy *per particle* of $-\frac{e^2}{2}\frac{4\pi}{\mu^2}\frac{1}{V}$. Such a contribution cancels in the limit $L \to \infty$, $\mu \to 0$ (is this clear?). Hence we may now safely set $\mu = 0$.

Remark II: We can now transform the full Hamiltonian to the following dimensionless form

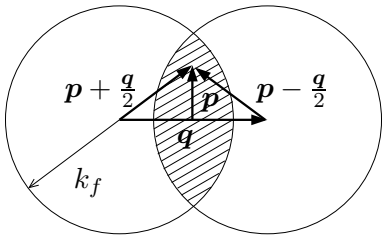
$$H = \frac{e^2}{a_0 r_s^2}\left(\sum_{\bar{\boldsymbol{k}}} \frac{\bar{\boldsymbol{k}}^2}{2} c^\dagger_{\bar{\boldsymbol{k}}} c_{\bar{\boldsymbol{k}}} + \frac{r_s}{2\bar{V}} \sum_{\bar{\boldsymbol{k}},\bar{\boldsymbol{p}},\bar{\boldsymbol{q}}\neq 0} \frac{4\pi}{\bar{\boldsymbol{q}}^2} c^\dagger_{\bar{\boldsymbol{k}}+\bar{\boldsymbol{k}}} c^\dagger_{\bar{\boldsymbol{p}}-\bar{\boldsymbol{q}}} c_{\bar{\boldsymbol{p}}} c_{\bar{\boldsymbol{k}}} \right), \tag{12}$$

where $a_0 = 1/me^2$ is the Bohr radius and $r_s = r_0/a_0$ characterizes the density of the system, for r_0 is defined in terms of the volume per particle $V \equiv \frac{4}{3}\pi r_0^3 N$ and hence corresponds to the inter-particle spacing. Moreover, we introduced $\bar{V} = r_0^{-3}V$, $\bar{\boldsymbol{k}} = r_0\boldsymbol{k}$, $\bar{\boldsymbol{p}} = r_0\boldsymbol{p}$ and $\bar{\boldsymbol{q}} = r_0\boldsymbol{q}$.

This is an important result, for it implies the potential energy becomes a small perturbation as $r_s \to 0$, corresponding to the high density limit ($r_0 \to 0$). Thus, the leading term in the interaction energy of a high-density electron gas **can be obtained with first-order perturbation theory**.



(a) First-order proper self-energy for the electron gas.



(b) Integration region in momentum space for F_1. The marked region is such that $k_F > |\boldsymbol{p} + \frac{\boldsymbol{q}}{2}|$ and $k_F > |\boldsymbol{p} - \frac{\boldsymbol{q}}{2}|$

(d) One can show that within first-order perturbation theory the free energy of a generic interacting system is given by

$$F(T, V, \mu) = F_0 + 2V \int \frac{d^3k}{(2\pi)^3} \frac{1}{\beta} \sum_n e^{i\omega_n \delta} \Sigma^*_{(1)}(\boldsymbol{k}, \omega_n) \tilde{G}^{(0)}(\boldsymbol{k}, \omega_n), \tag{13}$$

with F_0 the kinetic energy contribution, $\Sigma^*_{(1)}$ the first-order approximation to the proper self-energy and $\tilde{G}^{(0)}$ the free-particle (Matsubara) Green's function. Use Feynman rules to calculate $\Sigma^*_{(1)}$ for the electron gas and show the integral above (which we defined as F_1) simplifies to

$$F_1 = -2V \iint \frac{d^3k}{(2\pi)^3} \frac{d^3q}{(2\pi)^3} V(\boldsymbol{k} - \boldsymbol{q}) n_F(\epsilon^{(0)}_{\boldsymbol{q}}) n_F(\epsilon^{(0)}_{\boldsymbol{k}}), \tag{14}$$

where $V(\boldsymbol{k})$ is the $\boldsymbol{k}$ component of the Coulomb potential you computed in (b) (with $\mu = 0$, of course).

(HINT: Remember that for the electron gas the $\boldsymbol{q} = 0$ component of the interaction, i.e. the Hartree term, cancels the positive background contribution. The proper self-energy is therefore given by Fig.1a)

Remark III: In the limit of low temperatures one replaces the Fermi functions in eq. 14 by Heaviside functions and writes the first-order contribution to the interaction energy as

$$E_1 = -Ve^2 4\pi \int \frac{d^3q}{(2\pi)^3} \frac{1}{q^2} \int \frac{d^3p}{(2\pi)^3} \Theta(k_f - |\boldsymbol{p} - \frac{\boldsymbol{q}}{2}|) \Theta(k_f - |\boldsymbol{p} + \frac{\boldsymbol{q}}{2}|), \tag{15}$$

where $k_f = (\frac{3\pi^2 N}{V})^{1/3} = (\frac{9\pi}{4})^{1/3} r_0^{-1}$ is the Fermi momentum.

(Note: To get eq. 15 we first shifted $\boldsymbol{q} = \boldsymbol{q} + \boldsymbol{k}$ and then made the change of variables $\boldsymbol{k} = \boldsymbol{p} - \frac{\boldsymbol{q}}{2}$).

(e) Show that eq. 15 yields

$$E_1 = -\frac{e^2}{2a_0} N \frac{0.916}{r_s} \tag{16}$$

(HINT: the integral over $\boldsymbol{p}$ is simply the volume of the marked region in figure 1b).

(f) Finally, show the non-interacting (kinetic) energy of the electron gas

$$E_0 = V \int \frac{d^3k}{(2\pi)^3} \frac{\boldsymbol{k}^2}{2m} \Theta(k_f - k)$$

is given by

$$E_0 = \frac{e^2}{2a_0} N \frac{2.21}{r_s^2}. \tag{17}$$

FINAL REMARK: You have then showed the ground-state energy per particle in the high-density limit is given approximately by

$$\frac{E}{N} = \frac{e^2}{2a_0} \left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + ... \right) \tag{18}$$

(g) Plot $\frac{E}{N}$ as a function of r_s.

Unfortunately, the second-order term in the perturbative expansion goes as $r_s^2 \ln r_s$ and hence diverges in the high-density limit.