Exercise-sheet 9 (December 22, 2017)

1 Homework - due date: January 5, 2018 (55 points).

1.1 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

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

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

The total Hamiltonian of the system reads

$$H = H_{el} + H_b + H_{el-b}, \tag{2}$$

where

$$H_{el} = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m} + \frac{e^2}{2} \sum_{i\neq j}^{N} \frac{e^{-\mu|\boldsymbol{r}_i - \boldsymbol{r}_j|}}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}, \tag{3}$$

is the electronic Hamiltonian,

$$H_b = \frac{e^2}{2} \iint d^3x\, d^3x'\, n(\boldsymbol{x}) n(\boldsymbol{x}') \frac{e^{-\mu|\boldsymbol{x}-\boldsymbol{x}'|}}{|\boldsymbol{x}-\boldsymbol{x}'|}, \tag{4}$$

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

$$H_{el-b} = -e^2 \sum_{i=1}^{N} \int d^3x\, n(\boldsymbol{x}) \frac{e^{-\mu|\boldsymbol{x}-\boldsymbol{r}_i|}}{|\boldsymbol{x}-\boldsymbol{r}_i|}, \tag{5}$$

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

The exponential convergence factor in equations (3) - (5) 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. 4)

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

$$H_{el} = \sum_{\boldsymbol{k},\boldsymbol{k}'} \langle \boldsymbol{k}| \frac{p^2}{2m} |\boldsymbol{k}'\rangle c^\dagger_{\boldsymbol{k}} c_{\boldsymbol{k}'} + \frac{e^2}{2} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} \langle \boldsymbol{k}_1\boldsymbol{k}_2| \frac{e^{-\mu|\boldsymbol{x}-\boldsymbol{y}|}}{|\boldsymbol{x}-\boldsymbol{y}|} |\boldsymbol{k}_3\boldsymbol{k}_4\rangle c^\dagger_{\boldsymbol{k}_1} c^\dagger_{\boldsymbol{k}_2} c_{\boldsymbol{k}_4} c_{\boldsymbol{k}_3}, \tag{6}$$

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

Evaluate the matrix elements in equation (6) (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

$$H = \sum_{\boldsymbol{k}} \frac{k^2}{2m} c^\dagger_{\boldsymbol{k}} c_{\boldsymbol{k}} + \frac{1}{V}\frac{e^2}{2} \sum_{\boldsymbol{kpq}} \frac{4\pi}{q^2+\mu^2} c^\dagger_{\boldsymbol{k}+\boldsymbol{p}} c^\dagger_{\boldsymbol{p}-\boldsymbol{q}} c_{\boldsymbol{p}} c_{\boldsymbol{k}} - \frac{e^2}{2}\frac{N^2}{V}\frac{4\pi}{\mu^2}. \tag{7}$$

(c) Show the $\boldsymbol{q} = 0$ term in the second sum of equation (7) 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

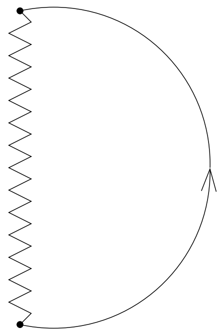
$$H = \frac{e^2}{a_0 r_s^2} \left(\sum_{\bar{\boldsymbol{k}}} \frac{\bar{\boldsymbol{k}}^2}{2} c^\dagger_{\bar{\boldsymbol{k}}} c_{\bar{\boldsymbol{k}}} + \frac{r_s}{2\bar{V}} \sum_{\bar{\boldsymbol{k}},\bar{\boldsymbol{p}},\bar{\boldsymbol{q}}\neq 0} \frac{4\pi}{\bar{\boldsymbol{q}}^2} c^\dagger_{\bar{\boldsymbol{k}}+\bar{\boldsymbol{k}}} c^\dagger_{\bar{\boldsymbol{p}}-\bar{\boldsymbol{q}}} c_{\bar{\boldsymbol{p}}} c_{\bar{\boldsymbol{k}}} \right), \tag{8}$$

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 $\bar{\boldsymbol{q}} = r_0 \boldsymbol{q}$.

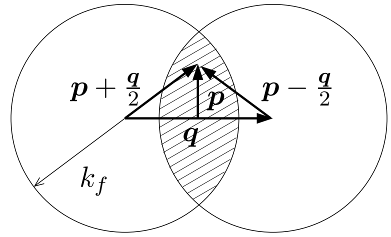
This is an important result, for it implies the potential energy becomes a small perturbation as $r_s \to 0$, corresponding to the high density limit ($r_0 \to 0$). Thus, the leading term in the interaction energy of a high-density electron gas **can be obtained with first-order perturbation theory**.

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

$$F(T,V,\mu) = F_0 + 2V \int \frac{d^3k}{(2\pi)^3} \frac{1}{\beta} \sum_n e^{i\omega_n \delta} \Sigma^*_{(1)}(\boldsymbol{k},\omega_n) \tilde{G}^{(0)}(\boldsymbol{k},\omega_n), \tag{9}$$

$\Sigma^*_{(1)} \quad =$ 

(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 $k_F > |\boldsymbol{p}-\frac{\boldsymbol{q}}{2}|$

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

$$F_1 = -2V \iint \frac{d^3k}{(2\pi)^3}\frac{d^3q}{(2\pi)^3} V(\boldsymbol{k}-\boldsymbol{q}) n_F(\epsilon^{(0)}_{\boldsymbol{q}}) n_F(\epsilon^{(0)}_{\boldsymbol{k}}), \tag{10}$$

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. 10 by Heaviside functions and writes the first-order contribution to the interaction energy as

$$E_1 = -Ve^2 4\pi \int \frac{d^3q}{(2\pi)^3}\frac{1}{q^2}\int \frac{d^3p}{(2\pi)^3}\Theta(k_f - |\boldsymbol{p}-\frac{\boldsymbol{q}}{2}|)\Theta(k_f - |\boldsymbol{p}+\frac{\boldsymbol{q}}{2}|), \tag{11}$$

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. 11 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. 11 yields

$$E_1 = -\frac{e^2}{2a_0} N \frac{0.916}{r_s} \tag{12}$$

(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

$$E_0 = \frac{e^2}{2a_0} N \frac{2.21}{r_s^2}. \tag{13}$$

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

$$\frac{E}{N} = \frac{e^2}{2a_0}\left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + ...\right) \tag{14}$$

(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.

1.2 Sommerfeld expansion (10 points)

Consider the following integral

$$I = \int_0^\infty \frac{f(\epsilon) d\epsilon}{e^{\beta(\epsilon-\mu)} + 1}. \tag{15}$$

where $f(\epsilon)$ is such that I converges and $\beta = 1/T$

(a) Perform the change of variables $z = \beta(\epsilon - \mu)$ and show that the integral (15) can be rewritten as

$$I = T \int_0^{\mu/T} \frac{f(\mu - Tz)}{e^{-z} + 1}\, dz + T \int_0^\infty \frac{f(\mu + Tz)}{e^z + 1}\, dz. \tag{16}$$

(b) Further, rewrite I as follows

$$I = T \int_0^{\mu/T} f(\mu - Tz)\, dz - T \int_0^{\mu/T} \frac{f(\mu - Tz)}{e^z + 1}\, dz + T \int_0^\infty \frac{f(\mu + Tz)}{e^z + 1}\, dz. \tag{17}$$

After replacing the upper limit in the second integral above by ∞ (such a replacement makes sense at temperatures for which $\mu/T \gg 1$ and thus amount to neglecting exponentially small terms) one gets

$$I = \int_0^\mu f(\epsilon)\, d\epsilon + T \int_0^\infty \frac{f(\mu + Tz) - f(\mu - Tz)}{e^z + 1}\, dz. \tag{18}$$

(c) Expand the numerator of the integrand in the equation above as a Taylor series of z to get

$$I = \int_0^\mu f(\epsilon)\, d\epsilon + 2T^2 f'(\mu) \int_0^\infty \frac{z}{e^z + 1}\, dz + O(T^4). \tag{19}$$

(d) (BONUS+5) Show the integral

$$I_2 = \int_0^\infty \frac{z^{x-1} dz}{e^z + 1} = \int_0^\infty z^{x-1} \sum_{n=0}^{\infty} (-1)^n e^{-(n+1)z} dz, \tag{20}$$

and perform the change of variables $y = nz$ to write

$$I_2 = (1 - 2^{1-x}) \Gamma(x) \zeta(x), \tag{21}$$

where $\Gamma(x)$ is the gamma function and $\zeta(x)$ the Riemann zeta function.

Comment: The result (21) allows to perform the integrals in equation (19) to yield the final expression

$$I = \int_0^\mu f(\epsilon)\, d\epsilon + \frac{\pi^2}{6} T^2 f'(\mu) + O(T^4). \tag{22}$$

1.3 Entropy and specific heat of the free electron gas (10 points)

Given the expression for the Free energy

$$F = -T \sum_{\boldsymbol{p}\sigma} \ln(1 + e^{\beta(\mu - \epsilon_{\boldsymbol{p}\sigma})}) \tag{23}$$

(a) Show that replacing the sum in equation (23) by and integral over energy and integrating by parts yields

$$F = -\frac{2}{3} \frac{V}{\pi^2} 2^{1/2} m^{3/2} \int_0^\infty \frac{\epsilon^{3/2} d\epsilon}{e^{\beta(\epsilon - \mu)} + 1} \tag{24}$$

(b) Use Sommerfeld's expansion to show

$$F = F_0 - \frac{V T^2 \sqrt{2\mu} m^{3/2}}{6}, \tag{25}$$

where F_0 denotes the value of F at absolute zero.

(c) At low temperatures we can approximate the chemical potential by $\mu = \frac{p_f^2}{2m}$. Use eq. (25) to calculate the entropy and specific heat for the non-interacting electron gas. How do your results compare with the ones obtained within Landau's Fermi-liquid theory?