Theory of Quantum Matter

Lecturer: Prof. Otfried Gühne (Mon 14:00, Fri 10:00, Room D120)
Exercises: Chau Nguyen (Fri 12:30, Room D201) **Sheet 8**

Hand in: Mon 10.12.2018 *(questions marked as $*$ are optional)*
Discussion date: Fri 14.12.2018

11. The grand potential of the electron gas: perturbation theory

We start with the free electron gas (spin ignored) with the grand canonical density operator

$$\rho_0 = \frac{1}{Z_0} \exp\{-\beta(H_0 - \mu N)\}, \tag{1}$$

where $\beta = 1/T$, $H_0 = \sum_{\vec{k}} \epsilon_k n_{\vec{k}}$ with $\epsilon_k = (\hbar k)^2/(2m)$, $n_{\vec{k}} = a^\dagger_{\vec{k}} a_{\vec{k}}$, $N = \sum_{\vec{k}} n_{\vec{k}}$ and Z_0 is the partition function $Z_0 = \mathrm{Tr}[e^{-\beta(H_0-\mu N)}]$. We set $k_B = 1$ throughout. The grand potential is defined by $G_0 = -T \ln Z_0$. The zero subscripts indicate that the gas is non-interacting.

(a) (10pts) Show that $G_0 = -T \sum_{\vec{k}} \ln[1 + e^{-\beta(\epsilon_k - \mu)}]$.

Hint: Compute the trace in the occupation number basis (both H and N are diagonal). In particular, figure out how $H_0 - \mu N$ acts on $\left|\cdots, n_{\vec{k}}, \cdots\right\rangle$ where $n_{\vec{k}} = 0, 1$.

(b) (10pts) *Fermi–Dirac distribution.* With $\langle n_{\vec{k}} \rangle_0 = \mathrm{Tr}(\rho_0 n_{\vec{k}})$, show that

$$\langle n_{\vec{k}} \rangle_0 = \frac{1}{e^{\beta(\epsilon_{\vec{k}} - \mu)} + 1}. \tag{2}$$

Hint: Study **Sheet 0** to find a trick to compute $\langle n_{\vec{k}} \rangle_0$ from G_0.

(c) (10pts) *Example of Wick's theorem.* Show that

$$\langle a^\dagger_{\vec{k}_4} a^\dagger_{\vec{k}_3} a_{\vec{k}_2} a_{\vec{k}_1} \rangle_0 = -\langle n_{\vec{k}_1} \rangle_0 \langle n_{\vec{k}_2} \rangle_0 \delta_{\vec{k}_4 \vec{k}_2} \delta_{\vec{k}_3 \vec{k}_1} + \langle n_{\vec{k}_1} \rangle_0 \langle n_{\vec{k}_2} \rangle_0 \delta_{\vec{k}_4 \vec{k}_1} \delta_{\vec{k}_3 \vec{k}_2} \tag{3}$$

Hint: Show that the term vanishes if: $\vec{k}_1 = \vec{k}_2$ or $\vec{k}_3 = \vec{k}_4$ or $\{\vec{k}_1, \vec{k}_2\} \neq \{\vec{k}_3, \vec{k}_4\}$; then you are left with only two cases $\vec{k}_1 = \vec{k}_3$, $\vec{k}_2 = \vec{k}_4$, $\vec{k}_1 \neq \vec{k}_2$ and $\vec{k}_1 = \vec{k}_4$, $\vec{k}_2 = \vec{k}_3$, $\vec{k}_1 \neq \vec{k}_2$.

Now we turn on the interaction between electrons so that the Hamiltonian becomes

$$H = H_0 + \lambda V, \tag{4}$$

where $V = \frac{1}{2\Omega} \sum_{\vec{k}_1, \vec{k}_2, \vec{q} \neq 0} V(q) a^\dagger_{\vec{k}_2 - \vec{q}} a^\dagger_{\vec{k}_1 + \vec{q}} a_{\vec{k}_1} a_{\vec{k}_2}$ with Ω being the volume of the system, $V(q) = 4\pi e^2/q^2$, and λ is a variable to track the perturbative expansion. The density operator is given by

$$\rho = \frac{1}{Z} \exp\{-\beta(H - \mu N)\}, \tag{5}$$

where $Z = \mathrm{Tr}[e^{-\beta(H-\mu N)}]$. The grand potential is again $G = -T \ln Z$. In the lecture, we have derived the Hartree–Fock correction from the variational principle. Here we will derive the correction from the perturbation theory. Regarding λ as being small, we expand $Z = Z_0 + \lambda Z_1 + \lambda^2 Z_2 + \cdots$. Accordingly the grand potential is also expanded as $G = G_0 + \lambda G_1 + \lambda^2 G_2 + \cdots$.

(d) (10pts) Show that $G_1 = \langle V \rangle_0$, where $\langle V \rangle_0 = \mathrm{Tr}(\rho_0 V)$.

Hint: First compute G_1 in terms of Z_1 and Z_0. Note that one cannot easily expand $e^{-\beta(H_0 - \mu N + \lambda V)}$ in λ since V does not commute with $H_0 - \mu N$. However, to get Z_1, it is still rather easy: expand the exponential $\mathrm{Tr}[e^{-\beta(H_0 - \mu N + \lambda V)}]$ in β, take the derivative with respect to λ at $\lambda = 0$ for every term, take the trace and resume the series.

(e) (10pts) Using Wick's theorem to find again the Hartree–Fock correction to the grand potential, and then convert the sums over momenta to integrals to obtain

$$G_1 = -\frac{1}{2}\frac{\Omega}{(2\pi)^6}\int\int \mathrm{d}\,\vec{k}_1\,\mathrm{d}\,\vec{k}_2 V(|\vec{k}_1 - \vec{k}_2|)\langle n_{\vec{k}_1}\rangle_0 \langle n_{\vec{k}_2}\rangle_0. \tag{6}$$

Using elementary dimensional analysis (i.e., analyse the unit) to show that at $T = 0$, $G_1 \propto \Omega e^2 k_F^4$.

(f) ($*$) Show that for an arbitrary system, $G = E - TS - \mu N$, where E is the energy, S is the entropy of the system.

Remark: With Wick's theorem, one can actually track all higher order terms in the perturbation series. In fact, certain subseries can be resummed to yield sophisticated corrections to the thermodynamics potential and physical observables.