# Problem Set 6: Thermodynamical Potential

## 1. Thermodynamical Potential of a gas of noninteracting fermions.

Consider a many-particle system of non-interacting fermions with Hamiltonian

$$\hat{H}_o = \sum_k \varepsilon_k \, c_k^\dagger c_k \,. \tag{1}$$

Its grandcanonical thermodynamic potential $\Omega = -T \ln Z$ is given by (see textbooks on Statistical Physics)

$$\Omega = -T \sum_k \log\left[1 + e^{-\beta(\varepsilon_k - \mu)}\right] \ , \tag{2}$$

where $\mu$ is the chemical potential. In this problem, we consider a toy model, described by $\hat{H} = \hat{H}_0 + \hat{V}$, with a perturbation

$$\hat{V} = \lambda \sum_k \varepsilon_k' c_k^\dagger c_k \tag{3}$$

where $\lambda$ is a small parameter. We will consider two different ways to derive an expansion of the corresponding thermodynamic potential $\Omega(\lambda)$ in powers of $\lambda$ by using (a) a clever short-cut which is often used in thermodynamics (calculating $\partial_\lambda \Omega(\lambda)$), (b) Feynman diagrams. The purpose of it all is simply to practice diagrammatic perturbation theory.

### 1(a) A Clever Shortcut

Use the relation

$$\partial_\lambda \Omega = \frac{1}{\lambda} \langle \hat{V} \rangle \,, \tag{4}$$

and verify (by integration $\int_0^\lambda d\lambda'$) that $\Omega(\lambda)$ is given by Eq.(2), with $\varepsilon_k$ replaced by $\tilde{\varepsilon}_k = \varepsilon_k + \lambda \varepsilon_k'$. Taylor-expand this in powers of $\lambda$ to obtain:

$$\Omega(\lambda) = \Omega(0) + \sum_n \left( \sum_k \frac{(\lambda {\varepsilon'}_k)^n}{n!} \partial_{\varepsilon_k}^{n-1} f(\varepsilon_k) \right) \,. \tag{5}$$

### 1(b) Diagrammatic perturbation theory

Let us derive the same result, Eq.(5), using thermodynamic perturbation theory. Start from the general relation

$$-\beta(\Omega(\lambda) - \Omega(0)) = \langle U_I(\beta) \rangle_C - 1 \ , \tag{6}$$

where the evolution operator in the interaction representation w.r.t. $\hat{V}$ is

$$U_I(\beta) = T_\tau \exp\left\{-\int_0^\beta \hat{V}(\tau)\mathrm{d}\tau\right\} \tag{7}$$

and $\langle \ldots \rangle_C$ denotes a sum over all *connected* diagrams. A proof of this relation in discussed below in the optional problem No.2.
Now, we have to sum up the perturbation series for $\langle U_I(\beta)\rangle_C$ to all orders in $\lambda$:

1. Show that, at every order of perturbation theory in $\lambda$ for $\langle U_I(\beta)\rangle_C$, there is only one connected diagram.

2. Draw this diagram for the general case of order $n$, and using the appropriate Feynman rules, write down the corresponding algebraic expression.

3. Calculate combinatorial factors for the $n$-th order diagram.

4. Evaluate this $n$-th order expression, i.e., perform the Matsubara sum.

   **Warning**: the tricks for doing Matsubara sums, as exemplified in Rickayzen's Appendix B, are derived for the case when the summand contains only poles of order one. You will have to generalize these methods to be able to handle a summand containing $G^n(\varepsilon_k, \xi_m)$, which has poles of order n. The following identity for computing residues will be useful:

$$\mathrm{Res}(h; z_o) = \lim_{z\to z_o} \frac{1}{(n-1)!}\partial_z^{n-1}\Big((z-z_o)^n h(z)\Big)\ .$$

5. Verify that the perturbation expansion of $\langle U_I(\beta)\rangle_C - 1$ matches the Taylor expansion, Eq.(5), term for term.

**2. Perturbation Theory for Thermodynamical Potential.** (challenging, optional)
Consider a generic system with the Hamiltonian

$$\hat{H} = \hat{H}_o + \hat{H}'\ . \tag{8}$$

Here $\hat{H}'$ describes interactions. The difference in thermodynamical potentials between interacting and noninteracting systems is given by

$$-\beta(\Omega - \Omega_o) = \log\left[\langle U_I(\beta)\rangle\right]\ ; \quad U_I(\beta) = T_\tau \exp\left\{-\int_0^\beta \hat{H}'(\tau)\mathrm{d}\tau\right\}\ . \tag{9}$$

1. Taylor expand $\langle U_I(\beta)\rangle$ in powers of $\hat{H}'$ and use Wick's theorem to show that any $n$-th order term yields connected ("loops") and disconnected diagrams, the latter consist of separate loops.

2. Diagrams generated by the $n$-th order term can be classified by a number of loops, $p_j$, containing a given number of vertices, $m_j$. Note that $\sum_{j=1}^{k} p_j m_j = n$, where $k$ is a number of different loops.

   (a) Consider the disconnected diagram where all loops are different, i.e. $m_1 \neq m_2 \neq \ldots \neq m_k$, and $p_j = 1$. Calculate combinatorial factors for given set of $\{m_j\}$ at $p_j = 1$.

   *Hint*: use an answer of well-know combinatorial problem of a distribution of $n$ balls over $k$ different boxes, each box containing $m_j$ empty positions.

   (b) Consider the disconnected diagram where some loops contain the same number of vertices. One can describe it by using "degeneracy factors" $p_j \neq 1$. Calculate combinatorial factors for given set of $\{m_j, p_j\}$.

   *Hint*: use an answer of another combinatorial problem of a distribution of $n$ balls over $\sum_j p_j$ boxes, each box containing $m_j$ empty positions. Take into account that, for given $m_j$, there are $p_j$ equivalent boxes.

3. Rewrite the perturbative expansion for $\langle U_I(\beta)\rangle$ as sums over $\{p_j\}$, calculate these sums and, thus, prove the identity

$$-\beta(\Omega - \Omega_o) = \langle U_I(\beta)\rangle_C - 1 \; . \tag{10}$$

*Remark*: The proof of Eq.(10) evidently involves relatively lengthy combinatorial analysis and a clever rearrangement of the perturbative expansion. This is a typical example of diagrammatic calculations and the cumbersome combinatorics is one of their main difficulties. A solution to the problem No.2 can be found, for example, in Sect. 15 (perturbation theory for the thermodynamic potential) of the book "*Methods of quantum field theory in statistical physics*" by A.A. Abrikosov, L.P. Gorkov and I.E. Dzyaloshinski (1962 – in Russian, 1963 – translated in English).