Lecture 3-7: General formalism at finite temperature

Reference: Negele & Orland (N&O) Chapter 2

Lecture 5

- Perturbation theory (continued)
  - Frequency and momentum representation (Home reading)
  - Some key results
    - \[ g_\alpha(\tau) = \sum_{\omega_n} \frac{-1}{\beta} e^{-i\omega_n \tau} \frac{1}{i\omega_n - (\epsilon_\alpha - \mu)} \]
    - \[ \omega_n = \frac{2\pi n}{\beta} \text{ for Bosons and } \omega_n = \frac{(2n+1)\pi}{\beta} \text{ for Fermions} \]
    - \[ \oint_{\alpha, \omega_n} = \tilde{g}_\alpha(\omega_n) = \frac{-1}{i\omega_n - (\epsilon_\alpha - \mu)} \]
  - The linked cluster theorem
    - The linked cluster theorem: \( \ln Z \) is in fact given by the sum of all connected diagrams.
    - Proof: We shall derive the theorem using the replica technique. The basic idea is to evaluate \( Z^n \) by replicating the system \( n \) times and expand the results as follows
      \[ Z^n = e^{n\ln Z} = 1 + n\ln Z + \sum_{m=2}^{\infty} \frac{(n\ln Z)^m}{m!} \]
    - Since
      \[ \frac{Z}{Z_0} = \frac{1}{Z_0} \int_{\psi_\alpha(\tau) = \psi_\alpha(0)} D(\psi_\alpha^*(\tau), \psi_\alpha(\tau)) e^{-\int_0^\beta dt (\sum_\alpha \psi_\alpha(\tau)^*(\partial_\tau + \epsilon_\alpha - \mu)\psi_\alpha(\tau) - V(\psi_\alpha^*(\tau), \psi_\alpha(\tau)))} \]
    - We may write \( Z^n \) as a functional integral over \( n \) set of fields \( \{\psi_\alpha^\sigma, \psi_\alpha^\sigma\} \), \( \sigma = 1, \cdots, n \),
Then \( \ln Z \) will be given by the coefficient of the graphs proportional to \( n \). The Feynman rules for \( \left( \frac{Z}{Z_0} \right)^n \) are the same as those for \( \frac{Z}{Z_0} \), except that each propagator now carries an index \( \sigma \), and all direct lines entering or leaving a given vertex have the same index \( \sigma \). It is evident that each connected part of a diagram must carry a single index \( \sigma \) and \( \sigma \) runs from 1 to \( n \) in the sum. Thus a graph with \( n_c \) connected parts is proportional to \( n^{n_c} \), and the graphs proportional to \( n \) are those with only one connected part. As a consequence, we obtain the linked cluster theorem

\[
\Omega - \Omega_0 = -\frac{1}{\beta} \sum (\text{all connected graphs})
\]

where

\[
\Omega_0 = \frac{\xi}{\beta} \sum_{\alpha} \ln(1 - \xi e^{-\beta(\epsilon_\alpha - \mu)})
\]

QED.

➢ Another way to derive the linked cluster theorem is to evaluate the exponential of the sum of all linked graphs, as Problem 2.10

➢ The replica technique can be used in many other contexts, such as disordered systems.

➢ The condition when the replica technique is applicable should be examined more carefully.
Calculation of observables and Green’s functions

We should use the replica technique to do linked expansion for the expectation value of any n-body operator \( R \) too. In such a marvelous way, the symmetry factors are simplified. In terms of unperturbed thermal average, the expectation value of \( R \) may be written

\[
\langle R \rangle = \frac{\int D(\psi_{a}, \psi_{a}') e^{-\int dt \sum_{a} \psi_{a}'(t) L_{a}(\psi_{a}(t))} R(\psi_{a}(0), \psi_{a}(0))}{\int D(\psi_{a}, \psi_{a}') e^{-\int dt \sum_{a} \psi_{a}'(t) L_{a}(\psi_{a}(t))}}
\]

\[
= \frac{\langle e^{-\int dt V(\psi_{a}(t), \psi_{a}(t))} R(\psi_{a}(0), \psi_{a}(0)) \rangle_{0}}{\langle e^{-\int dt V(\psi_{a}(t), \psi_{a}(t))} \rangle_{0}}. \tag{2.13}
\]

Let us again introduce \( \{ \psi_{a}, \psi_{a}' \} \), \( n \) \( \sigma = 1, \ldots, n \) and define

\[
R_{n} = Z_{n}^{-n} \prod_{\sigma=1}^{n} D(\psi_{a}^{\sigma}(t), \psi_{a}(t)) R(\psi_{a}^{1}(0), \psi_{a}(0))
\]

\[
\times \langle e^{-\int dt V(\psi_{a}(t), \psi_{a}(t))} \rangle_{0} \langle e^{-\int dt V(\psi_{a}(t), \psi_{a}(t))} \rangle_{0}^{n-1}
\]

Separating the \( \sigma = 1 \) component from the \((n-1)\) other component, we have that

\[
R_{n} = \langle e^{-\int dt V(\psi_{a}(t), \psi_{a}(t))} \rangle_{0} \langle e^{-\int dt V(\psi_{a}(t), \psi_{a}(t))} \rangle_{0}^{n-1}
\]

and thus the expectation value \( \langle R \rangle \) is obtained for \( n = 0 \).

The perturbation expansion reads

\[
R_{n} = \sum_{p=0}^{\infty} \frac{(-1)^{p}}{p!} \prod_{\sigma_{1}=1}^{n} \cdots \prod_{\sigma_{p}=1}^{n} \int_{0}^{\beta} d\tau_{1} \cdots d\tau_{p} \tag{2}
\]

\[
\times \langle V(\psi_{a}^{\sigma_{1}}(\tau_{1}), \psi_{a}^{\sigma_{1}}(\tau_{1})) \cdots V(\psi_{a}^{\sigma_{p}}(\tau_{p}), \psi_{a}^{\sigma_{p}}(\tau_{p})) R(\psi_{a}^{1}(0), \psi_{a}^{1}(0)) \rangle_{0}
\]

Diagrams rule can be developed straightforward.

The expansion series consist of all distinct diagrams containing one vertex \((\alpha\beta|\psi_{a}^{\sigma}|\psi_{a})\) at time \( \tau = 0 \) and any number of vertices \((\alpha\beta|\psi_{a}^{\sigma}|\psi_{a})\) at other times which
are integrated from 0 to $\beta$.

- All propagators carry an index $\sigma$, all propagators entering or leaving a vertex have the same index, and all indices are summed from 1 to $n$.

- The index associated with $R$ is one so that all the propagators entering and leaving $R$ are restricted to $\sigma = 1$.

- Consider a diagram composed of a set of interaction vertex $v$ connected to $R$ and one or more additional unconnected parts. In the portion of the diagram linked to $R$, $\sigma = 1$ everywhere. In the additional unconnected parts, there is at least one free summation over $\sigma$ leading to an overall factor of at least one power of $n$.

- When $n = 0$, all the diagrams with disconnected part vanish.

- The indices are constrained to be $\sigma = 1$ in all components linked to $R$ and can be omitted from the final diagram rules.

  - Unlabeled Feynman diagrams for a two-body operator

- Two types of vertices

  $v$-vertex

  $R$-vertex

- The symmetry factors are constrained to be $S = 1$ or $S = 2$.

- Some examples and the general rule
• The rule for calculating the $p$-th order contribution using unlabeled diagrams

> Rule 1:

**Draw** all distinct unlabeled connected diagrams composed of one $R$-vertex and $p$ $v$-vertices connected by directed lines. Two diagrams are distinct if they cannot be deformed so as to coincide completely including the direction of arrows on propagators. For each distinct unlabeled diagram, evaluate the contribution as follows.

> Rule 2:

Calculate the symmetry factor $S$ for the diagram. If the exchange of the extremities of $R$ combined with some time permutation and exchange of interaction extremities yields a deformation of the original diagram, $S = 2$. Otherwise, $S = 1$.

> Rule 3:

Assign a time label $\tau_i$ to each of the $p$ $v$-vertices, associate the time $\tau = 0$ with the $R$-vertex, and assign a single-particle index to each directed line. For each directed line include the factor

\[ \tau \int_a = g_a(\tau - \tau') = e^{-\left(\epsilon_a - \mu\right)(\tau' - \tau')} \left[ (1 + \zeta n_a) \theta(\tau - \tau' - \eta) + \zeta n_a \theta(\tau' - \tau - \eta) \right] . \]

> Rule 4:

For each $v$-vertex include the factor

\[ \gamma \delta \] = (\alpha \beta | v | \gamma \delta) \]

and for the $R$-vertex include the factor

\[ \gamma \delta \] = (\alpha \beta | R | \gamma \delta) .

> Rule 5:

Sum over all single particle indices and integrate the $p$ times over the interval $[0, \beta]$.

> Rule 6:

Multiply the result by the factor $\frac{(-1)^p}{S} \zeta^{n_L}$ where $n_L$ is the number of closed loops and $S$ is the symmetry factor.
Unlabeled Feynman diagrams for $\langle R \rangle$ with factor $1/S$ in order $p = 0, 1$

(A) $\frac{1}{2}$  
(B) $\frac{1}{2}$  
(C) $\frac{1}{2}$  
(D) $\frac{1}{2}$

(E) $\frac{1}{2}$  
(F) $\frac{1}{2}$  
(G) $\frac{1}{2}$  
(H) $\frac{1}{2}$

0-th order contribution from diagrams (A) and (B)

$$\langle R \rangle^{(0)} = \frac{1}{2} \sum_{\alpha, \beta} |(\alpha \beta | R | \alpha \beta) + \zeta(\alpha \beta | R | \beta \alpha)| n_\alpha n_\beta$$

The contribution from diagram (E)

$$\langle R \rangle^{(E)} = -\frac{1}{2} \sum_{\alpha \beta \gamma \delta} \int_0^\beta d\tau (\alpha \beta | R | \gamma \delta)(\gamma \delta | \alpha \beta) g_\alpha (-\tau) g_\beta (-\tau) g_\gamma (\tau) g_\delta (\tau)$$

Unlabeled Feynman diagrams for Green's function (Home reading)

The derivation of the diagrammatic expansion for the imaginary-time Green's function is completely analogous to the expectation $\langle R \rangle$,

$$g^{(n)} (\alpha_1 \beta_1, \ldots , \alpha_n \beta_n | \alpha'_1 \beta'_1, \ldots , \alpha'_n \beta'_n)$$

$$\left\langle \frac{e^{-\int d\tau V(\psi^*_\alpha (\tau), \psi_\alpha (\tau))} \psi_{\alpha_1} (\beta_1) \ldots \psi_{\alpha_n} (\beta_n) \psi^*_{\alpha'_1} (\beta'_1) \ldots \psi^*_{\alpha'_n} (\beta'_n)}{e^{-\int d\tau V(\psi^*_\alpha (\tau), \psi_\alpha (\tau))}} \right\rangle_0$$

Homework: Problem 2.10, 2.11