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Chapter 1

Useful formulas

1.1 Gaussian Integrals

For a positive number a ,

$$\int_{-\infty}^{\infty} dx e^{-ax^2} = \sqrt{\frac{\pi}{a}}, \quad \int \frac{dz^* dz}{2\pi i} e^{-z^* az} = \frac{1}{a} \quad . \quad (1.1.1)$$

For real multi-dimensional integrals,

$$\int \frac{dx_1 \cdots dx_n}{(2\pi)^{\frac{n}{2}}} e^{-\frac{1}{2} \sum_{ij} x_i A_{ij} x_j + \sum_i x_i J_i} = [\det A]^{-\frac{1}{2}} e^{\frac{1}{2} \sum_{ij} J_i A_{ij}^{-1} J_j} \quad . \quad (1.1.2)$$

For complex multi-dimensional integrals,

$$\int \left(\prod_{i=1}^n \frac{dz_i^* dz_i}{2\pi i} \right) e^{-\sum_{ij} z_i^* H_{ij} z_j + \sum_i (J_i^* z_i + z_i^* J_i)} = [\det H]^{-1} e^{\sum_{ij} J_i^* H_{ij}^{-1} J_j} \quad . \quad (1.1.3)$$

For Grassmann variables integrals,

$$\int \left(\prod_{i=1}^n d\eta_i^* d\eta_i \right) e^{-\sum_{ij} \eta_i^* H_{ij} \eta_j + \sum_i (\xi_i^* \eta_i + \eta_i^* \xi_i)} = [\det H] e^{\sum_{ij} \xi_i^* H_{ij}^{-1} \xi_j} \quad . \quad (1.1.4)$$

1.2 Gaussian Distribution

1.2.1 Gaussian Distribution for One Variable

The Gaussian distribution for one variable can be written as

$$w(x) = A e^{-\frac{1}{2} \beta x^2} \quad . \quad (1.2.1)$$

The normalization constant A is given by the condition $\int w(x) dx = 1$, thus

$$w(x) = \sqrt{\frac{\beta}{2\pi}} e^{-\frac{1}{2} \beta x^2} \quad . \quad (1.2.2)$$

The mean square fluctuation is

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 w(x) dx = \frac{1}{\beta}, \quad (1.2.3)$$

thus we can write the Gaussian distribution in the form

$$w(x) = \frac{1}{\sqrt{2\pi \langle x^2 \rangle}} \exp \left(-\frac{x^2}{2 \langle x^2 \rangle} \right) \quad . \quad (1.2.4)$$

1.2.2 Gaussian Distribution for More Than One Variable

The Gaussian distribution for more than one variable is

$$w(x_1, \dots, x_n) = Ae^{-\frac{1}{2}\beta_{ik}x_ix_k}, \quad (1.2.5)$$

where $\beta_{ik} = \beta_{ki}$ and normalization condition for A is

$$\int w dx_1 \cdots dx_n = 1. \quad (1.2.6)$$

The linear transformation

$$x_i = a_{ik}x'_k \quad (1.2.7)$$

of x_1, \dots, x_n converts the quadratic form β_{ik} into a sum of squares $x'_i x'_i$. In order that

$$\beta_{ik}x_ix_k = x'_i x'_i = x'_i x'_k \delta_{ik} \quad (1.2.8)$$

should be valid, the transformation coefficients must satisfy the relations

$$\beta_{ik}a_{il}a_{km} = \delta_{lm}. \quad (1.2.9)$$

The determinant of the matrix on the left of this equation is the product of the determinant $\beta = |\beta_{ik}|$ and two determinants $a = |a_{ik}|$. The determinant $\delta_{ik} = 1$. The above relation therefore shows that

$$\beta a^2 = 1. \quad (1.2.10)$$

The Jacobian of the linear transformation from the variables x_i to x'_i is the determinant a . After the transformation, therefore, the normalization integral separates into a product of n identical integrals

$$Aa \left[\int_{-\infty}^{\infty} \exp\left(-\frac{1}{2}x'^2\right) dx' \right]^n = \frac{A}{\sqrt{\beta}} (2\pi)^{\frac{n}{2}} = 1. \quad (1.2.11)$$

Thus we obtain finally the Gaussian distribution for more than one variables in the form

$$w = \frac{\sqrt{\beta}}{(2\pi)^{\frac{n}{2}}} \exp\left(-\frac{1}{2}\beta_{ik}x_ix_k\right). \quad (1.2.12)$$

Now let $S = -\frac{1}{2}\beta_{ik}x_ix_k$ and define the quantities

$$X_i = -\frac{\partial S}{\partial x_i} = \beta_{ik}x_k, \quad (1.2.13)$$

which we refer to as conjugate¹ to the x_i . From the definition the mean value \bar{x}_i is

$$\bar{x}_i = \frac{\beta}{(2\pi)^{\frac{n}{2}}} \int \cdots \int x_i \exp\left(-\frac{1}{2}\beta_{ik}(x_i - \bar{x}_i)(x_k - \bar{x}_k)\right) dx_1 \cdots dx_n, \quad (1.2.14)$$

differentiating this equation with respect to \bar{x}_k and then putting all \bar{x}_i to zero, we have

$$\langle x_i X_k \rangle = \delta_{ik}. \quad (1.2.15)$$

Since $X_k = \beta_{kl}x_l = x_l\beta_{lk}$, the above equation can be written as $\langle x_i x_l \rangle \beta_{lk} = \delta_{ik}$, whence

$$\langle x_i x_k \rangle = \beta_{ik}^{-1}. \quad (1.2.16)$$

Similarly,

$$\langle X_i X_k \rangle = \beta_{il} \langle x_l X_k \rangle = \beta_{il} \delta_{lk}, \quad (1.2.17)$$

i.e.

$$\langle X_i X_k \rangle = \beta_{ik}. \quad (1.2.18)$$

¹when apply to thermodynamics we call it thermodynamically conjugate.

1.3 Fourier Transform of Delta Function

The δ function can be expressed as

$$\delta(x - \alpha) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ip(x-\alpha)} dp. \quad (1.3.1)$$

1.4 Euler Integral

1.4.1 Euler Integral of The First Kind: Beta Function

Euler integral of the first kind: the Beta function:

$$B(a, b) = \int_0^1 x^{a-1} (1-x)^{b-1} dx. \quad (1.4.1)$$

The Beta function has the following properties:

(i) Substitute x with $x = 1 - t$ and it is easy to get

$$B(a, b) = B(b, a). \quad (1.4.2)$$

(ii) When $b > 1$, integrate by parts (note that $x^a = x^{a-1} - x^{a-1}(1-x)$)

$$\begin{aligned} B(a, b) &= \int_0^1 (1-x)^{b-1} d\frac{x^a}{a} \\ &= \frac{x^a(1-x)^{b-1}}{a} \Big|_0^1 + \frac{b-1}{a} \int_0^1 x^a (1-x)^{b-2} dx \\ &= \frac{b-1}{a} \int_0^1 x^{a-1} (1-x)^{b-2} dx - \frac{b-1}{a} \int_0^1 x^{a-1} (1-x)^{b-1} dx \\ &= \frac{b-1}{a} B(a, b-1) - \frac{b-1}{a} B(a, b), \end{aligned} \quad (1.4.3)$$

thus

$$B(a, b) = \frac{b-1}{a+b-1} B(a, b-1). \quad (1.4.4)$$

For $a > 1$, it is similar that

$$B(a, b) = \frac{a-1}{a+b-1} B(a-1, b). \quad (1.4.5)$$

Let n be a positive integer,

$$B(n, a) = B(a, n) = \frac{1 \cdot 2 \cdot 3 \cdots (n-1)}{a \cdot (a+1) \cdot (a+2) \cdots (a+n-1)}. \quad (1.4.6)$$

Let m, n be two positive integers,

$$B(m, n) = \frac{(n-1)!(m-1)!}{(m+n-1)!}. \quad (1.4.7)$$

(iii) Substitute x with $x = \frac{y}{1+y}$, here y is a new variable runs from 0 to ∞ , then

$$B(a, b) = \int_0^{\infty} \frac{y^{a-1}}{(1+y)^{a+b}} dy. \quad (1.4.8)$$

(iv) If $b = 1 - a$ and $0 < a < 1$ then

$$B(a, 1 - a) = \int_0^1 \frac{y^{a-1}}{1+y} dy, \quad (1.4.9)$$

this is also a Euler integral,

$$B(a, 1 - a) = \frac{\pi}{\sin a\pi} \quad (0 < a < 1), \quad (1.4.10)$$

especially we have

$$B\left(\frac{1}{2}, \frac{1}{2}\right) = \pi. \quad (1.4.11)$$

1.4.2 Euler Integral of The Second Kind: Gamma Function

Euler integral of the second kind: the Gamma function is defined as

$$\Gamma(a) = \int_0^{\infty} x^{a-1} e^{-x} dx. \quad (1.4.12)$$

The Euler-Gauss formula:

$$\Gamma(a) = \lim_{n \rightarrow \infty} n^a \frac{1 \cdot 2 \cdot 3 \cdots (n-1)}{a \cdot (a+1) \cdot (a+2) \cdots (a+n-1)}. \quad (1.4.13)$$

The Gamma Function has the following properties:

(i) For $a > 0$, $\Gamma(a)$ is smooth.

(ii) Integrate by parts we shall get

$$\Gamma(a+1) = a\Gamma(a), \quad (1.4.14)$$

repeat this formula

$$\Gamma(a+n) = (a+n-1)(a+n-2) \cdots (a+1)\Gamma(a). \quad (1.4.15)$$

Let n be a positive integer, then

$$\Gamma(n+1) = n! \quad . \quad (1.4.16)$$

(iii) If $a \rightarrow +0$ then

$$\Gamma(a) = \frac{\Gamma(a+1)}{a} \rightarrow +\infty. \quad (1.4.17)$$

If $a > n+1$ the

$$\Gamma(a) > n! \quad . \quad (1.4.18)$$

(iv) Relation to Beta function:

$$B(a, b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}. \quad (1.4.19)$$

(v) if $0 < a < 1$ then

$$\Gamma(a)\Gamma(1-a) = \frac{\pi}{\sin a\pi}, \quad (1.4.20)$$

and

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}. \quad (1.4.21)$$

(vi)

$$\prod_{\nu=1}^{n-1} \Gamma\left(\frac{\nu}{n}\right) = \frac{(2\pi)^{\frac{n-1}{2}}}{\sqrt{n}}. \quad (1.4.22)$$

(vii) Raabe's formula:

$$\int_a^{a+1} \ln \Gamma(t) dt = \frac{1}{2} \ln 2\pi + a \ln a - a, \quad a > 0, \quad (1.4.23)$$

in particular, if $a = 0$ then

$$\int_0^1 \ln \Gamma(t) dt = \frac{1}{2} \ln 2\pi. \quad (1.4.24)$$

(viii) Legendre formula:

$$\Gamma(a)\Gamma(a + \frac{1}{2}) = \frac{\sqrt{\pi}}{2^{2a-1}} \Gamma(2a). \quad (1.4.25)$$

1.5 Baker-Campbell-Hausdorff Formula

Baker-Campbell-Hausdorff Formula is

$$e^A B e^{-A} = \sum_{n=0}^{\infty} \frac{1}{n!} [A, B]_n = B + [A, B] + \frac{1}{2} [A, [A, B]] + \frac{1}{6} [A, [A, [A, B]]] + \cdots, \quad (1.5.1)$$

this formula can be proved by defining $B(\tau) = e^{\tau A} B e^{-\tau A}$ and formally integrating its equation of motion $dB/d\tau = [A, B(\tau)]$.

1.6 Feynman Result

The Feynman result reads

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}, \quad (1.6.1)$$

which is true only if $[A, B]$ commutes with both A and B .

To prove it, recall that

$$e^{\tau(A+B)} = e^{\tau A} T_{\tau} \exp \left[\int_0^{\tau} d\tau' e^{-\tau' A} B e^{\tau' A} \right] \quad (1.6.2)$$

and evaluate the integral for $\tau = 1$.

1.7 Laguerre Polynomials

The Laguerre polynomials are solution of Laguerre's equation:

$$xy'' + (1-x)y' + ny = 0, \quad (1.7.1)$$

where n is non-negative integer. The Laguerre polynomials is

$$L_n(x) = \frac{e^x}{n!} \frac{d^n}{dx^n} (e^{-x} x^n) = \sum_{k=0}^n \frac{(-x)^k}{k!} \frac{n!}{k!(n-k)!}. \quad (1.7.2)$$

The generating function is

$$\frac{e^{-xt/(1-t)}}{1-t} = \sum_{n=0}^{\infty} L_n(x) t^n. \quad (1.7.3)$$

1.8 Cramer's Rule

Consider a system of n linear equations of n unknowns, represented in matrix multiplication form:

$$Ax = b, \quad (1.8.1)$$

where the $n \times n$ matrix A has a nonzero determinant, and the vector $x = (x_1, \dots, x_n)^T$ is the column vector of the variables. Then Cramer's rule states that the system has a unique solution, whose individual values are given by:

$$x_i = \frac{\det A_i}{\det A}, \quad (1.8.2)$$

where A_i is the matrix formed by replacing the i -th column of A by the column vector b .

1.9 Sherman-Morrison Formula

Suppose A is an invertible square matrix and u, v are column vectors. Suppose that $1 + v^T A^{-1} u \neq 0$, then the Sherman-Morrison formula states that

$$(A + uv^T)^{-1} = A^{-1} - \frac{A^{-1}uv^T A^{-1}}{1 + v^T A^{-1}u}. \quad (1.9.1)$$

Here uv^T is the outer product of two vectors u and v .

1.10 Simple Impurity Model at Zero Temperature

The Hamiltonian of simple impurity model is defined as

$$H = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_k V_k (c_k^\dagger d + d^\dagger c_k) + \varepsilon_0 d^\dagger d, \quad (1.10.1)$$

let $H = H_0 + V$, where

$$H_0 = \sum_k \varepsilon_k c_k^\dagger c_k + \varepsilon_0 d^\dagger d, \quad V = \sum_k V_k (c_k^\dagger d + d^\dagger c_k). \quad (1.10.2)$$

The Green's function is

$$G(t) = -i \langle 0 | T d(t) d^\dagger | 0 \rangle = -i \langle 0 | d(t) d^\dagger | 0 \rangle, \quad (1.10.3)$$

apply Fourier transform on it, then

$$G(\omega) = \langle 0 | d \frac{1}{\omega + i0 - H} d^\dagger | 0 \rangle. \quad (1.10.4)$$

Notice that

$$\begin{aligned} \frac{1}{\omega - H} &= \frac{1}{\omega - H_0} + \frac{1}{\omega - H_0} V \frac{1}{\omega - H} \\ &= \frac{1}{\omega - H_0} + \frac{1}{\omega - H_0} V \frac{1}{\omega - H_0} + \frac{1}{\omega - H_0} V \frac{1}{\omega - H_0} V \frac{1}{\omega - H}, \end{aligned} \quad (1.10.5)$$

the second term produce just 0, thus

$$\begin{aligned} G(\omega) &= \langle 0 | d \frac{1}{\omega - H_0} d^\dagger | 0 \rangle + \langle 0 | d \frac{1}{\omega - H_0} V \frac{1}{\omega - H_0} V \frac{1}{\omega - H} d^\dagger | 0 \rangle \\ &= \frac{1}{\omega - \varepsilon_0} + \frac{1}{\omega - \varepsilon_0} \langle 0 | d V \frac{1}{\omega - H_0} V \frac{1}{\omega - H} d^\dagger | 0 \rangle \\ &= \frac{1}{\omega - \varepsilon_0} + \frac{1}{\omega - \varepsilon_0} \langle 0 | d \sum_k d^\dagger c_k \frac{V_k^2}{\omega - H_0} c_k^\dagger d \frac{1}{\omega - H} d^\dagger | 0 \rangle \\ &= \frac{1}{\omega - \varepsilon_0} + \frac{1}{\omega - \varepsilon_0} \sum_k \frac{V_k^2}{\omega - \varepsilon_k} G(\omega). \end{aligned} \quad (1.10.6)$$

Therefore

$$G^{-1}(\omega) = \omega - \varepsilon_0 - \sum_k \frac{V_k^2}{\omega - \varepsilon_k}, \quad (1.10.7)$$

it can be written as

$$G^{-1}(\omega) = \omega - \varepsilon_0 - \int_{-\infty}^{\infty} d\varepsilon \frac{\Delta(\varepsilon)}{\omega - \varepsilon}, \quad (1.10.8)$$

where

$$\Delta(\varepsilon) = \sum_k V_k^2 \delta(\varepsilon - \varepsilon_k). \quad (1.10.9)$$

Now consider V is in site representation:

$$V = \sum_i (t_{io} c_i^\dagger d + t_{oi} d^\dagger c_i), \quad (1.10.10)$$

then we have that

$$\begin{aligned} G(\omega) &= \frac{1}{\omega - \varepsilon_0} + \frac{1}{\omega - \varepsilon_0} \sum_{ij} t_{oi} t_{jo} \langle 0 | d d^\dagger c_i \frac{1}{\omega - H_0} c_j^\dagger d \frac{1}{\omega - H} d^\dagger | 0 \rangle \\ &= \frac{1}{\omega - \varepsilon_0} + \frac{1}{\omega - \varepsilon_0} \sum_{ij} t_{oi} t_{jo} G_{ij}^{(o)}(\omega) G(\omega), \end{aligned} \quad (1.10.11)$$

thus

$$G^{-1}(\omega) = \omega - \varepsilon_0 - \sum_{ij} t_{oi} t_{jo} G_{ij}^{(o)}(\omega), \quad (1.10.12)$$

where $G_{ij}^{(o)}$ is the Green's function with one site removed.

1.11 Green's Function for Simple Cubic Lattice

The first Brillouin zone for the simple cubic lattice is the cube

$$-\pi/a \leq k_x < \pi/a, \quad -\pi/a \leq k_y < \pi/a, \quad -\pi/a \leq k_z < \pi/a, \quad (1.11.1)$$

where a is the lattice constant. The diagonal matrix element of Green's function is

$$G(\omega) = \frac{a^3}{(2\pi)^3} \int_{-\pi/a}^{\pi/a} dk_x \int_{-\pi/a}^{\pi/a} dk_y \int_{-\pi/a}^{\pi/a} dk_z \frac{1}{\omega - 2t(\cos k_x a + \cos k_y a + \cos k_z a)}, \quad (1.11.2)$$

introducing the variable $x = k_x a, y = k_y a, z = k_z a$ we obtain

$$G(\omega) = \frac{1}{(2\pi)^3} \int_{-\pi}^{\pi} dx \int_{-\pi}^{\pi} dy \int_{-\pi}^{\pi} dz \frac{1}{\omega - 2t(\cos x + \cos y + \cos z)}. \quad (1.11.3)$$

This function can be expressed by complete elliptic integral. The complete elliptic integral of the first kind $K(k)$ as complex function of the complex modulus k is defined by

$$K(k) = \int_0^{\pi/2} d\theta (1 - k^2 \sin^2 \theta)^{-\frac{1}{2}}, \quad (1.11.4)$$

this function is an even function and $K(k^*) = K(k)^*$.

After the integration over y and z , the integral (1.11.3) yields

$$G(\omega) = \frac{1}{2\pi^2 t} \int_0^\pi k K(k) dx, \quad (1.11.5)$$

where

$$k = \frac{4t}{\omega - 2t \cos x}. \quad (1.11.6)$$

For simple cubic lattice, $\text{Re}G$ is an odd function of ω and $\text{Im}G$ is an even function:

$$\text{Re } G(\omega) = -\text{Re } G(\omega), \quad \text{Im } G(\omega) = \text{Im } G(\omega), \quad (1.11.7)$$

hence we have only to consider the range $0 \leq \omega \leq 6t$ in the following. The Green's function can be calculated numerically, when $0 < \omega < 2t$,

$$\begin{aligned} \text{Re } G(\omega) &= -\frac{1}{2\pi^2 t} \int_0^{\cos^{-1}(\omega/2t)} dx K\left(\frac{1}{|k|}\right) + \frac{1}{2\pi^2 t} \int_{\cos^{-1}(\omega/2t)}^{\pi} K\left(\frac{1}{k}\right), \\ \text{Im } G(\omega) &= \frac{1}{\pi^2} \int_0^{\pi} dx K\left(\frac{\sqrt{k^2 - 1}}{k}\right), \end{aligned} \quad (1.11.8)$$

when $2t \leq \omega < 6t$,

$$\begin{aligned} \text{Re } G(\omega) &= \frac{1}{2\pi^2 t} \int_0^{\cos^{-1}[(\omega-4t)/2t]} dx K\left(\frac{1}{k}\right) + \frac{1}{2\pi^2 t} \int_{\cos^{-1}[(\omega-4t)/2t]}^{\pi} dx K(k), \\ \text{Im } G(\omega) &= \frac{1}{2\pi^2 t} \int_0^{\cos^{-1}[(\omega-4t)/2t]} dx K\left(\frac{\sqrt{k^2 - 1}}{k}\right). \end{aligned} \quad (1.11.9)$$

Chapter 2

Coherent States

Coherent states is defined as the eigenstates of annihilation operator:

$$a_\alpha |\phi\rangle = \phi_\alpha |\phi\rangle. \quad (2.0.1)$$

2.1 Boson Coherent States

Boson coherent states:

$$|\phi\rangle = e^{\sum_\alpha \phi_\alpha a_\alpha^\dagger} |0\rangle, \quad \langle\phi| = \langle 0| e^{\sum_\alpha \phi_\alpha^* a_\alpha} \quad , \quad (2.1.1)$$

where ϕ_α is complex number.

The overlap of two coherent states:

$$\langle\phi|\phi'\rangle = e^{\sum_\alpha \phi_\alpha^* \phi'_\alpha} \quad . \quad (2.1.2)$$

The overcompleteness in the Fock space:

$$\int \left(\prod_\alpha \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} \right) e^{-\sum \phi_\alpha^* \phi_\alpha} |\phi\rangle \langle\phi| = 1, \quad (2.1.3)$$

where

$$\frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} = \frac{d(\text{Re}\phi_\alpha) d(\text{Im}\phi_\alpha)}{\pi} \quad . \quad (2.1.4)$$

The trace of an operator A in Fock space can be written as

$$\text{Tr} A = \int \left(\prod_\alpha \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} \right) e^{-\sum \phi_\alpha^* \phi_\alpha} \langle\phi| A |\phi\rangle \quad . \quad (2.1.5)$$

The average particle number of a coherent state is

$$\bar{N} = \frac{\langle\phi| N |\phi\rangle}{\langle\phi|\phi\rangle} = \frac{\langle\phi| \sum_\alpha a_\alpha^\dagger a_\alpha |\phi\rangle}{\langle\phi|\phi\rangle} = \sum_\alpha \phi_\alpha^* \phi_\alpha, \quad (2.1.6)$$

and the variance is

$$\sigma^2 = \frac{\langle\phi| N^2 |\phi\rangle}{\langle\phi|\phi\rangle} - \bar{N}^2 = \bar{N} \quad . \quad (2.1.7)$$

2.2 Grassmann Algebra

The Grassmann numbers is defined to be anticommuting numbers:

$$\xi_\alpha \xi_\beta + \xi_\beta \xi_\alpha = 0, \quad \xi_\alpha^2 = 0 \quad . \quad (2.2.1)$$

The conjugation of a Grassmann number is defined as

$$(\xi_\alpha)^* = \xi_\alpha^*, \quad (\xi_\alpha^*)^* = \xi_\alpha \quad . \quad (2.2.2)$$

If λ is a complex number,

$$(\lambda \xi_\alpha)^* = \lambda^* \xi_\alpha, \quad (2.2.3)$$

and for any product of Grassmann numbers:

$$(\xi_1 \cdots \xi_n)^* = \xi_n^* \xi_{n-1}^* \cdots \xi_1^* \quad , \quad (2.2.4)$$

and for combinations of Grassmann variables and creation and annihilation operators

$$\xi a + a \xi = 0, \quad (\xi a)^\dagger = a^\dagger \xi^* \quad . \quad (2.2.5)$$

Because of property (2.2.3),

$$f(\xi) = f_0 + f_1 \xi, \quad A(\xi^*, \xi) = a_0 + a_1 \xi + \bar{a}_1 \xi^* + a_{12} \xi^* \xi, \quad (2.2.6)$$

in particular,

$$e^{-\lambda \xi} = 1 - \lambda \xi \quad . \quad (2.2.7)$$

A derivative can be defined for Grassmann variable function,

$$\frac{\partial}{\partial \xi}(\xi^* \xi) = \frac{\partial}{\partial \xi}(-\xi \xi^*) = -\xi^* \quad . \quad (2.2.8)$$

And a integral can be defined as

$$\int d\xi 1 = 0, \quad \int d\xi \xi = 1, \quad \int d\xi^* 1 = 0, \quad \int d\xi^* \xi^* = 1, \quad (2.2.9)$$

to remember,

$$\int d\xi = \frac{\partial}{\partial \xi}, \quad \int d\xi^* = \frac{\partial}{\partial \xi^*} \quad . \quad (2.2.10)$$

2.3 Fermion Coherent States

Fermion Coherent States is defined as

$$|\xi\rangle = e^{-\sum_\alpha \xi_\alpha a_\alpha^\dagger} |0\rangle = \prod_\alpha (1 - \xi_\alpha a_\alpha^\dagger) |0\rangle, \quad (2.3.1)$$

we can verify that $a_\alpha |\xi\rangle = \xi_\alpha |\xi\rangle$ by using

$$\xi_\alpha |0\rangle = \xi_\alpha (1 - \xi_\alpha a_\alpha^\dagger) |0\rangle \quad . \quad (2.3.2)$$

Similarly, the adjoint of the coherent states is

$$\langle \xi | = \langle 0 | e^{-\sum_\alpha a_\alpha \xi_\alpha^*} = \langle 0 | e^{\sum_\alpha \xi_\alpha^* a_\alpha} \quad . \quad (2.3.3)$$

The overlap of two coherent states is

$$\langle \xi | \xi' \rangle = \prod_\alpha (1 + \xi_\alpha^* \xi'_\alpha) = e^{\sum_\alpha \xi_\alpha^* \xi'_\alpha} \quad . \quad (2.3.4)$$

The closure relation can be written as

$$\int \left(\prod_{\alpha} d\xi_{\alpha}^* d\xi_{\alpha} \right) e^{-\sum_{\alpha} \xi_{\alpha}^* \xi_{\alpha}} |\xi\rangle \langle \xi| = 1 \quad . \quad (2.3.5)$$

The trace of an operator A in Fock space can be written as

$$\text{Tr} A = \int \left(\prod_{\alpha} d\xi_{\alpha}^* d\xi_{\alpha} \right) e^{-\sum_{\alpha} \xi_{\alpha}^* \xi_{\alpha}} \langle -\xi | A | \xi \rangle, \quad (2.3.6)$$

note the anti periodic condition here.

Chapter 3

Linear Response

3.1 Perturbations Depending on Time

We now seek the solution of the perturbed equation

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = [H_0 + V(t)]\Psi(t), \quad (3.1.1)$$

in the form of a sum

$$\Psi(t) = \sum_k a_k(t) \psi_k(t), \quad (3.1.2)$$

where the expansion coefficients $a_k(t)$ are functions of time, and $\psi_k(t)$ are unperturbed stationary wave functions:

$$i\hbar \frac{\partial \psi_k(t)}{\partial t} = H_0 \psi_k(t) = E_k^{(0)} \psi_k(t). \quad (3.1.3)$$

Therefore we obtain that

$$i\hbar \sum_k \psi_k(t) \frac{da_k(t)}{dt} = \sum_k a_k(t) V(t) \psi_k(t), \quad (3.1.4)$$

multiplying both sides of this equation on the left by $\psi_m(t)$ and integrating then

$$i\hbar \frac{da_m(t)}{dt} = \sum_k V_{mk}(t) a_k(t), \quad (3.1.5)$$

where

$$V_{mk}(t) = \langle m | V | k \rangle e^{i\omega_{mk}t} = V_{mk} e^{i\omega_{mk}t}, \quad \omega_{mk} = \frac{E_m^{(0)} - E_k^{(0)}}{\hbar}. \quad (3.1.6)$$

Let the unperturbed wave function be $\psi_n(t)$, i.e. $a_n^{(0)} = 1$ and $a_k^{(0)} = 0$ for $k \neq n$. To find the first approximation, we seek $a_k = a_k^{(0)} + a_k^{(1)}$, substituting $a_k = a_k(0)$ we find

$$i\hbar \frac{da_k^{(1)}(t)}{dt} = V_{kn}(t), \quad (3.1.7)$$

integrating it gives

$$a_{kn}^{(1)}(t) = -\frac{i}{\hbar} \int V_{kn} e^{i\omega_{kn}t} dt. \quad (3.1.8)$$

3.2 Fermi Golden Rule

Let the perturbation be

$$V(t) = V e^{-i\omega t}, \quad (3.2.1)$$

then

$$a_{fi} = -\frac{i}{\hbar} \int_0^t V_{fi}(t) dt = -V_{fi} \frac{e^{i(\omega_{fi}-\omega)t} - 1}{\hbar(\omega_{fi} - \omega)}. \quad (3.2.2)$$

Therefore the squared modulus of a_{fi} is

$$|a_{fi}|^2 = |V_{fi}|^2 \frac{4 \sin^2[\frac{1}{2}(\omega_{fi} - \omega)t]}{\hbar^2(\omega_{fi} - \omega)^2}, \quad (3.2.3)$$

noticing that $\lim_{t \rightarrow \infty} \frac{\sin^2 \alpha t}{\pi t \alpha^2} = \delta(\alpha)$ we have

$$|a_{fi}|^2 = \frac{2\pi}{\hbar} |V_{fi}|^2 \delta(E_f - E_i - \hbar\omega) t. \quad (3.2.4)$$

Thus the probability dw_{fi} of the transition rate per unit time is

$$dw_{fi} = \frac{2\pi}{\hbar} |V_{fi}|^2 \delta(E_f - E_i - \hbar\omega). \quad (3.2.5)$$

Another method to derive the above formula is that let

$$V(t) = V e^{-i\omega t + \eta t}, \quad (3.2.6)$$

and integrating from $t = -\infty$ to $t = 0$, then

$$|a_{fi}|^2 = \frac{1}{\hbar^2} |V_{fi}|^2 \frac{e^{2\eta t}}{(\omega_{fi} - \omega)^2 + \eta^2} \quad (3.2.7)$$

Then the transition rate is [note that $\lim_{\eta \rightarrow 0} \frac{\eta}{\pi(\alpha^2 + \eta^2)} = \delta(\alpha)$]

$$\frac{d}{dt} |a_{fi}|^2 = \frac{2\pi}{\hbar} |V_{fi}|^2 \delta(E_f - E_i - \hbar\omega). \quad (3.2.8)$$

3.3 The Generalized Susceptibility

When there exists an external interaction, the perturbing operator can be written as

$$V = -x f(t), \quad (3.3.1)$$

where x is the operator of the physical quantity concerned, and the perturbing generalized force f is a given function of time.

The quantum mean value $\bar{x}(t)$ is given by a formula of the type

$$\bar{x}(t) = \int_0^\infty \alpha(\tau) f(t - \tau) d\tau, \quad (3.3.2)$$

where $\alpha(\tau)$ being a function of time which depends on the properties of the body.

Applying fourier transform on both sides of this formula

$$\int_0^\infty \bar{x}(t) e^{i\omega t} dt = \int_0^\infty \alpha(\tau) f(t - \tau) e^{i\omega t} d\tau dt, \quad (3.3.3)$$

we obtain that

$$\bar{x}(\omega) = \alpha(\omega) f(\omega). \quad (3.3.4)$$

If the function f is purely monochromatic and is given by the real expression

$$f(t) = \frac{1}{2}(f_0 e^{-i\omega t} + f_0^* e^{i\omega t}), \quad (3.3.5)$$

then we shall have

$$\bar{x}(t) = \frac{1}{2}[\alpha(\omega) f_0 e^{-i\omega t} + \alpha(-\omega) f_0^* e^{i\omega t}] \quad (3.3.6)$$

The function $\alpha(\omega)$ has the similar properties as retarded Green's function:

$$\alpha(-\omega) = \alpha^*(\omega), \quad (3.3.7)$$

i.e.,

$$\operatorname{Re} \alpha(-\omega) = \operatorname{Re} \alpha(\omega), \quad \operatorname{Im} \alpha(-\omega) = -\operatorname{Im} \alpha(\omega). \quad (3.3.8)$$

And the Kramers-Kronig relations:

$$\operatorname{Re} \alpha(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\operatorname{Im} \alpha(\varepsilon)}{\omega - \varepsilon} d\varepsilon, \quad \operatorname{Im} \alpha(\omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\operatorname{Re} \alpha(\varepsilon)}{\omega - \varepsilon} d\varepsilon. \quad (3.3.9)$$

The energy change per unit time of the system is just $dE/dt = \overline{\partial H / \partial t}$, since only the perturbation V in Hamiltonian depends on explicitly on time, we have

$$\frac{dE}{dt} = -\bar{x} \frac{df}{dt}. \quad (3.3.10)$$

Substituting \bar{x} and f from (3.3.5) and (3.3.6) and averaging over time, the terms containing $e^{2i\omega t}$ vanish, and we obtain

$$Q = \frac{1}{4} i\omega (\alpha^* - \alpha) |f_0|^2 = \frac{1}{2} \omega \operatorname{Im} \alpha(\omega) |f_0|^2, \quad (3.3.11)$$

where Q is the mean energy dissipated per unit time.

3.4 The Fluctuation Dissipation Theorem

Let us now assume that the system is at state $|n\rangle$ and is subject to a periodic perturbation, described by the operator

$$V = -xf = -\frac{1}{2}x(f_0 e^{-i\omega t} + f_0^* e^{i\omega t}). \quad (3.4.1)$$

Using Fermi Golden Rule, the transition rate from state n to state m per unit time is given by

$$w_{mn} = \frac{\pi |f_0|^2}{2\hbar^2} |x_{mn}|^2 [\delta(\omega + \omega_{mn}) + \delta(\omega + \omega_{nm})]. \quad (3.4.2)$$

The dissipation per unit time is given by

$$Q = \sum_m w_{mn} \hbar \omega_{mn} = \frac{\pi}{2\hbar} |f_0|^2 \sum_m |x_{mn}|^2 [\delta(\omega + \omega_{mn}) + \delta(\omega + \omega_{nm})] \omega_{mn}, \quad (3.4.3)$$

or, since the delta function zero except when their argument is zero,

$$Q = \frac{\pi}{2\hbar} \omega |f_0|^2 \sum_m |x_{mn}|^2 [\delta(\omega + \omega_{nm}) - \delta(\omega + \omega_{mn})], \quad (3.4.4)$$

thus

$$\operatorname{Im} \alpha(\omega) = \frac{\pi}{\hbar} \sum_m |x_{mn}|^2 [\delta(\omega + \omega_{nm}) - \delta(\omega + \omega_{mn})]. \quad (3.4.5)$$

Now define

$$(x^2)_\omega = \int_{-\infty}^{\infty} \frac{1}{2} \langle x(t)x(0) + x(0)x(t) \rangle e^{i\omega t} dt, \quad (3.4.6)$$

in canonical ensemble it is

$$(x^2)_\omega = \pi \sum_{nm} \rho_n |x_{mn}|^2 [\delta(\omega + \omega_{nm}) + \delta(\omega + \omega_{mn})], \quad (3.4.7)$$

where $\rho_n = e^{(F-E_n)/T}$, E_n denotes the energy levels and F is free energy. Since the summation is now over both m and n , these can be interchanged:

$$\begin{aligned} (x^2)_\omega &= \pi \sum_{mn} (\rho_n + \rho_m) |x_{mn}|^2 \delta(\omega + \omega_{nm}) \\ &= \pi \sum_{mn} \rho_n (1 + e^{-\hbar\omega_{mn}/T}) |x_{mn}|^2 \delta(\omega + \omega_{nm}) \\ &= \pi (1 + e^{-\hbar\omega/T}) \sum_{mn} \rho_n |x_{mn}|^2 \delta(\omega + \omega_{nm}). \end{aligned} \quad (3.4.8)$$

Similarly, in canonical ensemble

$$\text{Im } \alpha(\omega) = \frac{\pi}{\hbar} (1 - e^{-\hbar\omega/T}) \sum_{mn} \rho_n |x_{nm}|^2 \delta(\omega + \omega_{nm}), \quad (3.4.9)$$

a comparison of these two expressions gives

$$(x^2)_\omega = \hbar \text{Im } \alpha(\omega) \coth \frac{\hbar\omega}{2T}. \quad (3.4.10)$$

The mean square of the fluctuating quantity is given by the integration

$$\langle x^2 \rangle = \frac{\hbar}{\pi} \int_0^\infty \text{Im } \alpha(\omega) \coth \frac{\hbar\omega}{2T} d\omega. \quad (3.4.11)$$

3.5 Kubo Greenwood Formula

Now write the perturbing operator as

$$V = - \int \vec{j} \cdot \vec{A} dx, \quad (3.5.1)$$

let $\alpha(\omega)$ denotes the corresponding generalized susceptibility then the mean energy dissipated per unit time and per unit volume is

$$Q = \frac{1}{2} \omega \text{Im } \alpha(\omega) |\vec{A}|^2. \quad (3.5.2)$$

However, this generalized susceptibility is not the conductivity, to get the conductivity, recall that

$$\vec{E}(t) = - \frac{\partial \vec{A}}{\partial t}, \quad (3.5.3)$$

therefore

$$\vec{E}(\omega) = i\omega \vec{A}, \quad (3.5.4)$$

which means

$$j(\omega) = \alpha(\omega) A(\omega) = \frac{\alpha(\omega)}{i\omega} E(\omega), \quad (3.5.5)$$

or

$$\sigma(\omega) = \frac{\alpha(\omega)}{i\omega}. \quad (3.5.6)$$

Thus the dissipated term written in conductivity is just

$$Q = \frac{1}{2} \text{Im } \alpha(\omega) |A|^2 = \frac{1}{2} \text{Re } \sigma(\omega) |E|^2, \quad (3.5.7)$$

and

$$\operatorname{Re} \sigma = \frac{\operatorname{Im} \alpha}{\omega} = \frac{\pi}{\hbar \omega} \sum_{mn} (\rho_n - \rho_m) |j_{mn}|^2 \delta(\omega + \omega_{nm}). \quad (3.5.8)$$

Now there comes an assumption which is called “independent particle approximation”: we replace ρ by single electron distribution function f and recall that $j = -ev$ then

$$\operatorname{Re} \sigma = \frac{\hbar \pi e^2}{V} \sum_{mn} \frac{f_n - f_m}{\hbar \omega_{mn}} |v_{mn}|^2 \delta(E_n + \hbar \omega - E_m), \quad (3.5.9)$$

where V is the volume which acts as normalized factor. Notice that

$$\frac{f_n - f_m}{\hbar \omega_{mn}} \delta(E_n + \hbar \omega - E_m) = \int dE \frac{f(E) - f(E + \hbar \omega)}{\hbar \omega} \delta(E - E_n) \delta(E_n + \hbar \omega - E_m), \quad (3.5.10)$$

then the formula of $\operatorname{Re} \sigma$ become

$$\begin{aligned} \operatorname{Re} \sigma(\omega) &= \frac{\hbar \pi e^2}{V} \int dE \frac{f(E) - f(E + \hbar \omega)}{\hbar \omega} \sum_{nm} v_{nm} \delta(E_n + \hbar \omega - E_m) v_{mn} \delta(E - E_n) \\ &= \frac{\hbar e^2}{\pi V} \int dE \frac{f(E) - f(E + \hbar \omega)}{\hbar \omega} \operatorname{Tr}[v \operatorname{Im} G^R(E + \hbar \omega) v \operatorname{Im} G^R(E)]. \end{aligned} \quad (3.5.11)$$

For static conductivity, we have

$$\lim_{\omega \rightarrow 0} \operatorname{Re} \sigma(\omega) = \frac{\hbar e^2}{\pi V} \int dE \left(-\frac{\partial f}{\partial E} \right) \sum_k |\langle k | v | k \rangle|^2 |\operatorname{Im} G^R(E, k)|^2, \quad (3.5.12)$$

or in three dimension

$$\lim_{\omega \rightarrow 0} \operatorname{Re} \sigma(\omega) = \frac{\hbar e^2}{\pi} \int dE \left(-\frac{\partial f}{\partial E} \right) \int \frac{d^3 k}{(2\pi)^3} v^2(k) |\operatorname{Im} G^R(E, k)|^2. \quad (3.5.13)$$

3.6 Green Kubo Formula

Let $\Psi_n^{(0)}$ be the wave function of the unperturbed system, then applying equations of perturbations depending on time in first approximation we have

$$\Psi_n = \Psi_n^{(0)} + \sum_m a_m \Psi_m^{(0)}, \quad (3.6.1)$$

where a_m satisfy the equation

$$i\hbar \frac{da_m}{dt} = V_{mn} e^{i\omega_{mn}t} = -\frac{1}{2} x_{mn} e^{i\omega_{mn}t} (f_0 e^{-i\omega t} + f_0^* e^{i\omega t}). \quad (3.6.2)$$

In solving this, we must assume that the perturbation is “adiabatically” applied until the time t from $t = -\infty$, this means that we must put $\omega \rightarrow \omega \mp i0$ in factors $e^{\pm i\omega t}$. Then

$$a_m = \frac{1}{2\hbar} x_{mn} e^{i\omega_{mn}t} \left[\frac{f_0 e^{-i\omega t}}{\omega_{mn} - \omega - i0} + \frac{f_0^* e^{i\omega t}}{\omega_{mn} + \omega - i0} \right]. \quad (3.6.3)$$

Accordingly,

$$\begin{aligned} \bar{x} &= \int \Psi_n^* x \Psi_n dq \\ &= \sum_m (a_m x_{nm} e^{i\omega_{nm}t} + a_m^* x_{mn} e^{i\omega_{mn}t}) \\ &= \frac{1}{2\hbar} \sum_m x_{mn} x_{nm} \left[\frac{1}{\omega_{mn} - \omega - i0} + \frac{1}{\omega_{mn} + \omega - i0} \right] f_0 e^{-i\omega t} + \text{c.c.}, \end{aligned} \quad (3.6.4)$$

it can be seen that

$$\begin{aligned}\alpha(\omega) &= \frac{1}{\hbar} \sum_m |x_{mn}|^2 \left[\frac{1}{\omega_{mn} - \omega - i0} + \frac{1}{\omega_{mn} + \omega + i0} \right] \\ &= \frac{1}{\hbar} \sum_m |x_{mn}|^2 \left[-\frac{1}{\omega_{nm} + \omega + i0} + \frac{1}{\omega_{mn} + \omega + i0} \right].\end{aligned}\quad (3.6.5)$$

This expression is the Fourier transform of the function

$$\alpha(t) = \frac{i}{\hbar} \theta(t) \langle x(t)x(0) - x(0)x(t) \rangle = -G^R(t), \quad (3.6.6)$$

thus the we have the final result

$$\alpha(\omega) = \frac{i}{\hbar} \int_0^\infty e^{i\omega t} \langle x(t)x(0) - x(0)x(t) \rangle dt. \quad (3.6.7)$$

Similarly, if the generalized susceptibility of another physical quantity y is needed, we can write

$$\begin{aligned}\bar{y} &= \int \Psi_n^* y \Psi_n dq \\ &= \sum_m (a_m y_{nm} e^{i\omega_{nm}t} + a_m^* y_{mn} e^{i\omega_{mn}t}) \\ &= \frac{1}{2\hbar} \sum_m \left[\frac{x_{mn} y_{nm}}{\omega_{mn} - \omega - i0} + \frac{x_{nm} y_{mn}}{\omega_{mn} + \omega + i0} \right] f_0 e^{-i\omega t} + \text{c.c.},\end{aligned}\quad (3.6.8)$$

therefore

$$\begin{aligned}\alpha(\omega) &= \frac{1}{\hbar} \sum_m \left[\frac{x_{mn} y_{nm}}{\omega_{mn} - \omega - i0} + \frac{x_{nm} y_{mn}}{\omega_{mn} + \omega + i0} \right] \\ &= \frac{1}{\hbar} \sum_m \left[-\frac{x_{mn} y_{nm}}{\omega_{nm} + \omega + i0} + \frac{x_{nm} y_{mn}}{\omega_{mn} + \omega + i0} \right].\end{aligned}\quad (3.6.9)$$

This expression is the Fourier transform of the function

$$\alpha(t) = \frac{i}{\hbar} \theta(t) \langle y(t)x(0) - x(0)y(t) \rangle, \quad (3.6.10)$$

i.e.,

$$\alpha(\omega) = \frac{i}{\hbar} \int_0^\infty e^{i\omega t} \langle y(t)x(0) - x(0)y(t) \rangle dt. \quad (3.6.11)$$

Chapter 4

Fluctuations

4.1 Gaussian Distribution

The probability for a quantity x to have a value in the interval from x to $x + dx$ is proportional to $e^{S(x)}$, where $S(x)$ is the entropy formally regarded as a function of the exact value of x , namely

$$w(x) = \text{constant} \times e^{S(x)}. \quad (4.1.1)$$

The entropy S has a maximum for $x = \bar{x} = 0$. Hence $\partial S / \partial x = 0$ and $\partial^2 S / \partial x^2 < 0$ for $x = 0$. Expanding $S(x)$ in powers of x and retaining only terms of up to the second order, we obtain

$$S(x) = S(0) - \frac{1}{2}\beta x^2, \quad (4.1.2)$$

where β is a positive constant. Thus the probability distribution can be written in the form

$$w(x) = A e^{-\frac{1}{2}\beta x^2} = \sqrt{\frac{\beta}{2\pi}} e^{-\frac{1}{2}\beta x^2}. \quad (4.1.3)$$

The mean square fluctuation is

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 w(x) dx = \frac{1}{\beta}. \quad (4.1.4)$$

In similar manner we can determine the probability of a simultaneous deviation of several thermodynamic quantities from their mean values. Let these deviations be denoted by x_1, x_2, \dots, x_n . We define the entropy $S(x_1, \dots, x_n)$ as a function of the quantities x_1, \dots, x_n . Let S be expanded in powers of the x_i , as far as the second order terms, the difference $S - S_0$ is a negative-definite quadratic form:

$$S - S_0 = -\frac{1}{2}\beta_{ik}x_i x_k, \quad (4.1.5)$$

where $\beta_{ik} = \beta_{ki}$. Thus the probability distribution can be written as

$$w = A e^{-\frac{1}{2}\beta_{ik}x_i x_k} = \frac{\sqrt{\beta}}{(2\pi)^{\frac{n}{2}}} e^{-\frac{1}{2}\beta_{ik}x_i x_k}, \quad (4.1.6)$$

where β is the determinant of β_{ik} .

Let us define the quantities

$$X_i = -\frac{\partial S}{\partial x_i} = \beta_{ik}x_k, \quad (4.1.7)$$

which we refer as thermodynamically conjugate to the x_i . According to Gaussian distribution properties, we find that

$$\langle x_i X_k \rangle = \delta_{ik}, \quad \langle x_i x_k \rangle = \beta_{ik}^{-1}, \quad \langle X_i X_k \rangle = \beta_{ik}. \quad (4.1.8)$$

4.2 Fluctuations of The Fundamental Thermodynamic quantities

The probability w of a fluctuations is proportional to e^{S_t} , where S_t is the total entropy of a closed system. We can equally say that w is proportional to $e^{\Delta S_t}$, where ΔS_t is the change in entropy in the fluctuation. Thus

$$w \propto \exp \left(-\frac{\Delta E - T\Delta S + P\Delta V}{T} \right), \quad (4.2.1)$$

where $\Delta E, \Delta S, \Delta V$ are the changes in the energy, entropy and volume of the small part of the body in the fluctuation, and T, P the temperature and pressure of the medium.

Expanding ΔE in series, we obtain

$$\Delta E - T\Delta S + P\Delta V = \frac{1}{2} \left[\frac{\partial^2 E}{\partial S^2} (\Delta S)^2 + 2 \frac{\partial^2 E}{\partial S \partial V} \Delta S \Delta V + \frac{\partial^2 E}{\partial V^2} (\Delta V)^2 \right]. \quad (4.2.2)$$

It is easily seen that this expression may be written as

$$\frac{1}{2} \left[\Delta S \Delta \left(\frac{\partial E}{\partial S} \right)_V + \Delta V \Delta \left(\frac{\partial E}{\partial V} \right)_S \right] = \frac{1}{2} (\Delta S \Delta T - \Delta P \Delta V). \quad (4.2.3)$$

Thus we obtain the fluctuation probability in the form

$$w \propto \exp \left(\frac{\Delta P \Delta V - \Delta T \Delta S}{2T} \right). \quad (4.2.4)$$

From this general formula we can find the fluctuation of various thermodynamic quantities. Let us take V and T as independent variables, then

$$\begin{aligned} \Delta S &= \left(\frac{\partial S}{\partial T} \right)_V \Delta T + \left(\frac{\partial S}{\partial V} \right)_T \Delta V = \frac{C_V}{T} \Delta T + \left(\frac{\partial P}{\partial T} \right)_V \Delta V, \\ \Delta P &= \left(\frac{\partial P}{\partial T} \right)_V \Delta T + \left(\frac{\partial P}{\partial V} \right)_T \Delta V; \end{aligned} \quad (4.2.5)$$

therefore the distribution function becomes

$$w \propto \exp \left[-\frac{C_V}{2T^2} (\Delta T)^2 + \frac{1}{2T} \left(\frac{\partial P}{\partial V} \right)_T (\Delta V)^2 \right]. \quad (4.2.6)$$

Applying the general formula for the Gaussian distribution, we find the following expressions for the mean square fluctuations of temperature and volume:

$$\langle \Delta T \Delta V \rangle = 0, \quad \langle (\Delta T)^2 \rangle = \frac{T^2}{C_V}, \quad \langle (\Delta V)^2 \rangle = -T \left(\frac{\partial V}{\partial P} \right)_T. \quad (4.2.7)$$

These quantities are positive by virtue of the thermodynamic inequalities $C_V > 0$ and $(\partial P / \partial V)_T < 0$.

Let us now take P and S as the independent variables, then

$$\begin{aligned} \Delta V &= \left(\frac{\partial V}{\partial P} \right)_S \Delta P + \left(\frac{\partial V}{\partial S} \right)_P \Delta S = \left(\frac{\partial V}{\partial P} \right)_S \Delta P + \left(\frac{\partial T}{\partial P} \right)_S \Delta S; \\ \Delta T &= \left(\frac{\partial T}{\partial S} \right)_P \Delta S + \left(\frac{\partial T}{\partial P} \right)_S \Delta P = \frac{T}{C_P} \Delta S + \left(\frac{\partial T}{\partial P} \right)_S \Delta P. \end{aligned} \quad (4.2.8)$$

Therefore the distribution function becomes

$$w \propto \exp \left[\frac{1}{2T} \left(\frac{\partial V}{\partial P} \right)_S (\Delta P)^2 - \frac{1}{2C_P} (\Delta S)^2 \right], \quad (4.2.9)$$

and the mean square fluctuations are

$$\langle \Delta S \Delta P \rangle = 0, \quad \langle (\Delta S)^2 \rangle = C_P, \quad \langle (\Delta P)^2 \rangle = -T \left(\frac{\partial P}{\partial V} \right)_S. \quad (4.2.10)$$

Since $\langle(\Delta V)^2\rangle = -T(\partial V/\partial P)_T$, dividing both sides by N^2 we find the volume fluctuation per particle:

$$\langle(\Delta(V/N))^2\rangle = -\frac{T}{N^2} \left(\frac{\partial V}{\partial P} \right)_T. \quad (4.2.11)$$

We can find the fluctuation of the number of particles in a fixed volume. Since V is then constant, we must put $\Delta(V/N) = V\Delta(1/N) = -(V/N^2)\Delta N$, then

$$\langle(\Delta N)^2\rangle = -T \frac{N^2}{V^2} \left(\frac{\partial V}{\partial P} \right)_T. \quad (4.2.12)$$

Since $(\partial V/\partial P)_T$ is regarded as taken with N constant, we write

$$-\frac{N^2}{V^2} \left(\frac{\partial V}{\partial P} \right)_{T,N} = N \left(\frac{\partial}{\partial P} \frac{N}{V} \right). \quad (4.2.13)$$

The function N/V is a function of P and T only, and therefore does not matter whether N/V is differentiated at constant N or constant V , hence we can write

$$N \left(\frac{\partial}{\partial P} \frac{N}{V} \right)_{T,N} = \frac{N}{V} \left(\frac{\partial N}{\partial P} \right)_{T,V} = \left(\frac{\partial N}{\partial P} \right)_{T,V} \left(\frac{\partial P}{\partial \mu} \right)_{T,V} = \left(\frac{\partial N}{\partial \mu} \right)_{T,V}, \quad (4.2.14)$$

where we have used the equation $N/V = (\partial P/\partial \mu)_{T,V}$, which follows from formula $d\Omega = -VdP = -SdT - Nd\mu$. Thus we have for the fluctuation of the number of particles the formula

$$\langle(\Delta N)^2\rangle = T \left(\frac{\partial N}{\partial \mu} \right)_{T,V}. \quad (4.2.15)$$

For ideal gas, substituting $PV = NT$ gives

$$\langle(\Delta N)^2\rangle = N. \quad (4.2.16)$$

Let us consider an assembly of n_k particles in the k th quantum state, then

$$\langle(\Delta n_k)^2\rangle = T \frac{\partial \bar{n}_k}{\partial \mu}. \quad (4.2.17)$$

For a Fermi gas we must substitute

$$\bar{n}_k = \frac{1}{e^{(\varepsilon_k - \mu)/T} + 1}, \quad (4.2.18)$$

the differentiation gives

$$\langle(\Delta n_k)^2\rangle = \bar{n}_k(1 - \bar{n}_k). \quad (4.2.19)$$

Similarly, for a Bose gas

$$\langle(\Delta n_k)^2\rangle = \bar{n}_k(1 + \bar{n}_k). \quad (4.2.20)$$

For a Boltzmann gas the substitution $\bar{n}_k = e^{(\mu - \varepsilon_k)/T}$ gives

$$\langle(\Delta n_k)^2\rangle = \bar{n}_k, \quad (4.2.21)$$

where $\bar{n}_k \ll 1$.

Chapter 5

Small Polaron

5.1 Holstein Model

The Hamiltonian of Holstein Model is

$$H = - \sum_{\langle i,j \rangle} t_{ij} c_i^\dagger c_j + g \sum_i c_i^\dagger c_i (a_i + a_i^\dagger) + \omega_0 \sum_i a_i^\dagger a_i, \quad (5.1.1)$$

where c_i^\dagger (c_i) is creation (annihilation) operator for electron, and a_i^\dagger (a_i) is creation (annihilation) operator for phonon.

The model possesses two independent control parameters:

$$\lambda = g^2 / \omega_0 t, \quad (5.1.2)$$

$$\gamma = \omega_0 / t. \quad (5.1.3)$$

A third parameter can be conveniently introduced as a combination of the above ones:

$$\alpha = \lambda / \gamma = g / \omega_0. \quad (5.1.4)$$

It is worth defining the following regimes and limits, which are relevant to the Holstein model:

- (i) weak (strong) couplings $\lambda < 1$ ($\lambda > 1$);
- (ii) small (large) phonon frequency $\gamma < 1$ ($\gamma > 1$);
- (iii) multiphonon regime $\alpha^2 > 1$;
- (iv) adiabatic limit $\omega_0 = 0$, finite λ .

5.2 Weak Coupling Limit

Consider zero density ($n = 0$) and zero temperature ($T = 0$) limits, Green's function for a single electron can be defined as

$$G_{ij}(t) = -i \langle 0 | T c_i(t) c_j^\dagger(0) | 0 \rangle, \quad (5.2.1)$$

where $|0\rangle$ is the vacuum for phonons and electrons. There is only one possible ordering ($t > 0$), so the function is purely retarded.

Let $g \sum_i c_i^\dagger c_i (a_i + a_i^\dagger)$ acts as perturbation, we have that

$$G_{ij}(t) = -i \langle 0 | T c_i(t) c_j(0)^\dagger S | 0 \rangle, \quad (5.2.2)$$

where

$$S = T e^{-i \int dt [g \sum_i c_i^\dagger c_i (a_i + a_i^\dagger)]} \quad (5.2.3)$$

The expansion of S to second order of g gives

$$\begin{aligned} G_{ij}(t) &= -i \langle 0 | T c_i(t) c_j^\dagger | 0 \rangle \\ &\quad - i \frac{g^2}{2} \int dt' dt'' \sum_{kl} \langle 0 | T c_i(t) c_j^\dagger c_k^\dagger(t') c_k(t') c_l^\dagger(t'') c_l(t'') [a_k(t') a_l^\dagger(t'') + a_k^\dagger(t') a_l(t'')] | 0 \rangle, \end{aligned} \quad (5.2.4)$$

apply Wick's theorem and recall that (D is the Green's function for phonon)

$$\begin{aligned} \langle 0 | a_k^\dagger(t') a_l(t'') | 0 \rangle &= 0, \\ \langle 0 | a_k(t') a_l^\dagger(t'') | 0 \rangle &= D_{kl}(t' - t'') = \delta_{kl} D_{kk}(t' - t''), \end{aligned} \quad (5.2.5)$$

we can obtain that

$$G_{ij}(t) = G_{ij}^{(0)}(t) + ig^2 \sum_k \int dt' dt'' G_{ik}^{(0)}(t - t') G_{kk}^{(0)}(t' - t'') D_{kk}(t' - t'') G_{kj}(t''), \quad (5.2.6)$$

in frequency space, (note that $D_{kk}(t' - t'') = -ie^{-i\omega_0(t' - t'')}$)

$$G_{ij}(\omega) = G_{ij}^{(0)}(\omega) + g^2 \sum_k G_{ik}^{(0)}(\omega) G_{kk}^{(0)}(\omega - \omega_0) G_{kj}^{(0)}(\omega). \quad (5.2.7)$$

Compare with the Dyson equation

$$G_{ij} = G_{ij}^{(0)} + \sum_{kl} G_{ik}^{(0)} \Sigma_{kl} G_{lj} = G_{ij}^{(0)} + \sum_{kl} G_{ik}^{(0)} \Sigma_{kl} G_{lj}^{(0)} + \dots, \quad (5.2.8)$$

it is clear to see that second order perturbation gives a local (k -independent) self energy:

$$\Sigma_2(\omega) = g^2 G^{(0)}(\omega - \omega_0). \quad (5.2.9)$$

The electron effective mass, in the case of a local self-energy, is easily calculated via

$$\frac{m^*}{m} = \left. \frac{d(\omega - \text{Re}\Sigma(\omega))}{d\omega} \right|_{E_0} = 1 - \left. \frac{d\text{Re}\Sigma(\omega)}{d\omega} \right|_{E_0}, \quad (5.2.10)$$

where E_0 is the ground-state energy.

5.3 Atomic Limit (Zero Temperature)

The atomic limit is defined as the zero hopping case ($t = 0$). In this case, Hamiltonian (5.1.1) can be diagonalized by the unitary Lang-Firsov transformation

$$U = e^{-S}, \quad S = -\alpha \sum_i c_i^\dagger c_i (a_i - a_i^\dagger). \quad (5.3.1)$$

With the aid of Baker-Campbell-Hausdorff formula we have

$$\begin{aligned} \bar{c}_i &= e^S c_i e^{-S} = c_i X_i, \quad X_i = e^{\alpha(a_i - a_i^\dagger)}; \\ \bar{c}_i^\dagger &= e^S c_i^\dagger e^{-S} = c_i^\dagger X_i^\dagger, \quad X_i^\dagger = e^{\alpha(a_i^\dagger - a_i)}; \\ \bar{a}_i &= e^S a_i e^{-S} = a_i - \alpha c_i^\dagger c_i; \\ \bar{a}_i^\dagger &= e^S a_i^\dagger e^{-S} = a_i^\dagger - \alpha c_i^\dagger c_i; \\ \bar{H} &= e^S H e^{-S} = -\frac{g^2}{\omega_0} \sum_i c_i^\dagger c_i + \omega_0 \sum_i a_i^\dagger a_i. \end{aligned} \quad (5.3.2)$$

After the transformation, we can see that the ground energy is $\varepsilon_p = -g^2/\omega_0$, the excited state energy is $\varepsilon_p + n\omega_0$.

The static electron-displacement correlation function is defined as $C_0 = \langle n_i(a_i + a_i^\dagger) \rangle$, apply Lang-Firsov transformation it reads

$$C_0 = \langle n_i(a_i + a_i^\dagger) \rangle - 2\alpha \langle n_i \rangle = -2\alpha \langle n_i \rangle, \quad (5.3.3)$$

at the ground state $n_i = 1$, thus $C_0 = -2\alpha$. Meanwhile,

$$\langle e^S a^\dagger a e^{-S} \rangle = \langle a^\dagger a \rangle + \alpha^2 \langle c^\dagger c \rangle = \alpha^2. \quad (5.3.4)$$

The electron Green's function can also be calculated after the Lang-Firsov transformation¹:

$$\begin{aligned} G(t) &= -i \langle 0 | c(t) c^\dagger | 0 \rangle \\ &= -i \langle 0 | c X e^{-i\bar{H}t} c^\dagger X^\dagger | 0 \rangle \\ &= -i \sum_{mn} \langle 0 | c X | m \rangle \langle m | e^{-i\bar{H}t} | n \rangle \langle n | c^\dagger X^\dagger | 0 \rangle, \end{aligned} \quad (5.3.5)$$

where $|m\rangle$ is the phonon state corresponding to m phonons.

Using the Feynman result ($e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}$), we have that

$$X^\dagger = e^{-\alpha^2/2} e^{\alpha a^\dagger} e^{-\alpha a}, \quad X = e^{-\alpha^2/2} e^{-\alpha a^\dagger} e^{\alpha a}, \quad (5.3.6)$$

accordingly,

$$\begin{aligned} \langle m | X^\dagger | 0 \rangle &= e^{-\alpha^2/2} \langle m | e^{\alpha a^\dagger} | 0 \rangle = e^{-\alpha^2/2} \sum_n \langle m | \frac{\alpha^n}{\sqrt{n!}} | n \rangle = e^{-\alpha^2/2} \frac{\alpha^m}{\sqrt{m!}}, \\ \langle 0 | X | m \rangle &= e^{-\alpha^2/2} \frac{\alpha^m}{\sqrt{m!}}. \end{aligned} \quad (5.3.7)$$

Finally the electron Green's function is

$$G(\omega) = \sum_n \frac{\alpha^{2n} e^{-\alpha^2}}{n!} \frac{1}{\omega - n\omega_0 - \varepsilon_p}. \quad (5.3.8)$$

Let us now consider the action of the hopping. After the Lang-Firsov transformation, the hopping term becomes

$$t_{ij} c_i^\dagger c_j \rightarrow t_{ij} X_i^\dagger X_j c_i^\dagger c_j, \quad (5.3.9)$$

consider Holstein approximation, which neglect phonon emission and absorption during the hopping process, we have

$$t_{ij} \langle 0 | X_i^\dagger X_j | 0 \rangle = t_{ij} \langle 0 | X^\dagger | 0 \rangle \langle 0 | X | 0 \rangle = t_{ij} e^{-\alpha^2}. \quad (5.3.10)$$

5.4 Atomic Limit (Finite Temperature)

The Lang-Firsov transformation is the same as zero temperature case. Here we need to calculate $\langle n | X^\dagger | n \rangle$. We have that

$$\begin{aligned} e^{-\alpha a} | n \rangle &= \sum_{m=0}^{\infty} \frac{(-\alpha)^m}{m!} a^m | n \rangle \\ &= \sum_{m=0}^n \frac{(-\alpha)^m}{m!} \left[\frac{n!}{(n-m)!} \right]^{\frac{1}{2}} | n-m \rangle, \end{aligned} \quad (5.4.1)$$

and

$$\langle n | e^{\alpha a^\dagger} = \sum_{m=0}^n \frac{\alpha^m}{m!} \left[\frac{n!}{(n-m)!} \right]^{\frac{1}{2}} \langle n-m |, \quad (5.4.2)$$

¹Mahan's Many-Particle Physics, page 221

therefore

$$\langle n | e^{\alpha a^\dagger} e^{-\alpha a} | n \rangle = \sum_{m=0}^n \frac{(-\alpha^2)^m}{m!} \frac{n!}{m!(n-m)!} = L_n(\alpha^2), \quad (5.4.3)$$

where $L_n(x)$ is Laguerre polynomial. Thus

$$\langle n | X^\dagger | n \rangle = \langle n | X | n \rangle = e^{-\alpha^2/2} L_n(\alpha^2). \quad (5.4.4)$$

At finite temperature, the assumption is that we only average on phonon according to temperature. (“cold” electron in a thermalized phonon bath). So at finite temperature the effective hopping amplitude is

$$\begin{aligned} & t_{ij} (1 - e^{-\beta\omega_0})^2 \sum_{mn} e^{-\beta m\omega_0} \langle m | X_i^\dagger | m \rangle e^{-\beta n\omega_0} \langle n | X_j | n \rangle \\ &= t_{ij} e^{-\alpha^2} \left[(1 - e^{-\beta\omega_0}) \sum_{n=0}^{\infty} e^{-n\beta\omega_0} L_n(\alpha^2) \right]^2. \end{aligned} \quad (5.4.5)$$

Recall that the generating function of Laguerre polynomials:

$$\frac{e^{-xt/(1-t)}}{1-t} = \sum_{n=0}^{\infty} L_n(x) t^n, \quad (5.4.6)$$

let $t = e^{-\beta\omega_0}$ and $x = \alpha^2$ we find that the effective hopping amplitude is

$$t_{ij} e^{-S_T}, \quad S_T = \alpha^2 (1 + 2\langle n \rangle_T). \quad (5.4.7)$$

Now let us turn to electron Green’s function, now defined as

$$\begin{aligned} G(t) &= -i(1 - e^{-\beta\omega_0}) \sum_n e^{-\beta n\omega_0} \langle n | c(t) c^\dagger | n \rangle \\ &= -i(1 - e^{-\beta\omega_0}) \sum_n e^{-\beta n\omega_0} \langle 0 | c(t) X(t) c^\dagger X^\dagger | 0 \rangle \\ &= -i(1 - e^{-\beta\omega_0}) \langle 0 | c(t) c^\dagger | 0 \rangle \sum_n e^{-\beta n\omega_0} \langle n | X(t) X^\dagger | n \rangle. \end{aligned} \quad (5.4.8)$$

According to Heisenberg equation of motion (with Hamiltonian \bar{H}), we have that

$$\begin{aligned} c(t) &= c e^{-i\varepsilon_p t}, & c^\dagger(t) &= c^\dagger e^{i\varepsilon_p t}; \\ a(t) &= a e^{-i\omega_0 t}, & a^\dagger(t) &= a^\dagger e^{i\omega_0 t}, \end{aligned} \quad (5.4.9)$$

thus

$$X(t) = e^{-\alpha^2} e^{-\alpha a^\dagger e^{i\omega_0 t}} e^{\alpha a e^{-i\omega_0 t}} = e^{-\alpha^2} e^{-\alpha a^\dagger(t)} e^{\alpha a(t)} \quad (5.4.10)$$

and

$$X(t) X^\dagger = e^{-\alpha^2} e^{-\alpha a^\dagger(t)} e^{\alpha a(t)} e^{\alpha a^\dagger} e^{-\alpha a}. \quad (5.4.11)$$

Now we write $e^{\alpha a(t)} e^{\alpha a^\dagger}$ as²

$$e^{\alpha a(t)} e^{\alpha a^\dagger} = e^{\alpha a^\dagger} [e^{-\alpha a^\dagger} e^{\alpha a(t)} e^{\alpha a^\dagger}], \quad (5.4.12)$$

using Baker-Campbell-Hausdorff formula we get

$$e^{-\alpha a^\dagger} e^{\alpha a(t)} e^{\alpha a^\dagger} = e^{\alpha^2 e^{-i\omega_0 t}} e^{\alpha a(t)}. \quad (5.4.13)$$

²see Mahan’s Many-Particle Physics, page 222

Finally the electron Green's function is arranged into the desired form:

$$G(t) = -i(1 - e^{-\beta\omega_0})e^{-\alpha^2(1-e^{-i\omega_0 t})}\langle 0|c(t)c^\dagger|0\rangle \sum_n e^{-\beta n\omega_0} \langle n|e^{\alpha a^\dagger(1-e^{-i\omega_0 t})}e^{-\alpha a(1-e^{-i\omega_0 t})}|n\rangle, \quad (5.4.14)$$

again using Laguerre polynomials we can prove that

$$(1 - e^{-\beta\omega_0}) \sum_n e^{-\beta n\omega_0} \langle n|e^{u^* a^\dagger}e^{-ua}|n\rangle = e^{-|u|^2/(e^{\beta\omega_0}-1)}, \quad (5.4.15)$$

thus

$$G(t) = -ie^{-i\varepsilon_p t} \exp\left[-\alpha^2[(N+1)(1-e^{-i\omega_0 t}) + N(1-e^{i\omega_0 t})]\right], \quad (5.4.16)$$

where

$$N = \frac{1}{e^{\beta\omega_0} - 1}. \quad (5.4.17)$$

Recall the generating function of Bessel functions of complex argument,

$$e^{z \cos \theta} = \sum_{n=-\infty}^{\infty} I_n(z) e^{in\theta}, \quad (5.4.18)$$

let [note $(N+1)/N = e^{\beta\omega_0}$, $\sqrt{(N+1)/N} = e^{\beta\omega_0/2}$]

$$z = 2\alpha^2 \sqrt{N(N+1)}, \quad \theta = \omega_0(t + i\beta/2) \quad (5.4.19)$$

then (note that $I_n = I_{-n}$)

$$G(t) = -ie^{-(2N+1)\alpha^2} e^{-i\varepsilon_p t} \sum_{n=-\infty}^{\infty} e^{-in\omega_0 t} e^{\beta n\omega_0/2} I_n\{2\alpha^2 \sqrt{N(N+1)}\}, \quad (5.4.20)$$

in frequency space

$$G(\omega) = e^{-(2N+1)\alpha^2} \sum_{n=-\infty}^{\infty} e^{\beta n\omega_0/2} I_n\{2\alpha^2 \sqrt{N(N+1)}\} \frac{1}{\omega - n\omega_0 - \varepsilon_p}. \quad (5.4.21)$$

5.5 The Impurity Analogy for A Single Electron

The Hamiltonian for impurity model is

$$H_{\text{imp}} = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_k V_k (c_k^\dagger d + d^\dagger c_k) + \omega_0 a^\dagger a + g d^\dagger d (a + a^\dagger), \quad (5.5.1)$$

here V_k and E_k is related to G_0 by

$$G_0^{-1}(\omega) = \omega - \int_{-\infty}^{\infty} d\varepsilon \frac{\Delta(\varepsilon)}{\omega - \varepsilon}, \quad (5.5.2)$$

where

$$\Delta(\varepsilon) = \sum_k V_k^2 \delta(\varepsilon - \varepsilon_k). \quad (5.5.3)$$

Let us separate the Hamiltonian into two parts H_0 and V , where

$$H_0 = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_k V_k (c_k^\dagger d + d^\dagger c_k) + \omega_0 a^\dagger a, \quad V = g d^\dagger d (a + a^\dagger). \quad (5.5.4)$$

5.5.1 The Zero Temperature Formalism

The Green's function for one electron at zero temperature is

$$G(t) = -i\theta(t)\langle 0|d(t)d^\dagger|0\rangle, \quad (5.5.5)$$

after Fourier transformation:

$$G(\omega) = \langle 0|d\frac{1}{\omega + i0 - H}d^\dagger|0\rangle. \quad (5.5.6)$$

An operator identity holds:

$$\frac{1}{\omega - H} = \frac{1}{\omega - H_0} + \frac{1}{\omega - H_0}V\frac{1}{\omega - H}. \quad (5.5.7)$$

To proceed further one needs to introduce the generalized matrix elements:

$$G_{nm} = \langle 0|\frac{a^n}{\sqrt{n!}}d\frac{1}{\omega - H}d^\dagger\frac{(a^\dagger)^m}{\sqrt{m!}}|0\rangle, \quad (5.5.8)$$

now introduce a set of zero electron p -phonon states and a set of one electron p -phonon states

$$|0, p\rangle = \frac{(a^\dagger)^p}{\sqrt{p!}}|0\rangle, \quad |1, p\rangle = \frac{(a^\dagger)^p}{\sqrt{p!}}d^\dagger|0\rangle, \quad (5.5.9)$$

one can write

$$\begin{aligned} G_{nm} &= \langle 0|\frac{a^n}{\sqrt{n!}}d\frac{1}{\omega - H_0}d^\dagger\frac{(a^\dagger)^m}{\sqrt{m!}}|0\rangle + \langle 0|\frac{a^n}{\sqrt{n!}}d\frac{1}{\omega - H_0}V\frac{1}{\omega - H}d^\dagger\frac{(a^\dagger)^m}{\sqrt{m!}}|0\rangle \\ &= G_{nm}^{(0)} + g \sum_{p_1, p_2} \langle 0|\frac{a^n}{\sqrt{n!}}d\frac{1}{\omega - H_0}d^\dagger|0, p_1\rangle \langle 0, p_1|d(a + a^\dagger)|1, p_2\rangle \langle 0, p_2|d\frac{1}{\omega - H}d^\dagger\frac{(a^\dagger)^m}{\sqrt{m!}}|0\rangle \\ &= G_{nm}^{(0)} + g \sum_{p_1, p_2} G_{n, p_1}^{(0)} X_{p_1, p_2} G_{p_2, m} \\ &= G_{nn}^{(0)} \delta_{nm} + g \sum_p G_{nn}^{(0)} X_{np} G_{pm}, \end{aligned} \quad (5.5.10)$$

where $G_{nn}^{(0)}(\omega) = G_{00}^{(0)}(\omega - n\omega_0)$ is the diagonal element of the free Green's function, X_{np} are the phonon displacement matrix elements:

$$X_{np} = \sqrt{p+1}\delta_{n, p+1} + \sqrt{p}\delta_{n, p-1}. \quad (5.5.11)$$

Equation (5.5.10) can be solved in matrix notation:

$$G^{-1} = G_0^{-1} - gX, \quad (5.5.12)$$

it is easy to that G^{-1} is a tridiagonal matrix.

Now define T_k as the determinant of G^{-1} with first k rows and columns removed, using Cramer's rule we find that

$$G_{00} = \frac{T_1}{T_0}, \quad (5.5.13)$$

and define D_k as the determinant comprising the first $k+1$ rows and columns of G^{-1} and $D_{-1} = 1, D_{-2} = 0$, then

$$\begin{aligned} D_0 &= [G^{(0)}]_{00}^{-1}, \\ D_1 &= [G^{(0)}]_{11}^{-1} [G^{(0)}]_{00}^{-1} - g^2 = [G^{(0)}]_{11}^{-1} D_0 - g^2, \\ D_2 &= \dots = [G^{(0)}]_2^{-1} D_1 - 2g^2 D_0, \end{aligned} \quad (5.5.14)$$

and, for the general case, the recurrence relations

$$D_k = [G^{(0)}]_{k,k}^{-1} D_{k-1} - kg^2 D_{k-2}. \quad (5.5.15)$$

What's more, we have that

$$T_k = [G^{(0)}]_{kk}^{-1} T_{k+1} - (k+1)g^2 T_{k+2}, \quad \text{or} \quad \frac{T_k}{T_{k+1}} = [G^{(0)}]_{kk}^{-1} - (k+1)g^2 \frac{T_{k+2}}{T_{k+1}}, \quad (5.5.16)$$

therefore

$$\frac{T_1}{T_0} = \frac{1}{[G^{(0)}]_{00}^{-1} - g^2 \frac{T_2}{T_1}} = \dots, \quad (5.5.17)$$

or

$$G(\omega) = \frac{1}{G_0^{-1}(\omega) - \frac{g^2}{G_0^{-1}(\omega - \omega_0) - \frac{2g^2}{G_0^{-1}(\omega - 2\omega_0) - \frac{3g^2}{G_0^{-1}(\omega - 3\omega_0) - \dots}}}} \quad (5.5.18)$$

Now use Dyson equation $\Sigma = G_0^{-1} - G^{-1}$ and we shall get

$$\Sigma(\omega) = \frac{g^2}{G_0^{-1}(\omega - \omega_0) - \frac{2g^2}{G_0^{-1}(\omega - 2\omega_0) - \frac{3g^2}{G_0^{-1}(\omega - 3\omega_0) - \dots}}} \quad (5.5.19)$$

The self-energy can be defined recursively,

$$\Sigma^{(p)}(\omega) = \frac{pg^2}{G_0^{-1}(\omega - p\omega_0) - \Sigma^{(p+1)}} \quad (5.5.20)$$

5.5.2 The Finite Temperature Formalism

At finite temperature, the trace performed over free phonon states gives

$$G(\omega) = (1 - e^{\beta\omega_0}) \sum_n e^{-\beta n\omega_0} G_{nn}(\omega). \quad (5.5.21)$$

Now we need to calculate $G_{nn}(\omega)$, according to $G^{-1}G = I$ we have such a recurrence relation (recall that G^{-1} is a tridiagonal matrix):

$$G_{nn} = G_n^{(0)} + gG_n^{(0)}(\sqrt{n}G_{n-1,n} + \sqrt{n+1}G_{n+1,n}), \quad (5.5.22)$$

which we seek to write in a form as

$$G_{nn} = G_n^{(0)} + G_n^{(0)}(AG_{nn} + BG_{nn}). \quad (5.5.23)$$

Again according to Cramer's rule,

$$G_{n-1,n} = \sqrt{n}g \frac{D_{n-2}T_{n+1}}{T_0}, \quad G_{nn} = \frac{D_{n-1}T_{n+1}}{T_0}, \quad (5.5.24)$$

recall the recurrence relation for D :

$$D_k = [G_k^{(0)}]^{-1} D_{k-1} - kg^2 D_{k-2}, \quad (5.5.25)$$

or

$$\frac{D_{k-1}}{D_k} = \frac{1}{[G_k^{(0)}]^{-1} - kg^2 \frac{D_{k-2}}{D_{k-1}}} \quad (5.5.26)$$

Therefore

$$G_{n-1,n} = \sqrt{n}g \frac{D_{n-2}}{D_{n-1}} \frac{D_{n-1}T_{n+1}}{T_0} = \sqrt{n}g \frac{D_{n-2}}{D_{n-1}} G_{nn}, \quad (5.5.27)$$

i.e.,

$$A = ng^2 \frac{D_{n-2}}{D_{n-1}} = \frac{ng^2}{[G_n^{(0)}(\omega + \omega_0)]^{-1} - \frac{(n-1)g^2}{[G_n^{(0)}(\omega + 2\omega_0)]^{-1} - \frac{(n-2)g^2}{\ddots - \frac{g^2}{[G_n^{(0)}(\omega + n\omega_0)]^{-1}}}} \quad (5.5.28)$$

Similarly,

$$G_{n+1,n} = \sqrt{n+1}g \frac{D_{n-1}T_{n+2}}{T_0} = \sqrt{n+1}g \frac{T_{n+2}}{T_{n+1}} G_{nn}, \quad (5.5.29)$$

recall the recurrence relation for T :

$$T_k = [G_k^{(0)}]^{-1} T_{k+1} - (k+1)g^2 T_{k+2}, \quad (5.5.30)$$

or

$$\frac{T_{k+1}}{T_k} = \frac{1}{[G_k^{(0)}]^{-1} - (k+1)g^2 \frac{T_{k+2}}{T_{k+1}}}. \quad (5.5.31)$$

Therefore

$$B = (n+1)g^2 \frac{T_{n+2}}{T_{n+1}} = \frac{(n+1)g^2}{[G_n^{(0)}(\omega - \omega_0)]^{-1} - \frac{(n+2)g^2}{[G_n^{(0)}(\omega - 2\omega_0)]^{-1} - \frac{(n+3)g^2}{[G_n^{(0)}(\omega - 3\omega_0)]^{-1} - \dots}}, \quad (5.5.32)$$

finally

$$G_{nn} = \frac{1}{[G_n^{(0)}]^{-1} - A - B}. \quad (5.5.33)$$

5.5.3 Dynamical Mean Field

If we want to apply dynamical mean field theory, then a self consistent condition is needed. Basically it is (see the solution for simple impurity model)

$$G^{-1}(\omega) = \omega - \sum_{ij} t_{oi} t_{jo} G_{ij}^{(o)}(\omega), \quad (5.5.34)$$

where $G_{ij}^{(o)}$ is the Green's function with one site removed. For Bethe lattice, it is very simple, in this case it is restricted $i = j$, and in limit of infinite connectivity $G_{ii}^{(o)} = G_{ii}$. Therefore for Bethe lattice

$$G^{-1}(\omega) = \omega - t^2 G(\omega). \quad (5.5.35)$$

For a general lattice, the relation between the cavity and full Green's functions reads

$$G_{ij}^{(o)} = G_{ij} - \frac{G_{io} G_{oj}}{G_{oo}}. \quad (5.5.36)$$

Therefore equation (5.5.34) become

$$G^{-1} = \omega - \sum_{ij} t_{oi} t_{jo} G_{ij} + \frac{(\sum_i G_{oi})^2}{G_{oo}}, \quad (5.5.37)$$

recall that

$$G(\omega, k) = \frac{1}{\omega - \varepsilon_k - \Sigma(\omega)}, \quad (5.5.38)$$

we have that

$$G^{-1} = \omega - \int d\varepsilon \frac{\rho(\varepsilon)\varepsilon^2}{\zeta - \varepsilon} - \left(\int d\varepsilon \frac{\rho(\varepsilon)\varepsilon}{\zeta - \varepsilon} \right)^2 / \int d\varepsilon \frac{\rho(\varepsilon)}{\zeta - \varepsilon}, \quad (5.5.39)$$

where $\zeta = \omega - \Sigma(\omega)$. This can be simplified further using the following relations:

$$\int d\varepsilon \frac{\rho(\varepsilon)\varepsilon^2}{\zeta - \varepsilon} = \zeta \int d\varepsilon \frac{\rho(\varepsilon)\varepsilon}{\zeta - \varepsilon}, \quad \int d\varepsilon \frac{\rho(\varepsilon)}{\zeta - \varepsilon} = -1 + \zeta \int d\varepsilon \frac{\rho(\varepsilon)}{\zeta - \varepsilon}. \quad (5.5.40)$$

We have used $t_{oo} = \sum_k t_k = \int \rho(\varepsilon)\varepsilon = 0$, finally

$$G_0^{-1} = \Sigma + G^{-1}. \quad (5.5.41)$$

Chapter 6

Physical Constants

- The speed of light in vacuum, $c = 299,792,458 \text{ m/s} \approx 3 \times 10^8 \text{ m/s}$.
- Electric charge $e = -1.602 \times 10^{-19} \text{ C}$.
- energy in SI unit, joule $J = \text{kg} \cdot (\text{m/s})^2 = \text{N} \cdot \text{m} = \text{C} \cdot \text{V}$.
- Planck constant $h = 6.62607004 \times 10^{-34} \text{ J} \cdot \text{s} = 4.135667662 \times 10^{-15} \text{ eV} \cdot \text{s}$.
- reduced Planck constant $\hbar = 1.0545718 \times 10^{-34} \text{ J} \cdot \text{s} = 6.582119514 \times 10^{-16} \text{ eV} \cdot \text{s}$.
- Boltzmann constant $k_B = 1.38064852 \times 10^{-23} \text{ J} \cdot \text{K}^{-1} = 8.6173324 \times 10^{-5} \text{ eV} \cdot \text{K}^{-1}$.
- Bohr magneton $\mu_B = 9.27400968 \times 10^{-24} \text{ J} \cdot \text{T}^{-1} = 5.7883818066 \times 10^{-5} \text{ eV} \cdot \text{T}^{-1}$.
- Bohr radius $a_0 = 5.29 \times 10^{-11} \text{ m}$.
- Electron mass $m_e = 9.10938215 \times 10^{-31} \text{ kg} = 8.18710438 \times 10^{-14} \text{ J/c}^2 = 0.51099891 \text{ MeV/c}^2$.
- Ohm $\Omega = \frac{\text{V}}{\text{A}} = \frac{\text{V} \cdot \text{s}}{\text{C}} = \frac{\text{J} \cdot \text{s}}{\text{C}^2} = \frac{\text{J}}{\text{s} \cdot \text{A}^2}$.