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# Chapter 1

## Useful formulas

### 1.1 Gaussian Integrals

For a positive number  $a$ ,

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

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  $\beta_{ik}$  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 conjugate<sup>1</sup> 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.

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

---

<sup>1</sup>when apply to thermodynamics we call it thermodynamically conjugate.

## 1.3 Delta Function

The  $\delta$  function satisfies the following properties.

$$\int \delta(x - a)f(x) = f(a). \quad (1.3.1)$$

And  $\delta$  function is an even function:

$$\delta(-x) = \delta(x). \quad (1.3.2)$$

For a non-zero scalar  $\alpha$

$$\delta(\alpha x) = \frac{\delta(x)}{|\alpha|} \quad (1.3.3)$$

The  $\delta$  function can be expressed as

$$\delta(x - \alpha) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ip(x-\alpha)} dp = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ip(x-\alpha)} dp. \quad (1.3.4)$$

## 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  $\infty$ , 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

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

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:

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

## 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 Kubo Identity

The Kubo Identity states that

$$[e^{-\beta H}, A] = e^{-\beta H} \int_0^{\beta} e^{\lambda H} [A, H] e^{-\lambda H} d\lambda. \quad (1.7.1)$$

To derive this relation, let us consider a quantity

$$S = e^{\lambda H} [A, e^{-\lambda H}] = e^{\lambda H} A e^{-\lambda H} - A, \quad (1.7.2)$$

differentiating it with respect to  $\lambda$  yields

$$\frac{dS}{d\lambda} = e^{\lambda H} [H, A] e^{-\lambda}. \quad (1.7.3)$$

Therefore

$$S(\beta) = S(0) + \int_0^{\beta} \frac{dS}{d\lambda} d\lambda = \int_0^{\beta} e^{\lambda H} [H, A] e^{-\lambda H} d\lambda, \quad (1.7.4)$$

and accordingly

$$[e^{-\beta H}, A] = -e^{-\beta H} S(\beta) = e^{-\beta H} \int_0^{\beta} e^{\lambda H} [A, H] e^{-\lambda H} d\lambda. \quad (1.7.5)$$

## 1.8 Laguerre Polynomials

The Laguerre polynomials are solution of Laguerre's equation:

$$xy'' + (1-x)y' + ny = 0, \quad (1.8.1)$$

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

$$L_n(x) = \frac{e^x}{n!} \frac{d^n}{dx^n} (e^{-x} x^n) = \sum_{k=0}^n \frac{(-x)^k}{k!} \frac{n!}{k!(n-k)!}. \quad (1.8.2)$$

The generating function is

$$\frac{e^{-xt/(1-t)}}{1-t} = \sum_{n=0}^{\infty} L_n(x) t^n. \quad (1.8.3)$$

## 1.9 Cramer's Rule

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

$$Ax = b, \quad (1.9.1)$$

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:

$$x_i = \frac{\det A_i}{\det A}, \quad (1.9.2)$$

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

## 1.10 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

$$(A + uv^T)^{-1} = A^{-1} - \frac{A^{-1} u v^T A^{-1}}{1 + v^T A^{-1} u}. \quad (1.10.1)$$

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

## 1.11 Simple Impurity Model at Zero Temperature

The Hamiltonian of simple impurity model is defined as

$$H = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_k V_k (c_k^\dagger d + d^\dagger c_k) + \varepsilon_0 d^\dagger d, \quad (1.11.1)$$

let  $H = H_0 + V$ , where

$$H_0 = \sum_k \varepsilon_k c_k^\dagger c_k + \varepsilon_0 d^\dagger d, \quad V = \sum_k V_k (c_k^\dagger d + d^\dagger c_k). \quad (1.11.2)$$

The Green's function is

$$G(t) = -i \langle 0 | T d(t) d^\dagger | 0 \rangle = -i \langle 0 | d(t) d^\dagger | 0 \rangle, \quad (1.11.3)$$

apply Fourier transform on it, then

$$G(\omega) = \langle 0 | d \frac{1}{\omega + i0 - H} d^\dagger | 0 \rangle. \quad (1.11.4)$$



Notice that

$$\begin{aligned}\frac{1}{\omega - H} &= \frac{1}{\omega - H_0} + \frac{1}{\omega - H_0} V \frac{1}{\omega - H} \\ &= \frac{1}{\omega - H_0} + \frac{1}{\omega - H_0} V \frac{1}{\omega - H_0} + \frac{1}{\omega - H_0} V \frac{1}{\omega - H_0} V \frac{1}{\omega - H},\end{aligned}\quad (1.11.5)$$

the second term produce just 0, thus

$$\begin{aligned}G(\omega) &= \langle 0 | d \frac{1}{\omega - H_0} d^\dagger | 0 \rangle + \langle 0 | d \frac{1}{\omega - H_0} V \frac{1}{\omega - H_0} V \frac{1}{\omega - H} d^\dagger | 0 \rangle \\ &= \frac{1}{\omega - \varepsilon_0} + \frac{1}{\omega - \varepsilon_0} \langle 0 | d V \frac{1}{\omega - H_0} V \frac{1}{\omega - H} d^\dagger | 0 \rangle \\ &= \frac{1}{\omega - \varepsilon_0} + \frac{1}{\omega - \varepsilon_0} \langle 0 | d \sum_k d^\dagger c_k \frac{V_k^2}{\omega - H_0} c_k^\dagger d \frac{1}{\omega - H} d^\dagger | 0 \rangle \\ &= \frac{1}{\omega - \varepsilon_0} + \frac{1}{\omega - \varepsilon_0} \sum_k \frac{V_k^2}{\omega - \varepsilon_k} G(\omega).\end{aligned}\quad (1.11.6)$$

Therefore

$$G^{-1}(\omega) = \omega - \varepsilon_0 - \sum_k \frac{V_k^2}{\omega - \varepsilon_k}, \quad (1.11.7)$$

it can be written as

$$G^{-1}(\omega) = \omega - \varepsilon_0 - \int_{-\infty}^{\infty} d\varepsilon \frac{\Delta(\varepsilon)}{\omega - \varepsilon}, \quad (1.11.8)$$

where

$$\Delta(\varepsilon) = \sum_k V_k^2 \delta(\varepsilon - \varepsilon_k). \quad (1.11.9)$$

Now consider  $V$  is in site representation:

$$V = \sum_i (t_{io} c_i^\dagger d + t_{oi} d^\dagger c_i), \quad (1.11.10)$$

then we have that

$$\begin{aligned}G(\omega) &= \frac{1}{\omega - \varepsilon_0} + \frac{1}{\omega - \varepsilon_0} \sum_{ij} t_{oi} t_{jo} \langle 0 | d d^\dagger c_i \frac{1}{\omega - H_0} c_j^\dagger d \frac{1}{\omega - H} d^\dagger | 0 \rangle \\ &= \frac{1}{\omega - \varepsilon_0} + \frac{1}{\omega - \varepsilon_0} \sum_{ij} t_{oi} t_{jo} G_{ij}^{(o)}(\omega) G(\omega),\end{aligned}\quad (1.11.11)$$

thus

$$G^{-1}(\omega) = \omega - \varepsilon_0 - \sum_{ij} t_{oi} t_{jo} G_{ij}^{(o)}(\omega), \quad (1.11.12)$$

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

## 1.12 Green's Function for Simple Cubic Lattice

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

$$-\pi/a \leq k_x < \pi/a, \quad -\pi/a \leq k_y < \pi/a, \quad -\pi/a \leq k_z < \pi/a, \quad (1.12.1)$$

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

$$G(\omega) = \frac{a^3}{(2\pi)^3} \int_{-\pi/a}^{\pi/a} dk_x \int_{-\pi/a}^{\pi/a} dk_y \int_{-\pi/a}^{\pi/a} dk_z \frac{1}{\omega - 2t(\cos k_x a + \cos k_y a + \cos k_z a)}, \quad (1.12.2)$$

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

$$G(\omega) = \frac{1}{(2\pi)^3} \int_{-\pi}^{\pi} dx \int_{-\pi}^{\pi} dy \int_{-\pi}^{\pi} dz \frac{1}{\omega - 2t(\cos x + \cos y + \cos z)}. \quad (1.12.3)$$

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

$$K(k) = \int_0^{\frac{\pi}{2}} d\theta (1 - k^2 \sin^2 \theta)^{-\frac{1}{2}}, \quad (1.12.4)$$

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

After the integration over  $y$  and  $z$ , the integral (1.12.3) yields

$$G(\omega) = \frac{1}{2\pi^2 t} \int_0^{\pi} k K(k) dx, \quad (1.12.5)$$

where

$$k = \frac{4t}{\omega - 2t \cos x}. \quad (1.12.6)$$

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

$$\text{Re } G(\omega) = -\text{Re } G(\omega), \quad \text{Im } G(\omega) = \text{Im } G(\omega), \quad (1.12.7)$$

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  $0 < \omega < 2t$ ,

$$\begin{aligned} \text{Re } G(\omega) &= -\frac{1}{2\pi^2 t} \int_0^{\cos^{-1}(\omega/2t)} dx K\left(\frac{1}{|k|}\right) + \frac{1}{2\pi^2 t} \int_{\cos^{-1}(\omega/2t)}^{\pi} K\left(\frac{1}{k}\right), \\ \text{Im } G(\omega) &= \frac{1}{\pi^2} \int_0^{\pi} dx K\left(\frac{\sqrt{k^2 - 1}}{k}\right), \end{aligned} \quad (1.12.8)$$

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

$$\begin{aligned} \text{Re } G(\omega) &= \frac{1}{2\pi^2 t} \int_0^{\cos^{-1}[(\omega-4t)/2t]} dx K\left(\frac{1}{k}\right) + \frac{1}{2\pi^2 t} \int_{\cos^{-1}[(\omega-4t)/2t]}^{\pi} dx K(k), \\ \text{Im } G(\omega) &= \frac{1}{2\pi^2 t} \int_0^{\cos^{-1}[(\omega-4t)/2t]} dx K\left(\frac{\sqrt{k^2 - 1}}{k}\right). \end{aligned} \quad (1.12.9)$$

## 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  $\phi_\alpha$  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  $\lambda$  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

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

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  $\rho$  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 (recall that  $\frac{1}{\pi} \operatorname{Im} G$  is the density of states)

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

For static conductivity, we have

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

or in three dimension

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

## 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

$$\alpha(t) = \frac{i}{\hbar} \theta(t) \sum_m [y_{nm}(t)x_{mn} - x_{nm}y_{mn}(t)]. \quad (3.6.10)$$

If the system in canonical distribution, then

$$\alpha(t) = \frac{i}{\hbar} \theta(t) \sum_{nm} \rho_n [y_{nm}(t)x_{mn} - x_{nm}y_{mn}(t)], \quad (3.6.11)$$

or we can write in a more compact way

$$\alpha(t) = \frac{i}{\hbar} \theta(t) \langle y(t)x(0) - x(0)y(t) \rangle. \quad (3.6.12)$$

Therefore

$$\alpha(\omega) = \frac{i}{\hbar} \int_0^\infty e^{i\omega t} \langle y(t)x(0) - x(0)y(t) \rangle dt. \quad (3.6.13)$$

With the aid of Kubo identity  $\alpha(t)$  can be written in another form. Let  $\rho = e^{-\beta H}/Z$ , where  $\beta = 1/T$  and  $Z$  is the partition function, then

$$\begin{aligned}\alpha(t) &= \frac{i}{\hbar} \theta(t) \langle y(t)x(0) - x(0)y(t) \rangle \\ &= \frac{i}{\hbar} \theta(t) \text{Tr}[\rho y(t)x(0) - \rho x(0)y(t)] \\ &= \frac{i}{\hbar} \theta(t) \text{Tr}[y(t)[x(0)\rho - \rho x(0)]].\end{aligned}\quad (3.6.14)$$

Substituting Kubo identity  $[e^{-\beta H}, x] = e^{-\beta H} \int_0^\beta e^{\lambda H} [x, H] e^{-\lambda H} d\lambda$  into the above formula we shall obtain that

$$\begin{aligned}
 \alpha(t) &= \frac{i}{\hbar} \theta(t) \text{Tr} \left[ y(t) \rho \int_0^\beta e^{\lambda H} [H, x(0)] e^{-\lambda H} d\lambda \right] \\
 &= \frac{i}{\hbar} \theta(t) \text{Tr} \left[ \rho \int_0^\beta e^{\lambda H} \dot{x}(0) e^{-\lambda H} y(t) d\lambda \right] \\
 &= \frac{i}{\hbar} \theta(t) \int_0^\beta \langle e^{\lambda H} \dot{x}(0) e^{-\lambda H} y(t) \rangle d\lambda.
 \end{aligned} \tag{3.6.15}$$



## 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  $\beta$  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  $\beta$  is the determinant of  $\beta_{ik}$ .

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  $\Delta S_t$  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  $\Delta E$  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  $\bar{n}_k \ll 1$ .

### 4.3 Correlations of Fluctuations in Time

There is some correlation between the values of  $x(t)$  at different instants, we define this correlation as

$$\phi(t - t') = \langle x(t)x(t') \rangle. \quad (4.3.1)$$

This correlation depends only on the difference  $t - t'$ , and the definition may therefore also be written

$$\phi(t) = \langle x(t)x(0) \rangle. \quad (4.3.2)$$

Note also that, because of the obvious symmetry of the definition as regards the interchange of  $t$  and  $t'$ , the function  $\phi(t)$  is even:

$$\phi(t) = \phi(-t). \quad (4.3.3)$$

The definition given above can be put in a form that is applicable to quantum variables also. To do this, we must consider in place of quantity  $x$  its Heisenberg operator  $x(t)$ . The operators  $x(t)$  and  $x(t')$  relating to different instants do not in general commute, and the correlation function must now be defined as

$$\phi(t - t') = \frac{1}{2} \langle x(t)x(t') + x(t')x(t) \rangle. \quad (4.3.4)$$

Let the quantity  $x$  have at some instants a value which is large compared with the mean fluctuation, i.e. the system be far from equilibrium. Then we can say that at subsequent instants the system will tend to reach equilibrium state. Under the assumption made, its rate of change will be at every instant entirely defined by the value of  $x$  at that instant:  $\dot{x} = -\lambda x$ . Expanding  $\dot{x}$  in powers of  $x$ , keeping only the linear term:

$$\frac{dx}{dt} = -\lambda x. \quad (4.3.5)$$

Returning to fluctuations in an equilibrium system, let us define a quantity  $\xi_x(t)$  as the mean value of  $x$  at an instant  $t > 0$  with the condition that it had some given value  $x$  at the prior instant  $t = 0$ . Evidently the correlation function  $\phi(t)$  may be written in terms of  $\xi_x(t)$  as

$$\phi(t) = \langle x\xi_x(t) \rangle, \quad (4.3.6)$$

where the averaging is only over the probabilities of the various values of  $x$  at the initial instant  $t = 0$ . For  $\xi_x(t)$  is an averaged quantity, we must expect that

$$\frac{d\xi_x(t)}{dt} = -\lambda\xi_x(t), \quad t > 0 \quad (4.3.7)$$

is true even when  $\xi_x(t)$  is not large. Since  $\xi_x(0) = x$  by definition, we have that

$$\xi_x(t) = xe^{-\lambda t}, \quad (4.3.8)$$

and finally we obtain a formula for the time correlation function

$$\phi(t) = \langle x^2 \rangle e^{-\lambda t}. \quad (4.3.9)$$

On the other hand, since  $\phi(t)$  is an even function, we can write the final formula as

$$\phi(t) = \langle x^2 \rangle e^{-\lambda|t|} = \frac{1}{\beta} e^{-\lambda|t|}. \quad (4.3.10)$$

The above theory can be also be formulated in another way that may have certain advantages. The equation  $\dot{x} = -\lambda x$  is valid only when  $x$  is large compared with the mean fluctuation of  $x$ . For arbitrary values of  $x$ , we write

$$\dot{x} = -\lambda x + y, \quad (4.3.11)$$

where  $y$  is the random force. The magnitude of the oscillations of  $y$  does not change with time, when  $x$  is large  $y$  is relatively small and may be neglected. The correlation function of the random force,  $\langle y(t)y(0) \rangle$ , must be specified in such a way as to lead the correct result for  $\langle x(t)x(0) \rangle$ . To do so, we must put

$$\langle y(t)y(0) \rangle = 2\lambda \langle x^2 \rangle \delta(t) = \frac{2\lambda}{\beta} \delta(t). \quad (4.3.12)$$

This is easily seen by writing the solution of equation (4.3.11)

$$x(t) = e^{-\lambda t} \int_{-\infty}^t y(\tau) e^{\lambda \tau} d\tau, \quad (4.3.13)$$

and averaging the product  $x(t)x(0)$  after expressing it as a double integral.

If there are several quantities  $x_1, \dots, x_n$  simultaneously deviate from their equilibrium values. The correlation functions for the fluctuations of these quantities are defined (in the classical theory) as

$$\phi_{ik}(t - t') = \langle x_i(t) x_k(t') \rangle. \quad (4.3.14)$$

By virtue of this definition, they have the obvious symmetry property

$$\phi_{ik}(t) = \phi_{ki}(-t). \quad (4.3.15)$$

Since there is also time reversal symmetry, there is

$$\phi_{ik}(t) = \phi_{ik}(-t), \quad (4.3.16)$$

combining these two symmetries we obtain that

$$\phi_{ik}(t) = \phi_{ki}(t). \quad (4.3.17)$$

The equations for  $\dot{x}_i$  now become

$$\dot{x}_i = -\lambda_{ik} x_k \quad (4.3.18)$$

with constant coefficients  $\lambda_{ik}$ . We define the mean values  $\xi_i(t)$  of the quantities  $x_i$  at a time  $t > 0$  for given values of all the  $x_1, \dots, x_n$  at the earlier time  $t = 0$ . These quantities satisfy the equation

$$\dot{\xi}_i = -\lambda_{ik} \xi_k. \quad (4.3.19)$$

Now the equation for correlation functions can be written as

$$\frac{d\phi_{il}(t)}{dt} = \frac{d\langle \xi_l(t) x_i \rangle}{dt} = -\lambda_{ik} \phi_{kl}(t), \quad (4.3.20)$$

with the initial conditions

$$\phi_{ik}(0) = \langle x_i x_k \rangle = \beta_{ik}^{-1}. \quad (4.3.21)$$

## 4.4 Onsager's Principle

Let us return to the macroscopic equations

$$\dot{x}_i = -\lambda_{ik} x_k. \quad (4.4.1)$$

These equations have a deep-lying internal symmetry, which becomes explicit only when the right-hand sides are expressed in terms of the thermodynamically conjugate quantities

$$X_i = -\frac{\partial S}{\partial x_i} = \beta_{ik} x_k, \quad (4.4.2)$$

with  $\beta_{ik} = \beta_{ki}$ .

If we express the quantities  $\dot{x}_i$  in terms of  $X_i$ , we obtain the relaxation equations in the form

$$\dot{x}_i = -\gamma_{ik} X_k, \quad (4.4.3)$$

where

$$\gamma_{ik} = \lambda_{il} \beta_{lk}^{-1} \quad (4.4.4)$$

are new constants called *kinetic coefficients*. We shall prove the *principle of the symmetry of the kinetic coefficients* or *Onsager's principle*, according to which

$$\gamma_{ik} = \gamma_{ki}. \quad (4.4.5)$$

We define mean values  $\xi_i(t)$  of the fluctuations quantities  $x_i$ , and mean values  $\Xi_i(t)$  of the  $X_i$ , then

$$\dot{\xi}_i = -\gamma_{ik}\Xi_k. \quad (t > 0) \quad (4.4.6)$$

We now make use of the symmetry  $\phi_{ik}(t) = \phi_{ik}(-t)$ , which may be written

$$\langle x_i(t)x_k(0) \rangle = \langle x_i(0)x_k(t) \rangle, \quad (4.4.7)$$

or, with  $\xi_i(t)$

$$\langle \xi_i(t)x_k \rangle = \langle x_i\xi_k(t) \rangle. \quad (4.4.8)$$

Differentiate this equation with respect to  $t$  and we obtain that

$$\gamma_{il}\langle \Xi_l x_k \rangle = \gamma_{kl}\langle x_i \Xi_l \rangle. \quad (4.4.9)$$

Putting  $t = 0$  in the above equation, we get

$$\gamma_{il}\langle X_l x_k \rangle = \gamma_{kl}\langle x_i X_l \rangle, \quad (4.4.10)$$

since  $\langle x_i X_k \rangle = \langle X_k x_i \rangle = \delta_{ik}$  the final result is arrived.

It has been assumed in the derivation that the quantities  $x_i$  and  $x_k$  are unaffected by time reversal. The relation remains valid if both quantities change sign under time reversal. But if one of  $x_i$  and  $x_k$  changes sign and the other remains unchanged<sup>1</sup>, the principle of the symmetry of the kinetic coefficients is formulated as

$$\gamma_{ik} = -\gamma_{ki}. \quad (4.4.11)$$

Exactly similar results are valid for kinetic coefficients  $\zeta_{ik} = \zeta_{ki}$  which appear in the relaxation equations when these are put in the form thermodynamically conjugate to equations:

$$\dot{X}_i = -\zeta_{ik}x_k, \quad \zeta_{ik} = \beta_{ik}\lambda_{kl}. \quad (4.4.12)$$

## 4.5 Spectral Resolution of Fluctuations

The spectral resolution of a fluctuating quantity  $x(t)$  is defined by the usual Fourier expansion formula:

$$x_\omega = \int_{-\infty}^{\infty} x(t)e^{i\omega t} dt, \quad (4.5.1)$$

and conversely

$$x(t) = \int_{-\infty}^{\infty} x_\omega e^{-i\omega t} \frac{d\omega}{2\pi}. \quad (4.5.2)$$

And the spectral resolution of correlation function  $\phi(t)$  is defined as

$$\phi(t) = \int_{-\infty}^{\infty} (x^2)_\omega \frac{\omega}{2\pi}, \quad (x^2)_\omega = \int_{-\infty}^{\infty} \phi(t)e^{i\omega t} dt, \quad (4.5.3)$$

and the spectral resolution of  $\phi(t - t')$  is

$$\phi(t - t') = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \langle x_\omega x_{\omega'} \rangle e^{-i(\omega t + \omega' t')} \frac{d\omega d\omega'}{(2\pi)^2}, \quad (4.5.4)$$

---

<sup>1</sup>For instance, one is the velocity  $v = \dot{x}$  and the other is  $x$ .

comparing the above two equations we obtain that

$$\langle x_\omega x_{\omega'} \rangle = 2\pi(x^2)_\omega \delta(\omega + \omega'). \quad (4.5.5)$$

Since  $\phi(t) = (1/\beta)e^{-\lambda|t|}$ , an integration of it would gives

$$(x^2)_\omega = \frac{1}{\beta} \left[ \frac{1}{\lambda - i\omega} + \frac{1}{\lambda + i\omega} \right] = \frac{2\lambda}{\beta(\omega^2 + \lambda^2)}. \quad (4.5.6)$$

In terms of the random force  $y(t)$ , the equation is  $\dot{x} = -\lambda x + y$ . Multiplying by  $e^{i\omega t}$  and integrating with respect to  $t$  from  $-\infty$  to  $\infty$  (the term  $\dot{x}e^{i\omega t}$  being integrated by parts), we obtain  $(\lambda - i\omega)x_\omega = y_\omega$ . Therefore

$$2\pi(y^2)_\omega \delta(\omega + \omega') = \langle y_\omega y_{\omega'} \rangle = (\lambda - i\omega)(\lambda - i\omega') \langle x_\omega x_{\omega'} \rangle = 2\pi(\omega^2 + \lambda^2)(x^2)_\omega \delta(\omega + \omega'), \quad (4.5.7)$$

i.e.,

$$(y^2)_\omega = (\omega^2 + \lambda^2)(x^2)_\omega = \frac{2\lambda}{\beta}. \quad (4.5.8)$$

The above expression can also be generalized to the simultaneous fluctuations of several thermodynamic variables. The components of their spectral resolution are

$$(x_i x_k)_\omega = \int_{-\infty}^{\infty} \phi_{ik}(t) e^{i\omega t} dt \equiv \int_{-\infty}^{\infty} \langle x_i(t) x_k(0) \rangle e^{i\omega t} dt, \quad (4.5.9)$$

and we have

$$\langle x_{i\omega} x_{k\omega'} \rangle = 2\pi(x_i x_k)_\omega \delta(\omega + \omega'). \quad (4.5.10)$$

A change in the sign of the time is equivalent to the change  $\omega \rightarrow -\omega$  in the spectral resolution, which in turn implies taking the complex conjugate of  $(x_i x_k)_\omega$ . The symmetry  $\phi_{ik}(t) = \phi_{ki}(-t)$  shows that

$$(x_i x_k)_\omega = (x_k x_i)_{-\omega} = (x_k x_i)_\omega^*. \quad (4.5.11)$$

The time reversal symmetry,  $\phi_{ik}(t) = \phi_{ik}(-t)$  or  $\phi_{ik}(t) = -\phi_{ik}(-t)$ , is written in terms of the spectral resolution as

$$(x_i x_k)_\omega = \pm (x_i x_k)_{-\omega} = \pm (x_i x_k)_\omega^*, \quad (4.5.12)$$

where the  $+$  and  $-$  signs respectively relate to cases where  $x_i$  and  $x_k$  behave similarly or differently under time reversal; in the former case,  $(x_i x_k)_\omega$  is real and symmetrical in the suffixes  $i$  and  $k$ , while in the latter case it is imaginary and antisymmetrical.

The equation for  $\phi_{ik}$  is

$$\frac{d\phi_{il}(t)}{dt} = -\lambda_{ik} \phi_{kl}(t), \quad (4.5.13)$$

after the Fourier transform (integrate respect to  $t$  from 0 to  $\infty$ ) it becomes

$$-\phi_{il}(0) - i\omega(x_i x_l)_\omega^{(+)} = -\lambda_{ik}(x_k x_l)_\omega^{(+)}, \quad (4.5.14)$$

with the notation

$$(x_k x_l)_\omega^{(+)} = \int_0^\infty \phi_{kl}(t) e^{i\omega t} dt. \quad (4.5.15)$$

Since  $\phi_{ik}(0) = \beta_{ik}^{-1}$ , we obtain that

$$(x_i x_k)_\omega = (x_i x_k)_\omega^{(+)} + (x_k x_i)_\omega^{(+)*} = (\zeta - i\omega\beta)_{ik}^{-1} + (\zeta + i\omega\beta)_{ki}^{-1}, \quad (4.5.16)$$

where  $\zeta_{ik} = \beta_{il}\lambda_{lk}$ .

If we use random force to formulate the theory, then

$$\dot{x}_i = -\lambda_{ik} x_k + y_i, \quad (4.5.17)$$

after the Fourier transform, it becomes

$$(\lambda_{ik} - i\omega\delta_{ik})x_{k\omega} = y_{i\omega}. \quad (4.5.18)$$

Then finally we get the formula

$$\begin{aligned} (y_i y_k)_\omega &= (\lambda_{il} - i\omega\delta_{il})(x_l x_m)_\omega (\lambda_{km} - i\omega\delta_{km}) \\ &= \gamma_{ik} + \gamma_{ki}, \end{aligned} \quad (4.5.19)$$

where  $\gamma_{ik} = \lambda_{il}\beta_{lk}^{-1}$ .

For a quantum variable, the spectral density  $(x^2)_\omega$  is defined by

$$\frac{1}{2}\langle x_\omega x_{\omega'} + x_{\omega'} x_\omega \rangle = 2\pi(x^2)_\omega \delta(\omega + \omega'). \quad (4.5.20)$$

According to fluctuation dissipation theorem,

$$(x^2)_\omega = \hbar \text{Im} \alpha(\omega) \coth \frac{\hbar\omega}{2T}, \quad (4.5.21)$$

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

$$\langle x^2 \rangle = \frac{\hbar}{\pi} \int_0^\infty \text{Im} \alpha(\omega) \coth \frac{\hbar\omega}{2T} d\omega. \quad (4.5.22)$$

At temperature  $T \gg \hbar\omega$ , we have  $\coth(\hbar\omega/2T) \approx 2T/\hbar\omega$ , then

$$(x^2)_\omega = (2T/\omega) \text{Im} \alpha(\omega), \quad (4.5.23)$$

and (using Kramers-Kronig relation here)

$$\langle x^2 \rangle = \frac{2T}{\pi} \int_0^\infty \frac{\text{Im} \alpha(\omega)}{\omega} d\omega = T \alpha(0). \quad (4.5.24)$$

If the body is subject to the action of a static force  $f$ , there would be a displacement  $\alpha(0)f = f/\beta T$  of  $\hbar x$ . The macroscopic equation of the relaxation then have the form

$$\dot{x} = -\lambda(x - f/\beta T). \quad (4.5.25)$$

Now let  $f$  is a time-dependent perturbation  $f(t)$ , then we obtain that

$$-i\omega\alpha(\omega)f_0 = \lambda\alpha(\omega)f_0 + (\lambda/\beta T)f_0, \quad (4.5.26)$$

whence

$$\alpha(\omega) = \frac{\lambda}{\beta T(\lambda - i\omega)}. \quad (4.5.27)$$

Therefore  $(x^2)_\omega$  becomes

$$(x^2)_\omega = \frac{2\lambda}{\beta(\lambda^2 + \omega^2)} \frac{\hbar\omega}{2T} \coth \frac{\hbar\omega}{2T}, \quad (4.5.28)$$

this expression differs from the classical one by a extra factor  $\frac{\hbar\omega}{2T} \coth \frac{\hbar\omega}{2T}$ . We can also formulate it with the random force  $y = \lambda f/\beta T$ , then

$$(y^2)_\omega = \frac{2\lambda}{\beta} \frac{\hbar\omega}{2T} \coth \frac{\hbar\omega}{2T}, \quad (4.5.29)$$

which differs from the classical one by the same factor. For several thermodynamic quantities

$$(y_i y_k)_\omega = (\gamma_{ik} + \gamma_{ki}) \frac{\hbar\omega}{2T} \coth \frac{\hbar\omega}{2T}. \quad (4.5.30)$$

### 4.5.1 Fluctuation of a One Dimensional oscillator

As an example of the use of the above formula, let us consider fluctuations of a one dimensional oscillator. We write its Hamiltonian in the form  $H = \frac{P^2}{2m} + \frac{1}{2}m\omega_0^2 Q^2$ . Then the distribution function for  $Q$  is

$$\sqrt{\frac{\beta}{2\pi}} e^{-\frac{1}{2}\beta x^2} = \sqrt{\frac{m\omega_0^2}{2\pi T}} e^{-\frac{1}{2}\frac{m\omega_0^2 Q^2}{T}}, \quad (4.5.31)$$

and the mean square fluctuation is

$$\langle Q^2 \rangle = \frac{T}{m\omega_0^2}. \quad (4.5.32)$$

The equation of motion of an oscillator with friction and random force are

$$\dot{Q} = \frac{P}{m}, \quad \dot{P} = -m\omega_0^2 Q - \gamma \frac{P}{m} + y, \quad (4.5.33)$$

represent the relations  $\dot{x}_i = -\gamma_{ik} X_k$ , so that

$$\gamma_{11} = 0, \quad \gamma_{12} = -\gamma_{21} = -T, \quad \gamma_{22} = \gamma T, \quad (4.5.34)$$

note that  $P$  is antisymmetrical under time reversal. Therefore we can write the spectral density of the fluctuations of the random force

$$(y^2)_\omega = \gamma_{22} + \gamma_{22} = 2\gamma T. \quad (4.5.35)$$

Because  $P = m\dot{Q}$ , we have that

$$m\ddot{Q} + \gamma\dot{Q} + m\omega_0^2 Q = y, \quad (4.5.36)$$

after Fourier transform it becomes

$$(-m\omega^2 - i\omega\gamma + m\omega_0^2)Q_\omega = y_\omega, \quad (4.5.37)$$

and hence finally

$$(Q^2)_\omega = \frac{2\gamma T}{m^2(\omega^2 - \omega_0^2)^2 + \omega^2\gamma^2}. \quad (4.5.38)$$

## 4.6 Thermoelectric Fluctuations

A particle current can be induced by external electric field and temperature gradient, the formula is

$$j = \sigma E - S\nabla T, \quad (4.6.1)$$

where  $S$  is the Seebeck coefficient (also known as the thermopower).

Similarly, the formula for heat current is

$$q - \mu j = \beta E - k\nabla T. \quad (4.6.2)$$

An electric field does mechanical work on the current-carrying particles, the work done per unit time and volume is equal to the scalar product  $j \cdot E$ . This is ‘‘Joule’s law’’. The evolution of heat results in an increase in the entropy of the body. When an amount of heat  $dQ = j \cdot E dV$  is involved, the entropy increases by  $dQ/T$ . The rate of change of the total entropy is therefore

$$\frac{ds}{dt} = \int \frac{j \cdot E}{T} dV. \quad (4.6.3)$$

And the entropy change due to heat current is

$$\frac{ds}{dt} = - \int \frac{\nabla(q - \mu j)}{T} dV = - \int \frac{(q - \mu j) \cdot \nabla T}{T^2} dV. \quad (4.6.4)$$

Therefore the total entropy change is

$$\frac{ds}{dt} = \int \frac{j \cdot E}{T} dV - \int \frac{(q - \mu j) \nabla T}{T^2} dV. \quad (4.6.5)$$

This formula can be derived in another way, writing the entropy change as  $ds/dt = -\int \nabla q/T dV$  and put  $\nabla j = 0$  then we have

$$\frac{\nabla q}{T} = \frac{1}{T} [\nabla(q - \mu j) + j \nabla \mu] = \frac{1}{T} \nabla(q - \mu j) - \frac{j \cdot E}{T}, \quad (4.6.6)$$

finally the same formula is obtained.

Let  $\dot{x}_i$  be  $j$  and  $q - \mu j$ , we find that  $X_i$  are  $-E/T$  and  $\nabla T/T^2$ . Accordingly in the relations

$$j = \sigma T \frac{E}{T} - ST^2 \frac{\nabla T}{T^2}, \quad q - \mu j = \beta T \frac{E}{T} - kT^2 \frac{\nabla T}{T^2}. \quad (4.6.7)$$

Let us label  $j$  as 1 and  $q - \mu j$  as 2, then

$$\gamma_{11} = \sigma T, \quad \gamma_{12} = -ST^2, \quad \gamma_{21} = \beta T, \quad \gamma_{22} = -kT^2. \quad (4.6.8)$$

According to Onsager's principle,  $\gamma_{12} = \gamma_{21}$ . If we write the equation of motion in form of random force,

$$\dot{x}_a = - \sum_b \gamma_{ab} X_b + y_a, \quad (4.6.9)$$

the coefficients  $\gamma_{ab}$  is immediately given by

$$\langle y_a(t_a) y_b(t_b) \rangle = (\gamma_{ab} + \gamma_{ba}) \delta(t_a - t_b), \quad \text{or} \quad (y_a y_b)_\omega = \gamma_{ab} + \gamma_{ba}. \quad (4.6.10)$$



# 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  $\lambda$ .

### 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 transformation<sup>1</sup>:

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

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

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

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<sup>1</sup>Mahan'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  $e^{\alpha a(t)} e^{\alpha a^\dagger}$  as<sup>2</sup>

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

using Baker-Campbell-Hausdorff formula we get

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

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<sup>2</sup>see 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

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

and, for the general case, the recurrence relations

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

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  $\Omega = \frac{\text{V}}{\text{A}} = \frac{\text{V} \cdot \text{s}}{\text{C}} = \frac{\text{J} \cdot \text{s}}{\text{C}^2} = \frac{\text{J}}{\text{s} \cdot \text{A}^2}$ .