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# Chapter 1

## Useful formulas

### 1.1 Guassian 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 Fourier Transform of Delta Function

The  $\delta$  function can be expressed as

$$\delta(x - \alpha) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ip(x-\alpha)} dp. \quad (1.2.1)$$

### 1.3 Euler Integral

#### 1.3.1 Euler Integral of The First Kind: Beta Function

Euler integral of the first kind: the Beta function:

$$B(a, b) = \int_0^1 x^{a-1} (1-x)^{b-1} dx. \quad (1.3.1)$$

The Beta function has the following properties:

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

$$B(a, b) = B(b, a). \quad (1.3.2)$$

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

$$\begin{aligned}
 B(a, b) &= \int_0^1 (1-x)^{b-1} d\frac{x^a}{a} \\
 &= \frac{x^a(1-x)^{b-1}}{a} \Big|_0^1 + \frac{b-1}{a} \int_0^1 x^a(1-x)^{b-2} dx \\
 &= \frac{b-1}{a} \int_0^1 x^{a-1}(1-x)^{b-2} dx - \frac{b-1}{a} \int_0^1 x^{a-1}(1-x)^{b-1} dx \\
 &= \frac{b-1}{a} B(a, b-1) - \frac{b-1}{a} B(a, b),
 \end{aligned} \tag{1.3.3}$$

thus

$$B(a, b) = \frac{b-1}{a+b-1} B(a, b-1). \tag{1.3.4}$$

For  $a > 1$ , it is similar that

$$B(a, b) = \frac{a-1}{a+b-1} B(a-1, b). \tag{1.3.5}$$

Let  $n$  be a positive integer,

$$B(n, a) = B(a, n) = \frac{1 \cdot 2 \cdot 3 \cdots (n-1)}{a \cdot (a+1) \cdot (a+2) \cdots (a+n-1)}. \tag{1.3.6}$$

Let  $m, n$  be two positive integers,

$$B(m, n) = \frac{(n-1)!(m-1)!}{(m+n-1)!}. \tag{1.3.7}$$

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

$$B(a, b) = \int_0^\infty \frac{y^{a-1}}{(1+y)^{a+b}} dy. \tag{1.3.8}$$

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

$$B(a, 1-a) = \int_0^\infty \frac{y^{a-1}}{1+y} dy, \tag{1.3.9}$$

this is also a Euler integral,

$$B(a, 1-a) = \frac{\pi}{\sin a\pi} \quad (0 < a < 1), \tag{1.3.10}$$

especially we have

$$B\left(\frac{1}{2}, \frac{1}{2}\right) = \pi. \tag{1.3.11}$$

### 1.3.2 Euler Integral of The Second Kind: Gamma Function

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

$$\Gamma(a) = \int_0^\infty x^{a-1} e^{-x} dx. \tag{1.3.12}$$

The Euler-Gauss formula:

$$\Gamma(a) = \lim_{n \rightarrow \infty} n^a \frac{1 \cdot 2 \cdot 3 \cdots (n-1)}{a \cdot (a+1) \cdot (a+2) \cdots (a+n-1)}. \tag{1.3.13}$$

The Gamma Function has the following properties:

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

(ii) Integrate by parts we shall get

$$\Gamma(a+1) = a\Gamma(a), \quad (1.3.14)$$

repeat this formula

$$\Gamma(a+n) = (a+n-1)(a+n-2)\cdots(a+1)\Gamma(a). \quad (1.3.15)$$

Let  $n$  be a positive integer, then

$$\Gamma(n+1) = n! \quad . \quad (1.3.16)$$

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

$$\Gamma(a) = \frac{\Gamma(a+1)}{a} \rightarrow +\infty. \quad (1.3.17)$$

If  $a > n+1$  the

$$\Gamma(a) > n! \quad . \quad (1.3.18)$$

(iv) Relation to Beta function:

$$B(a, b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}. \quad (1.3.19)$$

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

$$\Gamma(a)\Gamma(1-a) = \frac{\pi}{\sin a\pi}, \quad (1.3.20)$$

and

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}. \quad (1.3.21)$$

(vi)

$$\prod_{\nu=1}^{n-1} \Gamma\left(\frac{\nu}{n}\right) = \frac{(2\pi)^{\frac{n-1}{2}}}{\sqrt{n}}. \quad (1.3.22)$$

(vii) Raabe's formula:

$$\int_a^{a+1} \ln \Gamma(t) dt = \frac{1}{2} \ln 2\pi + a \ln a - a, \quad a > 0, \quad (1.3.23)$$

in particular, if  $a = 0$  then

$$\int_0^1 \ln \Gamma(t) dt = \frac{1}{2} \ln 2\pi. \quad (1.3.24)$$

(viii) Legendre formula:

$$\Gamma(a)\Gamma\left(a + \frac{1}{2}\right) = \frac{\sqrt{\pi}}{2^{2a-1}} \Gamma(2a). \quad (1.3.25)$$

## 1.4 Baker-Campbell-Hausdorff Formula

Baker-Campbell-Hausdorff Formula is

$$e^A B e^{-A} = \sum_{n=0}^{\infty} \frac{1}{n!} [A, B]_n = B + [A, B] + \frac{1}{2} [A, [A, B]] + \frac{1}{6} [A, [A, [A, B]]] + \cdots, \quad (1.4.1)$$

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

## 1.5 Feynman Result

The Feynman result reads

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}, \quad (1.5.1)$$

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

To prove it, recall that

$$e^{\tau(A+B)} = e^{\tau A} T_{\tau} \exp \left[ \int_0^{\tau} d\tau' e^{-\tau' A} B e^{\tau' A} \right] \quad (1.5.2)$$

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

## 1.6 Laguerre Polynomials

The Laguerre polynomials are solution of Laguerre's equation:

$$xy'' + (1-x)y' + ny = 0, \quad (1.6.1)$$

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

$$L_n(x) = \frac{e^x}{n!} \frac{d^n}{dx^n} (e^{-x} x^n) = \sum_{k=0}^n \frac{(-x)^k}{k!} \frac{n!}{k!(n-k)!}. \quad (1.6.2)$$

The generating function is

$$\frac{e^{-xt/(1-t)}}{1-t} = \sum_{n=0}^{\infty} L_n(x) t^n. \quad (1.6.3)$$

## 1.7 Cramer's Rule

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

$$Ax = b, \quad (1.7.1)$$

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:

$$x_i = \frac{\det A_i}{\det A}, \quad (1.7.2)$$

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

## 1.8 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

$$(A + uv^T)^{-1} = A^{-1} - \frac{A^{-1} u v^T A^{-1}}{1 + v^T A^{-1} u}. \quad (1.8.1)$$

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

## 1.9 Simple Impurity Model at Zero Temperature

The Hamiltonian of simple impurity model is defined as

$$H = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_k V_k (c_k^\dagger d + d^\dagger c_k) + \varepsilon_0 d^\dagger d, \quad (1.9.1)$$

let  $H = H_0 + V$ , where

$$H_0 = \sum_k \varepsilon_k c_k^\dagger c_k + \varepsilon_0 d^\dagger d, \quad V = \sum_k V_k (c_k^\dagger d + d^\dagger c_k). \quad (1.9.2)$$

The Green's function is

$$G(t) = -i \langle 0 | T d(t) d^\dagger | 0 \rangle = -i \langle 0 | d(t) d^\dagger | 0 \rangle, \quad (1.9.3)$$

apply Fourier transform on it, then

$$G(\omega) = \langle 0 | d \frac{1}{\omega + i0 - H} d^\dagger | 0 \rangle. \quad (1.9.4)$$

Notice that

$$\begin{aligned} \frac{1}{\omega - H} &= \frac{1}{\omega - H_0} + \frac{1}{\omega - H_0} V \frac{1}{\omega - H} \\ &= \frac{1}{\omega - H_0} + \frac{1}{\omega - H_0} V \frac{1}{\omega - H_0} + \frac{1}{\omega - H_0} V \frac{1}{\omega - H_0} V \frac{1}{\omega - H}, \end{aligned} \quad (1.9.5)$$

the second term produce just 0, thus

$$\begin{aligned} G(\omega) &= \langle 0 | d \frac{1}{\omega - H_0} d^\dagger | 0 \rangle + \langle 0 | d \frac{1}{\omega - H_0} V \frac{1}{\omega - H_0} V \frac{1}{\omega - H} d^\dagger | 0 \rangle \\ &= \frac{1}{\omega - \varepsilon_0} + \frac{1}{\omega - \varepsilon_0} \langle 0 | d V \frac{1}{\omega - H_0} V \frac{1}{\omega - H} d^\dagger | 0 \rangle \\ &= \frac{1}{\omega - \varepsilon_0} + \frac{1}{\omega - \varepsilon_0} \langle 0 | d \sum_k d^\dagger c_k \frac{V_k^2}{\omega - H_0} c_k^\dagger d \frac{1}{\omega - H} d^\dagger | 0 \rangle \\ &= \frac{1}{\omega - \varepsilon_0} + \frac{1}{\omega - \varepsilon_0} \sum_k \frac{V_k^2}{\omega - \varepsilon_k} G(\omega). \end{aligned} \quad (1.9.6)$$

Therefore

$$G^{-1}(\omega) = \omega - \varepsilon_0 - \sum_k \frac{V_k^2}{\omega - \varepsilon_k}, \quad (1.9.7)$$

it can be written as

$$G^{-1}(\omega) = \omega - \varepsilon_0 - \int_{-\infty}^{\infty} d\varepsilon \frac{\Delta(\varepsilon)}{\omega - \varepsilon}, \quad (1.9.8)$$

where

$$\Delta(\varepsilon) = \sum_k V_k^2 \delta(\varepsilon - \varepsilon_k). \quad (1.9.9)$$

Now consider  $V$  is in site representation:

$$V = \sum_i (t_{io} c_i^\dagger d + t_{oi} d^\dagger c_i), \quad (1.9.10)$$

then we have that

$$\begin{aligned} G(\omega) &= \frac{1}{\omega - \varepsilon_0} + \frac{1}{\omega - \varepsilon_0} \sum_{ij} t_{oi} t_{jo} \langle 0 | d d^\dagger c_i \frac{1}{\omega - H_0} c_j^\dagger d \frac{1}{\omega - H} d^\dagger | 0 \rangle \\ &= \frac{1}{\omega - \varepsilon_0} + \frac{1}{\omega - \varepsilon_0} \sum_{ij} t_{oi} t_{jo} G_{ij}^{(o)}(\omega) G(\omega), \end{aligned} \quad (1.9.11)$$

thus

$$G^{-1}(\omega) = \omega - \varepsilon_0 - \sum_{ij} t_{oi} t_{jo} G_{ij}^{(o)}(\omega), \quad (1.9.12)$$

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

## 1.10 Green's Function for Simple Cubic Lattice

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

$$-\pi/a \leq k_x < \pi/a, \quad -\pi/a \leq k_y < \pi/a, \quad -\pi/a \leq k_z < \pi/a, \quad (1.10.1)$$

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

$$G(\omega) = \frac{a^3}{(2\pi)^3} \int_{-\pi/a}^{\pi/a} dk_x \int_{-\pi/a}^{\pi/a} dk_y \int_{-\pi/a}^{\pi/a} dk_z \frac{1}{\omega - 2t(\cos k_x a + \cos k_y a + \cos k_z a)}, \quad (1.10.2)$$

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

$$G(\omega) = \frac{1}{(2\pi)^3} \int_{-\pi}^{\pi} dx \int_{-\pi}^{\pi} dy \int_{-\pi}^{\pi} dz \frac{1}{\omega - 2t(\cos x + \cos y + \cos z)}. \quad (1.10.3)$$

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

$$K(k) = \int_0^{\pi/2} d\theta (1 - k^2 \sin^2 \theta)^{-1/2}, \quad (1.10.4)$$

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

After the integration over  $y$  and  $z$ , the integral (1.10.3) yields

$$G(\omega) = \frac{1}{2\pi^2 t} \int_0^{\pi} k K(k) dx, \quad (1.10.5)$$

where

$$k = \frac{4t}{\omega - 2t \cos x}. \quad (1.10.6)$$

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

$$\text{Re } G(\omega) = -\text{Re } G(\omega), \quad \text{Im } G(\omega) = \text{Im } G(\omega), \quad (1.10.7)$$

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  $0 < \omega < 2t$ ,

$$\begin{aligned} \text{Re } G(\omega) &= -\frac{1}{2\pi^2 t} \int_0^{\cos^{-1}(\omega/2t)} dx K\left(\frac{1}{|k|}\right) + \frac{1}{2\pi^2 t} \int_{\cos^{-1}(\omega/2t)}^{\pi} K\left(\frac{1}{k}\right) dx, \\ \text{Im } G(\omega) &= \frac{1}{\pi^2} \int_0^{\pi} dx K\left(\frac{\sqrt{k^2 - 1}}{k}\right), \end{aligned} \quad (1.10.8)$$

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

$$\begin{aligned} \text{Re } G(\omega) &= \frac{1}{2\pi^2 t} \int_0^{\cos^{-1}[(\omega-4t)/2t]} dx K\left(\frac{1}{k}\right) + \frac{1}{2\pi^2 t} \int_{\cos^{-1}[(\omega-4t)/2t]}^{\pi} dx K(k), \\ \text{Im } G(\omega) &= \frac{1}{2\pi^2 t} \int_0^{\cos^{-1}[(\omega-4t)/2t]} dx K\left(\frac{\sqrt{k^2 - 1}}{k}\right). \end{aligned} \quad (1.10.9)$$



## 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

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



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

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

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

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

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

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

# Chapter 4

## Small Polaron

### 4.1 Holstein Model

The Hamiltonian of Holstein Model is

$$H = - \sum_{\langle i,j \rangle} t_{ij} c_i^\dagger c_j + g \sum_i c_i^\dagger c_i (a_i + a_i^\dagger) + \omega_0 \sum_i a_i^\dagger a_i, \quad (4.1.1)$$

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:

$$\lambda = g^2 / \omega_0 t, \quad (4.1.2)$$

$$\gamma = \omega_0 / t. \quad (4.1.3)$$

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

$$\alpha = \lambda / \gamma = g / \omega_0. \quad (4.1.4)$$

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  $\lambda$ .

### 4.2 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

$$G_{ij}(t) = -i \langle 0 | T c_i(t) c_j^\dagger(0) | 0 \rangle, \quad (4.2.1)$$

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

$$G_{ij}(t) = -i \langle 0 | T c_i(t) c_j(0)^\dagger S | 0 \rangle, \quad (4.2.2)$$

where

$$S = T e^{-i \int dt [g \sum_i c_i^\dagger c_i (a_i + a_i^\dagger)]} \quad (4.2.3)$$

The expansion of  $S$  to second order of  $g$  gives

$$\begin{aligned} G_{ij}(t) &= -i \langle 0 | T c_i(t) c_j^\dagger | 0 \rangle \\ &\quad - i \frac{g^2}{2} \int dt' dt'' \sum_{kl} \langle 0 | T c_i(t) c_j^\dagger c_k^\dagger(t') c_k(t') c_l^\dagger(t'') c_l(t'') [a_k(t') a_l^\dagger(t'') + a_k^\dagger(t') a_l(t'')] | 0 \rangle, \end{aligned} \quad (4.2.4)$$

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

$$\begin{aligned} \langle 0 | a_k^\dagger(t') a_l(t'') | 0 \rangle &= 0, \\ \langle 0 | a_k(t') a_l^\dagger(t'') | 0 \rangle &= D_{kl}(t' - t'') = \delta_{kl} D_{kk}(t' - t''), \end{aligned} \quad (4.2.5)$$

we can obtain that

$$G_{ij}(t) = G_{ij}^{(0)}(t) + ig^2 \sum_k \int dt' dt'' G_{ik}^{(0)}(t - t') G_{kk}^{(0)}(t' - t'') D_{kk}(t' - t'') G_{kj}(t''), \quad (4.2.6)$$

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

$$G_{ij}(\omega) = G_{ij}^{(0)}(\omega) + g^2 \sum_k G_{ik}^{(0)}(\omega) G_{kk}^{(0)}(\omega - \omega_0) G_{kj}^{(0)}(\omega). \quad (4.2.7)$$

Compare with the Dyson equation

$$G_{ij} = G_{ij}^{(0)} + \sum_{kl} G_{ik}^{(0)} \Sigma_{kl} G_{lj} = G_{ij}^{(0)} + \sum_{kl} G_{ik}^{(0)} \Sigma_{kl} G_{lj}^{(0)} + \dots, \quad (4.2.8)$$

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

$$\Sigma_2(\omega) = g^2 G^{(0)}(\omega - \omega_0). \quad (4.2.9)$$

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

$$\frac{m^*}{m} = \left. \frac{d(\omega - \text{Re}\Sigma(\omega))}{d\omega} \right|_{E_0} = 1 - \left. \frac{d\text{Re}\Sigma(\omega)}{d\omega} \right|_{E_0}, \quad (4.2.10)$$

where  $E_0$  is the ground-state energy.

### 4.3 Atomic Limit (Zero Temperature)

The atomic limit is defined as the zero hopping case ( $t = 0$ ). In this case, Hamiltonian (4.1.1) can be diagonalized by the unitary Lang-Firsov transformation

$$U = e^{-S}, \quad S = -\alpha \sum_i c_i^\dagger c_i (a_i - a_i^\dagger). \quad (4.3.1)$$

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

$$\begin{aligned} \bar{c}_i &= e^S c_i e^{-S} = c_i X_i, \quad X_i = e^{\alpha(a_i - a_i^\dagger)}; \\ \bar{c}_i^\dagger &= e^S c_i^\dagger e^{-S} = c_i^\dagger X_i^\dagger, \quad X_i^\dagger = e^{\alpha(a_i^\dagger - a_i)}; \\ \bar{a}_i &= e^S a_i e^{-S} = a_i - \alpha c_i^\dagger c_i; \\ \bar{a}_i^\dagger &= e^S a_i^\dagger e^{-S} = a_i^\dagger - \alpha c_i^\dagger c_i; \\ \bar{H} &= e^S H e^{-S} = -\frac{g^2}{\omega_0} \sum_i c_i^\dagger c_i + \omega_0 \sum_i a_i^\dagger a_i. \end{aligned} \quad (4.3.2)$$

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

$$C_0 = \langle n_i(a_i + a_i^\dagger) \rangle - 2\alpha \langle n_i \rangle = -2\alpha \langle n_i \rangle, \quad (4.3.3)$$

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

$$\langle e^S a^\dagger a e^{-S} \rangle = \langle a^\dagger a \rangle + \alpha^2 \langle c^\dagger c \rangle = \alpha^2. \quad (4.3.4)$$

The electron Green's function can also be calculated after the Lang-Firsov transformation<sup>1</sup>:

$$\begin{aligned} G(t) &= -i \langle 0 | c(t) c^\dagger | 0 \rangle \\ &= -i \langle 0 | c X e^{-i\bar{H}t} c^\dagger X^\dagger | 0 \rangle \\ &= -i \sum_{mn} \langle 0 | c X | m \rangle \langle m | e^{-i\bar{H}t} | n \rangle \langle n | c^\dagger X^\dagger | 0 \rangle, \end{aligned} \quad (4.3.5)$$

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

$$X^\dagger = e^{-\alpha^2/2} e^{\alpha a^\dagger} e^{-\alpha a}, \quad X = e^{-\alpha^2/2} e^{-\alpha a^\dagger} e^{\alpha a}, \quad (4.3.6)$$

accordingly,

$$\begin{aligned} \langle m | X^\dagger | 0 \rangle &= e^{-\alpha^2/2} \langle m | e^{\alpha a^\dagger} | 0 \rangle = e^{-\alpha^2/2} \sum_n \langle m | \frac{\alpha^n}{\sqrt{n!}} | n \rangle = e^{-\alpha^2/2} \frac{\alpha^m}{\sqrt{m!}}, \\ \langle 0 | X | m \rangle &= e^{-\alpha^2/2} \frac{\alpha^m}{\sqrt{m!}}. \end{aligned} \quad (4.3.7)$$

Finally the electron Green's function is

$$G(\omega) = \sum_n \frac{\alpha^{2n} e^{-\alpha^2}}{n!} \frac{1}{\omega - n\omega_0 - \varepsilon_p}. \quad (4.3.8)$$

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

$$t_{ij} c_i^\dagger c_j \rightarrow t_{ij} X_i^\dagger X_j c_i^\dagger c_j, \quad (4.3.9)$$

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

$$t_{ij} \langle 0 | X_i^\dagger X_j | 0 \rangle = t_{ij} \langle 0 | X^\dagger | 0 \rangle \langle 0 | X | 0 \rangle = t_{ij} e^{-\alpha^2}. \quad (4.3.10)$$

## 4.4 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

$$\begin{aligned} e^{-\alpha a} | n \rangle &= \sum_{m=0}^{\infty} \frac{(-\alpha)^m}{m!} a^m | n \rangle \\ &= \sum_{m=0}^n \frac{(-\alpha)^m}{m!} \left[ \frac{n!}{(n-m)!} \right]^{\frac{1}{2}} | n-m \rangle, \end{aligned} \quad (4.4.1)$$

and

$$\langle n | e^{\alpha a^\dagger} = \sum_{m=0}^n \frac{\alpha^m}{m!} \left[ \frac{n!}{(n-m)!} \right]^{\frac{1}{2}} \langle n-m |, \quad (4.4.2)$$

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<sup>1</sup>Mahan's Many-Particle Physics, page 221

therefore

$$\langle n | e^{\alpha a^\dagger} e^{-\alpha a} | n \rangle = \sum_{m=0}^n \frac{(-\alpha^2)^m}{m!} \frac{n!}{m!(n-m)!} = L_n(\alpha^2), \quad (4.4.3)$$

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

$$\langle n | X^\dagger | n \rangle = \langle n | X | n \rangle = e^{-\alpha^2/2} L_n(\alpha^2). \quad (4.4.4)$$

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

$$\begin{aligned} & t_{ij} (1 - e^{-\beta\omega_0})^2 \sum_{mn} e^{-\beta m\omega_0} \langle m | X_i^\dagger | m \rangle e^{-\beta n\omega_0} \langle n | X_j | n \rangle \\ &= t_{ij} e^{-\alpha^2} \left[ (1 - e^{-\beta\omega_0}) \sum_{n=0}^{\infty} e^{-n\beta\omega_0} L_n(\alpha^2) \right]^2. \end{aligned} \quad (4.4.5)$$

Recall that the generating function of Laguerre polynomials:

$$\frac{e^{-xt/(1-t)}}{1-t} = \sum_{n=0}^{\infty} L_n(x) t^n, \quad (4.4.6)$$

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

$$t_{ij} e^{-S_T}, \quad S_T = \alpha^2 (1 + 2\langle n \rangle_T). \quad (4.4.7)$$

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

$$\begin{aligned} G(t) &= -i(1 - e^{-\beta\omega_0}) \sum_n e^{-\beta n\omega_0} \langle n | c(t) c^\dagger | n \rangle \\ &= -i(1 - e^{-\beta\omega_0}) \sum_n e^{-\beta n\omega_0} \langle 0 | c(t) X(t) c^\dagger X^\dagger | 0 \rangle \\ &= -i(1 - e^{-\beta\omega_0}) \langle 0 | c(t) c^\dagger | 0 \rangle \sum_n e^{-\beta n\omega_0} \langle n | X(t) X^\dagger | n \rangle. \end{aligned} \quad (4.4.8)$$

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

$$\begin{aligned} c(t) &= c e^{-i\varepsilon_p t}, & c^\dagger(t) &= c^\dagger e^{i\varepsilon_p t}; \\ a(t) &= a e^{-i\omega_0 t}, & a^\dagger(t) &= a^\dagger e^{i\omega_0 t}, \end{aligned} \quad (4.4.9)$$

thus

$$X(t) = e^{-\alpha^2} e^{-\alpha a^\dagger e^{i\omega_0 t}} e^{\alpha a e^{-i\omega_0 t}} = e^{-\alpha^2} e^{-\alpha a^\dagger(t)} e^{\alpha a(t)} \quad (4.4.10)$$

and

$$X(t) X^\dagger = e^{-\alpha^2} e^{-\alpha a^\dagger(t)} e^{\alpha a(t)} e^{\alpha a^\dagger} e^{-\alpha a}. \quad (4.4.11)$$

Now we write  $e^{\alpha a(t)} e^{\alpha a^\dagger}$  as<sup>2</sup>

$$e^{\alpha a(t)} e^{\alpha a^\dagger} = e^{\alpha a^\dagger} [e^{-\alpha a^\dagger} e^{\alpha a(t)} e^{\alpha a^\dagger}], \quad (4.4.12)$$

using Baker-Campbell-Hausdorff formula we get

$$e^{-\alpha a^\dagger} e^{\alpha a(t)} e^{\alpha a^\dagger} = e^{\alpha^2 e^{-i\omega_0 t}} e^{\alpha a(t)}. \quad (4.4.13)$$

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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:

$$G(t) = -i(1 - e^{-\beta\omega_0})e^{-\alpha^2(1-e^{-i\omega_0 t})}\langle 0|c(t)c^\dagger|0\rangle \sum_n e^{-\beta n\omega_0} \langle n|e^{\alpha a^\dagger(1-e^{-i\omega_0 t})}e^{-\alpha a(1-e^{-i\omega_0 t})}|n\rangle, \quad (4.4.14)$$

again using Laguerre polynomials we can prove that

$$(1 - e^{-\beta\omega_0}) \sum_n e^{-\beta n\omega_0} \langle n|e^{u^* a^\dagger}e^{-ua}|n\rangle = e^{-|u|^2/(e^{\beta\omega_0}-1)}, \quad (4.4.15)$$

thus

$$G(t) = -ie^{-i\varepsilon_p t} \exp\left[-\alpha^2[(N+1)(1 - e^{-i\omega_0 t}) + N(1 - e^{i\omega_0 t})]\right], \quad (4.4.16)$$

where

$$N = \frac{1}{e^{\beta\omega_0} - 1}. \quad (4.4.17)$$

Recall the generating function of Bessel functions of complex argument,

$$e^{z \cos \theta} = \sum_{n=-\infty}^{\infty} I_n(z) e^{in\theta}, \quad (4.4.18)$$

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

$$z = 2\alpha^2 \sqrt{N(N+1)}, \quad \theta = \omega_0(t + i\beta/2) \quad (4.4.19)$$

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

$$G(t) = -ie^{-(2N+1)\alpha^2} e^{-i\varepsilon_p t} \sum_{n=-\infty}^{\infty} e^{-in\omega_0 t} e^{\beta n\omega_0/2} I_n\{2\alpha^2 \sqrt{N(N+1)}\}, \quad (4.4.20)$$

in frequency space

$$G(\omega) = e^{-(2N+1)\alpha^2} \sum_{n=-\infty}^{\infty} e^{\beta n\omega_0/2} I_n\{2\alpha^2 \sqrt{N(N+1)}\} \frac{1}{\omega - n\omega_0 - \varepsilon_p}. \quad (4.4.21)$$

## 4.5 The Impurity Analogy for A Single Electron

The Hamiltonian for impurity model is

$$H_{\text{imp}} = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_k V_k (c_k^\dagger d + d^\dagger c_k) + \omega_0 a^\dagger a + g d^\dagger d (a + a^\dagger), \quad (4.5.1)$$

here  $V_k$  and  $E_k$  is related to  $G_0$  by

$$G_0^{-1}(\omega) = \omega - \int_{-\infty}^{\infty} d\varepsilon \frac{\Delta(\varepsilon)}{\omega - \varepsilon}, \quad (4.5.2)$$

where

$$\Delta(\varepsilon) = \sum_k V_k^2 \delta(\varepsilon - \varepsilon_k). \quad (4.5.3)$$

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

$$H_0 = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_k V_k (c_k^\dagger d + d^\dagger c_k) + \omega_0 a^\dagger a, \quad V = g d^\dagger d (a + a^\dagger). \quad (4.5.4)$$

### 4.5.1 The Zero Temperature Formalism

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

$$G(t) = -i\theta(t)\langle 0|d(t)d^\dagger|0\rangle, \quad (4.5.5)$$

after Fourier transformation:

$$G(\omega) = \langle 0|d\frac{1}{\omega + i0 - H}d^\dagger|0\rangle. \quad (4.5.6)$$

An operator identity holds:

$$\frac{1}{\omega - H} = \frac{1}{\omega - H_0} + \frac{1}{\omega - H_0}V\frac{1}{\omega - H}. \quad (4.5.7)$$

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

$$G_{nm} = \langle 0|\frac{a^n}{\sqrt{n!}}d\frac{1}{\omega - H}d^\dagger\frac{(a^\dagger)^m}{\sqrt{m!}}|0\rangle, \quad (4.5.8)$$

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

$$|0, p\rangle = \frac{(a^\dagger)^p}{\sqrt{p!}}|0\rangle, \quad |1, p\rangle = \frac{(a^\dagger)^p}{\sqrt{p!}}d^\dagger|0\rangle, \quad (4.5.9)$$

one can write

$$\begin{aligned} G_{nm} &= \langle 0|\frac{a^n}{\sqrt{n!}}d\frac{1}{\omega - H_0}d^\dagger\frac{(a^\dagger)^m}{\sqrt{m!}}|0\rangle + \langle 0|\frac{a^n}{\sqrt{n!}}d\frac{1}{\omega - H_0}V\frac{1}{\omega - H}d^\dagger\frac{(a^\dagger)^m}{\sqrt{m!}}|0\rangle \\ &= G_{nm}^{(0)} + g \sum_{p_1, p_2} \langle 0|\frac{a^n}{\sqrt{n!}}d\frac{1}{\omega - H_0}d^\dagger|0, p_1\rangle \langle 0, p_1|d(a + a^\dagger)|1, p_2\rangle \langle 0, p_2|d\frac{1}{\omega - H}d^\dagger\frac{(a^\dagger)^m}{\sqrt{m!}}|0\rangle \\ &= G_{nm}^{(0)} + g \sum_{p_1, p_2} G_{n, p_1}^{(0)} X_{p_1, p_2} G_{p_2, m} \\ &= G_{nn}^{(0)}\delta_{nm} + g \sum_p G_{nn}^{(0)} X_{np} G_{pm}, \end{aligned} \quad (4.5.10)$$

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:

$$X_{np} = \sqrt{p+1}\delta_{n, p+1} + \sqrt{p}\delta_{n, p-1}. \quad (4.5.11)$$

Equation (4.5.10) can be solved in matrix notation:

$$G^{-1} = G_0^{-1} - gX, \quad (4.5.12)$$

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

$$G_{00} = \frac{T_1}{T_0}, \quad (4.5.13)$$

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

$$\begin{aligned} D_0 &= [G^{(0)}]_{00}^{-1}, \\ D_1 &= [G^{(0)}]_{11}^{-1}[G^{(0)}]_{00}^{-1} - g^2 = [G^{(0)}]_{11}^{-1}D_0 - g^2, \\ D_2 &= \dots = [G^{(0)}]_2^{-1}D_1 - 2g^2D_0, \end{aligned} \quad (4.5.14)$$

and, for the general case, the recurrence relations

$$D_k = [G^{(0)}]_{k,k}^{-1}D_{k-1} - kg^2D_{k-2}. \quad (4.5.15)$$



What's more, we have that

$$T_k = [G^{(0)}]_{kk}^{-1} T_{k+1} - (k+1)g^2 T_{k+2}, \quad \text{or} \quad \frac{T_k}{T_{k+1}} = [G^{(0)}]_{kk}^{-1} - (k+1)g^2 \frac{T_{k+2}}{T_{k+1}}, \quad (4.5.16)$$

therefore

$$\frac{T_1}{T_0} = \frac{1}{[G^{(0)}]_{00}^{-1} - g^2 \frac{T_2}{T_1}} = \dots, \quad (4.5.17)$$

or

$$G(\omega) = \frac{1}{G_0^{-1}(\omega) - \frac{g^2}{G_0^{-1}(\omega - \omega_0) - \frac{2g^2}{G_0^{-1}(\omega - 2\omega_0) - \frac{3g^2}{G_0^{-1}(\omega - 3\omega_0) - \dots}}}} \quad (4.5.18)$$

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

$$\Sigma(\omega) = \frac{g^2}{G_0^{-1}(\omega - \omega_0) - \frac{2g^2}{G_0^{-1}(\omega - 2\omega_0) - \frac{3g^2}{G_0^{-1}(\omega - 3\omega_0) - \dots}}} \quad (4.5.19)$$

The self-energy can be defined recursively,

$$\Sigma^{(p)}(\omega) = \frac{pg^2}{G_0^{-1}(\omega - p\omega_0) - \Sigma^{(p+1)}} \quad (4.5.20)$$

### 4.5.2 The Finite Temperature Formalism

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

$$G(\omega) = (1 - e^{\beta\omega_0}) \sum_n e^{-\beta n\omega_0} G_{nn}(\omega). \quad (4.5.21)$$

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):

$$G_{nn} = G_n^{(0)} + gG_n^{(0)}(\sqrt{n}G_{n-1,n} + \sqrt{n+1}G_{n+1,n}), \quad (4.5.22)$$

which we seek to write in a form as

$$G_{nn} = G_n^{(0)} + G_n^{(0)}(AG_{nn} + BG_{nn}). \quad (4.5.23)$$

Again according to Cramer's rule,

$$G_{n-1,n} = \sqrt{n}g \frac{D_{n-2}T_{n+1}}{T_0}, \quad G_{nn} = \frac{D_{n-1}T_{n+1}}{T_0}, \quad (4.5.24)$$

recall the recurrence relation for  $D$ :

$$D_k = [G_k^{(0)}]^{-1} D_{k-1} - kg^2 D_{k-2}, \quad (4.5.25)$$

or

$$\frac{D_{k-1}}{D_k} = \frac{1}{[G_k^{(0)}]^{-1} - kg^2 \frac{D_{k-2}}{D_{k-1}}} \quad (4.5.26)$$

Therefore

$$G_{n-1,n} = \sqrt{n}g \frac{D_{n-2}}{D_{n-1}} \frac{D_{n-1}T_{n+1}}{T_0} = \sqrt{n}g \frac{D_{n-2}}{D_{n-1}} G_{nn}, \quad (4.5.27)$$

i.e.,

$$A = ng^2 \frac{D_{n-2}}{D_{n-1}} = \frac{ng^2}{[G_n^{(0)}(\omega + \omega_0)]^{-1} - \frac{(n-1)g^2}{[G_n^{(0)}(\omega + 2\omega_0)]^{-1} - \frac{(n-2)g^2}{\ddots - \frac{g^2}{[G_n^{(0)}(\omega + n\omega_0)]^{-1}}}} \quad (4.5.28)$$

Similarly,

$$G_{n+1,n} = \sqrt{n+1}g \frac{D_{n-1}T_{n+2}}{T_0} = \sqrt{n+1}g \frac{T_{n+2}}{T_{n+1}} G_{nn}, \quad (4.5.29)$$

recall the recurrence relation for  $T$ :

$$T_k = [G_k^{(0)}]^{-1} T_{k+1} - (k+1)g^2 T_{k+2}, \quad (4.5.30)$$

or

$$\frac{T_{k+1}}{T_k} = \frac{1}{[G_k^{(0)}]^{-1} - (k+1)g^2 \frac{T_{k+2}}{T_{k+1}}}. \quad (4.5.31)$$

Therefore

$$B = (n+1)g^2 \frac{T_{n+2}}{T_{n+1}} = \frac{(n+1)g^2}{[G_n^{(0)}(\omega - \omega_0)]^{-1} - \frac{(n+2)g^2}{[G_n^{(0)}(\omega - 2\omega_0)]^{-1} - \frac{(n+3)g^2}{[G_n^{(0)}(\omega - 3\omega_0)]^{-1} - \dots}}, \quad (4.5.32)$$

finally

$$G_{nn} = \frac{1}{[G_n^{(0)}]^{-1} - A - B}. \quad (4.5.33)$$

### 4.5.3 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)

$$G^{-1}(\omega) = \omega - \sum_{ij} t_{oi} t_{jo} G_{ij}^{(o)}(\omega), \quad (4.5.34)$$

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

$$G^{-1}(\omega) = \omega - t^2 G(\omega). \quad (4.5.35)$$

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

$$G_{ij}^{(o)} = G_{ij} - \frac{G_{io} G_{oj}}{G_{oo}}. \quad (4.5.36)$$

Therefore equation (4.5.34) become

$$G^{-1} = \omega - \sum_{ij} t_{oi} t_{jo} G_{ij} + \frac{(\sum_i G_{oi})^2}{G_{oo}}, \quad (4.5.37)$$

recall that

$$G(\omega, k) = \frac{1}{\omega - \varepsilon_k - \Sigma(\omega)}, \quad (4.5.38)$$

we have that

$$G^{-1} = \omega - \int d\varepsilon \frac{\rho(\varepsilon)\varepsilon^2}{\zeta - \varepsilon} - \left( \int d\varepsilon \frac{\rho(\varepsilon)\varepsilon}{\zeta - \varepsilon} \right)^2 \bigg/ \int d\varepsilon \frac{\rho(\varepsilon)}{\zeta - \varepsilon}, \quad (4.5.39)$$

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

$$\int d\varepsilon \frac{\rho(\varepsilon)\varepsilon^2}{\zeta - \varepsilon} = \zeta \int d\varepsilon \frac{\rho(\varepsilon)\varepsilon}{\zeta - \varepsilon}, \quad \int d\varepsilon \frac{\rho(\varepsilon)}{\zeta - \varepsilon} = -1 + \zeta \int d\varepsilon \frac{\rho(\varepsilon)}{\zeta - \varepsilon}. \quad (4.5.40)$$

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

$$G_0^{-1} = \Sigma + G^{-1}. \quad (4.5.41)$$



## Chapter 5

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