Contents

Chapter 1

Useful formulas

1.1 Guassian Integrals

For a positive number a,

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

For real multi-dimensional integrals,

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

For complex multi-dimensional integrals,

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

For Grassmann variables integrals,

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

1.2 Fourier Transform of Delta Function

The δ function can be expressed as

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

1.3 Euler Integral

1.3.1 Euler Integral of The First Kind: Beta Function

Euler integral of the first kind: the Beta function:

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

The Beta function has the following properties:

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

$$B(a, b) = B(b, a). \tag{1.3.2}$$

(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 ∞, 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

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

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:

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

The Gamma Function has the following properties:

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

(ii) Integrate by parts we shall get

$$\Gamma(a+1) = a\Gamma(a), \tag{1.3.14}$$

repeat this formula

$$\Gamma(a+n) = (a+n-1)(a+n-1)\cdots(a+1)\Gamma(a). \tag{1.3.15}$$

Let n be a positive integer, then

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

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

$$\Gamma(a) = \frac{\Gamma(a+1)}{a} \to +\infty. \tag{1.3.17}$$

If $a > n+1$ the

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

(iv) Relation to Beta function:

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

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

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

and

$$\Gamma(\frac{1}{2}) = \sqrt{\pi}. \tag{1.3.21}$$

(vi)

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

(vii) Raabe's formula:

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

in particular, if $a = 0$ then

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

(viii) Legendre formula:

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

1.4 Baker-Campbell-Hausdorff Formula

Baker-Campbell-Hausdorff Formula is

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

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

1.5 Feynman Result

The Feynman result reads

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

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

To prove it, recall that

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

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

1.6 Laguerre Polynomials

The Laguerre polynomials are solution of Laguerre's equation:

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

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

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

The generating function is

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

1.7 Cramer's Rule

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

$$Ax = b, \tag{1.7.1}$$

where the $n \times n$ matrix A has a nonzero determinant, and the vector $x = (x_1, \cdots, x_n)^T$ 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:

$$x_i = \frac{\det A_i}{\det A}, \tag{1.7.2}$$

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

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

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

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

let $H = H_0 + V$, where

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

The Green's function is

$$G(t) = -i\langle 0|Td(t)d^\dagger|0\rangle = -i\langle 0|d(t)d^\dagger|0\rangle, \tag{1.9.3}$$

apply Fourier transform on it, then

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

Notice that

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

the second term produce just 0, thus

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

Therefore

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

it can be written as

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

where

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

Now consider V is in site representation:

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

then we have that

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

thus

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

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

$$-\pi/a \le k_x < \pi/a, \quad -\pi/a \le k_x < \pi/a, \quad -\pi/a \le k_x < \pi/a, \tag{1.10.1}$$

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

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

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

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

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

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

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

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

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

where

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

For simple cubic lattice, ReG is an odd function of ω and ImG is an even function:

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

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

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

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

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

Chapter 2

Coherent States

Coherent states is defined as the eigenstates of annihilation operator:

$$a_\alpha|\phi\rangle = \phi_\alpha|\phi\rangle. \tag{2.0.1}$$

2.1 Boson Coherent States

Boson coherent states:

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

where ϕ_α is complex number.

The overlap of two coherent states:

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

The overcompleteness in the Fock space:

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

where

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

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

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

The average particle number of a coherent state is

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

and the variance is

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

2.2 Grassmann Algebra

The Grassmann numbers is defined to be anticommuting numbers:

$$\xi_\alpha \xi_\beta + \xi_\beta \xi_\alpha = 0, \quad \xi_\alpha^2 = 0 \quad . \tag{2.2.1}$$

The conjugation of a Grassmann number is defined as

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

If λ is a complex number,

$$(\lambda \xi_\alpha)^* = \lambda^* \xi_\alpha, \tag{2.2.3}$$

and for any product of Grassmann numbers:

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

and for combinations of Grassmann variables and creation and annihilation operators

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

Because of property (2.2.3),

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

in particular,

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

A derivative can be defined for Grassmann variable function,

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

And a integral can be defined as

$$\int d\xi \, 1 = 0, \quad \int d\xi \, \xi = 1, \quad \int d\xi^* \, 1 = 0, \quad \int d\xi^* \, \xi^* = 1, \tag{2.2.9}$$

to remember,

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

2.3 Fermion Coherent States

Fermion Coherent States is defined as

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

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

$$\xi_\alpha |0\rangle = \xi_\alpha (1 - \xi_\alpha a^\dagger) |0\rangle \quad . \tag{2.3.2}$$

Similarly, the adjoint of the coherent states is

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

The overlap of two coherent states is

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

The closure relation can be written as

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

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

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

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

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

in the form of a sum

$$\Psi(t) = \sum_k a_k(t)\psi_k(t), \tag{3.1.2}$$

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

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

Therefore we obtain that

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

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

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

where

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

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

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

integrating it gives

$$a_{kn}^{(0)}(t) = -\frac{i}{\hbar}\int V_{kn}e^{i\omega_{kn}t}dt. \tag{3.1.8}$$

3.2 Fermi Golden Rule

Let the perturbation be

$$V(t) = Ve^{-i\omega t}, \tag{3.2.1}$$

then

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

Therefore the squared modulus of a_{fi} is

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

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

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

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

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

Another method to derive the above formula is that let

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

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

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

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

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

3.3 The Generalized Susceptibility

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

$$V = -xf(t), \tag{3.3.1}$$

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

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

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

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

we obtain that

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

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

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

then we shall have

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

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

$$\alpha(-\omega) = \alpha^*(\omega), \tag{3.3.7}$$

i.e.,

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

And the Kramers-Kronig relations:

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

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

$$\frac{dE}{dt} = -\bar{x}\frac{df}{dt}. \tag{3.3.10}$$

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

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

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

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

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

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

The dissipation per unit time is given by

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

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

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

thus

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

Now define

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

in canonical ensemble it is

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

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:

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

Similarly, in canonical ensemble

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

a comparison of these two expressions gives

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

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

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

3.5 Kubo Greenwood Formula

Now write the perturbing operator as

$$V = -\int \vec{j} \cdot \vec{A} dx, \tag{3.5.1}$$

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

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

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

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

therefore

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

which means

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

or

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

Thus the dissipated term written in conductivity is just

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

and

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

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

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

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

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

then the formula of $\mathrm{Re}\,\sigma$ become

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

For static conductivity, we have

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

or in three dimension (need correction)

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

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

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

where a_m satisfy the equation

$$i\hbar\frac{da_m}{dt} = V_{mn}e^{i\omega_{mn}t} = -\frac{1}{2}x_{mn}e^{i\omega_{mn}t}(f_0e^{-i\omega t} + f_0^*e^{i\omega t}). \tag{3.6.2}$$

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 $\omega \to \omega \mp i0$ in factors $e^{\pm i\omega t}$. Then

$$a_m = \frac{1}{2\hbar}x_{mn}e^{i\omega_{mn}t}\left[\frac{f_0e^{-i\omega t}}{\omega_{mn} - \omega - i0} + \frac{f_0^*e^{i\omega t}}{\omega_{mn} + \omega + i0}\right]. \tag{3.6.3}$$

Accordingly,

$$\begin{aligned}\bar{x} &= \int\Psi_n^*x\Psi_ndq\\ &= \sum_m(a_mx_{nm}e^{i\omega_{nm}t} + a_m^*x_{mn}e^{i\omega_{mn}t})\\ &= \frac{1}{2\hbar}\sum_m x_{mn}x_{nm}\left[\frac{1}{\omega_{mn} - \omega - i0} + \frac{1}{\omega_{mn} + \omega + i0}\right]f_0e^{-i\omega t} + \text{c.c},\end{aligned} \tag{3.6.4}$$

it can be seen that

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

This expression is the Fourier transform of the function

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

thus the we have the final result

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

Chapter 4

Small Polaron

4.1 Holstein Model

The Hamiltonian of Holstein Model is

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

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:

$$\lambda = g^2/\omega_0 t, \tag{4.1.2}$$

$$\gamma = \omega_0/t. \tag{4.1.3}$$

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

$$\alpha = \lambda/\gamma = g/\omega_0. \tag{4.1.4}$$

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 λ.

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

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

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

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

where

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

The expansion of S to second order of g gives

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

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

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

we can obtain that

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

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

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

Compare with the Dyson equation

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

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

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

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

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

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

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

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

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

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

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

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

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

The electron Green's function can also be calculated after the Lang-Firsov transformation[1]:

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

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

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

accordingly,

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

Finally the electron Green's function is

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

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

$$t_{ij}c_i^\dagger c_j \quad \to \quad t_{ij}X_i^\dagger X_j c_i^\dagger c_j, \tag{4.3.9}$$

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

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

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

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

and

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

[1] Mahan's Many-Particle Physics, page 221

therefore

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

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

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

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

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

Recall that the generating function of Laguerre polynomials:

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

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

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

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

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

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

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

thus

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

and

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

Now we write $e^{\alpha a(t)}e^{\alpha a^\dagger}$ as[2]

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

using Baker-Campbell-Hausdorff formula we get

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

[2] see Mahan's Many-Particle Physics, page 222

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

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

again using Laguerre polynomials we can prove that

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

thus

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

where

$$N = \frac{1}{e^{\beta\omega_0}-1}. \tag{4.4.17}$$

Recall the generating function of Bessel functions of complex argument,

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

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

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

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

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

in frequency space

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

4.5 The Impurity Analogy for A Single Electron

The Hamiltonian for impurity model is

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

here V_k and E_k is related to G_0 by

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

where

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

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

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

4.5.1 The Zero Temperature Formalism

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

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

after Fourier transformation:

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

An operator identity holds:

$$\frac{1}{\omega - H} = \frac{1}{\omega - H_0} + \frac{1}{\omega - H_0}V\frac{1}{\omega - H}. \tag{4.5.7}$$

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

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

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

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

one can write

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

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

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

Equation (4.5.10) can be solved in matrix notation:

$$G^{-1} = G_0^{-1} - gX, \tag{4.5.12}$$

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

$$G_{00} = \frac{T_1}{T_0}, \tag{4.5.13}$$

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

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

and, for the general case, the recurrence relations

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

What's more, we have that

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

therefore

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

or

$$G(\omega) = \cfrac{1}{G_0^{-1}(\omega) - \cfrac{g^2}{G_0^{-1}(\omega-\omega_0) - \cfrac{2g^2}{G_0^{-1}(\omega-2\omega_0) - \cfrac{3g^2}{G_0^{-1}(\omega-3\omega_0) - \cdots}}}}. \tag{4.5.18}$$

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

$$\Sigma(\omega) = \cfrac{g^2}{G_0^{-1}(\omega-\omega_0) - \cfrac{2g^2}{G_0^{-1}(\omega-2\omega_0) - \cfrac{3g^2}{G_0^{-1}(\omega-3\omega_0) - \cdots}}}. \tag{4.5.19}$$

The self-energy can be defined recursively,

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

4.5.2 The Finite Temperature Formalism

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

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

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):

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

which we seek to write in a form as

$$G_{nn} = G_n^{(0)} + G_n^{(0)} (A G_{nn} + B G_{nn}). \tag{4.5.23}$$

Again according to Cramer's rule,

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

recall the recurrence relation for D:

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

or

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

Therefore

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

i.e.,

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

Similarly,

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

recall the recurrence relation for T:

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

or

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

Therefore

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

finally

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

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)

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

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

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

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

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

Therefore equation (4.5.34) become

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

recall that

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

we have that

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

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

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

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

$$G_0^{-1} = \Sigma + G^{-1}. \tag{4.5.41}$$

Chapter 5

Physical Constants

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