Contents

Chapter 1

Useful formulas

1.1 Gaussian Integrals

For a positive number a,

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

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 Gaussian Distribution

1.2.1 Gaussian Distribution for One Variable

The Gaussian distribution for one variable can be written as

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

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

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

The mean square fluctuation is

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

thus we can write the Gaussian distribution in the form

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

1.2.2 Gaussian Distribution for More Than One Variable

The Gaussian distribution for more than one variable is

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

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

$$\int w \, dx_1 \cdots dx_n = 1. \tag{1.2.6}$$

The linear transformation

$$x_i = a_{ik}x'_k \tag{1.2.7}$$

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

$$\beta_{ik}x_ix_k = x'_ix'_i = x'_ix'_k\delta_{ik} \tag{1.2.8}$$

should be valid, the transformation coefficients must satisfy the relations

$$\beta_{ik}a_{il}a_{km} = \delta_{lm}. \tag{1.2.9}$$

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

$$\beta a^2 = 1. \tag{1.2.10}$$

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

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

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

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

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

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

which we refer to as conjugate[1] to the x_i. From the definition the mean value $\bar{x}_i$ is

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

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

$$\langle x_iX_k \rangle = \delta_{ik}. \tag{1.2.15}$$

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

$$\langle x_ix_k \rangle = \beta_{ik}^{-1}. \tag{1.2.16}$$

Similarly,

$$\langle X_iX_k \rangle = \beta_{il}\langle x_lX_k \rangle = \beta_{il}\delta_{lk}, \tag{1.2.17}$$

i.e.

$$\langle X_iX_k \rangle = \beta_{ik}. \tag{1.2.18}$$

[1] when apply to thermodynamics we call it thermodynamically conjugate.

1.3 Delta Function

The δ function satisfies the following properties.

$$\int \delta(x-a)f(x) = f(a). \tag{1.3.1}$$

And δ function is an even function:

$$\delta(-x) = \delta(x). \tag{1.3.2}$$

For a non-zero scalar α

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

The δ function can be expressed as

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

1.4 Euler Integral

1.4.1 Euler Integral of The First Kind: Beta Function

Euler integral of the first kind: the Beta function:

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

The Beta function has the following properties:

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

$$B(a,b) = B(b,a). \tag{1.4.2}$$

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

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

thus

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

For $a > 1$, it is similar that

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

Let n be a positive integer,

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

Let m, n be two positive integers,

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

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

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

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

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

this is also a Euler integral,

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

especially we have

$$B(\frac{1}{2}, \frac{1}{2}) = \pi. \tag{1.4.11}$$

1.4.2 Euler Integral of The Second Kind: Gamma Function

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

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

The Euler-Gauss formula:

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

The Gamma Function has the following properties:

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

(ii) Integrate by parts we shall get

$$\Gamma(a+1) = a\Gamma(a), \tag{1.4.14}$$

repeat this formula

$$\Gamma(a+n) = (a+n-1)(a+n-1)\cdots(a+1)\Gamma(a). \tag{1.4.15}$$

Let n be a positive integer, then

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

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

$$\Gamma(a) = \frac{\Gamma(a+1)}{a} \to +\infty. \tag{1.4.17}$$

If $a > n+1$ the

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

(iv) Relation to Beta function:

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

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

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

and

$$\Gamma(\frac{1}{2}) = \sqrt{\pi}. \tag{1.4.21}$$

(vi)

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

(vii) Raabe's formula:

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

in particular, if $a = 0$ then

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

(viii) Legendre formula:

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

1.5 Baker-Campbell-Hausdorff Formula

Baker-Campbell-Hausdorff Formula is

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

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

1.6 Feynman Result

The Feynman result reads

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

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

To prove it, recall that

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

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

1.7 Kubo Identity

The Kubo Identity states that

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

To derive this relation, let us consider a quantity

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

differentiating it with respect to λ yields

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

Therefore

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

and accordingly

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

1.8 Laguerre Polynomials

The Laguerre polynomials are solution of Laguerre's equation:

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

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

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

The generating function is

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

1.9 Cramer's Rule

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

$$Ax = b, \tag{1.9.1}$$

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:

$$x_i = \frac{\det A_i}{\det A}, \tag{1.9.2}$$

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

1.10 Sherman-Morrison Formula

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

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

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

1.11 Simple Impurity Model at Zero Temperature

The Hamiltonian of simple impurity model is defined as

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

let $H = H_0 + V$, where

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

The Green's function is

$$G(t) = -i\langle 0|Td(t)d^\dagger|0\rangle = -i\langle 0|d(t)d^\dagger|0\rangle, \tag{1.11.3}$$

apply Fourier transform on it, then

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

Notice that

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

the second term produce just 0, thus

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

Therefore

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

it can be written as

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

where

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

Now consider V is in site representation:

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

then we have that

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

thus

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

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

1.12 Green's Function for Simple Cubic Lattice

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

$$-\pi/a \le k_x < \pi/a, \quad -\pi/a \le k_x < \pi/a, \quad -\pi/a \le k_x < \pi/a, \tag{1.12.1}$$

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

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

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

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

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

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

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

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

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

where

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

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

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

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

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

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

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

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:

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

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

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

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

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

a comparison of these two expressions gives

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

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

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

3.5 Kubo Greenwood Formula

Now write the perturbing operator as

$$V = -\int \vec{j} \cdot \vec{A} d^3 r, \tag{3.5.1}$$

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

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

where $\mathcal{V}$ is the volume. 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

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

and applying "independent particle approximation" yields

$$\begin{aligned} Q &= \frac{\pi e^2}{2\hbar}\sum_{nm}\omega(f_n - f_m)|v_{nm}|^2|A|^2\delta(\omega+\omega_{nm}) \\ &= \frac{\pi e^2}{2\hbar\omega}\sum_{nm}(f_n - f_m)|v_{nm}|^2|E|^2\delta(\omega+\omega_{nm}). \end{aligned} \tag{3.5.8}$$

Therefore we have

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

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

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

For static conductivity, we have

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

or in three dimension

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

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,

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

it can be seen that

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

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

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

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

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

therefore

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

This expression is the Fourier transform of the function

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

If the system in canonical distribution, then

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

or we can write in a more compact way

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

Therefore

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

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

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

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

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

Chapter 4

Fluctuations

4.1 Gaussian Distribution

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

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

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

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

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

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

The mean square fluctuation is

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

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

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

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

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

where β is the determinant of β_{ik}.

Let us define the quantities

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

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

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

4.2 Fluctuations of The Fundamental Thermodynamic quantities

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

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

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

Expanding ΔE in series, we obtain

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

It is easily seen that this expression may be written as

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

Thus we obtain the fluctuation probability in the form

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

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

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

therefore the distribution function becomes

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

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

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

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

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

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

Therefore the distribution function becomes

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

and the mean square fluctuations are

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

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

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

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

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

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

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

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

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

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

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

For ideal gas, substituting $PV = NT$ gives

$$\langle(\Delta N)^2\rangle = N. \tag{4.2.16}$$

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

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

For a Fermi gas we must substitute

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

the differentiation gives

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

Similarly, for a Bose gas

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

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

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

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

4.3 Correlations of Fluctuations in Time

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

$$\phi(t-t') = \langle x(t)x(t')\rangle. \tag{4.3.1}$$

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

$$\phi(t) = \langle x(t)x(0)\rangle. \tag{4.3.2}$$

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

$$\phi(t) = \phi(-t). \tag{4.3.3}$$

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

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

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

$$\frac{dx}{dt} = -\lambda x. \tag{4.3.5}$$

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

$$\phi(t) = \langle x\xi_x(t)\rangle, \tag{4.3.6}$$

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

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

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

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

and finally we obtain a formula for the time correlation function

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

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

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

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

$$\dot{x} = -\lambda x + y, \tag{4.3.11}$$

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

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

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

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

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

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

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

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

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

Since there is also time reversal symmetry, there is

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

combining these two symmetries we obtain that

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

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

$$\dot{x}_i = -\lambda_{ik} x_k \tag{4.3.18}$$

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

$$\dot{\xi}_i = -\lambda_{ik} \xi_k. \tag{4.3.19}$$

Now the equation for correlation functions can be written as

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

with the initial conditions

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

4.4 Onsager's Principle

Let us return to the macroscopic equations

$$\dot{x}_i = -\lambda_{ik} x_k. \tag{4.4.1}$$

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

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

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

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

$$\dot{x}_i = -\gamma_{ik} X_k, \tag{4.4.3}$$

where

$$\gamma_{ik} = \lambda_{il} \beta_{lk}^{-1} \tag{4.4.4}$$

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

$$\gamma_{ik} = \gamma_{ki}. \tag{4.4.5}$$

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

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

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

$$\langle x_i(t)x_k(0)\rangle = \langle x_i(0)x_k(t)\rangle, \tag{4.4.7}$$

or, with $\xi_i(t)$

$$\langle \xi_i(t)x_k\rangle = \langle x_i\xi_k(t)\rangle. \tag{4.4.8}$$

Differentiate this equation with respect to t and we obtain that

$$\gamma_{il}\langle \Xi_l x_k\rangle = \gamma_{kl}\langle x_i \Xi_l\rangle. \tag{4.4.9}$$

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

$$\gamma_{il}\langle X_l x_k\rangle = \gamma_{kl}\langle x_i X_l\rangle, \tag{4.4.10}$$

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

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

$$\gamma_{ik} = -\gamma_{ki}. \tag{4.4.11}$$

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

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

4.5 Spectral Resolution of Fluctuations

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

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

and conversely

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

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

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

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

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

[1] For instance, one is the velocity $v = \dot{x}$ and the other is x.

comparing the above two equations we obtain that

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

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

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

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

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

i.e.,

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

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

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

and we have

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

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

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

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

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

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

The equation for ϕ_{ik} is

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

after the Fourier transform (integrate respect to t from 0 to ∞) it becomes

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

with the notation

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

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

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

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

If we use random force to formulate the theory, then

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

after the Fourier transform, it becomes

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

Then finally we get the formula

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

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

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

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

According to fluctuation dissipation theorem,

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

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

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

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

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

and (using Kramers-Kronig relation here)

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

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

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

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

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

whence

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

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

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

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

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

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

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

4.5.1 Fluctuation of a One Dimensional oscillator

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

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

and the mean square fluctuation is

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

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

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

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

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

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

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

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

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

after Fourier transform it becomes

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

and hence finally

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

4.6 Thermoelectric Fluctuations

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

$$j = \sigma E - S\nabla T, \tag{4.6.1}$$

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

Similarly, the formula for heat current is

$$q - \mu j = \beta E - k\nabla T. \tag{4.6.2}$$

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

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

And the entropy change due to heat current is

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

Therefore the total entropy change is

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

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

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

finally the same formula is obtained.

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

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

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

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

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

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

the coefficients γ_{ab} is immediately given by

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

Chapter 5

Coherent Potential Approximation

Perfect lattice have been studied intensively by physicist since the beginning of quantum mechanics. The periodicity of the lattice allows us to use Bloch waves to describe the wave function of electrons in lattice. However, in real world the perfect lattice does not exist and there are always some kinds of disorders in lattice. Usually weak disorder limit is described by the scattering of Bloch waves by impurities, and Boltzmann transport equation is enough to handle it. But in strong disorder limit, the situation becomes much more complicated. In this chapter we shall briefly review methods to deal with disordered electronic systems in lattice.

5.1 The Hamiltonian for Disordered Electronic Systems

In lattice, we use an unified tight-binding Hamiltonian to describe the disorders:

$$\hat{H} = \sum_{ij} W_{ij} \hat{c}_i^\dagger \hat{c}_j + \sum_i V_i \hat{c}_i^\dagger \hat{c}_i, \tag{5.1.1}$$

where $\hat{c}_i^\dagger$ ($\hat{c}_i$) are creation (annihilation) operators of electron at site i, and V_i is the on-site energy when there is an electron at site i. The quantity W_{ij} describe the hopping energy for transition of an electron from site j to site i, and hence $W_{ij} = 0$ when $i = j$. It is clear that V_i are diagonal elements of the Hamiltonian, while W_{ij} are off diagonal elements. If the diagonal elements V_i are random variables, then we call the system diagonal disorder system and the off diagonal elements W_{ij} is still transitional invariance. On the contrary, if V_i is a position independent constant while W_{ij} are random variables, such a system is called off diagonal disorder system.

In this chapter we shall focus on the diagonal disorder systems. First we split the Hamiltonian as

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \tag{5.1.2}$$

where the off diagonal elements

$$\hat{H}_0 = \sum_{ij} W_{ij} \hat{c}_i^\dagger \hat{c}_j \tag{5.1.3}$$

are the ordered terms in the Hamiltonian, while the diagonal elements

$$\hat{H}_1 = \sum_i V_i \hat{c}_i^\dagger \hat{c}_i \tag{5.1.4}$$

are disordered terms. This corresponds to the random potential. Since the hopping terms W_{ij} are ordered terms, $\hat{H}_0$ is just the usual Hamiltonian of tight binding model which can be diagonalized by Fourier transformation to $\boldsymbol{k}$-representation. Therefore sometimes $\hat{H}_0$ is also written as

$$\hat{H}_0 = \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} \hat{c}_{\boldsymbol{k}}^\dagger \hat{c}_{\boldsymbol{k}}, \tag{5.1.5}$$

where $\varepsilon_{\boldsymbol{k}}$ is dispersion relation of the energy band.

The Green's Function

The single particle Green's function in disordered system is defined as the retarded Green's function with respect to vacuum state

$$G_{ij}(t) = -\frac{i}{\hbar}\theta(t)\langle 0|\hat{c}_i(t)\hat{c}_j^\dagger(0) + \hat{c}_j^\dagger(0)\hat{c}_i(t)|0\rangle, \tag{5.1.6}$$

where $|0\rangle$ is the vacuum state. Because the Green's function is defined with respect to vacuum state, it is clear that

$$\langle 0|\hat{c}_j^\dagger(0)\hat{c}_i(t)|0\rangle = 0. \tag{5.1.7}$$

Therefore the Green's function reduces to

$$G_{ij}(t) = -\frac{i}{\hbar}\langle 0|\hat{c}_i(t)\hat{c}_j^\dagger(0)|0\rangle, \quad t \geq 0. \tag{5.1.8}$$

The physical meaning of the Green's function $G_{ij}(t)$ is clear: it creates an electron at site j then annihilates an electron after time t at site i, and gives the coefficient amplitude of an electron at site i. Thus the square modulus $|G_{ij}(t)|^2$ gives the probability of finding the electron at site i at time t with its initial position at site j at time 0. In other words, the Green's function acts as a propagator.

Now we move to the equation of motion of the Green's function. According to Heisenberg equation we have

$$i\hbar\frac{d\hat{c}_i(t)}{dt} = [\hat{c}_i(t), \hat{H}], \tag{5.1.9}$$

and substituting (5.1.1) in it and collaborating the commutation rule for fermions $\hat{c}_i\hat{c}_j^\dagger + \hat{c}_j^\dagger\hat{c}_i = \delta_{ij}$ we obtain

$$i\hbar\frac{d\hat{c}_i(t)}{dt} = V_i\hat{c}_i(t) + \sum_k W_{ik}\hat{c}_k(t). \tag{5.1.10}$$

Therefore the equation of motion of the Green's function is

$$\begin{aligned} \frac{dG_{ij}(t)}{dt} &= (-i/\hbar)^2\langle 0|[\hat{c}_i(t), \hat{H}]\hat{c}_j^\dagger(0)|0\rangle - \frac{i}{\hbar}\delta_{ij}(t) \\ &= (-i/\hbar)^2[\langle 0|V_i\hat{c}_i(t)\hat{c}_j^\dagger(0)|0\rangle + \sum_k \langle 0|W_{ik}\hat{c}_k(t)c_j^\dagger(0)|0\rangle] - \frac{i}{\hbar}\delta_{ij}(t), \end{aligned} \tag{5.1.11}$$

where the delta function $\delta_{ij}(t)$ comes from the discontinuity of the Green's function at time $t = 0$, thus we have for $t \geq 0$

$$i\hbar\frac{dG_{ij}(t)}{dt} = V_iG_{ij}(t) + \sum_k W_{ik}G_{kj}(t) + \delta_{ij}(t). \tag{5.1.12}$$

Apply Fourier transform on both sides we have the equation in energy representation as

$$EG_{ij}(E) = V_iG_{ij}(E) + \sum_k W_{ik}G_{kj}(E) + \delta_{ij}, \tag{5.1.13}$$

where, since $G_{ij}(t) = 0$ when $t < 0$,

$$G_{ij}(E) = \int_{-\infty}^{\infty} G_{ij}(t)e^{\frac{i}{\hbar}Et}dt = \int_0^{\infty} G_{ij}(t)e^{\frac{i}{\hbar}Et}dt, \tag{5.1.14}$$

and the inverse Fourier transform is

$$G_{ij}(t) = \int_{-\infty}^{\infty} G_{ij}(E)e^{-\frac{i}{\hbar}Et}\frac{dE}{2\pi\hbar}. \tag{5.1.15}$$

The equation (5.1.13) can be arranged as

$$\sum_k [(E - V_i)\delta_{ik} - W_{ik}]G_{kj}(E) = \delta_{ij}. \tag{5.1.16}$$

Now use notation $\hat{G}$ to denote the matrix $G_{ij}(E)$, $\hat{W}$ to denote the matrix W_{ij} and $\hat{V}$ to denote the matrix $V_i\delta_{ij}$. And write the identity matrix as $\hat{I}$. Thus the Hamiltonian can be written as $\hat{H} = \hat{W} + \hat{V}$ and the equation (5.1.16) can be written as

$$(E\hat{I} - \hat{V} - \hat{W})\hat{G}(E) = \hat{I}. \tag{5.1.17}$$

Hence the formal solution for the Green's function is written as

$$\hat{G}(E) = (E\hat{I} - \hat{H})^{-1} = (E\hat{I} - \hat{V} - \hat{W})^{-1}. \tag{5.1.18}$$

Now define the unperturbed Green's function as

$$\hat{G}_0(E) = (E\hat{I} - \hat{H}_0)^{-1} = (E\hat{I} - \hat{W})^{-1}, \tag{5.1.19}$$

then (5.1.17) may be written

$$(\hat{G}_0^{-1} - \hat{V})\hat{G} = \hat{I}, \tag{5.1.20}$$

or

$$\hat{G} = \hat{G}_0 + \hat{G}_0\hat{V}\hat{G}. \tag{5.1.21}$$

This is the required equation of motion of the Green's function in energy representation and it is just the Dyson equation.

5.2 Average T-Matrix Approximation

Since the system is disordered, it is impossible to obtain the exact Green's function. However, the statistical properties of the system are related to the average of the disorders, thus the studies of the disordered system mainly focus on the average of the Green's function with respect to all possible realization of disorders. In this section we shall introduce a method called the average T-matrix approximation to calculate the average Green's function.

Substituting (5.1.21) into the right side of itself iteratively we obtain an infinite series expression for $\hat{G}$ that

$$\hat{G} = \hat{G}_0 + \hat{G}_0\hat{V}\hat{G}_0 + \hat{G}_0\hat{V}\hat{G}_0\hat{V}\hat{G}_0 + \cdots . \tag{5.2.1}$$

Now define T-matrix as

$$\hat{G} = \hat{G}_0 + \hat{G}_0\hat{T}\hat{G}_0, \tag{5.2.2}$$

and a comparison of this definition with (5.2.1) just gives

$$\hat{T} = \hat{T}(E) = \hat{V} + \hat{V}\hat{G}_0\hat{V} + \hat{V}\hat{G}_0\hat{V}\hat{G}_0\hat{V} + \cdots . \tag{5.2.3}$$

This T-matrix is an infinite series and contains all the scattering of $\hat{G}_0$ caused by the off diagonal disorders $\hat{V}$.

Since there is no disorder in $\hat{G}_0$, the average of $\hat{G}$ can be expressed in terms of T-matrix as

$$\langle\hat{G}\rangle = \hat{G}_0 + \hat{G}_0\langle\hat{T}\rangle\hat{G}_0. \tag{5.2.4}$$

We can also define a matrix of self-energy for the average Green's function in the usual way as

$$\hat{\Sigma}(E) = \hat{G}_0^{-1} - \langle\hat{G}\rangle^{-1}, \tag{5.2.5}$$

or, in Dyson equation form,

$$\langle\hat{G}\rangle = \hat{G}_0 + \hat{G}_0\hat{\Sigma}\langle\hat{G}\rangle = \hat{G}_0 + \langle\hat{G}\rangle\hat{\Sigma}\hat{G}_0. \tag{5.2.6}$$

A comparison of (5.2.4) and (5.2.6) immediately gives the relation between the self-energy and T-matrix as

$$\hat{\Sigma} = \langle\hat{T}\rangle(1 + \hat{G}_0\langle\hat{T}\rangle)^{-1} = (1 + \langle\hat{T}\rangle\hat{G}_0)^{-1}\langle\hat{T}\rangle. \tag{5.2.7}$$

This expression states that the self-energy of the average Green's function can be determined by the average T-matrix $\langle\hat{T}\rangle$. However, single impurity scattering problem can be solved exactly, so here we shall introduce the single site t-matrix.

To introduce t-matrix, we first split the random potential matrix $\hat{V}$ into

$$\hat{V} = \sum_i \hat{V}_i, \tag{5.2.8}$$

where $\hat{V}$ is a diagonal matrix while $\hat{V}_i$ is also a diagonal matrix but only at site i it has value V_i. Explicitly,

$$\hat{V} = \begin{pmatrix} V_1 & 0 & 0 & 0 & \cdots \\ 0 & V_2 & 0 & 0 & \cdots \\ \vdots & 0 & \ddots & 0 & \vdots \\ \cdots & 0 & 0 & V_{n-1} & 0 \\ \cdots & 0 & 0 & 0 & V_n \end{pmatrix}, \qquad \hat{V}_i = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ 0 & \ddots & 0 & 0 & \cdots \\ \vdots & 0 & V_i & 0 & \vdots \\ \cdots & 0 & 0 & \ddots & 0 \\ \cdots & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{5.2.9}$$

The infinite series expression (5.2.3) can be treated as the power expansions of

$$\hat{T} = \hat{V}(1 - \hat{G}_0\hat{V})^{-1}, \tag{5.2.10}$$

or we write this expression as

$$\hat{T}(1 - \hat{G}_0\hat{V}) = \hat{V}. \tag{5.2.11}$$

Therefore we obtain a self-consistently formula for $\hat{T}$ as

$$\hat{T} = (1 + \hat{T}\hat{G}_0)\hat{V}. \tag{5.2.12}$$

Now write $\hat{T} = \sum_i \hat{T}_i$, where the matrix $\hat{T}_i$ represents the contribution of site i to T-matrix, and we have

$$\sum_i \hat{T}_i = [1 + (\sum_i \hat{T}_i)\hat{G}_0]\hat{V} = \sum_i [1 + (\sum_j \hat{T}_j)\hat{G}_0]\hat{V}_i, \tag{5.2.13}$$

or, comparing the both sides the expression,

$$\hat{T}_i = [1 + (\sum_j \hat{T}_j)\hat{G}_0]\hat{V}_i = (\hat{V}_i + \hat{T}_i\hat{G}_0\hat{V}_i) + \sum_{j\neq i} \hat{T}_j\hat{G}_0\hat{V}_i. \tag{5.2.14}$$

Now define the single site t-matrix at site i as

$$\hat{t}_i = \hat{V}_i(1 - \hat{G}_0\hat{V}_i)^{-1} = \hat{V}_i + \hat{V}_i\hat{G}_0\hat{V}_i + \hat{V}_i\hat{G}_0\hat{V}_i\hat{G}_0\hat{V}_i + \cdots . \tag{5.2.15}$$

This $\hat{t}_i$ includes all the scattering processes caused by site i. If we are dealing with the single impurity scattering problem where the system has only one impurity, then this $\hat{t}_i$ is also the full T-matrix. This $\hat{t}_i$ is clear solvable, thus the single impurity scattering problem is also solvable. Write (5.2.14) as

$$\hat{T}_i(1 - \hat{G}_0\hat{V}_i) = \hat{V}_i + \sum_{j\neq i} \hat{T}_j\hat{G}_0\hat{V}_i, \tag{5.2.16}$$

and then we have

$$\begin{aligned} \hat{T}_i &= \hat{V}_i(1 - \hat{G}_0\hat{V}_i) + \sum_{j\neq i} \hat{T}_j\hat{G}_0\hat{V}_i(1 - \hat{G}_0\hat{V}_i) \\ &= \hat{t}_i + \sum_{j\neq i} \hat{T}_j\hat{G}_0\hat{t}_i. \end{aligned} \tag{5.2.17}$$

This is the formal solution of $\hat{T}_i$, and it not only includes the contribution from the scattering at site i but also but the scattering effects from other sites. We also obtain an infinite series expression for $\hat{T}$ as

$$\hat{T} = \sum_i \hat{T}_i = \sum_i \hat{t}_i + \sum_i \sum_{j\neq i} \hat{t}_j\hat{G}_0\hat{t}_i + \sum_i \sum_{j\neq i} \sum_{k\neq i,j} \hat{t}_k\hat{G}_0\hat{t}_j\hat{G}_0\hat{t}_i + \cdots . \tag{5.2.18}$$

When calculating $\langle\hat{T}\rangle$, infinite correlation terms of t-matrix, such as $\langle\hat{t}_j\hat{G}_0\hat{t}_i\rangle$ and $\hat{t}_k\hat{G}_0\hat{t}_j\hat{G}_0\hat{t}_i$, are involved. In principle it is impossible to calculate all these terms, so we need some approximation.

The most common approximation is called the *single site approximation* which neglect the correlations between different site. Under such an approximation the average of (5.2.18) can be written as

$$\langle\hat{T}\rangle = \sum_i\langle\hat{t}_i\rangle + \sum_i\sum_{j\neq i}\langle\hat{t}_j\rangle\hat{G}_0\langle\hat{t}_i\rangle + \sum_i\sum_{j\neq i}\sum_{k\neq i,j}\langle\hat{t}_k\rangle\hat{G}_0\langle\hat{t}_j\rangle\hat{G}_0\langle\hat{t}_i\rangle + \cdots, \tag{5.2.19}$$

and the average of (5.2.17) can be written as

$$\begin{aligned}\langle\hat{T}_i\rangle &= \langle\hat{t}_i\rangle + \sum_{j\neq i}\langle\hat{T}_j\rangle\hat{G}_0\langle\hat{t}_i\rangle \\ &= (1+\langle\hat{T}\rangle\hat{G}_0)\langle\hat{t}_i\rangle - \langle\hat{T}_i\rangle\hat{G}_0\langle\hat{t}_i\rangle,\end{aligned} \tag{5.2.20}$$

or, moving the last term to the left side of the equation and then multiplying the inverse on both sides,

$$\langle\hat{T}_i\rangle = (1+\langle\hat{T}\rangle\hat{G}_0)\langle\hat{t}_i\rangle(1+\hat{G}_0\langle\hat{t}_i\rangle)^{-1}. \tag{5.2.21}$$

According to the above expression, we can also write

$$\langle\hat{T}\rangle = \sum_i\langle\hat{T}_i\rangle = (1+\langle\hat{T}\rangle\hat{G}_0)\sum_i\langle\hat{t}_i\rangle(1+\hat{G}_0\langle\hat{t}_i\rangle)^{-1}, \tag{5.2.22}$$

and substituting in (5.2.7) just gives the formula for self-energy under single site approximation as

$$\hat{\Sigma} = \sum_i\langle\hat{t}_i\rangle(1+\hat{G}_0\langle\hat{t}_i\rangle)^{-1}, \tag{5.2.23}$$

and the corresponding average Green's function matrix

$$\langle\hat{G}\rangle = (\hat{G}_0^{-1}-\hat{\Sigma})^{-1}. \tag{5.2.24}$$

5.3 Average T-Matrix Approximation for Binary Alloy

Let us apply the average T-matrix approximation to a binary alloy A_xB_{1-x}, where A and B are two types of atoms in the alloy and x is the concentration of atom A. In such a system, the random potential V_i can only have two values V_A and V_B, or explicitly, $V_i = V_A$ when site i is occupied by atom A while $V_i = V_B$ when site i is occupied by atom B.

It is clear that the only non zero element in $\hat{t}_i$ is

$$\langle i|\hat{t}_i|i\rangle = \langle i|\hat{V}_i(1-\hat{G}_0\hat{V}_i)^{-1}|i\rangle = \frac{V_i}{1-\langle i|\hat{G}_0|i\rangle V_i}, \tag{5.3.1}$$

where V_i can be V_A and V_B depending on the atom at site i. Since the ordered Green's function $\langle i|\hat{G}_0|i\rangle$ has transitional invariance, it is also the unperturbed Green's averaging over sites:

$$\langle i|\hat{G}_0|i\rangle = \frac{1}{N}\sum_i\langle i|\hat{G}_0|i\rangle, \tag{5.3.2}$$

where N is the number of sites. Now denote this average by $F(E)$ that $F(E) = \frac{1}{N}\sum_i\langle i|\hat{G}_0(E)|i\rangle$. If $\hat{H}_0$ is written in $\boldsymbol{k}$-representation that $\hat{H}_0 = \sum_{\boldsymbol{k}}\hat{c}^\dagger_{\boldsymbol{k}}\hat{c}_{\boldsymbol{k}}$, then we have

$$F(E) = \frac{1}{N}\sum_{\boldsymbol{k}}(E-\varepsilon_{\boldsymbol{k}})^{-1}. \tag{5.3.3}$$

Since the value of V_i can only be V_A and V_B, thus the mean value of $\langle i|\hat{t}_i|i\rangle$ is just

$$\overline{\langle i|\hat{t}_i|i\rangle} = xt_A + (1-x)t_B, \tag{5.3.4}$$

where

$$t_A = \frac{V_A}{1 - FV_A}, \quad t_B = \frac{V_B}{1 - FV_B}. \tag{5.3.5}$$

According to (5.2.23), the self-energy is a diagonal matrix and its diagonal elements are all equal to

$$\Sigma = \frac{[xt_A + (1-x)t_B]}{1 + F(E)[xt_A + (1-x)t_B]}. \tag{5.3.6}$$

Let $\hat{I}$ be the identity matrix, then we can write the self-energy matrix as

$$\hat{\Sigma} = \Sigma \hat{I}. \tag{5.3.7}$$

Defect of the Average T-Matrix Approximation

Using the single site approximation we can obtain the average self-energy and accordingly the average Green's function. However, there is a defect in this method that the calculation results depend on the reference crystal.

To see this, let us first choose atom B as reference crystal, thus the unperturbed Hamiltonian may be written

$$\hat{H}_0 = \sum_{\boldsymbol{k}} (\varepsilon_{\boldsymbol{k}} + V_B) \hat{c}^\dagger_{\boldsymbol{k}} \hat{c}_{\boldsymbol{k}}, \tag{5.3.8}$$

while the perturbation operator is

$$\hat{H}_1 = \sum_{i \in A} (V_A - V_B) \hat{c}^\dagger_{\boldsymbol{k}} \hat{c}_{\boldsymbol{k}}, \tag{5.3.9}$$

where the summation is over the sites occupied by atom A. In this case the scatterings occur at sites occupied by atom A, thus we have

$$t_A = \frac{(V_A - V_B)}{1 - F(E - V_B)(V_A - V_B)}, \quad t_B = 0, \tag{5.3.10}$$

where the average Green's function F is

$$F(E - V_B) = \frac{1}{N} \sum_{\boldsymbol{k}} [(E - V_B) - \varepsilon_{\boldsymbol{k}}]^{-1}. \tag{5.3.11}$$

Then according to (5.3.6) the self-energy with atom B as reference crystal is

$$\Sigma_B = \frac{x(V_A - V_B)}{1 - (1-x)F(E - V_B)(V_A - V_B)}. \tag{5.3.12}$$

Similarly, if we choose atom A as reference crystal, the unperturbed Hamiltonian would become

$$\hat{H}_0 = \sum_{\boldsymbol{k}} (\varepsilon_{\boldsymbol{k}} + V_A) \hat{c}^\dagger_{\boldsymbol{k}} \hat{c}_{\boldsymbol{k}}, \tag{5.3.13}$$

and accordingly

$$t_A = 0, \quad t_B = \frac{V_B - V_A}{1 - F(E - V_A)(V_B - V_A)}. \tag{5.3.14}$$

Hence the expression for the self-energy with atom A as reference crystal is

$$\Sigma_A = \frac{(1-x)(V_B - V_A)}{1 - xF(E - V_A)(V_B - V_A)}. \tag{5.3.15}$$

From the expression for Σ_B and Σ_A it is easy to see that they contradict each other, and

$$\Sigma_A \sim 1 - x, \quad \Sigma_B \sim x. \tag{5.3.16}$$

Therefore $\Sigma_B \sim x$ only applicable to small x region ($x \ll 1$) while $\Sigma_A \sim 1 - x$ is only applicable for $x \to 1$ region and neither of these two reference crystal alone can describe the properties of the system for all $0 \le x \le 1$. In practice, we need to choose a proper reference crystal first to apply the average T-matrix approximation.

Virtual Crystal Approximation

Sometimes we can choose a virtual crystal as the reference crystal, which means that we define a new potential as

$$\overline{V} = \langle V_i \rangle = xV_A + (1-x)V_B, \tag{5.3.17}$$

and choose a virtual lattice with this potential as the reference crystal. This is called the *Virtual Crystal Approximation*. Hence the unperturbed Hamiltonian become

$$\hat{H}_0 = \sum_{\boldsymbol{k}} (\varepsilon_{\boldsymbol{k}} + \overline{V}) \hat{c}^\dagger_{\boldsymbol{k}} \hat{c}_{\boldsymbol{k}}, \tag{5.3.18}$$

and accordingly we have

$$t_A = \frac{V_A - \overline{V}}{1 - F(E-\overline{V})(V_A - \overline{V})}, \quad t_B = \frac{V_B - \overline{V}}{1 - F(E-\overline{V})(V_B - \overline{V})}. \tag{5.3.19}$$

According to the above expressions we can write

$$\begin{aligned} xt_A + (1-x)t_B &= x(1-x)(V_A - V_B)\left[\frac{1}{1 - F(E-\overline{V})(V_A - V_B)} - \frac{1}{1 + F(E+\overline{V})(V_A - V_B)}\right] \\ &\approx x(1-x)F(E-\overline{V})(V_A - V_B)^2, \end{aligned} \tag{5.3.20}$$

and retaining the self-energy with virtual crystal approximation Σ_{VCA} up to second order of powers of $V_A - V_B$ gives

$$\Sigma_{\mathrm{VCA}}(E) \approx x(1-x)(V_A - V_B)^2 F(E - \overline{V}). \tag{5.3.21}$$

Since the Green's function defined in average T-matrix approximation is the retarded Green's function, we need to add an imaginary infinitesimal $i0$ to the energy E, so that

$$\Sigma_{\mathrm{VCA}}(E + i0) \approx x(1-x)(V_A - V_B)^2 F(E + i0 - \overline{V}), \tag{5.3.22}$$

and imaginary part of the self-energy is

$$\mathrm{Im}\,\Sigma_{\mathrm{VCA}}(E + i0) \approx x(1-x)(V_A - V_B)^2 \mathrm{Im}\,F(E + i0 - \overline{V}). \tag{5.3.23}$$

The imaginary part of the retarded Green's function F is proportional to the density of states and is negative, thus

$$\mathrm{Im}\,\Sigma_{\mathrm{VCA}}(E + i0) \sim -x(1-x)(V_A - V_B)^2. \tag{5.3.24}$$

As we know from Drude theory,

$$\mathrm{Im}\,\Sigma_{\mathrm{VCA}}(E + i0) = -\frac{\hbar}{2\tau(E)}, \tag{5.3.25}$$

where τ is the relaxation time. Since the electrical conductivity σ is proportional to the relaxation time so that

$$\sigma \propto -\frac{1}{\mathrm{Im}\,\Sigma_{\mathrm{VCA}}}, \tag{5.3.26}$$

or

$$\sigma \propto \frac{1}{x(1-x)}. \tag{5.3.27}$$

Therefore the resistivity $1/\sigma$ is proportional to $x(1-x)$, and this is just the *Nordheim's rule*.

5.4 Coherent Potential Approximation

According to the discussion in last section we find that the calculation of the average T-matrix approximation is heavily dependent on the choice of reference crystal, this makes it hard to control the results. The *coherent potential approximation* avoids such problems by using self consistent procedures to produce an effective lattice. The basic ideas of the coherent potential approximation was proposed by Paul Soven and David Taylor in 1967. However, the essential idea can be even dated back to James Maxwell in his effective medium approximation.

Note that although the Green's function $\hat{G}$ is disordered, the average Green's function $\langle\hat{G}\rangle$ is ordered and transitional invariant. Thus we try to use an uniform effective medium to replace all the scattering effects caused by disorders. Let $\Sigma(E)$ denote the uniform potential of the effective medium. It should be noted that this uniform potential of the virtual effective medium is energy dependent. Thus the effective Hamiltonian may be written as

$$\hat{H}_e = \sum_{\boldsymbol{k}} [\varepsilon_{\boldsymbol{k}} + \Sigma(E)] \hat{c}^\dagger_{\boldsymbol{k}} \hat{c}_{\boldsymbol{k}}, \tag{5.4.1}$$

and accordingly the average effective Green's function is

$$G_e(E) \equiv \frac{1}{N} \sum_{\boldsymbol{k}} [E - \varepsilon_{\boldsymbol{k}} - \Sigma(E)]^{-1}. \tag{5.4.2}$$

It is seen that the effective potential $\Sigma(E)$ acts as an energy dependent self-energy. Such a self-energy neglects all $\boldsymbol{k}$ dependence and thus is a local self-energy. This is the approximation made in this method.

Now the question becomes how to choose the effective medium so that the effective Green's function G_e can represent the average Green's function

$$\langle G \rangle = \frac{1}{N} \mathrm{Tr}\, \hat{G}. \tag{5.4.3}$$

According to (5.2.22) the T-matrix for the effective Hamiltonian can be written as

$$\langle \hat{T} \rangle = \sum_i \langle \hat{T}_i \rangle = (1 + \langle \hat{T} \rangle \hat{G}_e) \sum_i \langle \hat{t}_i \rangle (1 + \hat{G}_e \langle \hat{t}_i \rangle)^{-1}. \tag{5.4.4}$$

In principle, when this average T-matrix equal to zero, all the scattering effects are absorbed into the effective self-energy $\Sigma(E)$. In this case we can use the average effective Green's function G_e to replace $\langle G \rangle$. To make $\langle T \rangle = 0$ it is sufficient to require the average t-matrix equal to zero that

$$\langle t_i \rangle = \left\langle \frac{V_i - \Sigma}{1 - (V_i - \Sigma) G_e} \right\rangle = 0. \tag{5.4.5}$$

This condition can be expressed in a more useful form. Let us write it as

$$\left\langle \frac{1}{G_e} \left[1 - \frac{1}{1 - (V_i - \Sigma) G_e} \right] \right\rangle = 0, \tag{5.4.6}$$

which means

$$\left\langle \frac{1}{1 - (V_i - \Sigma) G_e} \right\rangle = 1. \tag{5.4.7}$$

From (5.4.7) it can be seen that the condition (5.4.5) can be rewritten as

$$\left\langle \frac{V_i}{1 - (V_i - \Sigma) G_e} \right\rangle = \left\langle \frac{\Sigma}{1 - (V_i - \Sigma) G_e} \right\rangle, \tag{5.4.8}$$

and since Σ is a constant for specific E, we finally have

$$\left\langle \frac{V_i}{1 - (V_i - \Sigma) G_e} \right\rangle = \Sigma. \tag{5.4.9}$$

This expression is just the self consistent condition which is needed when determining the effective potential (self-energy for effective Green's function) Σ.

Here we list the basic procedures of the coherent potential approximation:

1. choose an initial self-energy $\Sigma(E)$ for specific E;
2. use (5.4.2) to calculate the average effective Green's function G_e;

   It should be noted here that (5.4.2) is not practical in real calculation, and usually another form of this formula is used that
$$G_e = \int \frac{\rho_0(\varepsilon)}{E - \varepsilon - \Sigma} d\varepsilon, \tag{5.4.10}$$
   where $\rho_0(\varepsilon)$ is the density of states of unperturbed Hamiltonian. The above formula is essentially equivalent to (5.4.2) but it is more practical since the density of states can be calculated via other methods, for instance, for the cubic lattice there is analytic formulas for its density of states.
3. use (5.4.9) to calculate a new self-energy $\Sigma(E)$;
4. compare the new self-energy with the old self-energy, if they are close enough then finish the self consistent procedures, otherwise go to step 2 again.

The self-energy is determined self consistently, thus the difficulty of choosing a proper reference lattice in the average T-matrix approximation is avoided. The self-energy $\Sigma(E)$ obtained in this way is usually a complex number, and according the discussion in Drude theory its imaginary part is related to the relaxation time. Therefore we can use Drude formula to calculate the conductivity. We can also use this self-energy to apply Kubo-Greenwood formula with the Green's function in $\boldsymbol{k}$-representation

$$G_e(E, \boldsymbol{k}) = \frac{1}{E - \varepsilon_{\boldsymbol{k}} - \Sigma(E)}. \tag{5.4.11}$$

Coherent Potential Approximation for Binary Alloy

Here we shall use a cubic binary alloy $A_x B_{1-x}$ as an example. The Hamiltonian is

$$\hat{H} = W \sum_{\langle ij \rangle} \hat{c}_i^\dagger \hat{c}_j + \sum_i V_i \hat{c}_i^\dagger \hat{c}_i, \tag{5.4.12}$$

where the symbol $\langle\rangle$ indicates that summation is over the nearest neighbors and W is the hopping energy among nearest neighbors. And for potential V_i we have

$$V_i = \begin{cases} V_A & i \in A; \\ V_B & i \in B, \end{cases} \tag{5.4.13}$$

where $i \in A$ means that site i is occupied by atom A and similar rule is for atom B.

In a binary alloy $A_x B_{1-x}$ the self consistent condition (5.4.9) becomes simply

$$\Sigma = \frac{x V_A}{1 - (V_A - \Sigma) G_e} + \frac{(1-x) V_B}{1 - (V_B - \Sigma) G_e}. \tag{5.4.14}$$

To apply formula (5.4.10) we need the density of states of cubic lattice.

here should be numerical results

5.5 Anderson Localization

A lattice with perfect periodicity is transitional invariant, and the wave function of an electron in it can be represented by Bloch functions in $\boldsymbol{k}$-representation that

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = u_{\boldsymbol{k}}(\boldsymbol{r}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{5.5.1}$$

where $u_{\boldsymbol{k}}$ is a periodic function. Such a wave function is like the plane wave and extended in the whole space, thus the states represented by Bloch waves are called *extended states*. On the contrary, there also exist some states that the electron is not extended, i.e., localized in some regions. For example, the wave function of an electron in high barrier is exponential decay like

$$\psi(\boldsymbol{r}) =\sim e^{-|\boldsymbol{r}|/l_0}, \tag{5.5.2}$$

where l_0 is a positive constant. Clearly that the electron states represented by such kind of wave functions are not extended. And these states, which are different from extended states, are called *localized states*. The electrons in localized states have little contributions to electrical conductivity.

The classical theories, such as Boltzmann equation, treat the disorders in the lattice as scattering sources and formulate the impurity scattering theory. The T-matrix formalism and coherent potential approximation basically do the same thing. In such theoretical frame, the disorders scatter Bloch electron and decrease the relaxation time, and thus decrease the electrical conductivity. The conductivity in this frame can never reach zero unless the scattering strength is infinite large. However, Philip Anderson pointed out that even the scattering strength is finite, the randomness of the system may also cause localization states in 1957.

Anderson Disorder Model

Anderson use the tight-binding Hamiltonian with disorders to describe a diagonal disordered system, which is now called *Anderson disorder model*. The Hamiltonian for Anderson disordered model has the same form with (5.1.1) that

$$\hat{H} = \sum_{ij} W_{ij}\hat{c}_i^\dagger \hat{c}_j + \sum_i V_i \hat{c}_i^\dagger \hat{c}_i. \tag{5.5.3}$$

Note that the off diagonal elements W_{ij} of the Hamiltonian is ordered, the disorders only exist in diagonal elements. If only the nearest neighbors hopping are under consideration, the Hamiltonian reduces to

$$\hat{H} = W \sum_{\langle ij \rangle} \hat{c}_i^\dagger \hat{c}_j + \sum_i V_i \hat{c}_i^\dagger \hat{c}_i, \tag{5.5.4}$$

where W is some constant and the symbol $\langle\rangle$ indicates that the summation is over the nearest neighbors.

And the disordered potential V_i is assumed to be distributed uniformly in an energy range with width Γ, that the distribution probability density is given by

$$P(V_i) = \begin{cases} \dfrac{1}{\Gamma}, & |V_i| \leq \Gamma/2; \\ 0, & |V_i| \geq \Gamma/2. \end{cases} \tag{5.5.5}$$

The disorders formulated in this way is short ranged and is characterized by an important parameter Γ which represents the degree of randomness.

Anderson Localization

To investigate localization phenomena in the Anderson disordered model we need first find the criteria of localized states. Recall that the Green's function $G_{ij}(t)$ gives the amplitude of finding the electron at site i at time t with the initial position at site j at time 0, and its square modulus $|G_{ij}(t)|^2$ gives the corresponding probability of finding the electron at site i at time t. Therefore $|G_{ii}(t)|^2$ gives the probability that an electron returns to its original site i after time t. If t is sufficient long and $G_{ii}(t)$ is zero, then the electron would not return to the origin after a long time, which means that the electron leaves the origin and propagates in the whole system, thus it is in extended states. On the other hand, the probability of electron that not return to original site in future counting from an arbitrary time $t_0 > 0$ is

$$\prod_{t_i=t_0}^{\infty} [1 - |G_{ii}(t_i)|^2], \tag{5.5.6}$$

where this product is understand to take the limit over all the infinitesimal intervals δt between t_0 and $t \to \infty$. It is clear that this quantity tends to zero if $G_{ii}(t)$ is not zero for large t, which means that electron would certainly return to the origin at some time in the distant future. And thus the electron is in localized states.

The equation of motion for the Green's function in energy representation is same as (5.1.13) that

$$EG_{ij}(E) = V_i G_{ij}(E) + \sum_k W_{ik} G_{kj} + \delta_{ij}, \tag{5.5.7}$$

or

$$(E - V_i) G_{ij}(E) = \sum_k W_{ik} G_{kj} + \delta_{ij}. \tag{5.5.8}$$

Now define a quantity

$$g_i = \frac{1}{E - V_i}, \tag{5.5.9}$$

then (5.5.7) becomes

$$\begin{aligned} G_{ij}(E) &= g_i \delta_{ij} + \sum_k g_i W_{ik} G_{kj} \\ &= g_i \delta_{ij} + \sum_{kl} g_i \delta_{ik} W_{kl} G_{lj}. \end{aligned} \tag{5.5.10}$$

This expression is in Dyson equation form and it is clear that $g_i \delta_{ij}$ acts the unperturbed Green's function. And the equation for diagonal elements of the Green's function G_{ii} is then

$$G_{ii}(E) = g_i + \sum_k g_i W_{ik} G_{ki}. \tag{5.5.11}$$

The right side of this equation contains off diagonal elements of the Green's function, now pick the diagonal elements out and do iteratively substitution that (note that the diagonal terms $W_{ii} = 0$ according to definition)

$$\begin{aligned} G_{ii} &= g_i + g_i W_{ii} G_{ii} + \sum_{k \neq i} g_i W_{ik} G_{ki} \\ &= g_i + \sum_{k \neq i} g_i W_{ik} g_k W_{ki} G_{ii} + \sum_{k \neq i} \sum_{l \neq k, i} g_i W_{ik} g_k W_{kl} G_{li} + \cdots . \end{aligned} \tag{5.5.12}$$

Then we obtain the Dyson equation for diagonal Green's function G_{ii} in term of self-energy that

$$G_{ii} = g_i + g_i \Sigma_i G_{ii}, \tag{5.5.13}$$

where

$$\Sigma_i(E) = \sum_{k \neq i} W_{ik} g_k W_{ki} + \sum_{k \neq i} \sum_{l \neq k, i} W_{ik} g_k W_{kl} g_l W_{li} + \cdots . \tag{5.5.14}$$

According to the definition of g_i, the formal solution for $G_{ii}(E)$ can be written as

$$G_{ii}(E) = \frac{1}{E - V_i - \Sigma_i(E)}, \tag{5.5.15}$$

or, since the Green's function is essentially retarded Green's function,

$$G_{ii}(E) = \frac{1}{E + i0 - V_i - \Sigma_i(E)}. \tag{5.5.16}$$

Clearly the value of the self-energy determines the Green's function, and the Green's function in time representation with energy E is given by the inverse Fourier transform that

$$G_{ii}(t) = \int_{-\infty}^{\infty} G_{ii}(E) e^{-\frac{i}{\hbar} E t} \frac{dE}{2\pi\hbar} = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \frac{e^{-\frac{i}{\hbar} E t}}{E + i0 - V_i - \Sigma_i(E)} dE. \tag{5.5.17}$$

The inverse Fourier transform is an integration along a contour just above the real axis in the E-plane. If the self-energy $\Sigma_i(E)$ has a non-zero imaginary part, then $G_{ii}(t)$ acquires a exponentially decay factor $e^{\frac{1}{\hbar}\mathrm{Im},\Sigma_i t}$ and $G_{ii}(t)$ would tend to zero for large t. In another words, a necessary condition for localized states with energy E is that the imaginary part of corresponding self-energy $\Sigma_i(E)$ vanishes. The infinite series expression for self-energy Σ_i is just (5.5.14). When E is real, this infinite series must also be real if it has a limit. In other words, a sufficient condition that the state with energy E should be localized is that the infinite series (5.5.14) converges.

Now we rewrite the expression of self-energy (5.5.14), by writing W_{ik} as a constant since it is essentially an ordered quantity, as

$$\begin{aligned}\Sigma_i(E) &= \sum_{k\neq i} W g_k W + \sum_{k\neq i}\sum_{l\neq k,i} W g_k W g_l W + \cdots \\ &= W\sum_{L=1}^{\infty}\sum_j T_j^{(L)},\end{aligned} \tag{5.5.18}$$

where

$$T_j^{(L)} = \frac{W^L}{(E-V_{j_1})\cdots(E-V_{j_L})} = \prod_{i=1}^{L} W g_{j_i}. \tag{5.5.19}$$

It should be emphasized that after replacing the matrix W_{ik} by constant W the summation must be understood that it is over the "connected" sites, and the connection between site i and k means that the original matrix element W_{ik} is not zero. Therefore $T_j^{(L)}$ represents a path that starts from site i, passes L different sites $j_1, j_2, \cdots, j_L$ and then returns to site i. Note that sites $j_1, j_2, \cdots, j_L$ are all different, and such a path is generally called *self-avoiding walk*. Suppose each site has Z neighbors, then in the summation for Σ_i there are roughly Z^L terms $T_j^{(L)}$ for each L. Now we introduce a simple method given by John Ziman to estimate this summation.

Now define a quantity Q as the logarithm of $|T_j^{(L)}|$:

$$Q = \ln|T_j^{(L)}| = \ln\prod_{i=1}^{L}|W g_{j_i}| = \sum_{i=1}^{L}\ln|W g_{j_i}|. \tag{5.5.20}$$

Since g_{j_i} are random variables, we use the average value

$$\langle \ln|W g_{j_i}|\rangle = \int dV_i P(V_i)\ln\left|\frac{W}{E-V_i}\right| \tag{5.5.21}$$

to replace $\ln|W g_{j_i}|$. It is clear that the average value $\langle \ln|W g_{j_i}|\rangle$ is statistically site independent, thus we omit the subscript and write it simply as $\langle \ln|W g|\rangle$. Therefore after the average we write

$$Q = \sum_{i=1}^{L}\ln|W g_{j_i}| \approx L\langle \ln|W g|\rangle, \tag{5.5.22}$$

and

$$|T_j^{(L)}| = e^Q \approx \exp\left[L\langle \ln|W g|\rangle\right]. \tag{5.5.23}$$

Because in the summation for a specific L there are Z^L terms which have the same form with $T_j^{(L)}$, then we have

$$\sum_j |T_j^{(L)}| \approx \left[Z\exp(\langle \ln|W g|\rangle)\right]^L. \tag{5.5.24}$$

There is always an inequality for the series that

$$\sum_j T_j^{(L)} \le \sum_j |T_j^{(L)}|, \tag{5.5.25}$$

so if the geometric series

$$W \sum_{L=1}^{\infty} \left[Z \exp(\langle \ln |Wg| \rangle)\right]^L \tag{5.5.26}$$

converges then the original series (5.5.18) converges.

The convergence condition for geometric series is

$$Z \exp(\langle \ln |Wg| \rangle) < 1, \tag{5.5.27}$$

and this condition can also be used as the localization condition. Substituting the distribution function (5.5.5) we find

$$\begin{aligned} \langle \ln |Wg| \rangle &= \frac{1}{\Gamma} \int_{-\Gamma/2}^{\Gamma/2} \ln \left| \frac{W}{E - V} \right| dV \\ &= 1 - \frac{1}{2} \left[\left(1 + 2\frac{E}{\Gamma}\right) \ln \left| \frac{\Gamma}{2W} + \frac{E}{W} \right| + \left(1 - 2\frac{E}{\Gamma}\right) \ln \left| \frac{\Gamma}{2W} - \frac{E}{W} \right| \right]. \end{aligned} \tag{5.5.28}$$

For $E = 0$, we have

$$\langle \ln |Wg| \rangle = 1 - \ln \left| \frac{\Gamma}{2W} \right|, \tag{5.5.29}$$

and the localization condition for $E = 0$ is correspondingly

$$\frac{\Gamma}{2Z|W|} > e. \tag{5.5.30}$$

Note that the average value $\langle \ln |Wg| \rangle$ reaches its maximum when $E = 0$. Therefore if the localization condition is satisfied for $E = 0$ then all other states with $|E| > 0$ also satisfy the convergence condition $Z \exp(\langle \ln |Wg| \rangle) < 1$, which means that all states are localized states. The expression (5.5.30) is also called the *Anderson localization condition*.

Chapter 6

Small Polaron

6.1 Holstein Model

The Hamiltonian of Holstein Model is

$$H = -\sum_{\langle i,j \rangle} t_{ij} c_i^\dagger c_j + g \sum_i c_i^\dagger c_i (a_i + a_i^\dagger) + \omega_0 \sum_i a_i^\dagger a_i, \tag{6.1.1}$$

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:

$$\lambda = g^2/\omega_0 t, \tag{6.1.2}$$

$$\gamma = \omega_0/t. \tag{6.1.3}$$

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

$$\alpha = \lambda/\gamma = g/\omega_0. \tag{6.1.4}$$

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.

6.2 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

$$G_{ij}(t) = -i\langle 0|Tc_i(t)c_j^\dagger(0)|0\rangle, \tag{6.2.1}$$

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

$$G_{ij}(t) = -i\langle 0|Tc_i(t)c_j(0)^\dagger S|0\rangle, \tag{6.2.2}$$

where

$$S = Te^{-i\int dt[g\sum_i c_i^\dagger c_i(a_i+a_i^\dagger)]} \quad . \tag{6.2.3}$$

The expansion of S to second order of g gives

$$\begin{aligned} G_{ij}(t) &= -i\langle 0|Tc_i(t)c_j^\dagger|0\rangle \\ &\quad -i\frac{g^2}{2}\int dt'dt''\sum_{kl}\langle 0|Tc_i(t)c_j^\dagger c_k^\dagger(t')c_k(t')c_l^\dagger(t'')c_l(t'')[a_k(t')a_l^\dagger(t'')+a_k^\dagger(t')a_l(t'')]|0\rangle, \end{aligned} \tag{6.2.4}$$

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

$$\begin{aligned} &\langle 0|a_k^\dagger(t')a_l(t'')|0\rangle = 0, \\ &\langle 0|a_k(t')a_l^\dagger(t'')|0\rangle = D_{kl}(t'-t'') = \delta_{kl}D_{kk}(t'-t''), \end{aligned} \tag{6.2.5}$$

we can obtain that

$$G_{ij}(t) = G_{ij}^{(0)}(t) + ig^2\sum_k\int dt'dt''G_{ik}^{(0)}(t-t')G_{kk}^{(0)}(t'-t'')D_{kk}(t'-t'')G_{kj}(t''), \tag{6.2.6}$$

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

$$G_{ij}(\omega) = G_{ij}^{(0)}(\omega) + g^2\sum_k G_{ik}^{(0)}(\omega)G_{kk}^{(0)}(\omega-\omega_0)G_{kj}^0(\omega). \tag{6.2.7}$$

Compare with the Dyson equation

$$G_{ij} = G_{ij}^{(0)} + \sum_{kl}G_{ik}^{(0)}\Sigma_{kl}G_{lj} = G_{ij}^{(0)} + \sum_{kl}G_{ik}^{(0)}\Sigma_{kl}G_{lj}^{(0)} + \cdots \quad , \tag{6.2.8}$$

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

$$\Sigma_2(\omega) = g^2G^{(0)}(\omega-\omega_0). \tag{6.2.9}$$

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

$$\frac{m^*}{m} = \left.\frac{d(\omega-\mathrm{Re}\Sigma(\omega))}{d\omega}\right|_{E_0} = 1 - \left.\frac{d\mathrm{Re}\Sigma(\omega)}{d\omega}\right|_{E_0}, \tag{6.2.10}$$

where E_0 is the ground-state energy.

6.3 Atomic Limit (Zero Temperature)

The atomic limit is defined as the zero hopping case ($t = 0$). In this case, Hamiltonian (6.1.1) can be diagonalized by the unitary Lang-Firsov transformation

$$U = e^{-S}, \quad S = -\alpha\sum_i c_i^\dagger c_i(a_i - a_i^\dagger). \tag{6.3.1}$$

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

$$\begin{aligned} &\bar{c}_i = e^S c_i e^{-S} = c_i X_i, \quad X_i = e^{\alpha(a_i - a_i^\dagger)}; \\ &\bar{c}_i^\dagger = e^S c_i^\dagger e^{-S} = c_i^\dagger X_i^\dagger, \quad X_i^\dagger = e^{\alpha(a_i^\dagger - a_i)}; \\ &\bar{a}_i = e^S a_i e^{-S} = a_i - \alpha c_i^\dagger c_i; \\ &\bar{a}_i^\dagger = e^S a_i^\dagger e^{-S} = a_i^\dagger - \alpha c_i^\dagger c_i; \\ &\bar{H} = e^S H e^{-S} = -\tfrac{g^2}{\omega_0}\sum_i c_i^\dagger c_i + \omega_0\sum_i a_i^\dagger a_i. \end{aligned} \tag{6.3.2}$$

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

$$C_0 = \langle n_i(a_i + a_i^\dagger)\rangle - 2\alpha\langle n_i\rangle = -2\alpha\langle n_i\rangle, \tag{6.3.3}$$

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

$$\langle e^S a^\dagger a e^{-S}\rangle = \langle a^\dagger a\rangle + \alpha^2\langle c^\dagger c\rangle = \alpha^2. \tag{6.3.4}$$

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

$$\begin{aligned} G(t) &= -i\langle 0|c(t)c^\dagger|0\rangle \\ &= -i\langle 0|cXe^{-i\bar{H}t}c^\dagger X^\dagger|0\rangle \\ &= -i\sum_{mn}\langle 0|cX|m\rangle\langle m|e^{-i\bar{H}t}|n\rangle\langle n|c^\dagger X^\dagger|0\rangle, \end{aligned} \tag{6.3.5}$$

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

$$X^\dagger = e^{-\alpha^2/2}e^{\alpha a^\dagger}e^{-\alpha a}, \quad X = e^{-\alpha^2/2}e^{-\alpha a^\dagger}e^{\alpha a}, \tag{6.3.6}$$

accordingly,

$$\begin{aligned} &\langle m|X^\dagger|0\rangle = e^{-\alpha^2/2}\langle m|e^{\alpha a^\dagger}|0\rangle = e^{-\alpha^2/2}\sum_n\langle m|\frac{\alpha^n}{\sqrt{n!}}|n\rangle = e^{-\alpha^2/2}\frac{\alpha^m}{\sqrt{m!}}, \\ &\langle 0|X|m\rangle = e^{-\alpha^2/2}\frac{\alpha^m}{\sqrt{m!}}. \end{aligned} \tag{6.3.7}$$

Finally the electron Green's function is

$$G(\omega) = \sum_n^\infty \frac{\alpha^{2n}e^{-\alpha^2}}{n!}\frac{1}{\omega - n\omega_0 - \varepsilon_p}. \tag{6.3.8}$$

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

$$t_{ij}c_i^\dagger c_j \quad \to \quad t_{ij}X_i^\dagger X_j c_i^\dagger c_j, \tag{6.3.9}$$

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

$$t_{ij}\langle 0|X_i^\dagger X_j|0\rangle = t_{ij}\langle 0|X^\dagger|0\rangle\langle 0|X|0\rangle = t_{ij}e^{-\alpha^2}. \tag{6.3.10}$$

6.4 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

$$\begin{aligned} e^{-\alpha a}|n\rangle &= \sum_{m=0}^\infty \frac{(-\alpha)^m}{m!}a^m|n\rangle \\ &= \sum_{m=0}^n \frac{(-\alpha)^m}{m!}\left[\frac{n!}{(n-m)!}\right]^{\frac{1}{2}}|n-m\rangle, \end{aligned} \tag{6.4.1}$$

and

$$\langle n|e^{\alpha a^\dagger} = \sum_{m=0}^n \frac{\alpha^m}{m!}\left[\frac{n!}{(n-m)!}\right]^{\frac{1}{2}}\langle n-m|, \tag{6.4.2}$$

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

therefore

$$\langle n|e^{\alpha a^\dagger}e^{-\alpha a}|n\rangle = \sum_{m=0}^{n}\frac{(-\alpha^2)^m}{m!}\frac{n!}{m!(n-m)!} = L_n(\alpha^2), \tag{6.4.3}$$

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

$$\langle n|X^\dagger|n\rangle = \langle n|X|n\rangle = e^{-\alpha^2/2}L_n(\alpha^2). \tag{6.4.4}$$

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

$$\begin{aligned} & t_{ij}(1-e^{-\beta\omega_0})^2\sum_{mn}e^{-\beta m\omega_0}\langle m|X_i^\dagger|m\rangle e^{-\beta n\omega_0}\langle n|X_j|n\rangle \\ = \quad & t_{ij}e^{-\alpha^2}\left[(1-e^{-\beta\omega_0})\sum_{n=0}^{\infty}e^{-n\beta\omega_0}L_n(\alpha^2)\right]^2. \end{aligned} \tag{6.4.5}$$

Recall that the generating function of Laguerre polynomials:

$$\frac{e^{-xt/(1-t)}}{1-t} = \sum_{n=0}^{\infty}L_n(x)t^n, \tag{6.4.6}$$

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

$$t_{ij}e^{-S_T}, \quad S_T = \alpha^2(1+2\langle n\rangle_T). \tag{6.4.7}$$

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

$$\begin{aligned} G(t) &= -i(1-e^{-\beta\omega_0})\sum_n e^{-\beta n\omega_0}\langle n|c(t)c^\dagger|n\rangle \\ &= -i(1-e^{-\beta\omega_0})\sum_n e^{-\beta n\omega_0}\langle 0|c(t)X(t)c^\dagger X^\dagger|0\rangle \\ &= -i(1-e^{-\beta\omega_0})\langle 0|c(t)c^\dagger|0\rangle\sum_n e^{-\beta n\omega_0}\langle n|X(t)X^\dagger|n\rangle. \end{aligned} \tag{6.4.8}$$

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

$$\begin{aligned} c(t) = ce^{-i\varepsilon_p t}, \quad c^\dagger(t) = c^\dagger e^{i\varepsilon_p t}; \\ a(t) = ae^{-i\omega_0 t}, \quad a^\dagger(t) = a^\dagger e^{i\omega_0 t}, \end{aligned} \tag{6.4.9}$$

thus

$$X(t) = e^{-\alpha^2}e^{-\alpha a^\dagger e^{i\omega_0 t}}e^{\alpha a e^{-i\omega_0 t}} = e^{-\alpha^2}e^{-\alpha a^\dagger(t)}e^{\alpha a(t)} \tag{6.4.10}$$

and

$$X(t)X^\dagger = e^{-\alpha^2}e^{-\alpha a^\dagger(t)}e^{\alpha a(t)}e^{\alpha a^\dagger}e^{-\alpha a}. \tag{6.4.11}$$

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

$$e^{\alpha a(t)}e^{\alpha a^\dagger} = e^{\alpha a^\dagger}[e^{-\alpha a^\dagger}e^{\alpha a(t)}e^{\alpha a^\dagger}], \tag{6.4.12}$$

using Baker-Campbell-Hausdorff formula we get

$$e^{-\alpha a^\dagger}e^{\alpha a(t)}e^{\alpha a^\dagger} = e^{\alpha^2 e^{-i\omega_0 t}}e^{\alpha a(t)}. \tag{6.4.13}$$

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

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

$$G(t) = -i(1-e^{-\beta\omega_0})e^{-\alpha^2(1-e^{-i\omega_0 t})}\langle 0|c(t)c^\dagger|0\rangle \sum_n e^{-\beta n\omega_0}\langle n|e^{\alpha a^\dagger(1-e^{i\omega_0 t})}e^{-\alpha a(1-e^{-i\omega_0 t})}|n\rangle, \tag{6.4.14}$$

again using Laguerre polynomials we can prove that

$$(1-e^{-\beta\omega_0})\sum_n e^{-\beta n\omega_0}\langle n|e^{u^* a^\dagger}e^{-ua}|n\rangle = e^{-|u|^2/(e^{\beta\omega_0}-1)}, \tag{6.4.15}$$

thus

$$G(t) = -ie^{-i\varepsilon_p t}\exp\Big[-\alpha^2[(N+1)(1-e^{-i\omega_0 t})+N(1-e^{i\omega_0 t})]\Big], \tag{6.4.16}$$

where

$$N = \frac{1}{e^{\beta\omega_0}-1}. \tag{6.4.17}$$

Recall the generating function of Bessel functions of complex argument,

$$e^{z\cos\theta} = \sum_{n=-\infty}^{\infty} I_n(z)e^{in\theta}, \tag{6.4.18}$$

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

$$z = 2\alpha^2\sqrt{N(N+1)}, \quad \theta = \omega_0(t+i\beta/2) \tag{6.4.19}$$

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

$$G(t) = -ie^{-(2N+1)\alpha^2}e^{-i\varepsilon_p t}\sum_{n=-\infty}^{\infty} e^{-in\omega_0 t}e^{\beta n\omega_0/2}I_n\{2\alpha^2\sqrt{N(N+1)}\}, \tag{6.4.20}$$

in frequency space

$$G(\omega) = e^{-(2N+1)\alpha^2}\sum_{n=-\infty}^{\infty} e^{\beta n\omega_0/2}I_n\{2\alpha^2\sqrt{N(N+1)}\}\frac{1}{\omega - n\omega_0 - \varepsilon_p}. \tag{6.4.21}$$

6.5 The Impurity Analogy for A Single Electron

The Hamiltonian for impurity model is

$$H_{\text{imp}} = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_k V_k(c_k^\dagger d + d^\dagger c_k) + \omega_0 a^\dagger a + g d^\dagger d(a+a^\dagger), \tag{6.5.1}$$

here V_k and E_k is related to G_0 by

$$G_0^{-1}(\omega) = \omega - \int_{-\infty}^{\infty} d\varepsilon\frac{\Delta(\varepsilon)}{\omega-\varepsilon}, \tag{6.5.2}$$

where

$$\Delta(\varepsilon) = \sum_k V_k^2\delta(\varepsilon-\varepsilon_k). \tag{6.5.3}$$

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

$$H_0 = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_k V_k(c_k^\dagger d + d^\dagger c_k) + \omega_0 a^\dagger a, \quad V = g d^\dagger d(a+a^\dagger). \tag{6.5.4}$$

6.5.1 The Zero Temperature Formalism

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

$$G(t) = -i\theta(t)\langle 0|d(t)d^\dagger|0\rangle, \tag{6.5.5}$$

after Fourier transformation:

$$G(\omega) = \langle 0|d\frac{1}{\omega + i0 - H}d^\dagger|0\rangle. \tag{6.5.6}$$

An operator identity holds:

$$\frac{1}{\omega - H} = \frac{1}{\omega - H_0} + \frac{1}{\omega - H_0}V\frac{1}{\omega - H}. \tag{6.5.7}$$

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

$$G_{nm} = \langle 0|\frac{a^n}{\sqrt{n!}}d\frac{1}{\omega - H}d^\dagger\frac{(a^\dagger)^m}{\sqrt{m!}}|0\rangle, \tag{6.5.8}$$

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

$$|0,p\rangle = \frac{(a^\dagger)^p}{\sqrt{p!}}|0\rangle, \quad |1,p\rangle = \frac{(a^\dagger)^p}{\sqrt{p!}}d^\dagger|0\rangle, \tag{6.5.9}$$

one can write

$$\begin{aligned}
G_{nm} &= \langle 0|\frac{a^n}{\sqrt{n!}}d\frac{1}{\omega - H_0}d^\dagger\frac{(a^\dagger)^m}{\sqrt{m!}}|0\rangle + \langle 0|\frac{a^n}{\sqrt{n!}}d\frac{1}{\omega - H_0}V\frac{1}{\omega - H}d^\dagger\frac{(a^\dagger)^m}{\sqrt{m!}}|0\rangle \\
&= G^{(0)}_{nm} + g\sum_{p_1,p_2}\langle 0|\frac{a^n}{\sqrt{n!}}d\frac{1}{\omega - H_0}d^\dagger|0,p_1\rangle\langle 0,p_1|d(a+a^\dagger)|1,p_2\rangle\langle 0,p_2|d\frac{1}{\omega - H}d^\dagger\frac{(a^\dagger)^m}{\sqrt{m!}}|0\rangle \\
&= G^{(0)}_{nm} + g\sum_{p_1,p_2}G^{(0)}_{n,p_1}X_{p_1,p_2}G_{p_2,m} \\
&= G^{(0)}_{nn}\delta_{nm} + g\sum_{p}G^{(0)}_{nn}X_{np}G_{pm} \quad ,
\end{aligned} \tag{6.5.10}$$

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:

$$X_{np} = \sqrt{p+1}\delta_{n,p+1} + \sqrt{p}\delta_{n,p-1}. \tag{6.5.11}$$

Equation (6.5.10) can be solved in matrix notation:

$$G^{-1} = G_0^{-1} - gX, \tag{6.5.12}$$

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

$$G_{00} = \frac{T_1}{T_0}, \tag{6.5.13}$$

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

$$\begin{aligned}
&D_0 = [G^{(0)}]^{-1}_{00}, \\
&D_1 = [G^{(0)}]^{-1}_{11}[G^{(0)}]^{-1}_{00} - g^2 = [G^{(0)}]^{-1}_{11}D_0 - g^2, \\
&D_2 = \cdots = [G^{(0)}]^{-1}_{2}D_1 - 2g^2D_0,
\end{aligned} \tag{6.5.14}$$

and, for the general case, the recurrence relations

$$D_k = [G^{(0)}]^{-1}_{k,k}D_{k-1} - kg^2D_{k-2}. \tag{6.5.15}$$

What's more, we have that

$$T_k = [G^{(0)}]^{-1}_{kk} T_{k+1} - (k+1)g^2 T_{k+2}, \quad \text{or} \quad \frac{T_k}{T_{k+1}} = [G^{(0)}]^{-1}_{kk} - (k+1)g^2 \frac{T_{k+2}}{T_{k+1}}, \tag{6.5.16}$$

therefore

$$\frac{T_1}{T_0} = \frac{1}{[G^{(0)}]^{-1}_{00} - g^2 \frac{T_2}{T_1}} = \cdots, \tag{6.5.17}$$

or

$$G(\omega) = \cfrac{1}{G_0^{-1}(\omega) - \cfrac{g^2}{G_0^{-1}(\omega - \omega_0) - \cfrac{2g^2}{G_0^{-1}(\omega - 2\omega_0) - \cfrac{3g^2}{G_0^{-1}(\omega - 3\omega_0) - \cdots}}}}. \tag{6.5.18}$$

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

$$\Sigma(\omega) = \cfrac{g^2}{G_0^{-1}(\omega - \omega_0) - \cfrac{2g^2}{G_0^{-1}(\omega - 2\omega_0) - \cfrac{3g^2}{G_0^{-1}(\omega - 3\omega_0) - \cdots}}}. \tag{6.5.19}$$

The self-energy can be defined recursively,

$$\Sigma^{(p)}(\omega) = \frac{pg^2}{G_0^{-1}(\omega - p\omega_0) - \Sigma^{(p+1)}} \quad . \tag{6.5.20}$$

6.5.2 The Finite Temperature Formalism

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

$$G(\omega) = (1 - e^{\beta\omega_0}) \sum_n e^{-\beta n \omega_0} G_{nn}(\omega). \tag{6.5.21}$$

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):

$$G_{nn} = G_n^{(0)} + gG_n^{(0)}(\sqrt{n} G_{n-1,n} + \sqrt{n+1} G_{n+1,n}), \tag{6.5.22}$$

which we seek to write in a form as

$$G_{nn} = G_n^{(0)} + G_n^{(0)}(AG_{nn} + BG_{nn}). \tag{6.5.23}$$

Again according to Cramer's rule,

$$G_{n-1,n} = \sqrt{n} g \frac{D_{n-2}T_{n+1}}{T_0}, \quad G_{nn} = \frac{D_{n-1}T_{n+1}}{T_0}, \tag{6.5.24}$$

recall the recurrence relation for D:

$$D_k = [G_k^{(0)}]^{-1} D_{k-1} - kg^2 D_{k-2}, \tag{6.5.25}$$

or

$$\frac{D_{k-1}}{D_k} = \frac{1}{[G_k^{(0)}]^{-1} - kg^2 \dfrac{D_{k-2}}{D_{k-1}}} \quad . \tag{6.5.26}$$

Therefore

$$G_{n-1,n} = \sqrt{n} g \frac{D_{n-2}}{D_{n-1}} \frac{D_{n-1}T_{n+1}}{T_0} = \sqrt{n} g \frac{D_{n-2}}{D_{n-1}} G_{nn}, \tag{6.5.27}$$

i.e.,

$$A = ng^2 \frac{D_{n-2}}{D_{n-1}} = \cfrac{ng^2}{[G_n^{(0)}(\omega+\omega_0)]^{-1} - \cfrac{(n-1)g^2}{[G_n^{(0)}(\omega+2\omega_0)]^{-1} - \cfrac{(n-2)g^2}{\ddots - \cfrac{g^2}{[G_n^{(0)}(\omega+n\omega_0)]^{-1}}}}} \tag{6.5.28}$$

Similarly,

$$G_{n+1,n} = \sqrt{n+1} g \frac{D_{n-1} T_{n+2}}{T_0} = \sqrt{n+1} g \frac{T_{n+2}}{T_{n+1}} G_{nn}, \tag{6.5.29}$$

recall the recurrence relation for T:

$$T_k = [G_k^{(0)}]^{-1} T_{k+1} - (k+1) g^2 T_{k+2}, \tag{6.5.30}$$

or

$$\frac{T_{k+1}}{T_k} = \frac{1}{[G_k^{(0)}]^{-1} - (k+1) g^2 \frac{T_{k+2}}{T_{k+1}}}. \tag{6.5.31}$$

Therefore

$$B = (n+1) g^2 \frac{T_{n+2}}{T_{n+1}} = \cfrac{(n+1)g^2}{[G_n^{(0)}(\omega-\omega_0)]^{-1} - \cfrac{(n+2)g^2}{[G_n^{(0)}(\omega-2\omega_0)]^{-1} - \cfrac{(n+3)g^2}{[G_n^{(0)}(\omega-3\omega_0)]^{-1} - \cdots}}}, \tag{6.5.32}$$

finally

$$G_{nn} = \frac{1}{[G_n^{(0)}]^{-1} - A - B}. \tag{6.5.33}$$

6.5.3 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)

$$G^{-1}(\omega) = \omega - \sum_{ij} t_{oi} t_{jo} G_{ij}^{(o)}(\omega), \tag{6.5.34}$$

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

$$G^{-1}(\omega) = \omega - t^2 G(\omega). \tag{6.5.35}$$

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

$$G_{ij}^{(o)} = G_{ij} - \frac{G_{io} G_{oj}}{G_{oo}}. \tag{6.5.36}$$

Therefore equation (6.5.34) become

$$G^{-1} = \omega - \sum_{ij} t_{oi} t_{jo} G_{ij} + \frac{\left(\sum_i G_{oi}\right)^2}{G_{oo}}, \tag{6.5.37}$$

recall that

$$G(\omega, k) = \frac{1}{\omega - \varepsilon_k - \Sigma(\omega)}, \tag{6.5.38}$$

we have that

$$G^{-1} = \omega - \int d\varepsilon \frac{\rho(\varepsilon)\varepsilon^2}{\zeta - \varepsilon} - \left(\int d\varepsilon \frac{\rho(\varepsilon)\varepsilon}{\zeta - \varepsilon} \right)^2 \Bigg/ \int d\varepsilon \frac{\rho(\varepsilon)}{\zeta - \varepsilon}, \tag{6.5.39}$$

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

$$\int d\varepsilon \frac{\rho(\varepsilon)\varepsilon^2}{\zeta - \varepsilon} = \zeta \int d\varepsilon \frac{\rho(\varepsilon)\varepsilon}{\zeta - \varepsilon}, \quad \int d\varepsilon \frac{\rho(\varepsilon)}{\zeta - \varepsilon} = -1 + \zeta \int d\varepsilon \frac{\rho(\varepsilon)}{\zeta - \varepsilon}. \tag{6.5.40}$$

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

$$G_0^{-1} = \Sigma + G^{-1}. \tag{6.5.41}$$

Chapter 7

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 $h = 6.62607004 \times 10^{-34}\ \mathrm{J} \cdot \mathrm{s} = 4.135667662 \times 10^{-15}\ \mathrm{eV} \cdot \mathrm{s}$.
- reduced Plank constant $\hbar = 1.0545718 \times 10^{-34}\ \mathrm{J} \cdot \mathrm{s} = 6.582119514 \times 10^{-16}\ \mathrm{eV} \cdot \mathrm{s}$
- Boltzmann constant $k_B = 1.38064852 \times 10^{-23}\ \mathrm{J} \cdot \mathrm{K}^{-1} = 8.6173324 \times 10^{-5}\ \mathrm{eV} \cdot \mathrm{K}^{-1}$.
- Bohr magneton $\mu_B = 9.27400968 \times 10^{-24}\ \mathrm{J} \cdot \mathrm{T}^{-1} = 5.7883818066 \times 10^{-5}\ \mathrm{eV} \cdot \mathrm{T}^{-1}$.
- Bohr radius $a_0 = 5.29 \times 10^{-11}$ m.
- Electron mass $m_e = 9.10938215 \times 10^{-31}\ \mathrm{kg} = 8.18710438 \times 10^{-14}\ \mathrm{J/c^2} = 0.51099891\ \mathrm{MeV/c^2}$
- Ohm $\Omega = \frac{\mathrm{V}}{\mathrm{A}} = \frac{\mathrm{V \cdot s}}{\mathrm{C}} = \frac{\mathrm{J \cdot s}}{\mathrm{C^2}} = \frac{\mathrm{J}}{\mathrm{s \cdot A^2}}$.