

MENG SUN

NOTES ON: MANY PARTICLE
PHYSICS – BY D.
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1

Introductory Material

1.1 Harmonic oscillators and phonons

s1.1 First quantization in physics refers to the property of particles that certain operators do not commute

$$[x, p_x] = i\hbar \quad (1.1)$$

$$E \rightarrow i\hbar \frac{\partial}{\partial t} \quad (1.2)$$

For the second quantization, the basic idea is that forces are caused by the exchange of particle, and the number of particles is quantized, for example photons for electromagnetic force.

In solids the quantized vibrational modes of the atom are quantized because of the first quantization (1.1). This vibrational modes are called **phonons**. An electron can interact with a phonon, and this phonon can travel to another electron, interact, and thereby cause an indirect interaction between electrons. The induced interaction between electrons is an example of second quantization. They cause quantized interactions between electrons.

Phonons in solids can usually be described as harmonic oscillators.

$$H = \frac{p^2}{2m} + \frac{K}{2}x^2 \quad (1.3)$$

Introducing the dimensionless coordinate ξ

$$\omega^2 = \frac{K}{m} \quad (1.4)$$

$$\xi = x\sqrt{\frac{m\omega}{\hbar}} \quad (1.5)$$

$$-i\frac{\partial}{\partial \xi} = \frac{p}{\sqrt{\hbar m\omega}} \quad (1.6)$$

$$H = \frac{\hbar\omega}{2} \left(-\frac{\partial^2}{\partial \xi^2} + \xi^2 \right) \quad (1.7)$$

The harmonic oscillator Hamiltonian has a solution in terms of Hermit polynomials.

$$H\psi_n = \hbar\omega\left(n + \frac{1}{2}\right)\psi_n \quad (1.8)$$

Using the Dirac notation, the matrix elements for operators x and p

$$\begin{aligned} \langle n' | x | n \rangle &= \sqrt{\frac{\hbar}{2m\omega}} \left[\sqrt{n'} \delta_{n',n+1} + \sqrt{n} \delta_{n',n-1} \right] \\ \langle n' | p | n \rangle &= i\sqrt{\frac{m\hbar\omega}{2}} \left[\sqrt{n'} \delta_{n',n+1} - \sqrt{n} \delta_{n',n-1} \right] \end{aligned} \quad (1.9)$$

For creation operators

$$\begin{aligned} a &= \frac{1}{\sqrt{2}} \left(\xi + \frac{\partial}{\partial \xi} \right) = \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{ip}{m\omega} \right) \\ a^\dagger &= \frac{1}{\sqrt{2}} \left(\xi - \frac{\partial}{\partial \xi} \right) = \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{ip}{m\omega} \right) \end{aligned} \quad (1.10)$$

with commutation relations

$$[a, a^\dagger] = 1 \quad (1.11)$$

The eigenstate of (1.8) are

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle \quad (1.12)$$

and with

$$a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \quad a |n\rangle = \sqrt{n} |n-1\rangle \quad (1.13)$$

The time dependence of these operator is, in Heisenberg representation of quantum mechanics

$$O(t) = e^{iHt} O e^{-iHt} \quad \frac{\partial O(t)}{\partial t} = i[H, O(t)] \quad (1.14)$$

This suggest that

$$a(t) = a \exp(-i\omega t) \quad a^\dagger(t) = a^\dagger \exp(i\omega t) \quad (1.15)$$

The time development of the position operator can be represented as

$$x(t) = \sqrt{\frac{\hbar}{2m\omega}} \left(a e^{-i\omega t} + a^\dagger e^{i\omega t} \right) \quad (1.16)$$

Another problem is the charged harmonic oscillator in a constant electric field F

$$H = \frac{p^2}{2m} + \frac{K}{2} x^2 + eFx = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) + \lambda (a + a^\dagger) \quad (1.17)$$

$$\lambda = eF \sqrt{\frac{\hbar}{2m\omega}} \quad (1.18)$$

This Hamiltonian may be solved exactly. Consider the equation of motion for the time development

$$\frac{\partial a}{\partial t} = i [H, a] = -i (\omega a + \lambda) \quad (1.19)$$

The right hand side is no longer just proportional to a , however, by define the new operators

$$A = a + \frac{\lambda}{\omega} \quad (1.20)$$

$$A^\dagger = a^\dagger + \frac{\lambda}{\omega} \quad (1.21)$$

$$\frac{\partial A}{\partial t} = -i\omega A \quad (1.22)$$

$$A(t) = e^{-i\omega t} A \quad (1.23)$$

$$A^\dagger(t) = e^{i\omega t} A^\dagger \quad (1.24)$$

This new operators have same properties of the Harmonic oscillator ones

$$H = \omega \left(A^\dagger A + \frac{1}{2} \right) - \frac{\lambda^2}{\omega} \quad (1.25)$$

with the eigenstate

$$H |n\rangle = \left[\omega \left(n + \frac{1}{2} \right) - \frac{\lambda^2}{\omega} \right] |n\rangle \quad (1.26)$$

$$|n\rangle = \frac{(A^\dagger)^n}{\sqrt{n!}} |0\rangle \quad (1.27)$$

The position operator for this case is

$$x(t) = \sqrt{\frac{\hbar}{2m\omega}} \left(A e^{-i\omega t} + A^\dagger e^{i\omega t} - \frac{2\lambda}{\omega} \right) \quad (1.28)$$

The spring stretches to a new equilibrium point which is displaced a distance

$$x_0 = \sqrt{\frac{\hbar}{2m\omega}} \frac{2\lambda}{\omega} = -\frac{eF}{K} \quad (1.29)$$

from the original one. This oscillator is in new equilibrium with the same frequency ω as before and still quantized in the unit of ω . The energy $\frac{-\lambda^2}{\omega} = \frac{-e^2 F^2}{2K}$ is that gain by spring from the displacement along the electric field. One can also get the same result by rewrite the Hamiltonian as

$$H = \frac{p^2}{2m} + \frac{K}{2} \left(x + \frac{eF}{K} \right)^2 - \frac{e^2 F^2}{2K} \quad (1.30)$$

In a solid system, there are many atoms, which mutually interact. The vibrational modes are collective motions involving many atoms.

A simple introduction to this is by studying the normal modes of a one-dimensional harmonic chain

$$H = \sum_i \frac{p_i^2}{2m} + \frac{K}{2} \sum_i (x_i - x_{i+1})^2 \quad (1.31)$$

The classical solution is obtained by solving the equation of motion

$$-m\ddot{x}_j = m\omega^2 x_j = K(2x_j - x_{j+1} - x_{j-1}) \quad (1.32)$$

A solution is assumed of the form $x_j = x_0 \cos(kaj)$ and the force term becomes

$$2x_j - x_{j+1} - x_{j-1} = 2x_0 \cos(kaj) [1 - \cos(ka)] \quad (1.33)$$

The normal modes have the solution

$$\omega_k^2 = \frac{2K}{m} [1 - \cos(ka)] = \frac{4K}{m} \sin^2\left(\frac{ka}{2}\right) \quad (1.34)$$

The quantum mechanical solution begins by defining some normal coordinates, assuming periodic boundary condition

$$x_l = \frac{1}{\sqrt{N}} \sum_k e^{ikal} x_k; \quad x_k = \frac{1}{\sqrt{N}} \sum_l e^{-ikal} x_l \quad (1.35)$$

$$p_l = \frac{1}{\sqrt{N}} \sum_k e^{-ikal} p_k; \quad p_k = \frac{1}{\sqrt{N}} \sum_l e^{ikal} p_l \quad (1.36)$$

This choice maintains the desired commutation relations in either **real and wave vector** space

$$[x_l, p_m] = i\delta_{lm} \quad \text{realspace} \quad (1.37)$$

$$[x_k, p_p] = i\delta_{kp} \quad (1.38)$$

It is easy to show that the Hamiltonian may written in wave vector space as¹

$$H = \frac{1}{2m} \sum_k [p_k p_{-k} + m^2 \omega_k^2 x_k x_{-k}] \quad (1.39)$$

¹ Since, $\sum_l x_l x_{l+m} = \sum_k x_k x_{-k} e^{iamk}$ and $\sum_k p_l^2 = \sum_k p_k p_{-k}$ and the definition (1.34).

The Hamiltonian has the form of a simple harmonic oscillator for each wave vector. Define the creation and destruction operators as

$$a_k = \sqrt{\frac{m\omega_k}{2\hbar}} \left(x_k + \frac{i}{m\omega_k} p_{-k} \right) \quad (1.40)$$

$$a_k^\dagger = \sqrt{\frac{m\omega_k}{2\hbar}} \left(x_k - \frac{i}{m\omega_k} p_{-k} \right) \quad (1.41)$$

Where they obey the commutation relations and have the same Hamilton in the form of Harmonic oscillator. These collective modes of vibration are called **phonons**. They are the quantized version of

the classical vibrational modes in the solid. There are the same commutator relations and Hamiltonian as in the simple harmonic oscillator. Each wave vector state behaves independently, with a possible set of quantum numbers $n_k = 0, 1, 2, \dots$. The state of the system at any time is

$$\psi = |n_1, n_2, \dots, n_n\rangle = \prod_k |n_k\rangle = \prod_k \frac{(a_k^\dagger)^{n_k}}{\sqrt{n_k!}} |0\rangle \quad (1.42)$$

with expectation value of Hamiltonian

$$H = \sum_k \omega_k \left(n_k + \frac{1}{2} \right) \quad (1.43)$$

In thermal equilibrium the states have an average value of n_k

$$\langle n_k \rangle \equiv N_k = \frac{1}{e^{\beta\omega_k} - 1} \quad (1.44)$$

The position operator in wave vector and real space is

$$\begin{aligned} x_k(t) &= \sqrt{\frac{\hbar}{2m\omega_k}} \left(a_k e^{-i\omega_k t} + a_{-k}^\dagger e^{i\omega_k t} \right) \\ x_l(t) &= \sqrt{\frac{\hbar}{2mN\omega_k}} e^{ikal} \left(a_k e^{-i\omega_k t} + a_{-k}^\dagger e^{i\omega_k t} \right) \end{aligned} \quad (1.45)$$

Often the term mN is replaced by the quantity $mN = \rho V$, the mass density and volume. Where the following notations are well know

$$\lim_{V \rightarrow \infty} \frac{1}{V} \sum_{\mathbf{k}} f(\mathbf{k}) = \int \frac{d^3k}{8\pi^3} f(\mathbf{k}) \quad (1.46)$$

$$\lim_{V \rightarrow \infty} \delta_{\mathbf{k}, \mathbf{k}'} = \frac{8\pi^3}{V} \delta(\mathbf{k} - \mathbf{k}') \quad (1.47)$$

The quantum mechanical solution (1.39) has the same frequencies as found in the classical solution (1.32). Quantum mechanics only enters in a quantization of the amplitude of the oscillation. The phonons occur in discrete numbers with zero, one, two, ..., phonons in state \mathbf{k} .

In three-dimensional solids, the theory is nearly identical except there are more indices. Suppose there is a potential function between atoms or ions of the form

$$\sum_{ij} V(R_i - R_j) \quad (1.48)$$

where R_i is the position of an atom. Let R_i^0 as the equilibrium position and Q_i as the displacement from equilibrium. The potential function is expanded in a Taylor series about the equilibrium position

$$\begin{aligned} V(R_i - R_j) &= V(R_i^0 - R_j^0) + (Q_i - Q_j) \nabla V(R_i^0 - R_j^0) \\ &+ \frac{1}{2} (Q_i - Q_j)_\mu (Q_i - Q_j)_\nu \frac{\partial^2}{\partial R_\mu \partial R_\nu} V(R_i^0 - R_j^0) \\ &+ O(Q^3) \end{aligned} \quad (1.49)$$

The linear term in displacement vanishes, because of the definition of equilibrium point give the summation of forces is zero. The important term is the one which is quadratic in the displacement. It gives the potential eqnergy of the phonons

$$V_{ph} = \frac{1}{2} \sum_{ij} (Q_i - Q_j)_\mu (Q_i - Q_j)_\nu \Phi_{\mu\nu} (R_i^0 - R_j^0) \quad (1.50)$$

The interaction is evaluated in wave vector space by trying an expansion of the form

$$Q_i(t) = i \sum_{\mathbf{k}, \lambda} \sqrt{\frac{\hbar}{2MN\omega_{\mathbf{k}\lambda}}} \tilde{\zeta}_{\mathbf{k}, \lambda} \left(a_{\mathbf{k}, \lambda} e^{-i\omega_{\mathbf{k}\lambda}t} + a_{-\mathbf{k}, \lambda}^\dagger e^{i\omega_{\mathbf{k}\lambda}t} \right) e^{i\mathbf{k} \cdot \mathbf{R}_i^0} \quad (1.51)$$

where M is the ion mass. The faction of i on the right-hand side of the equation is required to make $Q_i^\dagger = Q_i$ since it represents a real displacement in space. To make (1.51) id Hermitian it requires that

$$\tilde{\zeta}_{\mathbf{k}, \lambda}^* = -\tilde{\zeta}_{-\mathbf{k}, \lambda} \quad (1.52)$$

The polarization vector $\tilde{\zeta}_{\mathbf{k}, \lambda}$ are assumed to be real but change sign with \mathbf{k} direction, $\tilde{\zeta}_{-\mathbf{k}} = -\tilde{\zeta}_{\mathbf{k}}$ and the above identity is satisfied. Since the displacement is in three diemnsions, there are $3L$ normal modes for each value of wave vector. Where L is the number of atoms per unit cell of the crystal. THhe index λ runs over these $3L$ values of normal mode. Each mode has its own eigenfrequency. It will also have a polarization vector $\tilde{\zeta}_{\mathbf{k}, \lambda}$ which specifies the bibrational direction of the ion for each wave vector and mode λ . If there are more than one atom per unit cell, one should add further subscripts to M and $\tilde{\zeta}_{\mathbf{k}, \lambda}$ to specify the values for each atom per unit cell.

The right-hand side of (1.49) may be written as

$$= \sum_{ij} V(R_i^0 - R_j^0) + \frac{M}{2} \sum_{\mathbf{k}, \lambda} Q_{\mathbf{k}, \lambda} Q_{-\mathbf{k}, \lambda} \omega_{\mathbf{k}\lambda}^2 \quad (1.53)$$

The first term is a constant which will be neglected in discussion of vibrational modes. The eigenvalues $\omega_{\mathbf{k}\lambda}$ are those solved in the harmonic approximation. In this approximation, one retains the quadratic term only in the displacements in the Hamiltonian. To be more careful, a third order anharmonic term V_3 can be added for the case of one atom per unit cell². The cubic terms V_3 permit on phonon to decay into two and vice versa.

² P10

1.2 Second Quantization for particle

Consider the Lagrangian density

$$L = i\hbar\psi^\dagger\dot{\psi} - \frac{\hbar^2}{2m}\nabla\psi^\dagger\nabla\psi - U(\mathbf{r}, t)\psi^\dagger\psi \quad (1.54)$$

The wave function is complex, with real and imaginary parts. These two parts can be treated as independent variables in the Lagrangian. An alternate choice is to treat ψ and ψ^\dagger as independent variable, then the variations give

$$\frac{\partial L}{\partial \psi} = -U\psi^\dagger \quad (1.55)$$

$$\frac{\partial L}{\partial \psi_x} = -\frac{\hbar^2}{2m}\psi^\dagger \quad (1.56)$$

$$\frac{\partial L}{\partial \dot{\psi}} = i\hbar\psi^\dagger \quad (1.57)$$

According to Euler-Lagrange equation of motion for a field³

$$\partial_\mu \left(\frac{\partial L}{\partial (\partial_\mu \phi)} \right) - \frac{\partial L}{\partial \phi} = 0 \quad (1.58)$$

³ We took the covariant way from Peskin's book. Where μ is the time and space coordinate.

One can get the Hermitian conjugate of Schrödinger's equation is recovered. In the Lagrangian formulation, the momentum which is conjugate to the variable ψ is

$$\omega = \frac{\partial}{\partial \dot{\psi}} = i\hbar\psi^\dagger \quad (1.59)$$

The Hamiltonian density

2

Green's Functions at Zero Temperature

The Green's function is a method trying to deduce the properties of some system described by a Hamiltonian H which may not be solved exactly. The usual approach is to set

$$H = H_0 + V \quad (2.1)$$

where H_0 is the Hamiltonian that can be solved exactly. The term V represents all remaining parts of H . One tries to choose H_0 so that the effects of V are small. The basic procedure is to start with a system completely described by H_0 . The effects of V are introduced, and then calculations are done to find how V changes the properties. These steps are the basic procedure in many-body theory.

2.1 *Interaction representation*

2.1.1 *Schrödinger*

In Schrödinger representation

$$i\partial_t\psi(t) = H\psi(t) \quad (2.2)$$

with the formal operator solution

$$\psi(t) = e^{-iHt}\psi(0) \quad (2.3)$$

The use of this formula requires:

- The wavefunction is time dependent.
- Operators such as the Hamiltonian H are taken to be independent of time.

2.1.2 *Heisenberg*

The Heisenberg representation has the following properties:

- The wavefunction is independent of the time
- The operators are time dependent and given by

$$O(t) = e^{iHt}O(0)e^{-iHt} \quad (2.4)$$

or, equivalently, the equation of motion is given by

$$i\partial_t O(t) = [O(t), H] \quad (2.5)$$

In physics, one is usually trying to evaluate matrix elements in order to determine the transition rates, in different representation

$$\langle \psi_1^\dagger(t) O \psi_2(t) \rangle_S = \langle \psi_1^\dagger O(t) \psi_2 \rangle_H = \langle \psi_1^\dagger(0) e^{iHt} O(0) e^{-iHt} \psi_2(0) \rangle \quad (2.6)$$

2.1.3 Interaction

The interaction representation is another way of doing things. **Here both the wavefunction and operators are time dependent.** The Hamiltonian is given by

$$H = H_0 + V \quad (2.7)$$

In the whole book the wavefunction and operator in interaction picture will represent by a caret. They have the following properties:

- The operators have a time dependence:

$$\hat{O}(t) = e^{iH_0 t} O_S e^{-iH_0 t} \quad i\partial_t \hat{O}(t) = [\hat{O}(t), H_0] \quad (2.8)$$

- The wavefunction have the time dependence:

$$\hat{\psi}(t) = e^{iH_0 t} e^{-iHt} \psi(0) \quad (2.9)$$

It is assumed that $[H_0, V] \neq 0$, which result a non-trivial problem.

Similarly, the matrix elements give the same result. The time dependence of the operator is relying on the unperturbed Hamiltonian as in (2.8). For the dependence of the wavefunction is governed by

$$\partial_t \hat{\psi}(t) = -i\hat{V}(t)\hat{\psi}(t) \quad (2.10)$$

As operator was introduced into (2.9), which can be defined as

$$U(t) = e^{iH_0 t} e^{-iHt} \quad (2.11)$$

Furthermore, it obeys a differential equation which can be written in the interaction representation:

$$\partial_t U(t) = -i\hat{V}(t)U(t) \quad (2.12)$$

By setting the initial condition $U(0) = 1$, we can have this iterated relation

$$\begin{aligned} U(t) &= 1 - i \int_0^t dt_1 \hat{V}(t_1) U(t_1) \\ &= \sum_{n=0}^{\infty} (-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \hat{V}(t_1) \hat{V}(t_2) \cdots \hat{V}(t_n) \end{aligned} \quad (2.13)$$

In this situation, it is convenient to introduce the time-ordering operator T , which works on a group of time-dependent operators. With the help of time-ordering operator, the expansion of $U(t)$ gives

$$U(t) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_0^t dt_1 \cdots \int_0^{t_{n-1}} dt_n T[\hat{V}(t_1) \cdots \hat{V}(t_n)] \quad (2.14)$$

This expansion may be abbreviated by writing it as

$$U(t) = T \exp \left[-i \int_0^t dt_1 \hat{V}(t_1) \right] \quad (2.15)$$

Always keep in minds that this is a short hand for the series definition.

2.2 *S Matrix*

It had been shown that the wavefunction in interaction representation had a time dependence at zero time:

$$\hat{\psi}(t) = U(t) \hat{\psi}(0) \quad (2.16)$$

Now define the S matrix as the operator $S(t, t')$ which changes the wavefunction in two different time

$$\hat{\psi}(t) = S(t, t') \hat{\psi}(t') \quad (2.17)$$

with the definition

$$S(t, t') = U(t) U^\dagger(t') \quad (2.18)$$

and some important properties of this operators

- $S(t, t) = 1$
- $S^\dagger(t, t') = S(t', t)$
- $S(t, t') S(t', t'') = S(t, t'')$

Finally, it can also be expressed as a time-ordered operator by

$$S(t, t') = T \exp \left[-i \int_{t'}^t dt_1 \hat{V}(t_1) \right] \quad (2.19)$$

In different representation, the wavefunction is identical at the $t = 0$, let $\psi(0)$ as the exact ground state wavefunction, and ϕ_0 as the

ground state of H_0 . The relationship between these two ground states at zero temperature was established by Gell-Mann and Low

$$\psi(0) = S(0, -\infty)\phi_0 \quad (2.20)$$

The result can be regarded as the following, since

$$\hat{\psi}(t) = S(t, 0)\psi(0) \quad (2.21)$$

operate by $S(0, t)$ we can get

$$\psi(0) = S(0, t)\hat{\psi}(t) \quad (2.22)$$

Let $t \rightarrow -\infty$, one get

$$\psi(0) = S(0, -\infty)\hat{\psi}(-\infty) \quad (2.23)$$

The important assertion is that $\hat{\psi}(-\infty) = \phi_0$. The traditional argument is that one starts in the long past with the wavefunction ϕ_0 which does not contain the effects of interaction V . The operator S brings this wavefunction *adiabatically* up to the present which with the interaction.

Additional property of these states which is needed for the discussion of Green's function is, as $t \rightarrow +\infty$,

$$\hat{\psi}(\infty) = S(\infty, 0)\psi(0) \quad (2.24)$$

One possible assumption is that $\hat{\psi}(\infty)$ must be related to ϕ_0 . If they are equal except for a phase factor L

$$\phi_0 e^{iL} = \hat{\psi}(\infty) = S(\infty, 0)\psi(0) = S(\infty, -\infty)\phi_0 \quad (2.25)$$

$$e^{iL} = \langle \phi_0 | S(\infty, -\infty) | \phi_0 \rangle \quad (2.26)$$

2.3 Green's Function

At zero temperature the electron Green's function is defined as

$$G(\lambda, t - t') = -i \langle | TC_\lambda(t) C_\lambda^\dagger(t') | \rangle \quad (2.27)$$

The quantum number λ can be anything depending on the problem¹. At zero temperature the state $| \rangle$ must be the ground state.

In the definition of Green's function the C_λ represent states of H_0 , while the ground state $| \rangle$ is an eigenstate of H . Furthermore, (2.27) is defined in Heisenberg picture, one has the usual dependence of time on operators (2.4).

To change the Green's function from Heisenberg picture to interaction one. Let $|\phi_0\rangle$ be the ground state of H_0 , so we have

$$| \rangle = S(0, -\infty) |\phi_0\rangle \quad (2.28)$$

¹ For free-electron gas $\lambda = (\mathbf{p}, \sigma)$, where \mathbf{p} is wave vector and σ is spin.

Next change the operators to interaction representation², we have the Green's function

$$\begin{aligned} G(\lambda, t - t') &= -i\Theta(t - t') \langle \phi_0 | S(-\infty, 0) S(0, t) \hat{C}_\lambda(t) S(t, 0) S(0, t') \\ &\quad \times \hat{C}_\lambda^\dagger(t') S(t', 0) S(0, -\infty) | \phi_0 \rangle \\ &\quad + i\Theta(t - t') \langle \phi_0 | S(-\infty, 0) S(0, t') \hat{C}_\lambda^\dagger(t') S(t', 0) S(0, t) \\ &\quad \times \hat{C}_\lambda(t) S(t, 0) S(0, -\infty) | \phi_0 \rangle \end{aligned}$$

The left-hand bracket can be changed by remembering (2.25) and (2.26)

$$\langle \phi_0 | S(-\infty, 0) = e^{-iL} \langle \phi_0 | S(\infty, -\infty) S(-\infty, 0) = \frac{\langle \phi_0 | S(\infty, 0)}{\langle \phi_0 | S(\infty, -\infty) | \phi_0 \rangle}$$

By introduce the time ordering operator T , it automatically sorts these segments so they act in their proper sequence. The total Green's function is expressed as

$$G(\lambda, t - t') = -i \frac{\langle \phi_0 | T \hat{C}_\lambda(t) \hat{C}_\lambda^\dagger(t') S(\infty, -\infty) | \phi_0 \rangle}{\langle \phi_0 | TS(\infty, -\infty) | \phi_0 \rangle} \quad (2.29)$$

A Green's function can also be defined for the special case where $V = 0$ where S matrix is unity. This Green's function is defined as

$$G^0(\lambda, t - t') = -i \langle \phi_0 | T \hat{C}_\lambda(t) \hat{C}_\lambda^\dagger(t') | \phi_0 \rangle \quad (2.30)$$

This G^0 is called the *unperturbed Green's function* or sometimes the *free propagator*.

For electronic systems there are two different types which have different ground states.

2.3.1 An empty band

Here the properties are studied of an electron in an energy band in which it is the only electron. An example is an electron in the conduction band of a semiconductor or an insulator. In this case the ground state is the particle vacuum denoted as $|0\rangle$. The stat has the property that

$$C_p |0\rangle = 0 \quad (2.31)$$

$$a_q |0\rangle = 0 \quad (2.32)$$

$$S(t, -\infty) |0\rangle = |0\rangle \quad (2.33)$$

Both of the ground state, ϕ_0 and ψ_0 are the vacuum state $|0\rangle$. The Green's function is only possible for this time ordering

$$G(\lambda, t - t') = -i\Theta(t - t') \langle 0 | \hat{C}_\lambda(t) \hat{C}_\lambda^\dagger(t) | 0 \rangle \quad (2.34)$$

The unperturbed Green's function is given

$$G^0(\lambda, t - t') = -i\Theta(t - t')e^{-i\varepsilon_\lambda(t-t')} \quad (2.35)$$

The Fourier transform is defined as

$$G(\lambda, E) = \int_{-\infty}^{\infty} dt e^{iEt} G(\lambda, t) \quad (2.36)$$

The unperturbed Green's function gives³

$$G^0(\lambda, E) = \frac{1}{E - \varepsilon_\lambda + i\delta} \quad (2.37)$$

³ To make the integral converge, add the infinitesimal quantity $i\delta$, which is

$$G^0(\lambda, E) = \int dt e^{i(E+i\delta)t} G^0(\lambda, t)$$

2.3.2 A degenerate electron gas

The second case is where electrons are in a Fermi sea at zero temperature. The standard example is a simple metal. The system has a chemical potential μ and all electron states with $E < \mu$ are occupied. If the unperturbed electrons, H_0 , are characterized by energy ε_k , the ground state $|\phi_0\rangle$ has all states $\varepsilon_k < \mu$ filled and others are empty. It is convenient and conventional to measure the electron's energy relative to the chemical potential, $\zeta_k = \varepsilon_k - \mu$. For a spherical Fermi surface,

$$\langle \phi_0 | C_k^\dagger C_k | \phi_0 \rangle = \Theta(p_F - k) \quad (2.38)$$

$$\langle \phi_0 | C_k C_k^\dagger | \phi_0 \rangle = \Theta(k - p_F) \quad (2.39)$$

This gives the Green's function

$$G^0(k, E) = \frac{1}{E - \zeta_k + i\delta \text{sgn}(\zeta_k)} \quad (2.40)$$

2.3.3 Phonons

The Green's function for phonons is defined as

$$D(\mathbf{q}, \lambda, t - t') = -i \langle | T A_{\mathbf{q}\lambda}(t) A_{-\mathbf{q}\lambda}(t') | \rangle \quad (2.41)$$

$$A_{\mathbf{q}\lambda} = a_{\mathbf{q}\lambda} + a_{-\mathbf{q}\lambda}^\dagger \quad (2.42)$$

The λ refer to the polarization of phonons. In the interaction picture

$$D(q, t - t') = -i \frac{\langle \phi_0 | T \hat{A}_{-q}(t) \hat{A}_{-q}(t') S(\infty, -\infty) | \phi_0 \rangle}{\langle \phi_0 | S(\infty, -\infty) | \phi_0 \rangle} \quad (2.43)$$

At zero temperature there are no phonons. The ground states $|\psi_0\rangle$ and $|\phi_0\rangle$ are the particle vacuum $|0\rangle$. The Green's function for phonon at zero temperature is

$$D^0(\mathbf{q}, t - t') = -i \left[\Theta(t - t') e^{-i\omega_q(t-t')} + \Theta(t' - t) e^{i\omega_q(t-t')} \right] \quad (2.44)$$

and

$$D^0(\mathbf{q}, \omega) = \frac{2\omega_{\mathbf{q}}}{\omega^2 - \omega_{\mathbf{q}}^2 + i\delta} \quad (2.45)$$

For nonzero temperature, we have

$$D^0(\mathbf{q}, t - t') = -i \left[(N_{\mathbf{q}} + 1)e^{-i\omega_{\mathbf{q}}|t-t'|} + N_{\mathbf{q}}e^{i\omega_{\mathbf{q}}|t-t'|} \right] \quad (2.46)$$

2.4 Wick's Theorem

For Green's function as defined in interaction picture such as (2.29) and (2.43). To evaluate these, the standard method is expanding the $S(\infty, -\infty)$ matrix in (2.19).

$$G(p, t - t') = \sum_{n=0}^{\infty} \frac{(-i)^{n+1}}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \frac{{}_0\langle T \hat{C}_p(t) \hat{V}(t_1) \cdots \hat{V}(t_n) \hat{C}_p^\dagger(t') \rangle_0}{{}_0\langle S(\infty, -\infty) \rangle_0} \quad (2.47)$$

We should follow the following rules

- The time ordering of each pair gives the proper time ordering to the entire result.
- For n creation and annihilation operators there are $n!$ possible combinations.
- Each pair should have the same eigenstate for nonzero result.
- Separation is always possible with different kinds of operators whenever operators commute.
- For the same time, destruction operator always goes to the right and give the number operator.
- For different time, one should get the unperturbed Green's function.
- Wick's theory is valid only when the Hamiltonian H_0 is bilinear form.

In summary, Wick's theorem states that a time-ordered bracket may be expanding into all possible pairings. Each of these pairings will be a time-ordered Green's function or a number operator. This Wick's theory is valid only when the Hamiltonian H_0 is bilinear in creation and destruction operators.

2.5 Feynman Diagrams

Feynman diagrams introduce the idea of representing the pairing terms by drawings. These diagrams can be drawn for the Green's

function depending on time and energy. An arrow is often include to represent the direction and does not imply time sequence. The phonon Green's function is represented by dashed line and doesn't have direction, because⁴

$$D^0(\mathbf{q}, t - t') = D^0(-\mathbf{q}, t' - t) \quad (2.48)$$

This term exist only if the phonon wave vector \mathbf{q} is nonzero, when it is zero a phonon is either a translation of the crystal or a permanent strain. In principle we have,

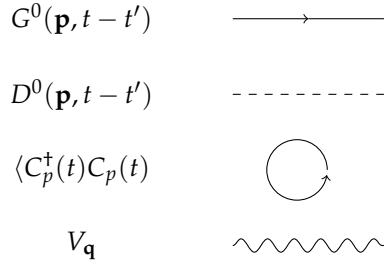


Figure 2.1: Elements of Feynman diagram.

2.6 Vacuum Polarization Graphs

The terms in the series of $\langle \phi_0 | S(\infty, -\infty) | \phi_0 \rangle$ are called *vacuum polarization terms*. The net result in calculating G , one needs only to evaluate the connected diagrams. The other contributions, from the disconnected diagrams and vacuum polarization diagrams, they exactly cancel one another⁵.

⁵ The theorem is explain in P83-P86.

2.7 Dyson's Equation

The Dyson's equation is obtained by formally summing the series⁶

$$G(\mathbf{p}, E) = \frac{G^0(\mathbf{p}, E)}{1 - G^0(\mathbf{p}, E)\Sigma(\mathbf{p}, E)} \quad (2.49)$$

where the self-energy is summation of all different self-energy contribution.

Dyson's equation is often written in a equivalent form. It is obtained by using the algebraic for G^0 , which gives

$$G(\mathbf{p}, E) = \frac{1}{E - \varepsilon_{\mathbf{p}} + i\delta - \Sigma(\mathbf{p}, E)} \quad (2.50)$$

and for the electron at Fermi sea in zero temperature⁷

$$G(\mathbf{p}, E) = \frac{1}{E - \xi_{\mathbf{p}} + i\delta \text{sgn}(p) - \Sigma(\mathbf{p}, E)} \quad (2.51)$$

⁶ P86-P88 in .

⁷ Note the energy spectrum is different with the single electron in a band case, we have μ here.

The self-energy has real and imaginary parts. The switching of signs of sgn_p was caused by the distinction between electron excitations with $\xi_p > 0$ and hole excitations with $\xi_p < 0$. This distinction is maintained even when self-energy is included and they have the same sign. The electron self-energy is sometimes called a *mass operator*.

For phonon Green's function, one have the same type of Dyson's equation

$$D(\mathbf{q}, \omega) = \frac{D^0(\mathbf{q}, \omega)}{1 - D^0(\mathbf{q}, \omega)\Pi(\mathbf{q}, \omega)} \quad (2.52)$$

Similarly, we have this form,

$$D(\mathbf{q}, \omega) = \frac{2\omega_{\mathbf{q}}}{\omega^2 - \omega_{\mathbf{q}}^2 + i\delta - 2\omega_{\mathbf{q}}\Pi(\mathbf{q}, \omega)} \quad (2.53)$$

The phonon self-energy term $\Pi(\mathbf{q}, \omega)$ is sometimes called a *polarization operator*, because the self-energy effects arise from the phons causing polarization in the medium.

2.8 Rules for Constructing Diagrams

The following rules should obey

- Draw the Feynman diagram for the self-energy term, with all phonon, Coulomb and electron lines.
- For each electron line, introduce the following Green's function

$$G_{\alpha\beta}^0(\mathbf{p}, E) = \frac{\delta_{\alpha\beta}}{E - \varepsilon_{\mathbf{p}} + i\delta_{\mathbf{p}}} \quad (2.54)$$

The $\delta_{\alpha\beta}$ conserves the spin index and indicates that the electron line must have the same spin at both ends of the propagator line.

- For each phonon line, introduce the following phonon propagator

$$D^0(\mathbf{q}, \omega) = \frac{2\omega_{\mathbf{q}}}{\omega^2 - \omega_{\mathbf{q}}^2 + i\delta} \quad (2.55)$$

Also add a factor of $|M_{\mathbf{q}}|^2$ for each phonon Green's function, where $M_{\mathbf{q}}$ is the matrix element for the electron-phonon interaction.

- Add Coulomb potential $v_q = 4\pi e^2/q^2$ for each Coulomb interaction. The Coulomb interaction is regarded as happening instantaneously in time.
- Conserve energy and momentum at each vertex.

- Sum over internal degree of freedom: momentum, energy and spin.
- Finally, multiply the result by the factor

$$\frac{i^m}{(2\pi)^{4m}} (-1)^F (2S+1)^F \quad (2.56)$$

where F is the number of closed fermion loops. The index m is chosen as follows:

- For electron self-energy, m is the number of internal phonon and Coulomb lines.
- For phonon self-energy, m is one-half the number of vertices.

The spin of the particle is S , and the factor $(2S+1)$ is from the summation over spin quantum number. The factor $(2\pi)^{4m}$ assumes taking the limit $v \rightarrow \infty$, for box normalization in a finite volume the factor is

$$\frac{i^m}{(2\pi v)^m} (-1)^F (2S+1)^F \quad (2.57)$$

and then the wave vector summations are discrete summations.

For photon Green's function, it is represented by dotted line. Charged particles interact with the photons through two terms in the interaction Hamiltonian. The first is $\mathbf{j} \cdot \mathbf{A}$ term. For free particles, this has the form

$$\frac{e}{c} \sum_i \mathbf{j}(\mathbf{r}_i) \cdot \mathbf{A}(\mathbf{r}_i) = \frac{e}{c} \sum_{\mathbf{q}\mu} j_\mu(\mathbf{q}) A_\mu(\mathbf{q}) = \frac{e}{mc} \sum_{\mathbf{q}\mu} A_\mu(\mathbf{q}) \sum_{\mathbf{k}\sigma} (\mathbf{k} + \frac{1}{2}\mathbf{q})_\mu C_{\mathbf{k}+\mathbf{q},\sigma}^\dagger C_{\mathbf{k},\sigma} \quad (2.58)$$

For this we have the rule

- For each photon line which interacts with particles through the $\mathbf{j} \cdot \mathbf{A}$ interaction, insert a factor

$$\frac{e^2}{m^2} \sum_{\mu\nu} (\mathbf{k} + \frac{1}{2}\mathbf{q})_\mu D_{\mu\nu}(\mathbf{q}, \omega) (\mathbf{k}' + \frac{1}{2}\mathbf{q})_\nu \quad (2.59)$$

where $D_{\mu\nu}$ is the photon Green's function and \mathbf{k} and \mathbf{k}' are the wave vectors of particles scattered at the two vertices.

- The other possible interaction of a charged particle with photons occurs through the terms

$$\frac{e^2}{2mc^2} \sum_i \mathbf{A}(\mathbf{r}_i)^2 = \frac{e^2}{2m} \sum_{\mathbf{k}\mu} \rho(\mathbf{q}) A_\mu(\mathbf{k}) A_\mu(\mathbf{q} - \mathbf{k})$$

latter this interaction can be shown that gives a contribution of self-energy term of $e^2 n_0 / m$ to photon, where n_0 is the density of charged particles.

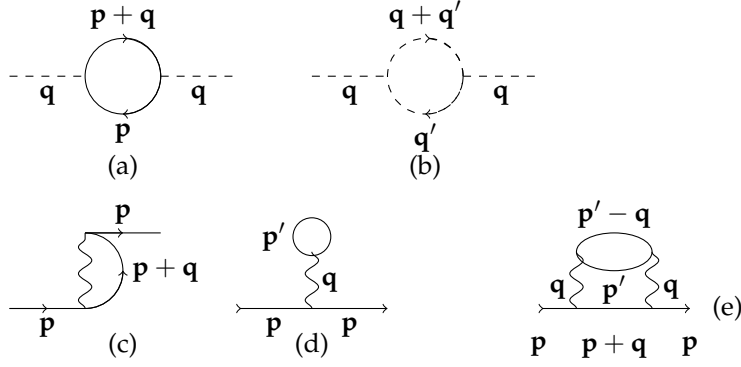


Figure 2.2: Phonon self-energies, (a) is due to electron-phonon interaction, and (b) is from lattice anharmonicity. (c) is **unscreend exchange energy**.

Now examine some example. For the first plot Fig. 2.2(a), we have $F = 1$, $S = \frac{1}{2}$ and $m = 1$, then⁸

$$\Pi(\mathbf{q}, \omega) = |M_{\mathbf{q}}|^2 P^1(\mathbf{q}, \omega) \quad (2.60)$$

$$P^1(\mathbf{q}, \omega) = \frac{i}{(2\pi)^4} (-1)(2) \int dE \int d\mathbf{p} G^0(\mathbf{p}, E) G^0(\mathbf{p} + \mathbf{q}, E + \omega)$$

The other phonon self-energy contribution arises from the lattice anharmonicity, which leads to interaction terms in the ion Hamiltonian proportional to the third power of the phonon displacement:

$$V = \sum_i V_i Q_i^3 = \sum_{\mathbf{q}\mathbf{q}'} M_{\mathbf{q},\mathbf{q}'} \mathbf{A}_{\mathbf{q}} \mathbf{A}_{\mathbf{q}'} \mathbf{A}_{-\mathbf{q}-\mathbf{q}'}$$

In this case, $F = 0$, $m = 1$ and $S = 0$, since phonon have zero spin, we have

$$\Pi^1(\mathbf{q}, \omega) = \frac{i}{(2\pi)^4} \int d\omega' \int d\mathbf{q}' |M_{\mathbf{q},\mathbf{q}'}|^2 D^0(\mathbf{q}', \omega') D^0(\mathbf{q} + \mathbf{q}', \omega + \omega') \quad (2.61)$$

The electron self-energy arising from electron-electron interaction. The self-energy term in Fig. 2.2(c) is called the *unscreend exchange energy* and is a very important contribution to the electron's energy. In this case, $F = 0$, $m = 1$ for one Coulomb line and $S = \frac{1}{2}$, we have

$$\Sigma_x(\mathbf{p}, E) = \frac{i}{(2\pi)^4} (-1)^0 (2)^0 \int d\omega \int d\mathbf{q} v_{\mathbf{q}} G^0(\mathbf{p} + \mathbf{q}, E + \omega) \quad (2.62)$$

There is a very important identity:

$$i \int \frac{d\omega}{2\pi} G^0(\mathbf{p} + \mathbf{q}, E + \omega) = -\eta_F(\xi_{\mathbf{p}+\mathbf{q}}) \quad (2.63)$$

with this we have

$$\Sigma_x(\mathbf{p}) = -\frac{1}{v} \sum_{\mathbf{q}} v_{\mathbf{q}} \eta_F(\xi_{\mathbf{p}+\mathbf{q}}) = - \int \frac{d^3q}{(2\pi)^3} v_{\mathbf{q}} \eta_F(\xi_{\mathbf{p}+\mathbf{q}}) \quad (2.64)$$

where subscript x denotes exchange.

Important identity: By Fourier transformation

$$i \int \frac{d\omega}{2\pi} \int dt e^{it(E+\omega)} G^0(\mathbf{p} + \mathbf{q}, t)$$

with the inverting the interaction order, the frequency integral gives a delta function $\delta(t)$, we then have

$$i \int \frac{d\omega}{2\pi} G^0(\mathbf{p} + \mathbf{q}, E + \omega) = i G^0(\mathbf{p} + \mathbf{q}, t = 0)$$

with different time approach, we have

$$G^0(\mathbf{p} + \mathbf{q}, t \rightarrow 0^+) = -i[1 - \eta_F(\xi_{\mathbf{p}+\mathbf{q}})]$$

$$G^0(\mathbf{p} + \mathbf{q}, t \rightarrow 0^-) = i\eta_F(\xi_{\mathbf{p}+\mathbf{q}})$$

by the definition of Green's function. Here we choose $t = 0^-$.

The next electron self-energy from electron-electron interactions is shown in Fig. 2.2(d). With $F = 1$, $m = 1$ and $S = \frac{1}{2}$:

$$\Sigma_H(\mathbf{p}, E) = -\frac{2i}{(2\pi)^4} \int dE' \int d\mathbf{p}' v_{\mathbf{q}=0} G^0(\mathbf{q}', E') \quad (2.65)$$

where the subscript "H" denotes "Hartree" approximation. This self-energy depends on neither \mathbf{p} nor E . The identity (2.63) can be used again to produce

$$\Sigma_H = 2v_{\mathbf{q}=0} \sum_{\mathbf{p}'} \eta_F(\xi_{\mathbf{p}'}) = v_{\mathbf{q}=0} N_e \quad (2.66)$$

where N_e is the number of electrons. In the limit $q \rightarrow 0$ gives $v_{q=0} \rightarrow \infty$. This term is the unscreened Coulomb energy from one electron interacting with all the other electrons in the system. This potential energy is truly a large number, which becomes infinity in the limit of an infinite system. But there must be an equal amount of positive charge in the system, and the electron interaction with the positive charge yields another large number which cancels the present divergence. *The Hartree energy is defined as the net interaction energy of an electron from both of the negative and positive charge sources.* It is zero in the jellium model of a metal, but is nonzero for actual system composed of ions and conduction electrons.

The third electron self-energy diagram is shown in Fig. 2.2(e). Its evaluation yields

$$\Sigma(\mathbf{p}, E) = \frac{1}{(2\pi)^4} \int d\omega \int d\mathbf{q} v_{\mathbf{q}}^2 P^1(\mathbf{q}, \omega) G^0(\mathbf{p} + \mathbf{q}, E + \omega) \quad (2.67)$$

2.9 Time-loop S Matrix

The S matrix is defined in Sec. 2.2. As time in (2.25) is taken over the whole interval. The state at $t = -\infty$ is well defined as the ground state of the noninteracting system ϕ_0 . The interaction are turned on slowly. At $t \approx 0$ the fully interacting ground state is $\psi(0) = S(0, -\infty)\phi_0$. In condensed matter physics the state at $t \rightarrow \infty$ must be defined carefully. One can require that the interactions turn off at large times, which returns the system to the ground state.

Schwinger suggested another method of handling the asymptotic limit $t \rightarrow \infty$. He proposed that the time integral in the S matrix has two pieces: one goes from $(-\infty, \tau)$ while the second goes from $(\tau, -\infty)$ and let $\tau \rightarrow \infty$. The integration path is a time loop. The advantage of this method is that one starts and ends the S matrix expansion with a known state ϕ_0 .

Considering the time-loop expansion for the S Matrix

$$S(-\infty, -\infty) = T_s \exp \left[-i \int_{loop} ds_1 \hat{V}(s_1) \right] \quad (2.68)$$

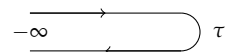


Figure 2.3: The time-loop integration path in the S matrix.

The integration path is the time loop in Fig. 2.3. The variable s_1 goes $(-\infty, \tau)$ and then $(\tau, -\infty)$. The operator T_s orders along the entire loop, with earliest value of s_1 occurring first. In expanding the S matrix, Green's functions are encountered of the form

$$G(\lambda, s_1 - s_2) = -i \langle \phi_0 | T_s C_\lambda(s_1) C_\lambda^\dagger(s_2) | \phi_0 \rangle \quad (2.69)$$

where s_1 and s_2 can be in different place of Fig. 2.3.

2.9.1 Six Green's Functions

For the time-loop expansion, it is necessary to define six different Green's function even though they are not independent. The six functions are

$$\begin{aligned} G^>(x_1, x_2) &= -i \langle \psi(x_1) \psi^\dagger(x_2) \rangle \\ G^<(x_1, x_2) &= i \langle \psi^\dagger(x_2) \psi(x_1) \rangle \\ G_t(x_1, x_2) &= \Theta(t_1 - t_2) G^>(x_1, x_2) + \Theta(t_2 - t_1) G^<(x_1, x_2) \\ G_{\bar{t}}(x_1, x_2) &= \Theta(t_2 - t_1) G^>(x_1, x_2) + \Theta(t_1 - t_2) G^<(x_1, x_2) \\ G_{ret}(x_1, x_2) &= G_t - G^< = G^> - G_{\bar{t}} \\ G_{adv}(x_1, x_2) &= G_{\bar{t}} - G^> = G^< - G_t \end{aligned} \quad (2.70)$$

For homogeneous systems in equilibrium, Green's function depend only upon the difference of the arguments. Then the important quantities are the Fourier transforms

$$G(\mathbf{k}, E) = \int d\mathbf{r} e^{-i\mathbf{k} \cdot \mathbf{r}} \int dt e^{-iEt} G(\mathbf{r}, t) \quad (2.71)$$

where G represents any of the six functions.

Often the Hamiltonian H can be solved exactly in terms of eigenfunctions $\phi_\lambda(\mathbf{r})$ and eigenvalues ε_λ . Two example are the electron in a magnetic field or a free particle. It is useful to have the expressions for the Green's function in terms of these eigenfunctions. They are derived by expanding the field operators in terms of eigenfunctions and creation and destruction operators⁹:

⁹ where we have $x_1 = (\mathbf{r}_1, t)$

$$\begin{aligned} \phi(x_1) &= \sum_\lambda C_\lambda \phi_\lambda(\mathbf{r}_1) e^{-i\varepsilon_\lambda t} \\ \phi^\dagger(x_1) &= \sum_\lambda C_\lambda^\dagger \phi_\lambda^*(\mathbf{r}_1) e^{i\varepsilon_\lambda t} \end{aligned} \quad (2.72)$$

Then the Green's function in (2.70) are evaluated with the occupation

faction $\eta_\lambda = \langle C_\lambda^\dagger C_\lambda \rangle$ and $t = t_1 - t_2$, we have

$$\begin{aligned}
G^>(x_1, x_2) &= -i \sum_\lambda (1 - \eta_\lambda) \phi_\lambda(\mathbf{r}_1) \phi_\lambda^*(\mathbf{r}_2) e^{-i\varepsilon_\lambda t} \\
G^<(x_1, x_2) &= i \sum_\lambda \eta_\lambda \phi_\lambda(\mathbf{r}_1) \phi_\lambda^*(\mathbf{r}_2) e^{-i\varepsilon_\lambda t} \\
G_t(x_1, x_2) &= -i \sum_\lambda [\Theta(t) - \eta_\lambda] \phi_\lambda(\mathbf{r}_1) \phi_\lambda^*(\mathbf{r}_2) e^{-i\varepsilon_\lambda t} \\
G_{\bar{t}}(x_1, x_2) &= -i \sum_\lambda [\Theta(-t) - \eta_\lambda] \phi_\lambda(\mathbf{r}_1) \phi_\lambda^*(\mathbf{r}_2) e^{-i\varepsilon_\lambda t} \\
G_{ret}(x_1, x_2) &= -i \Theta(t) \sum_\lambda \phi_\lambda(\mathbf{r}_1) \phi_\lambda^*(\mathbf{r}_2) e^{-i\varepsilon_\lambda t} \\
G_{adv}(x_1, x_2) &= i \Theta(-t) \sum_\lambda \phi_\lambda(\mathbf{r}_1) \phi_\lambda^*(\mathbf{r}_2) e^{-i\varepsilon_\lambda t} \tag{2.73}
\end{aligned}$$

at zero temperature $\eta_\lambda = \Theta(-\xi_\lambda)$ is the step function depending upon $\xi_\lambda = \varepsilon_\lambda - \mu$. However these formulas are also valid in equilibrium at nonzero temperature.

The starting point for any calculation, is the behavior of the Green's functions for system without interaction. Then the quantum number λ becomes the wave vector \mathbf{k} and spin index σ . The eigenvalue combination is $\phi_\lambda(\mathbf{r}_1) \phi_\lambda^*(\mathbf{r}_2) = \exp[i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}_2)]/v$. In noninteracting system in equilibrium, for (2.71), with Fourier transformation give the free-particle Green's functions

$$\begin{aligned}
G_0^>(\mathbf{k}, t) &= -i[1 - \eta_{\mathbf{k}}] e^{i\varepsilon_{\mathbf{k}} t} \\
G_0^<(\mathbf{k}, t) &= i\eta_{\mathbf{k}} e^{-i\varepsilon_{\mathbf{k}} t} \\
G_t^0(\mathbf{k}, t) &= -i[\Theta(t) - \eta_{\mathbf{k}}] e^{-i\varepsilon_{\mathbf{k}} t} \\
G_{\bar{t}}^0(\mathbf{k}, t) &= -i[\Theta(-t) - \eta_{\mathbf{k}}] e^{-i\varepsilon_{\mathbf{k}} t} \\
G_{ret}^0(\mathbf{k}, t) &= -i\Theta(t) e^{-i\varepsilon_{\mathbf{k}} t} \\
G_{adv}^0(\mathbf{k}, t) &= i\Theta(-t) e^{-i\varepsilon_{\mathbf{k}} t} \tag{2.74}
\end{aligned}$$

with Fourier transformation and $i\delta$ infinitesimal quantity

$$\begin{aligned}
G_0^>(\mathbf{k}, E) &= -2\pi i[1 - \eta_{\mathbf{k}}] \delta(E - \varepsilon_{\mathbf{k}}) \\
G_0^<(\mathbf{k}, E) &= 2\pi i\eta_{\mathbf{k}} \delta(E - \varepsilon_{\mathbf{k}}) \\
G_{ret}^0(\mathbf{k}, E) &= \frac{1}{E - \varepsilon_{\mathbf{k}} + i\delta} \\
G_{adv}^0(\mathbf{k}, E) &= \frac{1}{E - \varepsilon_{\mathbf{k}} - i\delta} \\
G_t^0(\mathbf{k}, E) &= G_{ret}^0 + G_0^< = \frac{1}{E - \varepsilon_{\mathbf{k}} + i\delta_{\mathbf{k}}} \\
G_{\bar{t}}^0(\mathbf{k}, E) &= G_0^< - G_{adv}^0 = \frac{-1}{E - \varepsilon_{\mathbf{k}} - i\delta_{\mathbf{k}}} \tag{2.75}
\end{aligned}$$

The time-order function G_t^0 is exactly the same on in (2.40). Note the two kinds of infinitesimal delta, where $\delta_{\mathbf{k}} \equiv \delta \text{sign}(\mathbf{k} - \mathbf{k}_F)$.

The above Green's functions are suitable for particles such as electrons or holes in semiconductors. Another type of Green's function is needed for boson fields such as photons and phonons. For phonons let $Q(x)$ be the displacement from equilibrium of the ions in the solid at position $x = (\mathbf{r}, t)$ in spacetime. The phonon Green's functions are defined as

$$\begin{aligned}
 D^>(x_1, x_2) &= -i\langle Q(x_1)Q(x_2) \rangle \\
 D^<(x_1, x_2) &= -i\langle Q(x_2)Q(x_1) \rangle \\
 D_t(x_1, x_2) &= \Theta(t_1 - t_2)D^>(x_1, x_2) + \Theta(t_2 - t_1)D^<(x_1, x_2) \\
 D_{\bar{t}}(x_1, x_2) &= \Theta(t_2 - t_1)D^>(x_1, x_2) + \Theta(t_1 - t_2)D^<(x_1, x_2) \\
 D_{ret} &= D_t - D^< = \Theta(t_1 - t_2)[D^> - D^<] \\
 D_{adv} &= D_t - D^> = -\Theta(t_2 - t_1)[D^> - D^<] \quad (2.76)
 \end{aligned}$$

These expressions are rather similar to those in (2.70) for particles. The main difference is that $D^<$ and $D^>$ have the same sign, since no change is made when interchanging the positions of boson operators. Also the displacement operator is Hermitian, $Q^\dagger = Q$, which introduces some redundancy such as $D^<(x_1, x_2) = D^>(x_2, x_1)$.

The displacement operators Q are usually represented in terms of phonon raising and lowering operators. Usually, we have $A_{\mathbf{q}} = a_{-\mathbf{q}}^\dagger + a_{\mathbf{q}}$ in the definition of the phonon Green's function. In this representation, the phonon Green's functions in equilibrium are expressed in terms of the phonon occupation number $N_{\mathbf{q}} = \langle a_{\mathbf{q}}^\dagger a_{\mathbf{q}} \rangle$. The noninteracting results are

$$\begin{aligned}
 D^>(\mathbf{q}, t) &= -i[(N_{\mathbf{q}} + 1)e^{-i\omega_{\mathbf{q}}t} + N_{\mathbf{q}}e^{i\omega_{\mathbf{q}}t}] \\
 D^<(\mathbf{q}, t) &= -i[(N_{\mathbf{q}} + 1)e^{i\omega_{\mathbf{q}}t} + N_{\mathbf{q}}e^{-i\omega_{\mathbf{q}}t}] \\
 D_{ret}(\mathbf{q}, t) &= -2\Theta(t) \sin(\omega_{\mathbf{q}}t) \\
 D_{adv}(\mathbf{q}, t) &= -2\Theta(-t) \sin(\omega_{\mathbf{q}}t) \quad (2.77) \\
 D_t(\mathbf{q}, t) &= -i\{(N_{\mathbf{q}} + \Theta(-t))e^{i\omega_{\mathbf{q}}t} + [N_{\mathbf{q}} + \Theta(t)]e^{-i\omega_{\mathbf{q}}t}\} \\
 D_{\bar{t}}(\mathbf{q}, t) &= -i\{(N_{\mathbf{q}} + \Theta(t))e^{i\omega_{\mathbf{q}}t} + [N_{\mathbf{q}} + \Theta(-t)]e^{-i\omega_{\mathbf{q}}t}\}
 \end{aligned}$$

2.9.2 Dyson's Equation

Each of the six Green's functions can be evaluated for an interacting system in terms of the S matrix in (2.68).

The potential V is composed of electron, phonon, or photon operators. The operators are paired using Wick's theorem. Each pair will have a time argument such as $G(s_i, s_j)$. If both s_i and s_j are in the top loop, the expression is just the time-ordered Green's function. If they are both in the return loop, the expression is the anti-time-ordered Green's function. If one s is on the top and other is in the bottom,

then T_s operator makes the expression be either $G^<$ or else $G^>$. These relationships are shown in Fig. 2.4. The n th term in the Green's function expansion is a product of $(n + 1)$ factors, where each factor is on the the four Green's functions in Fig. 2.4.

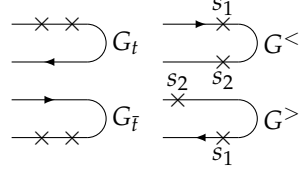


Figure 2.4: The four Green's function $G(s_1, s_2)$ depend on whether the time variable are on the outgoing or return parts of the time loop.

Considering an example. Below is given a potential term V of the type found for *electrons scattering from impurities*. The first term in the S -matrix expansion for $G^<$ with this interaction is

$$\begin{aligned} V &= \sum_{\alpha\beta} M_{\alpha\beta} C_{\alpha}^{\dagger} C_{\beta} \\ G^<(\lambda, t_1 - t_2) &= G_0^<(\lambda, t_1 - t_2) \\ &+ \sum_{\alpha\beta} M_{\alpha\beta} \int ds \langle \phi_0 | TC_{\lambda}^{\dagger}(t_2) C_{\beta}(s) | \phi_0 \rangle \langle \phi_0 | TC_{\alpha}^{\dagger}(s) C_{\lambda}(t_1) | \phi_0 \rangle \end{aligned} \quad (2.78)$$

The s integral runs over the time loop. For $G^<$ there are two possibilities, where s is on the top or below of the loop.

$$G^<(\lambda, t_1 - t_2) = G_0^<(\lambda, t_1 - t_2) + M_{\lambda\lambda} \int_{-\infty}^{\infty} ds [G_t^0(\lambda, t_1 - s) G_0^<(\lambda, s - t_2) - G_0^<(\lambda, t_1 - s) G_t^0(s - t_2)] \quad (2.79)$$

A sign change occurred in the last term when the direction of the time integration was changed from $(\infty, -\infty)$ to $(-\infty, \infty)$.

In the expansion of the S matrix, each time integral produces one set of terms for the outward s leg, and another for the return leg. The n th term in the S -matrix expansion produce 2^n arrangements. All of there terms can be managed by using a matrix formulation

$$G = \begin{bmatrix} G_t & -G^< \\ G^> & -G_{\bar{t}} \end{bmatrix} \quad \Sigma = \begin{bmatrix} \Sigma_t & -\Sigma^< \\ \Sigma^> & -\Sigma_{\bar{t}} \end{bmatrix} \quad (2.80)$$

For systems either in equilibrium or non-equilibrium, Dyson's equation is most easily expressed by using the matrix notation

$$\begin{aligned} G(x_1, x_2) &= G_0(x_1 - x_2) + \int_{-\infty}^{\infty} dx_3 \int_{-\infty}^{\infty} dx_4 G_0(x_1 - x_3) \\ &\times \Sigma(x_3, x_4) G(x_4, x_2) \end{aligned} \quad (2.81)$$

The matrix formulation comes directly from the time loop. Each s integral in the S matrix has an outward and return leg. Each of these legs gives a different Green's function. So each time integral generates two Green's function.

With a simple notation where the product of two functions implies an integration over the four variable dx , which condenses the Equation

$$G = G_0 + G_0 \Sigma G \quad (2.82)$$

Then the equation are iterated. The following exact expressions are:

$$\begin{aligned} G_{ret} &= G_{ret}^0 [1 + \Sigma_{ret} G_{ret}] \\ G_{adv} &= G_{adv}^0 [1 + \Sigma_{adv} G_{adv}] \\ G^> &= [1 + G_{ret} \Sigma_{ret}] G_0^> [1 + \Sigma_{adv} G_{adv}] + G_{ret} \Sigma^> G_{adv} \\ G^< &= [1 + G_{ret} \Sigma_{ret}] G_0^< [1 + \Sigma_{adv} G_{adv}] + G_{ret} \Sigma^< G_{adv} \\ G_t &= [1 + G_{ret} \Sigma_{ret}] G_t^0 [1 + \Sigma_{adv} G_{adv}] + G_{ret} \Sigma_t G_{adv} \\ G_{\bar{t}} &= [1 + G_{ret} \Sigma_{ret}] G_{\bar{t}}^0 [1 + \Sigma_{adv} G_{adv}] + G_{ret} \Sigma_{\bar{t}} G_{adv} \end{aligned} \quad (2.83)$$

With the Fourier transformation, and the spectral function, $A(\mathbf{k}, \omega) = -2ImG_{ret}(\mathbf{k}, \omega)$,

$$\begin{aligned} G_{ret}(k, \omega) &= \frac{1}{\omega - \varepsilon_k - \Sigma_{ret}}, \quad \sigma = \omega - \varepsilon_k - Re[\Sigma_{ret}] \\ G_{adv}(k, \omega) &= \frac{1}{\omega - \varepsilon_k - \Sigma_{adv}}, \quad \Sigma_{adv} = \Sigma_{ret}^* \\ A(k, \omega) &= -2Im[G_{ret}(k, \omega)] = \frac{2\Gamma}{\sigma^2 + \Gamma^2}, \quad \Gamma = -Im[\Sigma_{ret}] > 0 \\ \Sigma^< &= 2i\eta_F(\omega)\Gamma(k, \omega), \quad G^< = i\eta_F(\omega)A(k, \omega) \\ \Sigma^> &= -2i(1 - \eta_F)\Gamma, \quad G^> = -i(1 - \eta_F)A \end{aligned} \quad (2.84)$$

More will discussed in next chapter.

2.10 Photon Green's Functions

Considering the interaction of charges with themselves and with the photon field. The interaction Hamiltonian for spinless particles in the non-relativistic limit

$$H = \sum_i \frac{1}{2m} [\mathbf{p}_i - \frac{e}{c} \mathbf{A}(\mathbf{r}_i)]^2 + \frac{1}{2} \sum_{i \neq j} \frac{e_i e_j}{r_{ij}} + \sum_{\mathbf{k}\lambda} \omega_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda}^\dagger a_{\mathbf{k}\lambda} \quad (2.85)$$

With the vector potential is given by expansion

$$\frac{1}{c} A_\mu = \frac{1}{\sqrt{v}} \sum_{\mathbf{k}\lambda} e^{i\mathbf{k} \cdot \mathbf{r}} A_\mu(\mathbf{k}, \lambda, t) \quad (2.86)$$

$$A_\mu(\mathbf{k}, \lambda, t) = \left(\frac{2\pi}{\omega_{\mathbf{k}}}\right)^{\frac{1}{2}} \xi_\mu(\mathbf{k}, \lambda) (a_{\mathbf{k}\lambda} e^{-i\omega_{\mathbf{k}} t} + a_{-\mathbf{k}\lambda}^\dagger e^{i\omega_{\mathbf{k}} t}) \quad (2.87)$$

where \mathbf{k} is the wave vector and λ is the polarization and μ is x, y and z component. The operator $a_{\mathbf{k}\lambda}$ obey boson statistics. And Each state with \mathbf{k} and λ has its own harmonic oscillator statistics. The vector

potential represents the photon field. Two charges may interact via their common photon field or more directly through the instantaneous Coulomb interaction. **The division of the interaction between photons and Coulomb field is arbitrary— both interactions come from the same basic process.** The Hamiltonian (2.85) is written in the Coulomb gauge, $\nabla \cdot \mathbf{A} = 0$. Another choice of gauge will result in a different division between photon and Coulomb, The basic force between the particles are the same regardless of how the gauge is selected.

In terms of Green's function, for electron-electron interaction,

$$v_q = \frac{4\pi e^2}{q^2} \quad (2.88)$$

is in fact just the Green's function of the longitudinal potential. It has no frequency dependence because it is instantaneous.

Since v_q is a Green's function, it has a Dyson equation

$$v_q(\omega) = \frac{v_q}{1 - v_q P(\mathbf{q}, \omega)} \quad (2.89)$$

The factor $P(\mathbf{q}, \omega)$ is the **self-energy or polarization operator**. Consider the Maxwell's equations in a homogeneous material with an isotropic dielectric constant ϵ

$$\begin{aligned} \nabla \cdot \mathbf{B} &= 0 \\ \nabla \times \mathbf{E} &= 0 \\ \nabla \cdot \mathbf{E} &= \frac{4\pi\rho}{\epsilon} \\ \nabla \times \mathbf{B} &= \frac{\epsilon}{c} \partial_t \mathbf{E} + \frac{4\pi}{c} \mathbf{j} \end{aligned} \quad (2.90)$$

For the scalar and vector potentials

$$\begin{aligned} \psi(\mathbf{r}) &= \frac{1}{\epsilon} \int \frac{d^3\mathbf{r}' \rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \\ \nabla^2 \mathbf{A} - \frac{\epsilon}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{A} &= -\frac{4\pi}{c} \mathbf{j}_t \end{aligned} \quad (2.91)$$

Here the Coulomb Green's function is

$$\bar{v}_q = \frac{v_q}{\epsilon} \quad (2.92)$$

Regarding (2.89), it gives a formula for the dielectric function

$$\epsilon(\mathbf{q}, \omega) = 1 - v_q \mathbf{P}(\mathbf{q}, \omega) \quad (2.93)$$

This equation will serve as the definition of the longitudinal dielectric function. It arises from the self-energy parts of the Coulomb potential. The Green's function for the vector potential is

$$D_{\mu\nu}(\mathbf{k}, t - t') = -i \sum_{\lambda} \langle T A_{\mu}(\mathbf{k}, \lambda, t) A_{\nu}(-\mathbf{k}, \lambda, t') \rangle \quad (2.94)$$

Not quite understand here. Since, usually $\nabla \times \mathbf{E} = -\frac{1}{c} \partial_t \mathbf{B}$. For vacuum electromagnetic wave

$$\begin{aligned} \nabla \cdot \mathbf{E} &= 0 \\ \nabla \cdot \mathbf{B} &= 0 \\ \nabla \times \mathbf{E} &= -\partial_t \mathbf{B} \\ \nabla \times \mathbf{B} &= \mu_0 \epsilon_0 \partial_t \mathbf{E} \end{aligned}$$

where μ, ν are the x, y, z components, with vector potential in (2.87); the sum λ is the sum over the two transverse polarizations of the light, while ξ_μ are the polarization vectors for each component. At zero temperature,

$$D_{\mu\nu}^0(\mathbf{k}, t - t') = -\frac{2\pi i}{\omega_{\mathbf{k}}} e^{i\omega_{\mathbf{k}}|t-t'|} \sum_{\lambda} \xi_{\mu} \xi_{\nu} \quad (2.95)$$

and with Fourier transform is

$$D^0(\mathbf{k}, \omega) = \frac{4\pi}{\omega^2 - \omega_{\mathbf{k}}^2 + i\delta} \sum_{\lambda} \xi_{\mu} \xi_{\nu} = \frac{4\pi[\delta_{\mu\nu} - (k_{\mu}k_{\nu}/k^2)]}{\omega^2 - \omega_{\mathbf{k}}^2 + i\delta} \quad (2.96)$$

This expression is referred to as the **photon Green's function**. Keep in mind that the interaction between two charges occurs via both the scalar and vector potentials. How the interaction is divided between scalar and vector potentials is somewhat arbitrary and is determined by the gauge condition. After making this choice, the word "photon" is assigned to the vector potential part. This division between photon and Coulomb is arbitrary, and both parts should really be viewed as arising from photons.

The photon Green's function also obeys a Dyson equation.

$$D_{\mu\nu} = D_{\mu\nu}^0 + \sum_{\lambda\delta} D_{\mu\lambda}^0 \pi_{\lambda\delta} D_{\delta\nu} \quad (2.97)$$

where $\pi_{\lambda\delta}(\mathbf{k}, \omega)$ is the self-energy function, which is 3×3 matrix.

3

Nonzero Temperatures

3.1 Introduction

At nonzero temperature, whether electron, phonon, or spin, is interacting with a bath of other particles which have an average energy. The exact state of all these other particles is not known, since they are fluctuating between different configurations. All that is known is the temperature, which is related to the mean energy.

When defining the Green's function, one must average over all possible configurations of the system. A possible Green's function for electron is

$$\frac{\text{Tr} \left[e^{-\beta H} C_{\mathbf{p}\sigma}(t) C_{\mathbf{p}\sigma}^\dagger(t') \right]}{\text{Tr}(e^{-\beta H})} \quad (3.1)$$

$$C_{\mathbf{p}\sigma}(t) = e^{itH} C_{\mathbf{p}\sigma} e^{-itH} \quad (3.2)$$

where Tr denotes trace and is summation over some complete set of states.

The Matsubara method treats time as a complex temperature, the object is treat t and β as the real and imaginary parts of a complex variable, which will require only one S -matrix expansion.

The expansion of the series for bosons and fermions give

$$\eta_F(\xi_{\mathbf{p}}) = \frac{1}{e^{\beta \xi_{\mathbf{p}}} + 1} = \frac{1}{2} + \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \frac{1}{(2n+1)i\pi/\beta - \xi_{\mathbf{p}}} \quad (3.3)$$

$$\eta_B(\omega_{\mathbf{q}}) = \frac{1}{e^{\beta \omega_{\mathbf{q}}} - 1} = -\frac{1}{2} + \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \frac{1}{2ni\pi/\beta - \omega_{\mathbf{q}}} \quad (3.4)$$

These series can be derived from a theorem which states that any meromorphic function may be expanded as a summation over its poles and residues at those poles.¹ It is convenient to define the frequencies at the pole

$$p_n = (2n+1)\pi/\beta, \quad \omega_n = 2n\pi/\beta \quad (3.5)$$

In Matsubara method, time becomes a complex quantity which is usually called τ , where $\tau = it$. Green's functions are function of τ

Important knowledge, the expansion

$$\begin{aligned} & \frac{1}{e^x - 1} \\ = & \frac{1}{1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots - 1} \\ = & \frac{1}{x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots} \\ = & \frac{1}{x(1 + \frac{x}{2!} + \frac{x^2}{3!} + \dots)} \\ \approx & \frac{1}{x(1 + \frac{x}{2})} \\ \approx & \frac{1}{x} \left(1 - \frac{x}{2}\right) = \frac{1}{x} - \frac{1}{2} \end{aligned}$$

¹ Need to be more clear about this.

with domain

$$-\beta \leq \tau \leq \beta \quad (3.6)$$

Fourier transform theory states that if a function $f(\tau)$ is defined over such a range, then its Fourier expansion is

$$f(\tau) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} \left[a_n \cos\left(\frac{n\pi\tau}{\beta}\right) + b_n \sin\left(\frac{n\pi\tau}{\beta}\right) \right] \quad (3.7)$$

where

$$a_n = \frac{1}{\beta} \int_{-\beta}^{\beta} d\tau f(\tau) \cos\left(\frac{n\pi\tau}{\beta}\right) \quad (3.8)$$

$$b_n = \frac{1}{\beta} \int_{-\beta}^{\beta} d\tau f(\tau) \sin\left(\frac{n\pi\tau}{\beta}\right) \quad (3.9)$$

or **equivalently**. We have

$$f(i\omega_n) = \frac{1}{2}\beta(a_n + ib_n) \quad (3.10)$$

with

$$f(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-in\pi\tau/\beta} f(i\omega_n) \quad (3.11)$$

$$f(i\omega_n) = \frac{1}{2} \int_{-\beta}^{\beta} d\tau f(\tau) e^{in\pi\tau/\beta} \quad (3.12)$$

3.1.1 Boson

There is still a further simplification can be achieved. For boson Green's functions have the additional property that

$$\text{boson : } f(\tau) = f(\tau + \beta), \quad -\beta < \tau < 0 \quad (3.13)$$

Further we have

$$\begin{aligned} f(i\omega_n) &= \int_0^{\beta} d\tau e^{i\omega_n\tau} f(\tau) \\ f(\tau) &= \frac{1}{\beta} \sum_n e^{-i\omega_n\tau} f(i\omega_n) \\ \omega_n &= 2n\pi k_B T \end{aligned} \quad (3.14)$$

3.1.2 Fermion

Similarly, the fermion Green's function will have the property that

$$\text{fermions : } f(\tau) = -f(\tau + \beta), \quad -\beta < \tau < 0 \quad (3.15)$$

and the result give

$$\begin{aligned} f(i\omega_n) &= \int_0^{\beta} d\tau e^{i\omega_n\tau} f(\tau) \\ f(\tau) &= \frac{1}{\beta} \sum_n e^{-i\omega_n\tau} f(i\omega_n) \quad (3.16) \\ \omega_n &= (2n+1)\pi k_B T \end{aligned}$$

3.2 Matsubara Green's functions

The electron Green's function is defined as

$$\mathcal{G}(\mathbf{p}, \tau - \tau') = -\langle T_\tau C_{\mathbf{p}\sigma}(\tau) C_{\mathbf{p}\sigma}^\dagger(\tau') \rangle \quad (3.17)$$

$$\begin{aligned} \mathcal{G}(\mathbf{p}, \tau - \tau') &= -\text{Tr} \left[e^{-\beta(H - \mu N - \Omega)} T_\tau e^{\tau(H - \mu N)} C_{\mathbf{p}\sigma} e^{-(\tau - \tau')(H - \mu N)} \right. \\ &\quad \left. \times C_{\mathbf{p}\sigma}^\dagger e^{-\tau'(H - \mu N)} \right] \end{aligned} \quad (3.18)$$

$$e^{-\beta\Omega} = \text{Tr} \left(e^{-\beta(H - \mu N)} \right) \quad (3.19)$$

The definition is equivalent between (3.17) and (3.18), and it is the thermodynamic average, which is the trace over the complete set of states. The μ is the chemical potential and N is the particle number operator. A grand canonical ensemble is used, where the number of particles is variable. This many-particle system can be successfully used for one particle in an empty band. In this case, the analytical continuation is taken as $i\omega_n \rightarrow E + \mu + i\delta$, and the chemical potential will vanish from all expressions. One is not bothered by the fact that $\beta\mu \ll 0$ in one-particle systems at nonzero temperatures.

In a many-electron system, the chemical potential is retained in the formalism. The analytical continuation is $i\omega_n \rightarrow E + i\delta$ and energy is measured from the chemical potential.

With some derivation², we have the Green's functions

² P.112 P.114

$$\mathcal{G}(\mathbf{p}, \tau) = -\langle T_\tau C_{\mathbf{p}\sigma}(\tau) C_{\mathbf{p}\sigma}^\dagger(0) \rangle \quad (3.20)$$

$$= -\text{Tr} \left[e^{-\beta(K - \Omega)} T_\tau (e^{\tau K} C_{\mathbf{p}\sigma} e^{-\tau K} C_{\mathbf{p}\sigma}^\dagger) \right] \quad (3.21)$$

$$\mathcal{G}(\mathbf{p}, i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} \mathcal{G}(\mathbf{p}, \tau) \quad (3.22)$$

$$\mathcal{G}(\mathbf{p}, \tau) = \frac{1}{\beta} \sum_n e^{-i\omega_n \tau} \mathcal{G}(\mathbf{p}, i\omega_n) \quad (3.23)$$

For noninteracting Green's function, the τ evolution of the operators is³

$$C_{\mathbf{p}\sigma}(\tau) = e^{\tau K_0} C_{\mathbf{p}\sigma} e^{-\tau K_0} = e^{-\xi_{\mathbf{p}} \tau} C_{\mathbf{p}\sigma} \quad (3.24)$$

$$C_{\mathbf{p}\sigma}^\dagger(\tau) = e^{\tau K_0} C_{\mathbf{p}\sigma}^\dagger e^{-\tau K_0} = e^{\xi_{\mathbf{p}} \tau} C_{\mathbf{p}\sigma}^\dagger \quad (3.25)$$

³ Derived from the Baker-Hausdorff theorem

$$e^A C e^{-A} = C + [A, C] + \frac{1}{2!} [A, [A, C]] + \dots$$

Then the Green's function is

$$\mathcal{G}^0(\mathbf{p}, \tau) = -e^{-\xi_{\mathbf{p}} \tau} [\Theta(\tau) - \eta_F(\xi_{\mathbf{p}})] \quad (3.26)$$

and

$$\mathcal{G}^0(\mathbf{p}, i\omega_n) = \frac{1}{i\omega_n - \xi_{\mathbf{p}}} \quad (3.27)$$

The phonon and photon Green's functions are defined in the same fashion,

$$\mathcal{D}(\mathbf{q}, \tau - \tau') = -\langle T_\tau \mathbf{A}(\mathbf{q}, \tau) \mathbf{A}(-\mathbf{q}, \tau') \rangle \quad (3.28)$$

$$\mathbf{A}(\mathbf{q}, \tau) = e^{\tau H} (a_{\mathbf{q}} + a_{-\mathbf{q}}^\dagger) e^{-\tau H} \quad (3.29)$$

and with the relation in (3.13), we have

$$\mathcal{D}(\mathbf{q}, \tau) = \mathcal{D}(\mathbf{q}, \tau + \beta) \quad -\beta < \tau < 0 \quad (3.30)$$

For noninteracting system the Green's function of **phonons** is

$$\mathcal{D}^0(\mathbf{q}, i\omega_n) = -\frac{2\omega_{\mathbf{q}}}{\omega_n^2 + \omega_{\mathbf{q}}^2} \quad (3.31)$$

Notice that it is almost identical to the zero-temperature case (2.45).

The **photon** Green's function is also identical to its zero-temperature result, except for complex frequencies. The fundamental definition is

$$\mathcal{D}_{\mu\nu}(\mathbf{k}, \tau) = -\sum_{\lambda} \langle T_{\tau} \mathbf{A}_{\mu}(\mathbf{k}, \lambda, \tau) \mathbf{A}_{\nu}(-\mathbf{k}, \lambda, 0) \rangle \quad (3.32)$$

$$\mathbf{A}_{\mu}(\mathbf{k}, \lambda, 0) = \xi_{\mu}(\mathbf{k}, \lambda) \left(\frac{2\pi}{\omega_{\mathbf{k}}} \right) (a_{\mathbf{k}\lambda} + a_{\mathbf{k}\lambda}^{\dagger}) \quad (3.33)$$

$$\mathcal{D}_{\mu\nu}^0(\mathbf{k}, i\omega_n) = -\frac{4\pi(\delta_{\mu\nu} - k_{\mu}k_{\nu}/k^2)}{\omega_n^2 + \omega_{\mathbf{k}}^2} \quad (3.34)$$

3.3 Retarded and advance Green's functions

The retarded and advanced Green's functions were introduced in 2.9. All measurable quantities, such as conductivities or susceptibilities, are actually retarded correlation functions. The Green's function by Matsubara function can be easily convert to retarded and advanced Green's function.

The retarded Green's functions may be defined for both zero and nonzero temperature. The retarded Green's function for an electron in state \mathbf{p} is

$$\begin{aligned} G_{ret}(\mathbf{p}, t - t') &= G_t(\mathbf{p}, t - t') - G^<(\mathbf{p}, t - t') \\ &= -i\Theta(t - t') \langle [C_{\mathbf{p}\sigma}(t) C_{\mathbf{p}\sigma}^{\dagger}(t') + C_{\mathbf{p}\sigma}^{\dagger}(t') C_{\mathbf{p}\sigma}(t)] \rangle \end{aligned} \quad (3.35)$$

$$\begin{aligned} &= -i\Theta(t - t') \text{Tr} \{ e^{-\beta(K - \Omega)} [C_{\mathbf{p}\sigma}(t) C_{\mathbf{p}\sigma}^{\dagger}(t') + C_{\mathbf{p}\sigma}^{\dagger}(t') C_{\mathbf{p}\sigma}(t)] \} \\ K &= H - \mu N, \quad C_{\mathbf{p}\sigma}(t) = e^{iKt} C_{\mathbf{p}\sigma} e^{-iKt} \end{aligned} \quad (3.36)$$

The Green's function operates only for $t > t'$, which makes it **causal**. In the limit that times becomes equal, the anticommutator becomes unity. The plus sign in the middle of the two terms is an important feature for retarded Green's functions of fermion operators.

For phonons, the retarded Green's function is

$$D_{ret}(\mathbf{q}, t - t') = -i\Theta(t - t') \langle A(\mathbf{q}, t) A(-\mathbf{q}, t') - A(-\mathbf{q}, t') A(\mathbf{q}, t) \rangle \quad (3.37)$$

The sign in the middle is minus, which corresponding the bosons' commutation relations.

Retarded Green's functions are needed for many types of operators with products of electron or boson operators.

$$U = \sum_{ij} M_{ij} C_i^\dagger C_j \quad (3.38)$$

$$V = \sum_{ijk} M_{ijk} C_i^\dagger C_j C_k \quad (3.39)$$

The operator U is bilinear in operator C_i , this can be regarded as having boson properties. However, operator V can be regarded as fermion operators.

$$\bar{U}_{ret}(t-t') = -i\Theta(t-t') \langle [U(t)U^\dagger(t') - U^\dagger(t')U(t)] \rangle \quad (3.40)$$

$$\bar{V}_{ret}(t-t') = -i\Theta(t-t') \langle [V(t)V^\dagger(t') + V^\dagger(t')V(t)] \rangle \quad (3.41)$$

All these retarded function have the Fourier transforms defined by the usual convention:

$$G_{ret}(\mathbf{p}, E) = \int_{-\infty}^{\infty} dt e^{iE(t-t')} G_{ret}(\mathbf{p}, t-t') \quad (3.42)$$

The advanced Green's function for each is defined

$$\begin{aligned} G_{adv}(\mathbf{p}, t-t') &= i\Theta(t-t') \langle [C_{\mathbf{p}\sigma}(t)C_{\mathbf{p}\sigma}^\dagger(t') \\ &\quad + C_{\mathbf{p}\sigma}^\dagger(t')C_{\mathbf{p}\sigma}(t)] \rangle \end{aligned} \quad (3.43)$$

$$\begin{aligned} D_{adv}(\mathbf{q}, t-t') &= i\Theta(t-t') \langle A(\mathbf{q}, t)A(-\mathbf{q}, t') \\ &\quad - A(-\mathbf{q}, t')A(\mathbf{q}, t) \rangle \end{aligned} \quad (3.44)$$

The only two differences are the sign change in front and that the time domain is now $t' > t$, which is just opposite of that for retarded function.

The advanced functions of energy is defined as usual Fourier transform, and turn out to be *complex conjugate* of the corresponding retarded function.

$$U_{ret}(\omega) = U_{adv}^\dagger(\omega) \quad (3.45)$$

The Matsubara function can be changed to a retarded one with just this alteration:

$$i\omega_n \rightarrow \omega + i\delta \quad \mathcal{U}(i\omega_n) = U_{ret}(\omega) \quad (3.46)$$

This step is called an analytic continuation. The advanced Green's function can be changed by $i\omega_n \rightarrow \omega - i\delta$, since the advanced Green's function is the complex conjugate of the retarded one.

Another quantity is **spectral function**, it is imaginary part of any retarded function multiplied by 2:

$$A(\mathbf{p}, \omega) = -2 \text{Im}[G_{ret}(\mathbf{p}, \omega)] \quad (3.47)$$

An expression of this form is called **Lehmann representation**:

$$\begin{aligned} U_{ret}(\omega) &= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\omega')}{\omega - \omega' + i\delta} \\ \mathcal{U}(i\omega_n) &= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\omega')}{i\omega_n - \omega'} \end{aligned} \quad (3.48)$$

For fermions, the spectral density function is positive, $A(\mathbf{p}, \omega) > 0$. This positiveness is an important feature, since $A(\mathbf{p}, \omega)$ is interpreted as a probability function.

$$1 = \int \frac{d\omega}{2\pi} A(\mathbf{p}, \omega) \quad (3.49)$$

For bosons spectral function do not have this property, however, they are always positive for $\omega > 0$ and negative for $\omega < 0$.

For noninteracting electron the Green's function is

$$G_{ret}^0(\mathbf{p}, E) = \frac{1}{E - \xi_{\mathbf{p}} + i\delta} \quad (3.50)$$

It has one sign $\delta > 0$, even in many electron system with a Fermi surface. The retarded functions do not have $\delta_{\mathbf{p}}$ changing sign at the Fermi surface, which makes them easier to use than the zero-temperature Green's function.

The spectral function for the noninteracting Green's function is ⁴

$$A^0(\mathbf{p}, E) = 2\pi\delta(E - \xi_{\mathbf{p}}) \quad (3.51)$$

When $A(\mathbf{p}, E)$ is computed for interacting systems, there is a broad of the delta function. This means there is a band of E values for each \mathbf{p} . When the electron scatters, it has a nonzero mean free path, and there is some uncertainty in its momentum or energy or both. So \mathbf{p} and E are treated as separate variables and both are summed over when evaluating physical quantities.

Another quantity to evaluate, for an interacting electron system, is the number of electrons in a momentum state \mathbf{p} , which is

$$n_{\mathbf{p}} = \int \frac{dE}{2\pi} \eta_F(E) A(\mathbf{p}, E) \quad (3.52)$$

For phonons, the average number of phonons in a state \mathbf{q} is

$$2N_{\mathbf{q}} + 1 = \langle A_{\mathbf{q}}^\dagger A_{\mathbf{q}} \rangle = \int \frac{d\omega}{2\pi} \eta_B(\omega) A(\mathbf{q}, \omega) \quad (3.53)$$

The noninteracting phonon spectral function is

$$A^0(\mathbf{q}, \omega) = 2\pi[\delta(\omega - \omega_{\mathbf{q}}) - \delta(\omega + \omega_{\mathbf{q}})] \quad (3.54)$$

⁴

$$\frac{1}{E - \xi_{\mathbf{p}} + i\delta} = \frac{1}{E - \xi_{\mathbf{p}}} - 2\pi i\delta(E - \xi_{\mathbf{p}})$$

In later sections the Green's function in Matsubara form have a Dyson form

$$\mathcal{G}(\mathbf{p}, ip_n) = \frac{1}{ip_n - \xi_{\mathbf{p}} - \Sigma(\mathbf{p}, ip_n)} \quad (3.55)$$

$$\mathcal{D}(\mathbf{q}, i\omega_n) = \frac{-2\omega_{\mathbf{q}}}{\omega_n^2 + \omega_{\mathbf{q}}^2 + 2\omega_{\mathbf{q}}P(\mathbf{q}, i\omega_n)} \quad (3.56)$$

Define the retarded self-energies according to (3.46)

$$ip_n \rightarrow E + i\delta \quad \Sigma(\mathbf{p}, ip_n) \rightarrow \Sigma_{ret}(\mathbf{p}, E) = \text{Re } \Sigma_{ret} + i \text{Im } \Sigma_{ret} \quad (3.57)$$

Consider the retarded Green's function will have a Dyson equation

$$G_{ret}(\mathbf{p}, E) = \frac{1}{E + i\delta - \xi_{\mathbf{p}} - \Sigma_{ret}(\mathbf{p}, E)} \quad (3.58)$$

as derived from (3.46). The spectral function for the electron is rewritten in terms of the retarded self-energy,

$$A(\mathbf{p}, E) = \frac{-2 \text{Im } \Sigma_{ret}(\mathbf{p}, E)}{[E - \xi_{\mathbf{p}} - \text{Re } \Sigma_{ret}(\mathbf{p}, E)]^2 + [\text{Im } \Sigma_{ret}(\mathbf{p}, E)]^2} \quad (3.59)$$

Simple examples to distinguish Matsubara, retarded, and advanced Green's function. There are some simple functions which have the correct analytical properties. Considering a self-energy operator has the following functional form,

$$\Sigma(\mathbf{p}, Z) = C \ln[f(\mathbf{p}) - Z] \quad (3.60)$$

where Z is a complex variable representing the frequency. Take C as a constant and $f(\mathbf{p})$ as some function of momentum. The Matsubara self-energy is evaluated at the points

$$\Sigma(\mathbf{p}, ip_n) = C \ln[f(\mathbf{p}) - ip_n] \quad (3.61)$$

The analytic continuation $ip_n \rightarrow E \pm i\delta$ to the real axis has the following values. For retarded function ⁵, using $ip_n \rightarrow E + i\delta$

$$\Sigma_{ret}(\mathbf{p}, E) = C \ln |f(\mathbf{p}) - E| - i\pi C \Theta[E - f(\mathbf{p})] \quad (3.62)$$

and for advanced

$$\Sigma_{adv}(\mathbf{p}, E) = C \ln |f(\mathbf{p}) - E| + i\pi C \Theta[E - f(\mathbf{p})] \quad (3.63)$$

These two self-energies differ in the region $E > f(\mathbf{p})$, because their imaginary parts have the opposite sign. This difference agrees with the general theorem that

$$\Sigma_{ret}^*(\mathbf{p}, E) = \Sigma_{adv}(\mathbf{p}, E) \quad (3.64)$$

⁵ To get this relation

$$\begin{aligned} \Sigma_{ret} &= C \ln[f(\mathbf{p}) - E - i\delta] \\ &= C \int \frac{dE}{f(\mathbf{p}) - E - i\delta} + C \end{aligned}$$

and also implies that

$$\Sigma_{ret}^*(\mathbf{p}, E) = \Sigma_{adv}(\mathbf{p}, E) \quad (3.65)$$

There is a branch cut on the real axis for $E > f(\mathbf{p})$. This branch cut just expresses the fact that $\ln(f - Z)$ is not a continuous function of Z across the real axis.

Another example which has the similar analytical properties is

$$\Sigma(\mathbf{p}, Z) = C[f(\mathbf{p}) - Z]^{\frac{1}{2}} \quad (3.66)$$

This function also has a branch cut for $E > f(\mathbf{p})$, with $\text{Im } \Sigma < 0$ and $\text{Im } \Sigma > 0$. In fact, a branch cut is a necessary feature whenever $\text{Im } \Sigma \neq 0$, which gives

$$\Sigma(\mathbf{p}, E + i\delta) \neq \Sigma(\mathbf{p}, E - i\delta) \quad (3.67)$$

One should be aware that when self-energy functions are evaluated, they are often given by logarithmic or square root function.

When a branch cut occurs and $\text{Im } \Sigma \neq 0$, then the spectral function is given by (3.59). In other regions where there is no branch cut, then take the limit of $\text{Im} \rightarrow 0$ and obtain

$$\lim_{\text{Im } \Sigma=0} A(\mathbf{p}, E) = 2\pi\delta(E - \xi_{\mathbf{p}} - \text{Re } \Sigma_{ret}(\mathbf{p}, E)) \quad (3.68)$$

Here the spectral function is a delta function, but the real part of the self-energy may be nonzero, so that it affects the spectral function. Denote by $E(\mathbf{p})$ the solution to the equation

$$E(\mathbf{p}) - \mu = \xi_{\mathbf{p}} + \text{Re } \Sigma(\mathbf{p}, E(\mathbf{p}) - \mu) \quad (3.69)$$

Assume that there is a problem in which (3.69) is satisfied when $\text{Im } \Sigma = 0$. Then with the properties of delta function, the spectral function is written as

$$A(\mathbf{p}, E) = 2\pi Z(\mathbf{p})\delta(E - E(\mathbf{p}) + \mu) \quad (3.70)$$

$$Z(\mathbf{p}) = \frac{1}{\left| 1 - \frac{\partial}{\partial E} \Sigma_{ret}(\mathbf{p}, E) \right|_{E=E(\mathbf{p})-\mu}} \quad (3.71)$$

The factor $Z(\mathbf{p})$ is called **renormalization factor**. Because of (3.49) and $A(\mathbf{p}, E) > 0$, we have $Z(\mathbf{p}) < 1$. The strength of the delta function peak is always less than or equal to unity.

Equation (3.69) may be used to define the effective mass. Assume that the noninteracting states are free particles

$$\xi_{\mathbf{p}} = \frac{p^2}{2m} - \mu = \varepsilon_{\mathbf{p}} - \mu \quad (3.72)$$

Furthermore, assume at low momentum that $E(\mathbf{p})$ in (3.69) varies quadratically with momentum,

$$E(\mathbf{p}) = E_0 + \frac{p^2}{2m^*} + \mathcal{O}(p^4) \quad (3.73)$$

The proportionality constant is the inverse effective mass m^*

$$\frac{m}{m^*} = \frac{\partial E(\mathbf{p})}{\partial \varepsilon_{\mathbf{p}}} \quad (3.74)$$

from the definition of (3.69), we get

$$\frac{\partial E(\mathbf{p})}{\partial \varepsilon_{\mathbf{p}}} = \lim_{\varepsilon_{\mathbf{p}} \rightarrow 0} \left(1 + \frac{\partial}{\partial \varepsilon_{\mathbf{p}}} \text{Re} \Sigma_{ret}(\mathbf{p}, E) + \left[\frac{\partial}{\partial E} \text{Re} \Sigma_{ret}(\mathbf{p}, E) \right] \frac{\partial E(\mathbf{p})}{\partial \varepsilon_{\mathbf{p}}} \right) \quad (3.75)$$

With (3.74), the final term is arrived

$$\frac{m}{m^*} = \lim_{\varepsilon_{\mathbf{p}} \rightarrow 0} \left[\frac{1 + (\partial_{\varepsilon_{\mathbf{p}}}) \text{Re} \Sigma_{ret}(\mathbf{p}, E_0 - \mu)}{1 - (\partial_{E_0}) \text{Re} \Sigma_{ret}(\mathbf{p}, E_0 - \mu)} \right] \quad (3.76)$$

This formula will be frequently to obtain the effective mass from self-energy calculations.

3.4 Dyson's Equation

The Matsubara Green's functions are evaluated by the same method of Feynman diagram techniques. The ideas behind expanding the S matrix are presented, and Dyson's equation is rederived for the Matsubara Green's function in this section.

Consider the case of the electron Green's function:

$$\mathcal{G}(\mathbf{p}, \tau) = -e^{\beta\Omega} \text{Tr} \left[e^{-\beta K} T_{\tau} (e^{\tau K} C_{\mathbf{p}} e^{-\tau K} C_{\mathbf{p}}^{\dagger}) \right] \quad (3.77)$$

$$e^{-\beta\Omega} = \text{Tr} (e^{-\beta K}) \quad (3.78)$$

where we consider the general case

$$K = K_0 + V = H_0 - \mu N + V \quad (3.79)$$

where K_0 is a problem which can be solved. The Hamiltonians under consideration usually have the property that they commute with the number operator

$$[H_0, N] = [H, N] = 0 \quad (3.80)$$

where H and N can be defined in same eigenstates. Consider the evaluation operations in interaction picture (2.9), we have

$$U(\tau) = e^{\tau K_0} e^{\tau K} \quad U^{-1}(\tau) = e^{\tau K} e^{-\tau K_0} \quad (3.81)$$

ant the time dependence of operators

$$\hat{C}_{\mathbf{p}}(\tau) = e^{\tau K_0} C_{\mathbf{p}} e^{-\tau K_0} = e^{-\tau \xi_{\mathbf{p}}} C_{\mathbf{p}} \quad (3.82)$$

Then the Green's function in (3.77), is written for $\tau > 0$ as

$$\mathcal{G}(\mathbf{p}, \tau) = - \frac{\text{Tr} \left[e^{-\beta K_0} U(\beta) U^{-1}(\tau) \hat{C}_{\mathbf{p}}(\tau) U(\tau) C_{\mathbf{p}}^\dagger \right]}{\text{Tr} \left[e^{-\beta K_0} U(\beta) \right]} \quad (3.83)$$

The operator $U(\tau)$ can be solved in terms of τ -ordered products.

$$\partial_\tau U(\tau) = -\hat{V}(\tau) U(\tau) \quad (3.84)$$

This equation for $U(\tau)$ is given as

$$U(\tau) = T_\tau \exp \left[- \int_0^\tau d\tau_1 \hat{V}(\tau_1) \right] \quad (3.85)$$

Next consider the definition

$$S(\tau_1, \tau_2) = T_\tau \exp \left[- \int_{\tau_1}^{\tau_2} d\tau \hat{V}(\tau) \right] \quad (3.86)$$

as discussed in previous section. Then with the rearrange terms of (3.82),

$$\mathcal{G}(\mathbf{p}, \tau) = - \frac{\langle T_\tau S(\beta) \hat{C}_{\mathbf{p}}(\tau) \hat{C}_{\mathbf{p}}^\dagger \rangle_0}{\langle S(\beta) \rangle_0} \quad (3.87)$$

This form of the Green's function is similar to the zero-temperature result (2.29).

The Green's function is evaluated, at least formally, by expanding the S matrix in the numerator

$$\begin{aligned} & \langle T_\tau S(\beta) \hat{C}_{\mathbf{p}}(\tau) \hat{C}_{\mathbf{p}}^\dagger \rangle_0 \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \langle T_\tau \hat{C}_{\mathbf{p}}(\tau) \hat{V}(\tau_1) \cdots \hat{V}(\tau_n) \hat{C}_{\mathbf{p}}^\dagger \rangle_0 \end{aligned} \quad (3.88)$$

Each of the n th terms are evaluated by applying Wick's theorem.

The disconnected diagrams are canceled by the vacuum polarization diagrams which is $e^{-\beta \Omega}$.

Then the Matsubara Green's function can be reduced to an evaluation of all connected different diagrams

$$\mathcal{G}(\mathbf{p}, \tau) = - \sum_{n=0}^{\infty} (-1)^n \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \langle T_\tau \hat{C}_{\mathbf{p}}(\tau) \hat{V}(\tau_1) \cdots \hat{V}(\tau_n) \hat{C}_{\mathbf{p}}^\dagger(0) \rangle_0 \quad (3.89)$$

and the Green's function of energy is found by Fourier transform

$$\mathcal{G}(\mathbf{p}, ip_n) = \int_0^\beta d\tau e^{ip_n \tau} \mathcal{G}(\mathbf{p}, \tau) \quad \mathcal{G}(\mathbf{p}, \tau) = \frac{1}{\beta} \sum_{p_n} e^{-ip_n \tau} \mathcal{G}(\mathbf{p}, ip_n) \quad (3.90)$$

The terms in the series (3.89) yield self-energy diagrams, which may be collected into Dyson equation

$$\mathcal{G}(\mathbf{p}, ip_n) = \frac{\mathcal{G}^0(\mathbf{p}, ip_n)}{1 - \mathcal{G}^0(\mathbf{p}, ip_n)\Sigma(\mathbf{p}, ip_n)} \quad (3.91)$$

$$\mathcal{D}(\mathbf{q}, i\omega_n) = \frac{\mathcal{D}^0(\mathbf{q}, i\omega_n)}{1 - \mathcal{D}^0(\mathbf{q}, i\omega_n)\Pi(\mathbf{q}, i\omega_n)} \quad (3.92)$$

The rules for constructing diagrams, are similar in the non-zero temperature cases.

3.5 Frequency Summations

When using the Matsubara Green's functions, one must evaluate frequency summations over combinations of unperturbed Green's functions. The technique for evaluating these summations is discussed for both cases of unperturbed functions and also Green's functions with self-energies. There is a table of results for combinations which often occur.

$$\begin{aligned} -\frac{1}{\beta} \sum_m \mathcal{D}^0(\mathbf{q}, i\omega_m) \mathcal{G}^0(\mathbf{p}, ip_n + i\omega_m) &= \frac{N_{\mathbf{q}} + \eta_F(\xi_{\mathbf{p}})}{ip_n - \xi_{\mathbf{p}} + \omega_{\mathbf{q}}} \\ &+ \frac{N_{\mathbf{q}} + 1 - \eta_F(\xi_{\mathbf{p}})}{ip_n - \xi_{\mathbf{p}} - \omega_{\mathbf{q}}} \end{aligned} \quad (3.93)$$

$$\frac{1}{\beta} \sum_n \mathcal{G}^0(\mathbf{p}, ip_n) \mathcal{G}^0(\mathbf{k}, ip_n + i\omega_m) = \frac{\eta_F(\xi_{\mathbf{p}}) - \eta_F(\xi_{\mathbf{k}})}{i\omega_m + \xi_{\mathbf{p}} - \xi_{\mathbf{k}}} \quad (3.94)$$

$$-\frac{1}{\beta} \sum_n \mathcal{G}^0(\mathbf{p}, ip_n) \mathcal{G}^0(\mathbf{k}, i\omega_m - ip_n) = \frac{1 - \eta_F(\xi_{\mathbf{p}}) - \eta_F(\xi_{\mathbf{k}})}{i\omega_m - \xi_{\mathbf{p}} - \xi_{\mathbf{k}}} \quad (3.95)$$

$$\frac{1}{\beta} \sum_n \mathcal{G}^0(\mathbf{p}, ip_n) = \eta_F(\xi_{\mathbf{p}}) \quad (3.96)$$

First consider the summation over a boson series, considering (3.93), we have this term

$$S = \frac{1}{\beta} \sum_m \frac{2\omega_{\mathbf{q}}}{\omega_m^2 + \omega_{\mathbf{q}}^2} \frac{1}{ip_n + i\omega_m - \xi_{\mathbf{p}}} \quad (3.97)$$

Denote this equation as

$$S = -\frac{1}{\beta} \sum_m f(i\omega_m) \quad (3.98)$$

where $f(i\omega_m)$ is the product of Green's function in (3.97). This summation is evaluated by a contour integration. The integral has the form,

$$I = \lim_{R \rightarrow \infty} \oint \frac{dz}{2\pi i} f(z) \eta_B(z) \quad (3.99)$$

The function $\eta_B(z)$ is chosen to generate poles at the points $i\omega_m$ for all even integer m . The function $f(z)$ is

$$f(z) = \frac{2\omega_{\mathbf{q}}}{z^2 - \omega_{\mathbf{q}}^2} \frac{1}{ip_n + z - \xi_{\mathbf{p}}} \quad (3.100)$$

The corresponding poles and residues of integral I in (3.99) are

$$\begin{aligned} z_m &= i2\pi mk_B T, \quad R_i = \frac{1}{\beta} f(i\omega_m) \\ z_1 &= \omega_{\mathbf{q}}, \quad R_1 = \frac{N_{\mathbf{q}}}{ip_n - \xi_{\mathbf{p}} + \omega_{\mathbf{q}}} \\ z_2 &= -\omega_{\mathbf{q}}, \quad R_2 = \frac{N_{\mathbf{q}} + 1}{ip_n - \xi_{\mathbf{p}} - \omega_{\mathbf{q}}} \\ z_3 &= \xi_{\mathbf{p}} - ip_n, \quad R_3 = \frac{-2\omega_{\mathbf{q}}\eta_F(\xi_{\mathbf{p}})}{(ip_n - \xi_{\mathbf{p}})^2 - \omega_{\mathbf{q}}^2} \end{aligned} \quad (3.101)$$

Then, $I = \frac{1}{\beta} \sum_m f(i\omega) m + R_1 + R_2 + R_3$, and with (3.98).

$$S = R_1 + R_2 + R_3 \quad (3.102)$$

The method of evaluating these boson series is quite simple. To evaluate a series such as (3.98) one just finds all the simple poles of $f(z)$ which are at points z_j with residues r_j and then

$$S = \sum_j r_j \eta_B(z_j) \quad (3.103)$$

The same procedure is used to evaluate fermion series. Then the summations are of the form

$$S = - \sum_i r_i \eta_F(z_i) \quad (3.104)$$

The minus sign in front occurs because the residue of the fermion η_F is $-\frac{1}{\beta}$ and is $\frac{1}{\beta}$ for boson η_B .⁶

The last result in (3.96) is special

$$\frac{1}{\beta} \sum_n \mathcal{G}^0(\mathbf{p}, ip_n) = \eta_F(\xi_{\mathbf{p}})$$

Due to the definition, the left side is the Fourier transform of Matsubara Green's function. The result (3.50) is just the limit at $\tau \rightarrow 0$. This limit is ambiguous, since a different result is obtained if $\tau = 0$ is approached from the positive or negative direction

$$\mathcal{G}^0(\mathbf{p}, \tau = 0^+) = -[1 - \eta_F(\xi_{\mathbf{p}})] \quad (3.105)$$

$$\mathcal{G}^0(\mathbf{p}, \tau = 0^-) = \eta_F(\xi_{\mathbf{p}}) \quad (3.106)$$

The result (3.96) is merely the convention of adopting the limit $\tau = 0^-$.

6

$$\begin{aligned} & \text{Res}\left(\frac{1}{e^{-\beta z_0} - 1}\right) \\ &= \frac{g(z_0)}{f'(z_0)} \\ &= \left(-\beta e^{-\beta z_0}\right)^{-1} \\ &= -\frac{1}{\beta} \end{aligned}$$

Consider the example of evaluating the summation (3.93) except that the Green's function for the electron contains some self-energy terms:

$$\mathcal{G}(\mathbf{p}, ip_n) = \frac{1}{ip_n - \xi_{\mathbf{p}} - \Sigma(\mathbf{p}, ip_n)} \quad (3.107)$$

Letting $ip_n = z$ then the above function has branch cuts along the real Z axis. These branch cuts arise because of the self-energies $\Sigma(\mathbf{p}, ip_n)$ as discuss in 3.3. The contour integrals used to evaluate the frequency summations become more complicated because of the branch cut.

The most general possibility when evaluating a summation over Matsubara frequencies is to have all the Green's functions fully dressed. Then is is common to proceed by first expressing all the Green's functions in the **Lehmann representation**. For example, evaluate

$$S = -\frac{1}{\beta} \sum_m \mathcal{D}(\mathbf{q}, i\omega_m) \mathcal{G}(\mathbf{p}, ip_n + i\omega_m) \quad (3.108)$$

Express each Green's function as a frequency integral over its respective spectral function as shown in (3.48)

$$\mathcal{D}(\mathbf{q}, i\omega_m) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{B(\mathbf{q}, \omega)}{i\omega_m - \omega} \quad (3.109)$$

$$\mathcal{G}(\mathbf{p} + \mathbf{q}, ip_n + i\omega_m) = \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} \frac{A(\mathbf{p} + \mathbf{q}, \varepsilon)}{ip_n + i\omega_m - \varepsilon} \quad (3.110)$$

and the summation S becomes

$$S = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} B(\mathbf{q}, \omega) \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} A(\mathbf{p} + \mathbf{q}, \varepsilon) S_0(ip_n, \omega, \varepsilon)$$

and

$$S_0(ip_n, \omega, \varepsilon) = -\frac{1}{\beta} \sum_m \frac{1}{i\omega_m - \omega} \frac{1}{ip_n + i\omega_m - \varepsilon} = \frac{\eta_B(\omega) + \eta_F(\varepsilon)}{ip_n + \omega - \varepsilon}$$

The summation S_0 is now the easy type which is evaluated using noninteracting Green's functions. The final result provides for the most general case of fully interacting Green's functions. In general, any frequency summation can be done by expressing all Green's functions in their **Lehmann representation**.

3.6 Linked Cluster Expansions

Another method for evaluating correlation functions is called the linked cluster method or the cumulant expansion. It is the method used to evaluating the thermodynamic potential Ω . However, the method has also been applied to evaluating Green's function of time for a few problems as an alternative to Dyson equation approach.

3.6.1 Thermodynamic Potential

The thermodynamic potential is found from the equation

$$e^{-\beta\Omega} = \text{Tr}(e^{-\beta K}) = \text{Tr}[e^{-\beta K_0} S(\beta)] \quad (3.111)$$

This quantity is useful to evaluate by itself, for example, if N_e is the number of electrons

$$-\frac{\partial\Omega}{\beta\partial\mu} = \langle N_e \rangle \quad (3.112)$$

$$\frac{\partial(\beta\Omega)}{\partial\beta} = \langle K \rangle = U - \mu\bar{N}_e = \Omega + TS \quad (3.113)$$

$$m\frac{\partial\Omega}{\partial m} = \langle \sum_i \frac{p_i^2}{2m} \rangle = \sum_{\mathbf{p}} n_{\mathbf{p}} \frac{p^2}{2m} \quad (3.114)$$

where $n_{\mathbf{p}}$ is the number of electrons with momentum \mathbf{p} in (3.52).

For an interacting system

$$K = K_0 + V \quad (3.115)$$

For a system of electrons and phonons,

$$K_0 = \sum_{\mathbf{p},\sigma} \xi_{\mathbf{p}} C_{\mathbf{p}\sigma}^\dagger C_{\mathbf{p}\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} (a_{\mathbf{q}}^\dagger a_{\mathbf{q}} + \frac{1}{2}) \quad (3.116)$$

the trace is simple since the noninteracting eigenstates can be used to expand the trace eigenstates

$$e^{-\beta\Omega_0} = \Pi_{\mathbf{p}} (1 + e^{-\beta\xi_{\mathbf{p}}})^2 \Pi_{\mathbf{q}} \left(\frac{e^{-\beta\omega_{\mathbf{q}}/2}}{1 - e^{-\beta\omega_{\mathbf{q}}}} \right) \quad (3.117)$$

The logarithm of both sides of this equation

$$\beta\Omega_0 = -2 \sum_{\mathbf{p}} \ln(1 + e^{-\beta\xi_{\mathbf{p}}}) + \sum_{\mathbf{q}} [\ln(1 - e^{-\beta\omega_{\mathbf{q}}}) + \frac{1}{2}\beta\omega_{\mathbf{q}}] \quad (3.118)$$

The factor of 2 in front of electron is the spin degeneracy. The last term on the right is zero-point energy of phonons. Change the summations to integrals a factor appears of the volume v . The thermodynamic potential is proportional to the volume of the system. This result is also apparent from (3.112) to (3.114), since the right-hand side in each case is proportional to the volume or to the number of particles.

To calculate (3.111) including $S(\beta)$. The interaction V will add some correction terms to Ω_0 which changes it into Ω . The method of evaluating this correlation function is by the S -matrix expansion

$$e^{-\beta\Omega} = e^{-\beta\Omega_0} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \langle T_\tau \hat{V}(\tau_1) \cdots \hat{V}(\tau_n) \rangle_0 \quad (3.119)$$

In evaluating the right-hand side, all diagrams are included, whether connected or disconnected, since there is no other series at hand to cancel the disconnected diagrams. The way of doing this expansion is the linked cluster expansion.

The way to do this is stated here. First, introduce the parameter λ , to keep track of the number of times the potential occurs in each term in the S matrix. The S -matrix expansion in (3.119) may be written as

$$e^{-\beta\Omega} = e^{-\beta\Omega_0} \sum_{n=0}^{\infty} \lambda^n W_n \quad (3.120)$$

$$W_n = \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \langle T_\tau \hat{V}(\tau_1) \cdots \hat{V}(\tau_n) \rangle_0 \quad (3.121)$$

The basic linked cluster theorem is that this series can be resummed into

$$e^{-\beta\Omega} = \exp \left(-\beta\Omega_0 + \sum_{l=1}^{\infty} \lambda^l U_l \right) \quad (3.122)$$

$$U_l = \frac{(-1)^l}{l} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_l \langle T_\tau \hat{V}(\tau_1) \cdots \hat{V}(\tau_l) \rangle_0 \quad (3.123)$$

where U_l contains just different, connected diagrams: The thermodynamic potential is obtained by setting $\lambda = 1$ in (3.122),

$$\Omega = \Omega_0 - \frac{1}{\beta} \sum_{l=1}^{\infty} U_l \quad (3.124)$$

The basic theorem is that the thermodynamic potential is the summation of the different connected diagrams. With some discussion discussed in the book⁷, we have the identity

⁷ P144, Mahan

$$U_l = \frac{(-1)^k}{l!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_l \langle T_\tau \hat{V}(\tau_1) \cdots \hat{V}(\tau_l) \rangle_{connected} \quad (3.125)$$

In terms of the Green's functions, we have

$$U_l = \frac{1}{l!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_l \mathcal{G}(\mathbf{p}_1, \tau_1 - \tau_j) \mathcal{G}^0(\mathbf{p}_2, \tau_2 - \tau_k) \cdots \quad (3.126)$$

In prior section, the Green's function $\mathcal{G}(\mathbf{p}, \tau)$ was evaluated by a similar expansion technique. There the connected diagrams obeyed the counting rules that

$$\frac{1}{l!} \langle T_\tau \hat{C}_{\mathbf{p}\sigma}(\tau) \hat{V}(\tau_1) \cdots \hat{V}(\tau_l) \hat{C}_{\mathbf{p}\sigma}^\dagger(0) \rangle_{connected} = \langle T_\tau \hat{C}_{\mathbf{p}\sigma}(\tau) \hat{V}(\tau_1) \cdots \hat{V}(\tau_l) \hat{C}_{\mathbf{p}\sigma}^\dagger(0) \rangle_{different\ connected} \quad (3.127)$$

Here there are l arrangements which are identical. In the linked cluster method there are only $(l-1)!$.

Next consider the evaluation of the thermodynamic potential. It is obtained by evaluating the series of terms in (3.124). An example

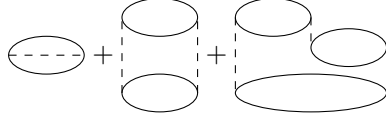


Figure 3.1: Link cluster diagram.

is shown here in Fig. 3.1 for the electron-phonon interaction. They can be summed to give an approximate simple answer. The rules for constructing diagrams for the terms in the thermodynamic potential are similar to those in Sec 3.4. One follows all those rules and then multiplies the result by $\frac{\beta}{T}$. The $\frac{1}{T}$ factor is just the one which occurs in (3.123). For the first bubble in Fig. 3.1,

$$U_2 = \frac{\beta}{2} \frac{\lambda^2}{\beta} \sum_{\mathbf{q}, iq_n} M_{\mathbf{q}}^2 \mathcal{D}^0(\mathbf{q}, iq_n) P^1(\mathbf{q}, iq_n) \quad (3.128)$$

where the polarization diagram $P^1(\mathbf{q}, iq_n)$ is for the single bubble, which was already evaluated

$$P^1(\mathbf{q}, iq_n) = \frac{2}{\beta V} \sum_{\mathbf{p}, ip_m} \mathcal{G}^0(\mathbf{p}, ip_m) \mathcal{G}^0(\mathbf{p} + \mathbf{q}, ip_m + iq_n) \quad (3.129)$$

The second term in Fig. 3.1 has two bubbles connected by two phonon lines. Using the rules for constructing diagrams gives

$$U_4 = \frac{\beta}{4} \frac{\lambda^4}{\beta} \sum_{\mathbf{q}, iq_m} \left[M_{\mathbf{q}}^2 \mathcal{D}^0(\mathbf{q}, iq_n) \mathcal{P}^1(\mathbf{q}, iq + n) \right]^2 \quad (3.130)$$

Momentum and frequency conservation requires both phonons to have the same variables (\mathbf{q}, iq_n) and both polarization diagrams are also just functions of combination. The term with n bubbles and n phonon lines is

$$U_{2n} = \frac{\beta}{2n} \frac{\lambda^{2n}}{\beta} \sum_{\mathbf{q}, iq_n} \left[M_{\mathbf{q}}^2 \mathcal{D}^0(\mathbf{q}, iq_n) \mathcal{P}^1(\mathbf{q}, iq_n) \right]^n \quad (3.131)$$

It is simple to sum the series

$$\Omega - \Omega_0 = -\frac{1}{\beta} \sum_{n=1}^{\infty} U_{2n} = \frac{1}{2\beta} \sum_{\mathbf{q}, iq_n} \ln \left[1 - \lambda^2 M_{\mathbf{q}}^2 \mathcal{D}^0(\mathbf{q}, iq_n) \mathcal{P}^1(\mathbf{q}, iq_n) \right] \quad (3.132)$$

This is the correction to the thermodynamic potential. The right-hand side is proportional to the volume V , as is obvious when the summation over \mathbf{q} is changed to an integration. The argument of the logarithm is not dependent on V , and V enters only by multiplying the result.

The answer in (3.132) is a logarithm. The summation over iq_n needs to be evaluated. A standard trick for eliminating the logarithm, although it does not eliminate it but just disguises it. Treat

$\eta = \lambda^2$ as a variable of integration

$$\int_0^{\lambda^2} d\eta \frac{\Lambda}{1 - \eta\Lambda} = -\ln [1 - \lambda^2\Lambda] \quad (3.133)$$

$$\Lambda = M_{\mathbf{q}}^2 \mathcal{D}^0(\mathbf{q}, iq_n) \mathcal{P}^1(\mathbf{q}, iq_n) \quad (3.134)$$

Then for $\lambda = 1$

$$\Omega - \Omega_0 = -\frac{V}{2\beta} \sum_{iq_n} \int \frac{d^3q}{(2\pi)^3} \int_0^1 d\eta \frac{M_{\mathbf{q}}^2 \mathcal{D}^0 \mathcal{P}^1}{1 - \eta M_{\mathbf{q}}^2 \mathcal{D}^0 \mathcal{P}^1} \quad (3.135)$$

The logarithm has been eliminated, but now the right-hand side must be evaluated for each value of η and then the integral is taken over η . Since η enters in the same way as a coupling constant, this step is called a **coupling constant integration**. The integration can be taken outside of the summation over iq_n , which makes this summation easier in some case.

Further, define the phonon self-energy as

$$\pi^1(\eta, \mathbf{q}, iq_n) = \eta M_{\mathbf{q}}^2 \mathcal{P}^1(\mathbf{q}, iq_n) \quad (3.136)$$

where the coupling constant η is included in the definition. The superscript indicates that this expression is an approximate self-energy, which only includes the single-electron bubble. The phonon Green's function is

$$\mathcal{D}^1(\eta, \mathbf{q}, iq_n) = \frac{\mathcal{D}^0}{1 - \mathcal{D}^0 \pi^1} \quad (3.137)$$

The Green's function is also a function of the coupling constant strength η . Equation (3.135) is rewritten as

$$\Omega - \Omega_0 = -\frac{V}{2\beta} \sum_{iq_n} \int \frac{d^3q}{(2\pi)^3} \int_0^1 \frac{d\eta}{\eta} \pi^{(1)}(\eta, \mathbf{q}, iq_n) \mathcal{D}^{(1)}(\eta, \mathbf{q}, iq_n) \quad (3.138)$$

This expression is an approximation to Ω since it employs an approximate self-energy $\pi^{(1)}$. According the ⁸, the exact correction to the thermodynamic potential from electron-phonon interactions is

$$\Omega - \Omega_0 = -\frac{V}{2\beta} \sum_{iq_n} \int \frac{d^3q}{(2\pi)^3} \int_0^1 \frac{d\eta}{\eta} \pi(\eta, \mathbf{q}, iq_n) \mathcal{D}(\eta, \mathbf{q}, iq_n) \quad (3.139)$$

where $\pi(\eta, \mathbf{q}, iq_n)$ is the exact phonon self-energy and $\mathcal{D}(\eta, \mathbf{q}, iq_n)$ is the exact phonon Green's function evaluated with the exact self-energy.



If electron-electron interactions are included, then the phonon self-energy can also contain internal Coulomb interactions, etc. The effect

Figure 3.2: The exact phonon self-energy $\pi(\eta, \mathbf{q}, iq_n)$ is the summation of this infinite number of diagrams. There are bubbles with internal phonon lines and also several bubbles connected by more than one phonon line.

of Coulomb interaction on the thermodynamic potential should also be included. The general theorem (3.123) and (3.124) is true for all interactions: Coulomb, phonon, or others.

It is possible to combine the effects of phonons and Coulomb interaction in a simple way. Consider electrons interacting by either or both interactions, and then the single-bubble diagram appears twice. The two electron vertices can be connected by a single Coulomb line or a single phonon line. The sum of these contributions is

It is possible to combine the effects of phonons and Coulomb interaction in a simple way. Consider electrons interacting by either or both interactions, and then the single-bubble diagram appears twice. The two electron vertices can be connected by a single Coulomb line or a single phonon line. The sum of these contributions is

$$U_2 = \frac{\eta}{2} \sum_{\mathbf{q}, iq_n} \mathcal{P}^{(1)}(\mathbf{q}, iq_n) \left[M_{\mathbf{q}}^2 \mathcal{D}^{(0)}(\mathbf{q}, iq_n) \right] \quad (3.140)$$

By introduce a combined interaction propagator, Coulomb plus phonon, which is

$$W^{(0)}(\mathbf{q}, iq_n) = v_q + M_{\mathbf{q}}^2 \mathcal{D}^{(0)}(\mathbf{q}, iq_n) \quad (3.141)$$

with the Dyson equation

$$W(\mathbf{q}, iq_n) = \frac{W^{(0)}(\mathbf{q}, iq_n)}{1 - W^{(0)}(\mathbf{q}, iq_n) \mathcal{P}^{(1)}} \quad (3.142)$$

The generalization of (3.139) to include both Coulomb and phonon effect is

$$\begin{aligned} \Omega - \Omega_0 &= -\frac{V}{2\beta} \sum_{iq_n} \int \frac{d^3q}{(2\pi)^3} \int_0^1 \frac{d\eta}{\eta} \pi(\eta, \mathbf{q}, iq_n) W(\eta, \mathbf{q}, iq_n) \\ &+ \frac{\eta}{2} \int \frac{d^3q}{(2\pi)^3} v_q \end{aligned} \quad (3.143)$$

The first term contains the Coulomb self-energy of an electron interacting with itself, and this unwanted contribution is subtracted out in the second term. The expression (3.139) is in the expression of phonon self-energies. It is also possible to use electron self-energy, considering (??)

$$U_2 = \frac{\lambda}{2} \sum_{ip_n, \mathbf{p}, \sigma} c g^{(0)}(\mathbf{p}, ip_n) \Sigma^{(1)}(\mathbf{p}, ip_n) \quad (3.144)$$

where $\Sigma^{(1)}$ is the electron self-energy from one-phonon processes, which gives

$$\Sigma^{(1)}(\mathbf{p}, ip_n) = \frac{1}{\beta V} \sum_{\mathbf{q}, iq_m} M_{\mathbf{q}}^2 \mathcal{G}^{(0)}(\mathbf{q} + \mathbf{p}, ip_n + iq_m) \mathcal{D}^{(0)}(\mathbf{q}, iq_m) \quad (3.145)$$

These formulas are often used to calculate the ground state energy in the limit of $T \rightarrow 0$. There are two limits which are taken: $V \rightarrow \infty$ and $T \rightarrow 0$. In studying the electron gas, to get the right answer one needs to take the limit of $V \rightarrow \infty$ first. The reverse order omits important terms,

$$\beta \eta_F(\xi_{\mathbf{p}}) [1 - \eta_f(\xi_{\mathbf{p}})] \quad (3.146)$$

If $V \neq \infty$, then all levels are discrete in finite volume and as $T \rightarrow 0$ these terms give zero since either η_F or $[1 - \eta_f]$ is zero. However, if one first takes $V \rightarrow \infty$, so that the levels are continuous, then the limit $T \rightarrow 0$ gives

$$\lim_{T \rightarrow 0} \beta \eta_F(\xi_{\mathbf{p}}) [1 - \eta_f(\xi_{\mathbf{q}})] = \lim_{T \rightarrow 0} \frac{d}{d\xi_{\mathbf{p}}} [-\eta_F(\xi_{\mathbf{p}})] = \delta(\xi_{\mathbf{p}}) \quad (3.147)$$

There are many terms of this kind in perurbation expansion for the ground state energy of the electron gas. They are called **dangerous diagrams**.

Here we show a simple example of evaluating the thermodynamic potntial. Assume that the onley effect of the phonon self-energy is to change the unperturbed frequencies $\omega_{\mathbf{q}}^2$ to a new set of renormalized frequencies $\Omega_{\mathbf{q}}^2$. Since the Green's function is

$$\mathcal{D} = \frac{2\omega_{\mathbf{q}}}{(i\omega_n)^2 - \omega_{\mathbf{q}}^2 - 2\omega_{\mathbf{q}}\pi(\mathbf{p}, i\omega_n)} = \frac{2\omega_{\mathbf{q}}}{(i\omega_n)^2 - \Omega_{\mathbf{q}}^2} \quad (3.148)$$

This form for \mathcal{D} can be accomplished choosing

$$2\omega_{\mathbf{q}}\pi(\eta, \mathbf{p}, i\omega_n) = \eta(\Omega_{\mathbf{q}}^2 - \omega_{\mathbf{q}}^2) \quad (3.149)$$

The choice (3.149) is not the only possible one to renormalize the frequencies. It is the choice one gets by assuming that the change from $\omega_{\mathbf{q}}$ to $\Omega_{\mathbf{q}}$ is accomplished by the one-bubble polarization diagram given in (3.136). Then the coupling constant η enters as just a multiplicative factor, as shown in (3.149). If further self-energy diagrams are needed to get a good phonon π , then η would enter in a more complicated fashion. But usually the single-bubble approximation is often adequate.

Consider the (3.139), the expression to be evaluated is

$$\Omega - \Omega_0 = -\frac{1}{2\beta} \sum_{\mathbf{q}, iq_n} \int_0^1 d\eta \frac{\Omega_{\mathbf{q}}^2 - \omega_{\mathbf{q}}^2}{(iq + n)^2 - \omega_{\mathbf{q}}^2 - \eta(\Omega_{\mathbf{q}}^2 - \omega_{\mathbf{q}}^2)} \quad (3.150)$$

Introduce the frequency

$$\Omega_{\eta}^2 = \omega_{\mathbf{q}}^2 + \eta(\Omega_{\mathbf{q}}^2 - \omega_{\mathbf{q}}^2) \quad (3.151)$$

The summation over Matsubara frequencies can be done easily since,

$$\frac{1}{\beta} \sum_{iq_n} \frac{1}{(iq_n)^2 - \Omega_{\eta}^2} = \frac{1}{2\Omega_{\eta}} \mathcal{D}_{\eta}(\tau = 0) = -\frac{1}{2\Omega_{\eta}} [2\eta_B(\Omega_{\eta}) + 1] \quad (3.152)$$

Then the evaluation of (3.150) is just the coupling constant integral,

$$\begin{aligned}
 \Omega - \Omega_0 &= \frac{1}{2} \sum_{\mathbf{q}} (\Omega_{\mathbf{q}}^2 - \omega_{\mathbf{q}}^2) \int_0^1 \frac{d\eta}{2\Omega_{\mathbf{q}}} \left(1 + \frac{2}{e^{\beta\Omega_{\mathbf{q}}} - 1} \right) \\
 &= \frac{1}{2} \sum_{\mathbf{q}} \left[\Omega_{\mathbf{q}} + \frac{2}{\beta} \ln \left(1 - e^{-\beta\Omega_{\mathbf{q}}} \right) \right]_{\eta=0}^{\eta=1} \\
 &= \sum_{\mathbf{q}} \left[\frac{1}{2} (\Omega_{\mathbf{q}} - \omega_{\mathbf{q}}) + \frac{1}{\beta} \ln \left(\frac{1 - \exp(-\beta\Omega_{\mathbf{q}})}{1 - \exp(-\beta\omega_{\mathbf{q}})} \right) \right] \quad (3.153)
 \end{aligned}$$

The right-hand side is the thermodynamic potential from the phonons at the new frequency $\Omega_{\mathbf{q}}$ minus the contribution from the phonons at the old frequencies $\omega_{\mathbf{q}}$. When this result is combined with (??) for Ω_0 , the terms with $\omega_{\mathbf{q}}$ all cancel. The final answer is

$$\Omega = -\frac{2V}{\beta} \int \frac{d^3p}{(2\pi)^3} \ln \left(1 + e^{-\beta\tilde{\epsilon}_{\mathbf{p}}} \right) + \frac{V}{\beta} \int \frac{d^3q}{(2\pi)^2} \left[\frac{1}{2} \beta \Omega_{\mathbf{q}} + \ln \left(1 - e^{-\beta\Omega_{\mathbf{q}}} \right) \right] \quad (3.154)$$

3.7 Real-Time Green's Function

For six different Green's function of time, the retarded and advanced function have been discussed at nonzero temperature. The usefulness of the real-time functions is in the treatment of non-equilibrium phenomena.

The Matsubara method is unsuitable for the non-equilibrium since there is no thermodynamic basis for a system out of equilibrium. The entire Matsubara method is based on temperature, and no method has been found so far for extending it to nonequilibrium processes.

The real-time functions at nonzero temperature have formal definitions very similar to those at zero temperature. Comparing with (2.70), the Green's functions for electrons of momentum \mathbf{p} are

$$\begin{aligned}
 \mathcal{G}^<(\mathbf{p}, t_1, t_2) &= i \langle C_{\mathbf{p}\sigma}^\dagger(t_2) C_{\mathbf{p}\sigma}(t_1) \rangle \\
 \mathcal{G}^>(\mathbf{p}, t_1, t_2) &= -i \langle C_{\mathbf{p}\sigma}(t_1) C_{\mathbf{p}\sigma}^\dagger(t_2) \rangle \\
 \mathcal{G}_t(\mathbf{p}, t_1, t_2) &= \Theta(t_1 - t_2) \mathcal{G}^>(\mathbf{p}, t_1, t_2) + \Theta(t_2 - t_1) \mathcal{G}^<(\mathbf{p}, t_1, t_2) \\
 \mathcal{G}_{\bar{t}}(\mathbf{p}, t_1, t_2) &= \Theta(t_2 - t_1) \mathcal{G}^>(\mathbf{p}, t_1, t_2) + \Theta(t_1 - t_2) \mathcal{G}^<(\mathbf{p}, t_1, t_2)
 \end{aligned} \quad (3.155)$$

These definitions appear to be identical to those at zero temperature. The definition of $\langle \dots \rangle$ have different meanings, depending on the circumstance:

- At zero temperature, and in equilibrium, $\langle \dots \rangle$ denote the ground state of the interacting system
- At nonzero temperature, and in equilibrium, the brackets denote the thermodynamic average as in (3.18) and (3.36)

- When not in equilibrium, the brackets denote an average over the accessible phase space. However, the available phase space depends upon the recent history of the system, and kinetic constraints such as energy conservation. The meaning of brackets is poorly understood for system out of equilibrium.

Note in (3.155) that the Green's functions are not expressed on the difference of the time. This is only true for equilibrium system.

In thermal equilibrium, the real-time functions each have a simple relation to the retarded function. Using the state $|n\rangle$ and $|m\rangle$, which are exact eigenstates of the Hamiltonian, we have⁹

$$\mathcal{G}^<(\mathbf{p}, \omega) = i\eta_F(\omega)A(\mathbf{p}, \omega) \quad (3.156)$$

$$\mathcal{G}^>(\mathbf{p}, \omega) = -i[1 - \eta_F(\omega)]A(\mathbf{p}, \omega) \quad (3.157)$$

$$\mathcal{G}_t(\mathbf{p}, \omega) = [1 - \eta_F(\omega)]\mathcal{G}_{ret}(\mathbf{p}, \omega) + \eta_F(\omega)\mathcal{G}_{adv}(\mathbf{p}, \omega) \quad (3.158)$$

$$\mathcal{G}_{\bar{t}}(\mathbf{p}, \omega) = -[1 - \eta_F(\omega)]\mathcal{G}_{adv}(\mathbf{p}, \omega) - \eta_F(\omega)\mathcal{G}_{ret}(\mathbf{p}, \omega) \quad (3.159)$$

These expression are identical to (2.84).

The primary usefulness of the real-time Green's functions is in the theory of non-equilibrium phenomena. The Dyson's equation is same as the result in zero temperature in (2.81), and the matrices have the definition as in (2.80).

Equation (2.81) is generally regarded as being the correct form for Dyson's equation, even for systems out of equilibrium. For systems in equilibrium, one can derive (2.81) at nonzero temperature by starting from Dyson's equation for the Matsubara Green's functions. Treating τ as a complex variable, one can deform the contour of integration, and end up with (2.81)¹⁰. Generally, (2.81) is used for Dyson's equation for nonzero temperature, for equilibrium and nonequilibrium, since there is nothing else available.

Nonequilibrium theory usually proceeds by deriving equations of motion for the Green's function, which is similar to Boltzmann equation. The first step is to find an equation of motion for the interacting Green's function when it is not in equilibrium. Such an equation can be found from (2.81) by operating by $\left(i\frac{\partial}{\partial t} - H\right)$ on both sides of equation. By the form (2.70) and (2.74), we have (by noting \tilde{G} and the matrix form)

$$\left(i\frac{\partial}{\partial t} - \varepsilon_{\mathbf{k}}\right)\tilde{G}_0(\mathbf{k}, t) = \delta(t)\tilde{I} \quad (3.160)$$

$$\left(i\frac{\partial}{\partial t} - H_0(x)\right)\tilde{G}_0(x) = \delta^4(x)\tilde{I} \quad (3.161)$$

On the right-hand side of (2.81), this operator acts only upon \tilde{G}_0 for

⁹ P120 and P155 in Mahan's book

The (2.80),

$$\tilde{G} = \begin{bmatrix} G_t & -G^< \\ G^> & -G_{\bar{t}} \end{bmatrix} \quad \tilde{\Sigma} = \begin{bmatrix} \Sigma_t & -\Sigma^< \\ \Sigma^> & -\Sigma_{\bar{t}} \end{bmatrix}$$

and (2.81)

$$\begin{aligned} \tilde{G}(x_1, x_2) &= \tilde{G}_0(x_1 - x_2) \\ &+ \int_{-\infty}^{\infty} dx_3 \int_{-\infty}^{\infty} dx_4 \tilde{G}_0(x_1 - x_3) \\ &\times \tilde{\Sigma}(x_3, x_4) \tilde{G}(x_4, x_2) \end{aligned}$$

we use the *tilde* to note this is a matrix.
¹⁰

which the above result is used to find

$$\left(i\frac{\partial}{\partial t} - H_0(x)\right) \tilde{G}(x_1, x_2) = \delta^4(x_1 - x_2) \tilde{I} + \int dx_3 \tilde{\Sigma}(x_1, x_3) \tilde{G}(x_3, x_2) \quad (3.162)$$

This formula provides the equation of motion for the interacting Green's function. **It is the basis for the nonequilibrium theory of interacting systems.** For (3.162), on the left-hand side, only the non-interacting terms are contained in the Hamiltonian H_0 . The contribution from the interactions is provided by the self-energy functions on the right-hand side.

It is useful to have an equation of motion for the variable x_2 . Since the definition (2.70) of the Green's functions contains the conjugate wave function $\phi^\dagger(x_2)$, the equation of motion on this variable is the complex conjugate of Schrodinger's equation. Further, Dyson's equation can be written in an alternate form

$$\tilde{G}(x_1, x_2) = \tilde{G}_0(x_1 - x_2) + \int dx_3 \int dx_4 \tilde{G}(x_1, x_3) \tilde{\Sigma}(x_3, x_4) \tilde{G}_0(x_4 - x_2) \quad (3.163)$$

and the alternate equation of motion for the Green's function

$$\left(-i\frac{\partial}{\partial t} - H_0(\mathbf{r}_2, -\mathbf{p}_2)\right) \tilde{G}(x_1, x_2) = \delta^4(x_1 - x_2) \tilde{I} + \int dx_3 \tilde{G}(x_1, x_3) \tilde{\Sigma}(x_3, x_2) \quad (3.164)$$

The sign change on \mathbf{p}_2 comes from the complex conjugate of Schrodinger's equation. The operator $\mathbf{p} = -i\nabla$ changes sign under complex conjugation. This behavior is different from the Hermitian conjugate, where H_0 acts to the left on $\phi^\dagger(x_2)$ and \mathbf{p} does not change sign. These two equations of motion will be used to develop a quantum Boltzmann equation for nonequilibrium phenomena.

3.7.1 Wigner Distribution Function

The traditional Boltzmann equation is expressed in terms of the distribution function $f(\mathbf{r}, \mathbf{v}, t)$. This is the semiclassical view since it is assumed that the position and velocity of the particle can be defined simultaneously. In order to use the distribution for quantum systems, it is necessary to perform some averaging in order to remove effects due to the uncertainty principle.

If quantum effects are important, it is necessary to introduce another variable into the distribution function. This is called **Wigner distribution function** $f(\mathbf{k}, \omega; \mathbf{r}, t)$. This distribution function is derived from the Green's function $G^<(x_1, x_2)$ defined in (2.70). The Wigner distribution is derived by center-of-mass coordinate system

$$(\mathbf{R}, T) = \frac{1}{2}(x_1 + x_2) \quad (3.165)$$

$$(\mathbf{r}, t) = x_1 - x_2 \quad (3.166)$$

with this notation

$$G^<(\mathbf{r}, t; \mathbf{R}, T) = i \langle \psi^\dagger(\mathbf{R} - \frac{1}{2}\mathbf{r}, T - \frac{1}{2}t) \psi(\mathbf{R} + \frac{1}{2}\mathbf{r}, T + \frac{1}{2}t) \rangle \quad (3.167)$$

with Fourier transformation

$$f(\mathbf{k}, \omega; \mathbf{R}, T) = -i G^<(\mathbf{k}, \omega; \mathbf{R}, T) \quad (3.168)$$

For the macroscopic quantities of particle density, particle current and energy density

$$n(\mathbf{R}, T) = \int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\mathbf{k}, \omega; \mathbf{R}, T) \quad (3.169)$$

$$j(\mathbf{R}, T) = \int \frac{d^3k}{(2\pi)^3} \frac{\mathbf{k}}{m} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\mathbf{k}, \omega; \mathbf{R}, T) \quad (3.170)$$

$$\begin{aligned} n_E(\mathbf{R}, T) &= \int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega f(\mathbf{k}, \omega; \mathbf{R}, T) \\ &= i \left[\frac{\partial}{\partial t} \langle \psi^\dagger(\mathbf{R}, T - \frac{1}{2}t) \psi(\mathbf{R}, T + \frac{1}{2}t) \rangle \right]_{t=0} \\ &= \langle \psi^\dagger(\mathbf{R}, T) H \psi(\mathbf{R}, T) \rangle \end{aligned} \quad (3.171)$$

Then the technique for solving nonequilibrium problems is simple. The equation of motion in 3.162 and 3.164 for $G^<(\mathbf{k}, \omega; \mathbf{R}, T)$ is just the **quantum Boltzmann equation**. With solving the equations, the Wigner distribution function is yielded and the macroscopic variables can be calculate by the integrals above.¹¹

The semiclassical Boltzmann distribution function $f(\mathbf{R}, \mathbf{v}, T)$ is found by taking the frequency integral

$$f(\mathbf{R}, \mathbf{v}, T) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(m\mathbf{v}, \omega; \mathbf{R}, T) \quad (3.172)$$

This method of deriving the semiclassical Boltzmann equation is an alternative to the usual technique of **coarse grain averaging**.

The matrix equation in (3.162) and (3.164) can be untangled to present the individual equation of motion for separate Green's function.¹²

The Wigner density function is not positive definite and can not interpreted as a probability density. This feature can be shown by a simple example, a particle in one dimensional box of length L . The eigenvalues and eigenfunction are

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin(k_n x), \quad \varepsilon_n = \varepsilon n^2 \quad (3.173)$$

$$k_n = \frac{n\pi}{L}, \quad \varepsilon = \frac{\pi^2}{2mL^2} \quad (3.174)$$

Using the representation in (2.73) and setting $t = t_1 - t_2$, gives

$$G^<(x_1, x_2, t) = \frac{2i}{L} \sum_n \eta_F(\varepsilon_n) \sin(k_n x_1) \sin(k_n x_2) e^{-it\varepsilon n^2} \quad (3.175)$$

¹¹ The current is 0 if the system in equilibrium state, since a system carrying current in steady state but not in equilibrium state.

¹² P159

With the Fourier transform of time gives the function of frequency. Since the system is equilibrium, write $G^< = i\eta_F(\omega)A$. In the center-of-mass notation

$$f(x, \omega; X) = \eta_F(\omega)A(x, \omega; X) \quad (3.176)$$

$$A(x, \omega; X) = \frac{2\pi}{L} \sum_n [\cos(k_n x) - \cos(2k_n X)] \delta(\omega - \epsilon n^2) \quad (3.177)$$

where $x = x_1 - x_2$ and $X = (x_1 + x_2)/2$. The function A is a sum of delta function with different sign.

3.8 Kubo Formula For Electrical Conductivity

Many Experiments in condensed matter physics measure the linear response to an external perturbation. Linear response means that the signal is directly proportional to the intensity of the external perturbation. Kubo formulas are the name applied to the correlation function which describes the linear response.

For conductivity response, as an example, the applied or external field E_α^{ext} induces currents which in turn make other electric fields. The summation of all these fields is the total electric field, which is called $E_\alpha(\mathbf{r}, t)$. The conductivity σ is the one which responds to the actual electric field in solid

$$J_\alpha(\mathbf{r}, t) = \sum_\beta \sigma_{\alpha\beta}(\mathbf{q}, \omega) E_\beta(\mathbf{r}, t) \quad (3.178)$$

$$E_\alpha(\mathbf{r}, t) = \Xi_\alpha \exp[i(\mathbf{q}\mathbf{r} - \omega t)] \quad (3.179)$$

Take (3.178) as the fundamental definition of the microscopic conductivity. And implies the spacetime response as

$$J_\alpha(\mathbf{r}, t) = \int d^3\mathbf{r}' \int_{-\infty}^t dt' \sigma_{\alpha\beta}(\mathbf{r} - \mathbf{r}', t - t') E_\beta(\mathbf{r}', t') \quad (3.180)$$

In solids, it is permissible to use (3.178) only when it is understood that the current is to be averaged over many unit cells of the solid. Usually it is applied when \mathbf{q} is small and long-wavelength excitations are being studied.

Considering the dc conductivity, where $\mathbf{q} \rightarrow 0$ and $\omega \rightarrow 0$ and assuming that the system is linear and perturbations at different frequencies act independently. Then the total current is the summation of the responses at different frequencies.

The Hamiltonian for the system is taken to have $H + H'$. The term H' contains the interaction between the total electric field and the particles of the system. Equation (2.85) is used as the basic form of the interaction between electromagnetic fields and charges, in the

expression of vector potential

$$H' = -\frac{1}{c} \int d^3r j_\alpha(\mathbf{r}) A_\alpha(\mathbf{r}, t) \quad (3.181)$$

$$\frac{1}{c} A_\alpha(\mathbf{r}, t) = -\frac{i}{\omega} E_\alpha(\mathbf{r}, t) \quad (3.182)$$

with the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$, also the electric and vector potential are taken to be transverse, so the scalar potential ϕ is set equal to zero. The terms in (2.85) with A^2 are dropped, since their effects are nonlinear in the electric field.¹³ The term H contains all the other terms and interactions in the solid or liquid. There are interactions such as electron-electron, electron-phonon, spin-spin, with impurities, etc. The goal is to calculate the electrical conductivity when all these interactions are present.

The current operator in (3.181) was discussed earlier in Chapter one.

$$j_\alpha = \frac{1}{2m} \sum_i e_i [\mathbf{p}_{i\alpha} \delta(\mathbf{r} - \mathbf{r}_i) + \delta(\mathbf{r} - \mathbf{r}_i) \mathbf{p}_{i\alpha}] \quad (3.183)$$

With (3.179), (3.181) and (3.182) we have

$$H' = \frac{i}{\omega} j_\alpha(\mathbf{q}) \Xi_\alpha e^{-i\omega t} \quad (3.184)$$

$$j_\alpha(\mathbf{q}) = \frac{1}{2m} \sum_i e_i [\mathbf{q}_{i\alpha} e^{i\mathbf{q}\mathbf{r}_i} + e^{i\mathbf{q}\mathbf{r}_i} \mathbf{p}_{i\alpha}] \quad (3.185)$$

In terms of creation and destruction operators, the current operator is conventionally written as

$$j_\alpha(\mathbf{q}) = \sum_{\lambda\delta} p_\alpha^{\lambda\delta} C_\lambda^\dagger C_\delta \quad (3.186)$$

where λ, δ are the states associated with some unperturbed Hamiltonian H_0 which is chosen as the basis for the perturbation expansion. A distinction is made between the current operator j_α in (3.185) and the induced current J_α in (3.178). The operator j_α is used in the Hamiltonian, while J_α is the actual current measured by experiment. The measured value of the current is the average value for the velocity of the particles in the system, which is taken as the summation over all the particle velocities divided by the volume

$$J_\alpha(\mathbf{r}, t) = \frac{e}{V} \langle \sum_i v_{i\alpha} \delta(\mathbf{r} - \mathbf{r}_i) \rangle = \frac{e}{V} \sum_i \langle v_{i\alpha} \rangle \quad (3.187)$$

When quantizing the particle velocity in (??), the velocity is momentum minus the vector potential

$$\mathbf{v}_i = \left[\mathbf{p}_i - \frac{e}{c} \mathbf{A}(\mathbf{r}_i) \right] \quad (3.188)$$

$$J_\alpha = \frac{e}{mV} \sum_i \langle p_{i\alpha} \rangle - \frac{e^2}{mcV} \sum_i A_\alpha(\mathbf{r}_i) \quad (3.189)$$

¹³ The equation (2.85)

$$H = \sum_i \frac{1}{2m} [\mathbf{p}_i - \frac{e}{c} \mathbf{A}(\mathbf{r}_i)]^2 + \frac{1}{2} \sum_{i \neq j} \frac{e_i e_j}{r_{ij}} + \sum_{\mathbf{k}\lambda} \omega_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda}^\dagger a_{\mathbf{k}\lambda}$$

The momentum operator \mathbf{p}_i is proportional to the current operator, $\mathbf{j} = e \frac{\mathbf{p}_i}{m}$. The last term uses the relationship (3.182) between the vector potential and the electric field. For the long-wavelength disturbance

$$J_\alpha(\mathbf{r}, t) = \langle j_\alpha(\mathbf{r}, t) \rangle + i \frac{n_0 e^2}{m\omega} E_\alpha(\mathbf{r}, t) \quad (3.190)$$

The second term in the current is proportional to the electric field and the first term given by the expectation value of the local current operator. Later it is shown that the constant of proportionality is given by the Kubo formula. Usually these two terms are called

$$\mathbf{J} = \mathbf{J}^{(1)} + \mathbf{J}^{(2)} \quad (3.191)$$

$$\mathbf{J}^{(1)} = \frac{in_0 e^2}{m\omega} \mathbf{E}(\mathbf{r}, t) \quad (3.192)$$

$$\mathbf{J}^{(2)} = \langle \mathbf{j}(\mathbf{r}, t) \rangle \quad (3.193)$$

3.8.1 Transverse Fields, Zero Temperature

The following derivation of the Kubo formula is valid at zero temperature. Consider the expectation value of the current operator as a function of time

$$J_\alpha^{(2)}(\mathbf{r}, t) = \langle \psi' | e^{i(H+H')t} j_\alpha(\mathbf{r}) e^{-i(H+H')t} | \psi \rangle \quad (3.194)$$

The **Heisenberg representation** is used here, as explained in 2.2.

Next go to the interaction representation, where H' is treated as the perturbation.

$$e^{-i(H+H')t} = e^{-itH} U(t) \quad (3.195)$$

$$U(t) = e^{itH} e^{-i(H+H')t} \quad (3.196)$$

$$J_\alpha^{(2)}(\mathbf{r}, t) = \langle \psi' | U^\dagger(t) e^{itH} j_\alpha(\mathbf{r}) e^{-itH} U(t) | \psi' \rangle \quad (3.197)$$

The operator $U(t)$ was defined in (2.11) and with a formal solution in (2.15) where the usual definitions are

$$H'(t) = e^{itH} H' e^{-itH} \quad (3.198)$$

$$j(t) = e^{itH} j e^{-itH}, \text{ etc} \quad (3.199)$$

The wave function $|\psi'\rangle$ in (3.194) is the Schrödinger wave function at $t = 0$ for an interacting system with both $H + H'$ as the Hamiltonian. As discussed in Sec. 3.1, the wave function $|\psi\rangle$ is accurate when H' is absent. Using the relation (2.20)

$$|\psi'\rangle = T \exp \left[-i \int_{-\infty}^0 dt' H'(t') \right] |\psi\rangle \quad (3.200)$$

Then the time development of the system is given by combining these result

$$U(t) |\psi'\rangle = T \exp \left[-i \int_{-\infty}^t dt' H'(t') \right] |\psi\rangle = S(t, -\infty) |\psi\rangle \quad (3.201)$$

The expectation value of the current is

$$J_\alpha^{(2)} = \langle \psi | S^\dagger(t, -\infty) j_\alpha(\mathbf{r}, t) S(t, -\infty) | \psi \rangle \quad (3.202)$$

For Kubo formula, only terms linear in H' is required, then

$$S(t, -\infty) | \psi \rangle = \left[1 - i \int_{-\infty}^t dt' H'(t') \right] | \psi \rangle + O(H')^2 \quad (3.203)$$

From (3.202), we have the expectation value of the current operator.

The first term is assumed to vanish

$$\langle \psi | j_\alpha(\mathbf{r}, t) | \psi \rangle = 0 \quad (3.204)$$

since there is usually no current in the solid in the absence of an electric field. The first nonzero term is the one linear in H' , which is the important contribution, and can be expressed as commutator

$$J_\alpha^{(2)}(\mathbf{r}, t) = -i \int_{-\infty}^t dt' \langle \psi | [j_\alpha(\mathbf{r}, t), H'(t')] | \psi \rangle \quad (3.205)$$

With H' given in (3.185), the integrand have

$$\begin{aligned} [j_\alpha(\mathbf{r}, t), H'(t')] &= \frac{i}{\omega} \Xi_\beta e^{-i\omega t'} [j_\alpha(\mathbf{r}, t), j_\beta(\mathbf{q}, t')] \\ &= \frac{i}{\omega} E_\beta(\mathbf{r}, t) e^{-i\mathbf{q}\mathbf{r}} e^{i\omega(t-t')} [j_\alpha(\mathbf{r}, t), j_\beta(\mathbf{q}, t')] \end{aligned} \quad (3.206)$$

Comparing the result with (3.178) shows that

$$\sigma_{\alpha\beta} = \frac{1}{\omega} e^{-i\mathbf{q}\mathbf{r}} \int_{-\infty}^t dt' e^{i\omega(t-t')} \langle \psi | [j_\alpha(\mathbf{r}, t), j_\beta(\mathbf{q}, t')] | \psi \rangle + i \frac{n_0 e^2}{m\omega} \delta_{\alpha\beta} \quad (3.207)$$

The final step is to average over the space variable \mathbf{r} in order to eliminate atomic fluctuations. Take this average by integrating over all volume d^3r and then divide by V . Take the r dependence of the expression¹⁴

$$\int d^3r e^{-i\mathbf{q}\mathbf{r}} j_\alpha(\mathbf{r}, t) = j_\alpha(-\mathbf{q}, t) = j_\alpha^\dagger(\mathbf{q}, t) \quad (3.208)$$

¹⁴ Not Fourier transformation, check (3.183) and (3.185).

Then by change the notation of t , the Kubo formula

$$\sigma_{\alpha\beta}(\mathbf{q}, \omega) = \frac{1}{\omega V} \int_0^\infty dt e^{i\omega t} \langle \psi | [j_\alpha^\dagger(\mathbf{q}, t), j_\beta(\mathbf{q}, 0)] | \psi \rangle + i \frac{n_0 e^2}{m\omega} \delta_{\alpha\beta} \quad (3.209)$$

The wave function $\ket{\psi}$ in (3.209) is the ground state of the many-body Hamiltonian H , which contains all the possible interaction in the solid except the interaction with the vector potential H' . In (3.209), the conductivity has no mention of photon field, since conductivity is an intrinsic property of the ground state of the system. Equation (3.178) can be viewed as a Taylor series in the applied electric field

$$J_\alpha(\Xi_\beta) = J_\alpha(0) + \left(\frac{\partial J_\alpha}{\partial \Xi_\beta} \right) \Xi_\beta^{(ext)} + O^2 \quad (3.210)$$

Where the conductivity is $\sigma_{\alpha\beta} = (\partial J_\alpha / \partial \Xi_\beta)$. It is a characteristic of all linear response correlation functions that they are ground state properties.

The Kubo formulas contain a retarded, two-particle correlation function. The retarded correlation function the current operator based on (3.40)

$$\Pi_{\alpha\beta}(\mathbf{q}, t - t') = -\frac{i}{v} \theta(t - t') \langle \psi | [j_\alpha^\dagger(\mathbf{q}, t), j_\beta(\mathbf{q}, t')] | \psi \rangle \quad (3.211)$$

With Fourier transformation,

$$\Pi_{\alpha\beta}(\mathbf{q}, \omega) = -\frac{i}{v} \int_{-\infty}^{\infty} dt e^{i\omega(t-t')} \theta(t - t') \langle \psi | [j_\alpha^\dagger(\mathbf{q}, t), j_\beta(\mathbf{q}, t')] | \psi \rangle \quad (3.212)$$

we have

$$\sigma_{\alpha\beta}(\mathbf{q}, \omega) = \frac{i}{\omega} \left[\Pi_{\alpha\beta}(\mathbf{q}, \omega) + \frac{n_0 e^2}{m} \delta_{\alpha\beta} \right] \quad (3.213)$$

The conductivity is the **retarded correlation function** of the current multiplied by i and divided by ω . The correlation function $\Pi_{\alpha\beta}(\mathbf{q}, \omega)$ is usually called the **current-current correlation function**. These quantities usually by the Matsubara method and with analytic extension.

The dc conductivity is obtained by taking the limit $\mathbf{q} \rightarrow 0$ and then the limit $\omega \rightarrow 0$. Be careful that wrong answer may be obtained if the order of these limits is reversed.

$$\lim_{\mathbf{q} \rightarrow 0} \begin{cases} \sigma_{\alpha\beta}(\mathbf{q}, \omega) &= \sigma_{\alpha\beta}(\omega) \\ \Pi_{\alpha\beta}(\mathbf{q}, i\omega_n) &= \Pi_{\alpha\beta}(i\omega_n) \\ \Pi_{\alpha\beta}(\mathbf{q}, \omega) &= \Pi_{\alpha\beta}(\omega) \\ j_\alpha(\mathbf{q}, \tau) &= j_\alpha(\tau) \end{cases} \quad (3.214)$$

The limit of $\omega \rightarrow 0$ is more delicate. Here the conductivity is real,

$$\text{Re } \sigma_{\alpha\beta} = - \lim_{\omega \rightarrow 0} \frac{1}{\omega} \text{Im} [\Pi_{\alpha\beta}(\omega)] \quad (3.215)$$

The right-hand side contains the imaginary part of the retarded correlation function which is related to the spectral function of that operator. One thing is that (3.209) is the right Kubo formula at nonzero temperatures.

The current-current correlation function is a **two-particle correlation function**. This correlation function describes how two particles are created and destroyed. The conductivity arises from correlations between these two events. Measure quantities always involve retarded correlation functions of at least two particles. The one-particle Green's function can never be measured in the rigorous sense, since real particles cannot be created or destroyed.

The two-particle correlation function, wherein a particle changes its state, is always found in the correlation functions of linear response. In elementary particle physics, a particle can be absolutely destroyed or created. But this event always happens in conjunction with some other event which involves other particles. For example, electron and positron can mutually annihilate and make several photons. Then one would have terms in the current operator involving the creation or destruction of two particles

$$j_\alpha(\mathbf{q}) = \sum \left[p_\alpha^{(\lambda\delta)} C_\lambda d_\delta + h.c. \right] \quad (3.216)$$

If the particles interact, then the correlation function may not be divided into two independent Green's function

$$\langle T_\tau C_\lambda(\tau) d_\delta(\tau) d_\delta^\dagger(0) C_\lambda^\dagger(0) \rangle \neq \langle T_\tau C_\lambda(\tau) C_\lambda^\dagger(0) \rangle \langle T_\tau d_\delta(\tau) d_\delta^\dagger(0) \rangle \quad (3.217)$$

When taking an electron from a filled band and moving it to an empty or partially filled band, then one has a current operator of the form (3.216), which is used to describe the electron-hole excitation process.

3.8.2 Nonzero Temperature

As time-varying perturbation $H'(t)$ is put into the system at nonzero temperature. The central question concerns the degree to which the thermodynamic averaging is influenced by the time-varying interaction. In Kubo's derivation, the density matrix $\rho_0 = \exp[\beta(\Omega - H + \mu N)]$ applies to the equilibrium system in the absence of $H'(t)$. It is assumed that the system is described by the density matrix at the initial point in the time, $t \rightarrow -\infty$. The perturbation H' is **adiabatically** switched on as the system is brought forward in time to the present. Now the time-dependent density matrix, have the following result

$$\frac{d}{dt}\rho(t) = -i[H + H'(t), \rho(t)] \quad (3.218)$$

$$J_\alpha^{(2)} = \text{Tr}[\rho(t) j_\alpha] \quad (3.219)$$

Kubo's starting point is tantamount to not including $H'(t)$ in the thermodynamic weighting factor. The density matrix is defined as $\rho(t) = \rho_0 + f(t)$, where ρ_0 is the density matrix in the absence of H' . The equilibrium density matrix ρ_0 is time independent,

$$i \frac{d}{dt} f = [H, \rho_0] + [H, f] + [H', \rho_0] + [H', f] \quad (3.220)$$

$$[H, \rho_0] = 0 \quad (3.221)$$

The objective is to solve for the term in $J^{(2)}$, which is proportional to H' , which is treated as infinitesimal. Since f is proportional to H' , it

follows that f is small. Terms proportional to $O(H')^2$, such as $[H', f]$ are neglected, then

$$e^{-itH} \left[i \frac{d}{dt} (e^{itH} f e^{-itH}) \right] e^{itH} = i \frac{d}{dt} f - [H, f] = [H', \rho_0] \quad (3.222)$$

The linear differential equation may be integrated to give

$$f(t) = -i e^{-itH} \left[\int_{-\infty}^t dt' [H'(t'), \rho_0] \right] e^{itH} \quad (3.223)$$

Then the evaluation of (3.219) is ¹⁵

$$J_{\alpha}^{(2)} = \text{Tr} [\rho_0 j_{\alpha}] + \text{Tr} [f(t) j_{\alpha}] \quad (3.224)$$

¹⁵ The derivation in P169 is not so clear to me still

The first term is zero, since it is equilibrium. By changing the terms in the trace, we get the Kubo formula (3.209)

$$J_{\alpha}^{(2)}(\mathbf{r}, t) = -i \int_{-\infty}^t dt' \langle [j_{\alpha}(\mathbf{r}, t), H'(t')] \rangle \quad (3.225)$$

4

Exactly Solvable Models

4.1 Potential Scattering

A very simple problem is an impurity potential $V(r)$ in an otherwise free-particle system. All other interactions are ignored except that of the free particles with the impurity, which is assumed to be at the origin. The potential is assumed to have no internal structure, and spherically symmetric.

The wave function for each particle may be obtained by solving a one-electron Schrödinger equation

$$H\psi_\lambda = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \psi_\lambda = \varepsilon_\lambda \psi_\lambda \quad (4.1)$$

In many-body theory, the impurity problem is usually encountered as a scattering center. The free-particle states are plane wave

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{v}} \sum_{\mathbf{k}} C_{\mathbf{k}\sigma} e^{i\mathbf{k}\mathbf{r}} \quad (4.2)$$

¹ Be careful about the notation of the Fourier transform (2.71).

The Hamiltonian is expressed (without spin index) ¹

$$H = \sum_{\mathbf{k}} C_{\mathbf{k}}^\dagger C_{\mathbf{k}} + \frac{1}{v} \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} C_{\mathbf{k}}^\dagger C_{\mathbf{k}'} \quad (4.3)$$

$$V_{\mathbf{k}\mathbf{k}'} = \int d^3r V(r) e^{-i\mathbf{r}(\mathbf{k}-\mathbf{k}')} = V(\mathbf{k}-\mathbf{k}') \quad (4.4)$$

The object is to diagonalize the Hamiltonian (4.3), which the solutions are of course given by (4.1). However, the problem is not entirely solved. Since the equation is second order, it has two solution. These may be chosen as the ingoing and outgoing waves, or by combination give standing waves. The choices must be related to the scattering problem implied in (4.3).

The integral equation for the wave function is

$$\psi_{\mathbf{k}}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) + \sum_{\mathbf{k}'} \frac{\phi_{\mathbf{k}'}(\mathbf{r})}{\varepsilon_k - \varepsilon_{k'}} \int d^3r' \phi_{\mathbf{k}'}^*(\mathbf{r}') V(r') \psi_{\mathbf{k}}(\mathbf{r}') \quad (4.5)$$

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{v}} e^{i\mathbf{k}\mathbf{r}} \quad (4.6)$$

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m} \quad (4.7)$$

This form of the integral equation is valid for the free-particle states with energy ε_k . For bound states, the energy is changed to the binding energy $\varepsilon_k \rightarrow -\varepsilon_B$ where $\varepsilon_B > 0$ and the term $\psi_{\mathbf{k}}$ on the right is absent.

To prove (4.5) is equivalent to (4.1). Operate on both sides of the equation by $H_0 - \varepsilon_k$,

$$(H_0 - \varepsilon_k) \psi_{\mathbf{k}} = (H_0 - \varepsilon_k) \phi_{\mathbf{k}} + \sum_{\mathbf{k}'} \frac{(H_0 - \varepsilon_k) \phi_{\mathbf{k}'}(\mathbf{r})}{\varepsilon_k - \varepsilon_{k'}} \int d^3r' \phi_{\mathbf{k}'}^*(\mathbf{r}') V(r') \psi_{\mathbf{k}}(\mathbf{r}) \quad (4.8)$$

this gives

$$(H_0 - \varepsilon_k) \psi_{\mathbf{k}} = - \sum_{\mathbf{k}'} \phi_{\mathbf{k}'}(\mathbf{r}) \int d^3r' \phi_{\mathbf{k}'}^*(\mathbf{r}') V(r') \psi_{\mathbf{k}}(\mathbf{r}') \quad (4.9)$$

The completeness relation for the summation over the set of states is

$$\sum_{\mathbf{k}'} \phi_{\mathbf{k}'}(\mathbf{r}) \phi_{\mathbf{k}'}^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \quad (4.10)$$

$$(H_0 - \varepsilon_k) \psi_{\mathbf{k}} = -V(r) \psi_{\mathbf{k}}(\mathbf{r}) \quad (4.11)$$

Then we have the desired answer

$$(H_0 + V - \varepsilon_k) \psi_{\mathbf{k}}(\mathbf{r}) = 0 \quad (4.12)$$

About the boundary conditions, the differential equation (4.1) is second order, so there are two independent solutions. One choice is to have the wave function a standing wave. This leads to the reaction matrix equation. The other choices are the have the wave function an incoming wave or an outgoing wave, which leads to T-matrix theory. The integral equation (4.5) is a convenient starting point for discussion of boundary conditions, since the various choices of standing, outgoing, or ingoing waves are determined only by the complex part of the energy denominator. The factor $\varepsilon_k - \varepsilon_{k'}$, for standing waves, so that the principal part is chosen for the denominator. The factor is $\varepsilon_k - \varepsilon_{k'} + i\delta$ for outgoing waves, and $\varepsilon_k - \varepsilon_{k'} - i\delta$ for ingoing waves.

4.1.1 Reaction Matrix

Here the energy denominator is chosen to be real and given by principal part. The free-particle Green's function is then defined as

$$G_0(\mathbf{k}, \mathbf{r} - \mathbf{r}') = P \sum_{\mathbf{k}'} \frac{\phi_{\mathbf{k}'}(\mathbf{r}) \phi_{\mathbf{k}'}^*(\mathbf{r}')}{\varepsilon_k - \varepsilon_{k'}} = \frac{P}{v} \sum_{\mathbf{k}'} \frac{e^{i\mathbf{k}'(\mathbf{r}-\mathbf{r}')}}{\varepsilon_k - \varepsilon_{k'}} \quad (4.13)$$

$$= P \int \frac{d^3k'}{(2\pi)^3} \frac{e^{i\mathbf{k}'(\mathbf{r}-\mathbf{r}')}}{\varepsilon_k - \varepsilon_{k'}} \quad (4.14)$$

The integral is standard and gives

$$G_0(\mathbf{k}, \mathbf{r} - \mathbf{r}') = \pi \rho(k) \frac{\cos[k|\mathbf{r} - \mathbf{r}'|]}{k|\mathbf{r} - \mathbf{r}'|} \quad (4.15)$$

Where the density of states of the particles

$$\rho(k) = \int \frac{d^3k'}{(2\pi)^3} \delta(\varepsilon_k - \varepsilon_{k'}) = \frac{mk}{2\hbar^2 \pi^2} \quad (4.16)$$

The Green's function may be expanded as a function of \mathbf{r} and \mathbf{r}'

$$G_0(\mathbf{k}, \mathbf{r} - \mathbf{r}') = \pi \rho(k) \sum_l (2l+1) P_l(\hat{\mathbf{r}} \cdot \hat{\mathbf{r}}') j_l(kr_<) \eta_l(kr_>) \quad (4.17)$$

where the notation $r_<$ is the smaller of \mathbf{r} and \mathbf{r}' . The $j_l(kr)$ and $\eta_l(kr)$ are the spherical Bessel functions of the first and second kind, and $P_l(\cos \theta)$ are the Legendre functions. ² With (4.5), we have

² [wiki:Bessel function](#) and [wiki:Legendre function](#)

$$\psi_{\mathbf{k}}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) + \int d^3r' G_0(\mathbf{k}, \mathbf{r} - \mathbf{r}') V(r') \psi_{\mathbf{k}}(\mathbf{r}') \quad (4.18)$$

An important identity is the following, introducing the **angular momentum components** l , the plane wave may be expanded as

$$e^{i\mathbf{k} \cdot \mathbf{r}} = \sum_l (2l+1) i^l P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}) j_l(kr) \quad (4.19)$$

for the actual wave function

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_l (2l+1) i^l P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}) R_l(kr) \quad (4.20)$$

The radial function $R_l(kr)$ satisfied the **radial Schrödinger equation** of the form

$$-\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial R}{\partial r} \frac{l(l+1)}{r^2} R \right] + [V(r) - \varepsilon_k] R = 0 \quad (4.21)$$

which does not determine the boundary conditions. Using the fact that,

$$\int d\Omega_r P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}) P_m(\hat{\mathbf{r}} \cdot \hat{\mathbf{p}}) = \frac{4\pi}{2l+1} \delta_{lm} P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{p}}) \quad (4.22)$$

to reduce the equation down to one which involves only the same angular momentum component,

$$\begin{aligned}
 R_l(kr) &= j_l(kr) + 4\pi^2\rho(k) \int_0^\infty r'^2 dr' j_l(kr_{<}) \eta_l(kr_{>}) V(r') R_l(kr') \\
 &= j_l(kr) + 4\pi^2\rho(k) \left[\eta_l(kr) \int_0^r r'^2 dr' j_l(kr') V(r') R_l(kr') \right. \\
 &\quad \left. + j_l(kr) \int_r^\infty r'^2 dr' \eta_l(kr') V(r') R_l(kr') \right] \quad (4.23)
 \end{aligned}$$

It is important that the potential is spherically symmetric. Otherwise the scattering term would mix angular momentum components, which make it hard to solve.

The solution is examined in the limit as $kr \rightarrow \infty$. From (4.21) it can be shown that the radial wave function must asymptotically approach the value

$$\lim_{kr \rightarrow \infty} R_l(kr) \rightarrow \frac{C_l(k)}{kr} \sin \left[kr + \delta_l(k) - \frac{l\pi}{2} \right] \quad (4.24)$$

The prefactor C_l is determined below. The asymptotic limit of the integral equation (4.23) is

$$\lim_{kr \rightarrow \infty} R_l(kr) \rightarrow j_l(kr) + D_l(k) \eta_l(kr) \rightarrow \frac{\sin(kr - l\pi/2)}{kr} - D_l \frac{\cos(kr - l\pi/2)}{kr} \quad (4.25)$$

where

$$D_l(k) = 4\pi^2\rho(k) \int_0^\infty r^2 dr j_l(kr) V(r) R_l(kr) \quad (4.26)$$

The potential $V(r)$ is assumed to be of short range: **It falls off faster than r^{-2} at large distance.** The scattering is then described by a phase shift $\delta_l(k)$ which depends on angular momentum and wave vector. The two asymptotic expansions (4.24) and (4.25) must be identical, which means

$$D_l = -\tan(\delta_l) = 4\pi^2\rho(k) \int_0^\infty r^2 dr j_l(kr) V(r) R_l(kr) \quad (4.27)$$

The complicated integral just defines the tangent of the phase shift.

Then (4.25) becomes

$$\lim_{kr \rightarrow \infty} R_l(kr) \rightarrow \frac{1}{kr \cos(\delta_l)} [\cos(\delta_l) \sin(kr - l\pi/2) + \sin(\delta_l) \cos(kr - l\pi/2)] = \frac{\sin(kr + \delta_l l\pi/2)}{kr \cos(\delta_l)} \quad (4.28)$$

The normalization coefficient in (4.24) is

$$C_l = \frac{1}{\cos(\delta_l)} \quad (4.29)$$

When solving the radial wave function (4.21), the solution is obtained which is well behaved at the origin. This solution is followed outward

in r until the region is reached where $V(r) \approx 0$ and the centrifugal barrier $\hbar^2 l(l+1)/(2mr^2)$ is small. Then the solution has the form (4.24) with $C_l = 1/\cos(\delta_l)$. The wave function is now properly normalized at large r , and by following it back toward the origin it is normalized everywhere. These steps provide the proper solution to the scattering equation (4.5) which was the starting point in the calculation.

The reaction matrix is defined as the quantity

$$R_{\mathbf{k}'\mathbf{k}} = \int d^3\mathbf{r} \phi_{\mathbf{k}'}^*(\mathbf{r}) V(r) \psi_{\mathbf{k}}(\mathbf{r}) \quad (4.30)$$

Expanding in angular momentum state by using the expansions for the wave function and the plane wave, the angular integrals give

$$R_{\mathbf{k}'\mathbf{k}} = 4\pi \sum_l (2l+1) P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}') R_l(k', k) \quad (4.31)$$

where the radial integral is

$$R_l(k', k) = \int_0^\infty r^2 dr j_l(k'r) V(r) R_l(kr) \quad (4.32)$$

It is defined for the general case where $k' \neq k$. And if they are equal, the answer is just (4.27)

$$R_l(k, k) = -\frac{\hbar^2 \tan(\delta_l)}{2mk} \quad (4.33)$$

The reaction matrix obeys an integral equation which is deduced by putting (4.30) into the integral equation (4.5) for $\psi_{\mathbf{k}}(\mathbf{r})$

$$R_{\mathbf{k}'\mathbf{k}} = V_{\mathbf{k}'\mathbf{k}} + P \sum_{\mathbf{k}_1} \frac{V_{\mathbf{k}'\mathbf{k}_1} R_{\mathbf{k}_1\mathbf{k}}}{\varepsilon_k - \varepsilon_{k_1}} \quad (4.34)$$

5

Homogeneous Electron Gas

5.1 Exchange and Correlation

The homogeneous electron gas is describe by the Hamiltonian

$$\begin{aligned}
 H &= \sum_{\mathbf{p}\sigma} \varepsilon_{\mathbf{p}} C_{\mathbf{p}\sigma}^{\dagger} C_{\mathbf{p}\sigma} + \frac{1}{2V} \sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'} \sum_{\mathbf{q}\neq 0} v_{\mathbf{q}} C_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger} C_{\mathbf{k}'-\mathbf{q}\sigma'}^{\dagger} C_{\mathbf{k}'\sigma'} C_{\mathbf{k}\sigma} \quad (5.1) \\
 \varepsilon_p &= \frac{p^2}{2m} \\
 v_q &= \frac{4\pi e^2}{q^2} \quad (5.2)
 \end{aligned}$$

which was derived in (??). The free electrons mutually interact by Coulomb's law. This N_e electrons in a volume V with the average density $n_0 = \frac{N_e}{V}$. A positive charge of density n_0 is spread uniformly through the volume make the system charge neutrality. The homogeneous electron gas is also called the **jellium model** of a solid.

The parameter r_s is universally used to describe the density of an electro gas,

$$\frac{4\pi n_0 a_0^3}{3} r_s^3 = 1 \quad (5.3)$$

where a_0 is the Bohr radius. r_s is small for high-density electron gas and it is large for a low-density gas. The density may related to the Fermi vector,

$$n_0 = 2 \int \frac{d^3 p}{(2\pi)^3} \eta_p = \frac{1}{\pi^2} \int_0^{k_F} p^2 dp = \frac{k_F^3}{3\pi^2} \quad (5.4)$$

so the Fermi wave vector and energy are related to r_s ,

$$\begin{aligned}
 k_F a_0 &= \frac{1.9192}{r_s} \\
 E_F &= \frac{3.6832}{r_s^2} E_{ry}, \quad E_{ry} = 13.60 eV \quad (5.5)
 \end{aligned}$$

The plasma frequency is

$$\hbar\omega_p = \hbar \sqrt{\frac{4\pi e^2 n_0}{m}} \quad (5.6)$$

In homogeneous electron gas, the average kinetic energy of the electrons is going to be proportional to $\langle E_F \rangle \sim k_F^2$. Which by dimension analysis, we have $\langle E_F \rangle \propto 1/r_s^2$. For the Coulomb energy $\langle v_p \rangle \propto 1/r_s$. When the electron gas is sufficiently high, r_s is small, the kinetic energy term will be larger than the potential energy term, which means electrons behaves like the free particles.

5.1.1 Kinetic energy

The first energy term is kinetic energy. The contribution to the ground state energy is obtained by summing over all particles in the ground state

$$\begin{aligned} E &= \sum_{p\sigma} \varepsilon_p n_p = 2V \int \frac{d^3p}{(2\pi)^3} \frac{p^2}{2m} \eta_p = \left(\frac{N_e}{n_0} \right) \frac{1}{2\pi^2 m} \int_0^{k_F} p^4 dp \\ &= \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} N_e = \frac{3}{5} E_F N_e = \frac{2.2099}{r_s^2} E_{ry} N_e \end{aligned} \quad (5.7)$$

The average kinetic energy is $\frac{3}{5} E_F$, which is given in terms of r_s .

5.1.2 Hartee

All the remaining terms in the energy come from the Coulomb interaction between the particles. *The first term which occurs is the Coulomb interaction between the electrons and the uniform positive background*, which is called the **Hartee interaction**. In the model of the homogeneous electron gas, the time-averaged electron density is uniform throughout the system, as is the positive background. These equal and opposite charge cancel each other, and Hartree energy is zero. The energy is

$$N_e E_0 = \frac{e^2}{2} \int \frac{d^3r_1 d^3r_2}{|\mathbf{r}_1 - \mathbf{r}_2|} [\rho_e(\mathbf{r}_1) - \rho_i(\mathbf{r}_1)] [\rho_e(\mathbf{r}_2) - \rho_i(\mathbf{r}_2)] \quad (5.8)$$

but the ion and electron are $\rho_e = \rho_i = n_0$, then the contribution is zero. This fact has already been used in (5.1) by omission of the $\mathbf{q} = 0$ term from the Coulomb interaction. The $\mathbf{q} = 0$ term is the direct Coulomb interaction among the electrons, and it is omitted because it is canceled by the direct interaction with the positive background.

5.1.3 Exchange

The Coulomb interaction in (5.1) provide other energy contributions in addition to the direct term. For Hartee term the corresponding H is given

$$\sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'} \langle C_{\mathbf{k}+\mathbf{q},\sigma}^\dagger C_{\mathbf{k}'-\mathbf{q},\sigma'}^\dagger C_{\mathbf{k}',\sigma'} C_{\mathbf{k},\sigma} \rangle \approx \delta_{\mathbf{q}=0} \sum_{\mathbf{k}\sigma} \langle C_{\mathbf{k},\sigma}^\dagger C_{\mathbf{k},\sigma} \rangle \sum_{\mathbf{k}'\sigma'} \langle C_{\mathbf{k}',\sigma'}^\dagger C_{\mathbf{k}',\sigma'} \rangle \quad (5.9)$$

Another way to pair the same operator gives

$$\approx - \sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'} \langle C_{\mathbf{k}+\mathbf{q},\sigma}^\dagger C_{\mathbf{k}',\sigma'} \rangle \langle C_{\mathbf{k}'-\mathbf{q},\sigma'}^\dagger C_{\mathbf{k},\sigma} \rangle = - \sum_{\mathbf{k}\sigma} n_{\mathbf{k}+\mathbf{q}} n_{\mathbf{k}} \quad (5.10)$$

This require that $\sigma' = \sigma$ and $\mathbf{k}' = \mathbf{k} + \mathbf{q}$. This term is called **exchange energy (Fock energy)**. *Retaining both terms is called Hartree-Fock*. The exchange term was derived in (2.64), it gives a contribution to the energy of an individual electron, as well as a contribution to the ground state energy of the collection of electrons. **For per electron,**

$$\Sigma_x(k) = - \frac{1}{V} \sum_{\mathbf{q}} v_{\mathbf{q}} n_{\mathbf{k}+\mathbf{q}} \quad (5.11)$$

$$E_{gx} = - \sum_{\mathbf{k}\mathbf{q}\sigma} \frac{v_{\mathbf{q}}}{2V} n_{\mathbf{k}+\mathbf{q}} n_{\mathbf{k}} = \frac{1}{2N_e} \sum_{\mathbf{k}\sigma} n_{\mathbf{k}} \Sigma_x(k) \quad (5.12)$$

The self-energy $\Sigma_x(k)$ depends only on the magnitude of the wave vector k of the particle and gives

$$\begin{aligned} \Sigma_x(k) &= - \int \frac{d^3p}{(2\pi)^3} \frac{4\pi e^2}{|\mathbf{p} - \mathbf{k}|^2} n_p \\ &= - \frac{e^2}{\pi} \int_0^{k_F} p^2 dp \int_{-1}^1 \frac{d \cos \theta}{k^2 + p^2 - 2pk \cos \theta} \\ &= - \frac{e^2 k_F}{\pi} \left(1 + \frac{1-y^2}{2y} \ln \left| \frac{1+y}{1-y} \right| \right) \end{aligned} \quad (5.13)$$

$$y = \frac{k}{k_F} \quad (5.14)$$

A particle at the Fermi energy $k = k_F$ has

$$\Sigma_x(k_F) = - \frac{e^2 k_F}{\pi} \quad (5.15)$$

It is convenient to write

$$\Sigma_x(k) = \frac{e^2 k_F}{\pi} S(y) \quad (5.16)$$

$$S(y) = - \left(1 + \frac{1-y^2}{2y} \ln \left| \frac{1+y}{1-y} \right| \right) \quad (5.17)$$

where $S(y)$ is a function which gives the wave vector dependence of the exchange energy. The behaviour of the function is in shown in Figure 5.1.

The derivative has a logarithmic divergence as $y \rightarrow 1$. This fact is interesting because it predicts that the effective mass is zero. The effective mass of a particle defined in (3.76). Since the exchange self-energy is not frequency dependent, the effective mass is

$$\left(\frac{m}{m^*} \right) = 1 + \partial_{\varepsilon_k} \Sigma_x(k) = \frac{e^2 m}{2\pi k_F} \frac{1}{y^2} \left(\frac{1+y^2}{y} \ln \left| \frac{1+y}{1-y} \right| - 1 \right) \quad (5.18)$$

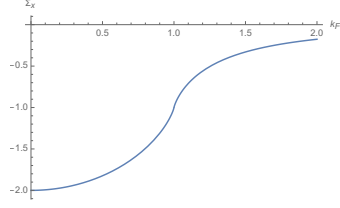


Figure 5.1: Exchange energy.

which diverges at Fermi energy $y \rightarrow 1$. If the inverse effective mass really diverged at the Fermi surface, it would have several observable consequences. The electron gas would be unstable at low temperatures, and the specific heat would diverge. Further terms in the perturbation theory produces another divergence in the effective mass which exactly cancels the one due to exchange. The effective mass and specific heat are not divergent.

The exchange energy contribution to the ground state energy is obtained from (5.12). Summing over spin gives an expression

$$\begin{aligned} E_{gx} &= \frac{1}{N_e} \sum_{\mathbf{k}} n_{\mathbf{k}} \Sigma_x(k) = \frac{1}{n_0} \int \frac{d^3k}{(2\pi)^3} n_{\mathbf{k}} \Sigma_x(k) \\ &= -\frac{3}{4} \frac{e^2 k_F}{\pi} \end{aligned} \quad (5.19)$$

The average exchange energy per electron is $\frac{3}{2}$ of the value at the Fermi energy. In terms of the parameter r_s , the total ground state exchange energy per electron is

$$E_{gx} = -\frac{3}{2\pi} (k_F a_0) \left(\frac{e^2}{2a_0} \right) = -\frac{0.9163}{r_s} \quad (5.20)$$

So far two terms have been found for the energy of the particle,

$$E(k) = \frac{\hbar^2 k^2}{2m} + \Sigma_x(k) + \dots \quad (5.21)$$

The corresponding two terms for the ground state energy per particle are,

$$E_g = \frac{2.2099}{r_s^2} - \frac{0.9163}{r_s} + \dots \quad (5.22)$$

The ground state energy has the appearance of a power series, in increasing powers of r_s . Although it is usually unsafe to extrapolate from just two terms, in fact E_g is a series in r_s . The next term will be of order $O(r_s^0)$. The zeroth power could be interpreted as either a constant or as $\ln(r_s)$. The series have the form

$$E_g = \frac{2.2099}{r_s^2} - \frac{0.9163}{r_s} - 0.094 + 0.0622 \ln(r_s) + \dots \quad (5.23)$$

The above energy terms comprise the Hartree-Fock theory. It is defined to be the kinetic energy, the Hartree energy which is zero,

and the exchange energy. The total ground state energy per particle is written with correlation energy,

$$E_g = \frac{2.2099}{r_s^2} - \frac{0.9163}{r_s} + E_c \quad (5.24)$$

where the correlation energy E_c needs to be determined. The result

$$E_c = -0.094 + 0.0622 \ln(r_s) + O(r_s) \quad (5.25)$$

is convergence when $r_s \leq 1$.

5.1.4 Seitz's Theorem

The theorem of Seitz relates the ground state energy to the chemical potential. The chemical potential is defined as the energy it takes to add or remove an electron from the material. It is the energy which divides the empty from the occupied states at zero temperature. Of course, it is just the Fermi energy of the metal. The chemical potential is the energy of an electron of momentum k_F

$$\mu = \frac{\hbar^2 k_F^2}{2m} + \Sigma_x(k_F) + \text{Re } \Sigma_c(k_F, 0) \quad (5.26)$$

where $ik_n = 0$ is the chemical potential. The chemical potential μ is only a function of the electron n_0 . The theorem of Seitz is

$$\mu(n_0) = \frac{d}{dn_0} [n_0 E_g(n_0)] = E_g + n_0 \frac{dE_g}{dn_0} \quad (5.27)$$

The proof, by definition of chemical potential

$$\mu = E_T(N_e + 1) - E_T(N_e) \quad (5.28)$$

The total energy for N_e particle system is $E_T = N_e E_g$ for a fixed volume since the E_g is the function of density,

$$\begin{aligned} E_T(N_e + 1) &= (N_e + 1) E_g(n_0 + 1/V) = (N_e + 1) \left(E_g(n_0) + \frac{1}{V} \frac{dE_g}{dn_0} \right) \\ &= N_e E_g + E_g(n_0) + n_0 \frac{dE_g}{dn_0} + O\left(\frac{1}{V}\right) \end{aligned} \quad (5.29)$$

In proving the theorem, the volume V is kept fixed, as is the amount of positive charge. The $N_e + 1$ particle system has a slight charge imbalance, but it is negligible to the contribution of energy. Considering a body of average dimension L is uniformly charged with on unit of charge, the Coulomb energy is of order e^2/L . This contribution is negligible when L is large.

The chemical potential is the negative of the work function. It is the energy required to remove an electron from the solid and take

it to infinity with zero kinetic energy. However, there is a surface correction to the work function, but not to volume part of the ground state energy per particle.

$$E_T = N_e E_g + A E_S \quad (5.30)$$

where A is the total surface area and E_S is the energy per unit surface area. For macroscopic bodies, E_g does not depend on the surface area. However, μ does have a term which depends on the surface—actually on the surface dipole layer, $\mu = \mu_B + \Delta\mu$. The theorem of Seitz actually just works on μ_B . In Hartree-Fock approximation the chemical potential gives for the bulk contribution,

$$\mu_{B,HF} = \frac{d}{dn_0} (n_0 E_{g,HF}) = E_F - \frac{e^2 k_F}{\pi} \quad (5.31)$$

5.1.5 Σ^{2a}

The exchange energy calculated involve one Coulomb line. The correlation energy is the sum of all contribution with two or more Coulomb lines. There are three diagrams with two Coulomb line.

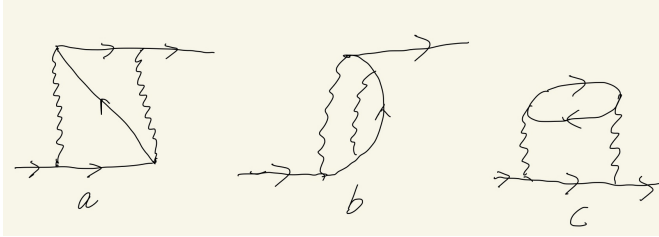


Figure 5.2: Diagrame

For Figure 5.2a, the self-energy contribution is

$$\Sigma^{2a}(k) = \frac{1}{V^2 \beta^2} \sum_{\mathbf{q}\mathbf{q}'} v_q v_{q'} \sum_{i\mathbf{q}_n, i\mathbf{q}_{n'}} \mathcal{G}^0(k+\mathbf{q}) \mathcal{G}^0(k+\mathbf{q}') \mathcal{G}^0(k+\mathbf{q}+\mathbf{q}') \quad (5.32)$$

according (3.94) and calculation, we have

$$\begin{aligned} \Sigma^{2a}(k) &= -\frac{1}{V^2} \sum_{\mathbf{q}\mathbf{q}'} \frac{v_q v_{q'}}{ik_n + \xi_{\mathbf{k}+\mathbf{q}+\mathbf{q}'} - \xi_{\mathbf{k}+\mathbf{q}'} - \xi_{\mathbf{k}+\mathbf{q}}} \\ &= \left[\eta_F(\xi_{\mathbf{k}+\mathbf{q}'}) \left(\eta_F(\xi_{\mathbf{k}+\mathbf{q}}) - \eta_F(\xi_{\mathbf{k}+\mathbf{q}+\mathbf{q}'}) \right) \right. \\ &\quad \left. + \eta_F(\xi_{\mathbf{k}+\mathbf{q}+\mathbf{q}'}) (1 - \eta_F(\xi_{\mathbf{k}+\mathbf{q}})) \right] \end{aligned} \quad (5.33)$$

The self-energy of a particle is needed on the Fermi surface. Set $k = k_F$ and $ik_n = \xi_{k_F} = k_F^2/2m - \mu = 0$. The terms in the energy denominator largely cancel,

$$\xi_{\mathbf{k}} + \xi_{\mathbf{k}+\mathbf{q}+\mathbf{q}'} - \xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}+\mathbf{q}'} = \frac{\mathbf{q} \cdot \mathbf{q}'}{m} \quad (5.34)$$

The self-energy is

$$\begin{aligned}\Sigma^{2a}(k_F, 0) &= -\frac{(4\pi e^2)^2 m}{(2\pi)^6} \int \frac{d^3 q}{q^2} \int \frac{d^3 q'}{(q')^2} \frac{1}{\mathbf{q} \cdot \mathbf{q}'} \\ &\times \left\{ \eta_F(\xi_{\mathbf{k}+\mathbf{q}}) \left[\eta_F(\xi_{\mathbf{k}+\mathbf{q}}) - \eta_F(\xi_{\mathbf{k}+\mathbf{q}+\mathbf{q}'}) \right] + \dots \right\} \quad (5.35)\end{aligned}$$

The quantity on the right is independent of the electron density.

The integral is convergent and give nonzero result. It contribute the constant term in E_c . With further calculation by Onsager, we have

$$\Sigma^{2a} = \frac{1}{3} \ln(2) - \frac{3}{2\pi^2} \zeta(3) = 0.0436 \quad (5.36)$$

5.1.6 Σ^{2b}

The second self-energy term involving two Coulomb lines is shown in Figure 5.2b, this contribution can be shown equal to zero. Consider the summation of the similar diagrams, all terms may be summed by evaluating the exchange energy with an electron Green's function in the self-energy which includes the exchange energy. This summation is given by the self-energy

$$\Sigma'_x(k) = -\frac{1}{V\beta} \sum_{\mathbf{q}, ik_n} v_q \mathcal{G}(\mathbf{k} + \mathbf{q}, ik_n) \quad (5.37)$$

$$\mathcal{G}(\mathbf{k} + \mathbf{q}, ik_n) = \frac{1}{ik_n - \xi_{\mathbf{k}+\mathbf{q}} - \Sigma_x(\mathbf{k} + \mathbf{q})} \quad (5.38)$$

where the Green's function has a self-energy due to exchange.

chapter Optical Properties of Solids

5.2 Wannier Excitons

5.2.1 The Model

Exciton states play an extremely important role in the understand of interband transitions in semiconductors. The word exciton is used to signify the modification of the *absorption rate of phonons due the the Coulomb interaction between the electron and the valence band hole*.

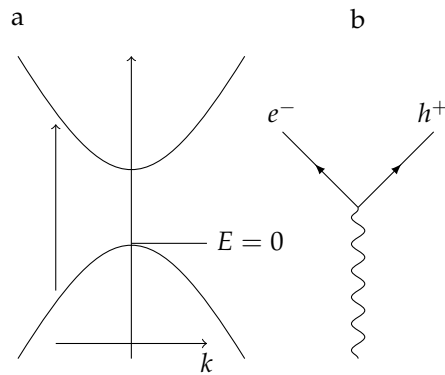


Figure 5.3: Optical transition in a semiconductor between occupied valence band and empty conduction band for a direct transition. (a) Conventional band picture; (b) Wannier picture where the photon makes an electron-hole.

The easiest case is shown in Fig. 5.3(a), the interband transition is direct. The valence band states are all filled and the conduction band states are all empty. The vertical arrow show a possible interband transition which can occur when a photon is absorbed in the solid. The valence state is shown as nondegenerate (except for spin) at $\mathbf{k} = 0$, although that is seldom the case; usually the band has an orbital degeneracy and is anisotropic.

The point of view in Fig. 5.3(a) is a single-particle picture of the transition process. The transition rate for the absorption of photons is given by golden rule

$$A(\omega) = \frac{2\pi}{\hbar V} \sum_{\mathbf{k}\mathbf{k}'} |\langle c, \mathbf{k}' | \hat{\epsilon} \cdot \mathbf{p} | v, \mathbf{k} \rangle|^2 \delta[\varepsilon_v(\mathbf{k}) + \hbar\omega - \varepsilon_c(\mathbf{k}')] \quad (5.39)$$

$$\varepsilon_v(\mathbf{k}) = -\frac{\hbar^2 k^2}{2m_v}, \quad \varepsilon_c(\mathbf{k}) = E_g + \frac{\hbar^2 k^2}{2m_c} \quad (5.40)$$

The energy zero is chosen to be the top of the valence band. The matrix element is between the one-electron initial and final states. The wave function are taken to be Bloch function $u_{\mathbf{k}}(\mathbf{r}) \otimes \exp(i\mathbf{k}\mathbf{r})$. For discussion reason assume the cell-periodic parts as independent of wave vector \mathbf{k} , and assumed that the valence band has p symmetry and conduction band has s symmetry. Then $u_v(\mathbf{r})$ is a periodic orbital with angular momentum $l = 1$, while $u_c(\mathbf{r})$ is $l = 0$. With these

approximations the optical matrix element is a constant except for wave vector conservation

$$|v, \mathbf{k}\rangle = u_v(\mathbf{r}) \frac{e^{i\mathbf{k}\mathbf{r}}}{\sqrt{V}} \quad (5.41)$$

$$|c, \mathbf{k}'\rangle = u_v(\mathbf{r}) \frac{e^{i\mathbf{k}'\mathbf{r}}}{\sqrt{V}} \quad (5.42)$$

$$\langle c, \mathbf{k}' | \hat{\mathbf{p}} | v, \mathbf{k} \rangle \equiv \hat{\mathbf{p}}_{cv} \delta_{\mathbf{k}\mathbf{k}'} \quad (5.43)$$

$$\hat{\mathbf{p}} = \frac{1}{V} \int_{cell} d^3r u_c^* \hat{\mathbf{p}} u_v \quad (5.44)$$

neglect the wave vector \mathbf{q} for photons since it is in the optical frequencies.

$$A(\omega) = |\hat{\mathbf{p}}_{cv}|^2 \frac{(2\mu)^{3/2}}{2\pi} \sqrt{\hbar\omega - E_g} \Theta(\hbar\omega - E_g) \quad (5.45)$$

with $\mu^{-1} = m_c^{-1} + m_v^{-1}$. Equation (5.43) predicts that the absorption rate begins at the energy gap of semiconductor and rise as the square root of factor of optical frequency. But this is not observed, in fact, the one-particle theory is totally inadequate.

Wannier observed that the interband transition in semiconductors was really a **two-particle process**, as in Fig.5.3(b). In this new picture, the electron and hole are particles with charges of opposite sign, so that there is a Coulomb attraction $-\frac{2}{\epsilon_0 r}$ between them, where ϵ_0 is the static dielectric function. The dielectric function is assumed to be a constant which is independent of the frequency.¹ The attractive Coulomb interaction between the electron and hole can cause hydrogenic bound states between them.

The optical absorption rate for this process was calculated by Elliott. The final state of the system is described by a two-particle Schödinger equation

$$\Psi(\mathbf{r}_e, \mathbf{r}_h) = u_c(\mathbf{r}_e) u_v(\mathbf{r}_h) \Phi(\mathbf{r}_e, \mathbf{r}_h) \quad (5.46)$$

$$0 = \left[-\frac{\hbar^2 \nabla_e^2}{2m_c} - \frac{\hbar^2 \nabla_h^2}{2m_v} - \frac{e^2}{\epsilon_0 |\mathbf{r}_e - \mathbf{r}_h|} - E \right] \Phi(\mathbf{r}_e, \mathbf{r}_h) \quad (5.47)$$

$\Phi(\mathbf{r}_e, \mathbf{r}_h)$ can be factored into relative $\mathbf{r} = \mathbf{r}_e - \mathbf{r}_h$ and center of mass coordinate $M = m_c + m_v$ in standard fashion

$$\mathbf{R} = \frac{m_c \mathbf{r}_e + m_v \mathbf{r}_h}{M} \quad (5.48)$$

$$\Phi(\mathbf{r}_e, \mathbf{r}_h) = \frac{e^{i\mathbf{P}\mathbf{R}}}{\sqrt{V}} \phi(\mathbf{r}) \quad (5.49)$$

$$0 = \left(-\frac{\hbar^2}{2\mu} \nabla^2 - \frac{e^2}{\epsilon_0 r} - \epsilon_r \right) \phi(\mathbf{r}) \quad (5.50)$$

$$E = E_g + \epsilon_r + \frac{p^2}{2M} \quad (5.51)$$

¹ This is a poor approximation, since most semiconductors are polar and dielectric function has significant dispersion at frequencies near the optical phonon frequencies, see ??

The center of mass motion is plane-wave-like, with a wave vector \mathbf{P} which in optical experiments is equal to the photon wave vector. This is usually small and set $\mathbf{P} = 0$. For relative energy $\varepsilon_r < 0$, the two particles form bound hydrogenic states with energy $\varepsilon_r = \varepsilon_n = -\frac{E_R}{n^2}$. For relative energy greater than zero, the form scattering states $\phi_{\mathbf{k}}(\mathbf{r})$. Elliott showed that the optical transition rate depends on the relative wave function $br = 0$. Instead of (5.43), the transition rate is

$$A(\omega) = \frac{2\pi}{\hbar} |\hat{\mathbf{p}}_{cv}|^2 \sum_j |\phi_j(0)|^2 \delta(\hbar\omega - E_g - \varepsilon_j) \quad (5.52)$$

The summation j run over the bound and continuum states.

The relative motions of electron and hole are in s-wave hydrogenic state, either bound or unbound, because of the angular momentum selection rule. The one-unit change in l , in the photon absorption, is take by the change of band symmetry, and the relative motion is not permitted any additional angular momentum. For s states, the bound states have an amplitude given by the principal quantum number n and the Bohr radius a_0 ,

$$\phi_n(0) = \frac{1}{\sqrt{\pi a_0^3 n^3}} \quad (5.53)$$

For continuum states, with energy $\varepsilon_k = \frac{k^2}{2\mu}$, the relative wave function at the origin is

$$\psi_{k,l=0}(0) = \frac{2\pi\eta}{V [2 - e^{-2\pi\eta}]} \quad (5.54)$$

where $\eta^{-1} = ka_0$. Then (5.51) predicts that the absorption is a constant in frequency at the energy gap E_g , and does not rise with a square root dependence. The absorption function now have a few sharp, distinct exciton lines at low frequency correspond to $1s$, $2s$, etc. These absorption bands are very strong, and all the light is attenuated before trasversing the sample. At higher frequencies, the ns stats are closer in frequency and are broadened and merges with the continuum absorption which starts at $\hbar\omega = E_g$.

5.2.2 Solution by Green's Functions

6

Superconductivity

The theory of superconductivity was formulated by Bardeen, Cooper, and Schrieffer (1957) and is called the BCS theory. It very successfully describes the superconducting properties of weak superconductors, such as aluminum, which are weak because of the small strength of electron-phonon interaction. Further refinement of the theory have led to strong coupling theory of Eliashberg, which describes the properties of superconductor lead. The distinction is roughly determined by the value of the electron-phonon mass enhancement factor λ shown by McMillan.

The basic idea of BCS theory is that the electrons in the metal form bound pairs. This bound states of electron pairs are not described by simple orbitals such as hydrogen atom. The pair state and entire ground state of the superconductor requires a many-body description.

Fröhlich was the first to realize that electrons could interact by exchanging phonons and that this interaction could be attractive. Another piece in theoretical puzzle was supplied by Schafroth, who shown that a charged boson gas, when undergoing a Bose-Einstein condensation would exhibit many of superconducting properties such as Meissner effect. In the BCS theory, the electron pairs behave in some respects as bosons.

6.1 Cooper Instability

Cooper pointed out that the ground state of a normal metal was unstable at zero temperature. A normal metal is defined as one which is neither superconducting nor magnetic. The demonstration of an instability does not provide a description of superconducting state, but it suggest that the instability was caused by the scattering between pairs of electrons, where the scattering potential is the exchange of phonons.

The scattering process as shown [6.1](#). The screened interaction

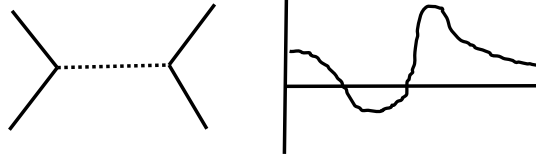


Figure 6.1: Scattering process and potential

between two electrons was derived before as

$$V_s(\mathbf{q}, \omega) = \frac{v_q}{\epsilon(\mathbf{q}, \omega)} + \frac{2\omega\lambda M_{\mathbf{q}}^2}{\epsilon(\mathbf{q})^2 [\omega^2 - \omega_{\lambda}(\mathbf{q})^2]} \quad (6.1)$$

The first is the screened Coulomb interaction. The theory of superconductivity is applied at low temperatures, where the energy exchanged between particles, while scattering, is also low. The requirements of crystal stability require that this interaction be repulsive at zero frequency.

The second term in (6.1) is the screened electron-phonon interaction. It is on the average weaker than the repulsive Coulomb interaction. However, for frequency near to Debye ($\omega < \omega_D$) the energy denominator becomes small and negative, which causes a relatively large interaction over this narrow range of frequency. It may be possible for two electrons to bind if they can construct a relative wave function which selectively uses the frequency region which is attractive.

For simplicity instead of (6.1) use a interaction model

$$V_s(\mathbf{q}, \omega) = \begin{cases} -V_0 & |\xi_q| < \omega_D \\ 0 & |\xi_q| > \omega_D \end{cases} \quad (6.2)$$

This potential is constant and attractive up to a cutoff energy which is of the order of the Debye energy ω_D of the solid.

The Cooper's model of a normal metal at low temperature was a free-electron system. The electrons are allowed to have a weak attractive interaction as in (6.2). Consider the mutual scattering of two electrons. Assume they initially have states of equal and opposite momentum, \mathbf{k} and $-\mathbf{k}$. It is also assumed the particles have opposite spin that exchange scattering does not occur¹. The interaction poten-

¹ P298 Hatree fock approximation

tial does not flip the electron spin and the spin states are preserved in the scattering process.

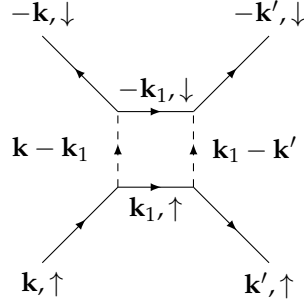


Figure 6.2: Scattering event between two electron lines.

In Figure 6.2 show a double scattering event between two electron lines which are moving in the same direction in time. This process is the scattering in the second **Born approximation**, where the first Born approximation is shown in Fig. 6.1. The effective scattering in the first and second Born approximation is

$$V_{eff}(\mathbf{k} - \mathbf{k}') = V(\mathbf{k} - \mathbf{k}') + \int \frac{d^3 k_1}{(2\pi)^3} \frac{V(\mathbf{k} - \mathbf{k}_1)V(\mathbf{k}_1 - \mathbf{k}')}{2\zeta_{\mathbf{k}} - 2\zeta_{\mathbf{k}_1}} \left([1 - \eta_F(\zeta_{\mathbf{k}_1})] [1 - \eta_F(\zeta_{\mathbf{k}})] - \eta_F(\zeta_{\mathbf{k}_1})^2 \right) \quad (6.3)$$

The second term on the right is the contribution of Fig. 6.2. The denominator contains the initial state energy minus the intermediate state energy. The factors $[1 - \eta_F(\zeta_{\mathbf{k}_1})]^2 - \eta_F(\zeta_{\mathbf{k}_1})^2 = 1 - 2\eta_F(\zeta_{\mathbf{k}_1})$, which occur because the two particle can scatter into the state when they are not occupied. The term $\eta_F(\zeta_{\mathbf{k}_1})^2$ represents the scattering back into this state, $|\mathbf{k}_1, \uparrow\rangle \rightarrow |\mathbf{k}_1, \uparrow\rangle$, since the result depends upon the net scattering. What is left are the remaining factors $1 - 2\eta_F(\zeta_{\mathbf{k}_1})$, these occupation factors play a crucial role in the theory and are the cause of instability.

The integral in (6.3) may be evaluated. The key is that the interaction acts only over a small energy interval near the Fermi energy. Over this Debye energy window, the electron density of states in most metal is nearly constant. One can change the integration variable

$$\int \frac{d^3 k_1}{(2\pi)^3} = \int d\zeta_1 N(\zeta_1) \quad (6.4)$$

and treat $N(\zeta \approx 0) \equiv N_F$ as a constant. At zero temperature the result is ($\zeta_{\mathbf{k}_1} = \zeta_1$)

$$V_{eff}(\mathbf{k} - \mathbf{k}') = V(\mathbf{k} - \mathbf{k}') + N_F V_0^2 \int_{-\omega_D}^{\omega_D} d\zeta_1 \frac{\frac{1}{2} - \eta_F(\zeta_1)}{\zeta - \zeta_1} \quad (6.5)$$

The factor 1/2 does not cause any singularity and may be ignored,

To under the (6.3), the correlation operator looks like this

$$\langle \psi(t_1)\psi^\dagger(t_2)\psi(t_3)\psi^\dagger(t_4)S \rangle$$

where S is the all possible interaction, like Green's function. The 'Dyson' equation looks



$$G = G_0 + G_0 \Sigma G$$



The Green function of electron gives the different combination of distribution function.

then in zero temperature

$$\int_{-\omega_D}^{\omega_D} d\zeta_1 \frac{\eta_F(\zeta_1)}{\zeta - \zeta_1} = -\ln\left(\frac{\zeta}{\omega_D}\right) \quad (6.6)$$

and

$$V_{eff} = -V_0 \left[1 - N_F V_0 \ln\left(\frac{\zeta}{\omega_D}\right) \right] \quad (6.7)$$

The term $-N_F V_0 \ln(\zeta/\omega_D)$ is regarded as the **vertex correction** which results from the additional scattering between electrons. This scattering become very large for electrons near the Fermi energy.

Further insight is gained by considering the sum of diagrams like these. Each additional interaction (dashed line) causes two more Green's function which are going parallel in the intermediate state. Each new set of intermediate stats has the same type of integrand, so that a term with $(n+1)$ ladder diagrams gives a net contribution of

$$-V_0 \left[-N_F V_0 \ln\left(\frac{\zeta}{\omega_D}\right) \right]^n \quad (6.8)$$

The summation of these terms produces the series

$$\begin{aligned} V_{eff} &= -V_0 \sum_{n=0}^{\infty} \left[-N_F V_0 \ln\left(\frac{\zeta}{\omega_D}\right) \right]^n \\ &= -\frac{V_0}{1 + N_F V_0 \ln(\zeta/\omega_D)} \end{aligned} \quad (6.9)$$

The denominator equals zero at ($V_{eff} = 0$)

$$\zeta_0 = \omega_D \exp\left[-\frac{1}{N_F V_0}\right] \quad (6.10)$$

This ζ_0 gives a pole in (6.9). In the vicinity of ζ_0 can be approximated by using $\zeta = \zeta_0 + (\zeta - \zeta_0)$ and the scattering has a pole

$$\begin{aligned} V_{eff} &= -\frac{1}{N_F} \frac{1}{\ln(\zeta/\zeta_0)} = -\frac{1}{N_F} \frac{1}{\ln[1 + (\zeta - \zeta_0)/\zeta_0]} \\ &\approx -\frac{\zeta_0}{N_F(\zeta - \zeta_0)} \end{aligned} \quad (6.11)$$

This pole is sufficient to cause the instability. The electrons near the Fermi energy will interact with their pair on the opposite side of the Fermi sea. The mutual scattering produces a pole in the scattering amplitude, which will make the pair of electrons try to bind together. The entire electron paires are doing this simultaneously, so that the entire metal undergoes a phase transition. The existence of this pole depended on the sharpness of the electron distribution. If all the electrons near the Fermi energy become paired, one must reconsider wheter this sharp distribution still exists. A theory of superconductivity must self-consistently determin the properties of bound electron pairs.

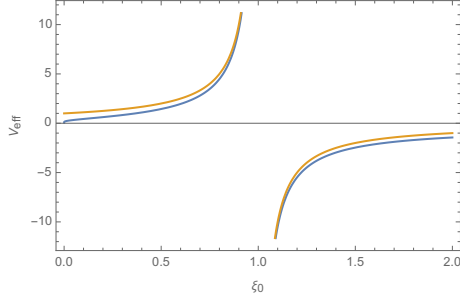


Figure 6.3: The behaviour of V_{eff} as the function of ξ_0 . The yellow line is the approximation one.

Another way to describe the instability is as a function of temperature. It enters into the electron distribution η_F by changing the step function into a smooth function with an energy width of several $k_B T$. By expressing the (6.6) as

$$\int_{-\omega_D}^{\omega_D} d\xi_1 \frac{\eta_F(\xi_1)}{\xi - \xi_1} \approx -\frac{1}{2} \ln \left[\frac{\xi^2 + (k_B T)^2}{\omega_D^2} \right] \quad (6.12)$$

Summation of all the ladder diagrams and the effective potential have the form

$$V_{eff} = -\frac{V_0}{1 + N_F V_0 \ln \left[\sqrt{\xi^2 + (k_B T)^2} / \omega_D \right]} \quad (6.13)$$

At zero energy, $\xi = 0$, V_{eff} becomes singular when the temperature is lower to the critical temperature T_c

$$k_B T_c = \omega_D \exp \left[-\frac{1}{N_F V_0} \right] \quad (6.14)$$

The theory of Cooper instability should be compared, for example, with the ordinary binding of two isolated particles. If two particles are isolated, they do not have to obey the statistics of a collection of identical particles. Then the scattering theory does not contain any of the occupation factors. all states may be used as intermediate state since there are no other particles. In theory of Wannier excitons 5.2, the multiple scattering theory may be described by a vertex function

$$\Gamma(\mathbf{k}, \mathbf{k}') = V(\mathbf{k} - \mathbf{k}') + \int \frac{d^3 k_1}{(2\pi)^3} \frac{V(\mathbf{k} - \mathbf{k}_1) \Gamma(\mathbf{k}_1, \mathbf{k}')}{2\xi_{\mathbf{k}} - 2\xi_{\mathbf{k}_1}} \quad (6.15)$$

The solution to this vertex function is equivalent to solving the two-particle Schrödinger equation in relative coordinates

$$\left[-\frac{1}{2m} (\nabla_1^2 + \nabla_2^2) + V(\mathbf{r}_1 - \mathbf{r}_2) - E \right] \psi(\mathbf{r}_1, \mathbf{r}_2) = 0 \quad (6.16)$$

The problem is factored into the relative and center of mass motions

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \quad \psi(\mathbf{r}_1, \mathbf{r}_2) = e^{i\mathbf{p} \cdot \mathbf{R}} \phi(\mathbf{r}) \quad (6.17)$$

$$\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2), \quad E = \frac{p^2}{2m} + \varepsilon \quad (6.18)$$

$$\left[-\frac{\nabla^2}{m} + V(\mathbf{r}) - \varepsilon \right] \phi(\mathbf{r}) = 0 \quad (6.19)$$

The center of mass motion is plane wave, and the relative motion becomes a one-body problem. Without the occupation factors, the relative scattering of two particles by an instantaneous potential is a trivial problem. When bound states occur, they are at negative binding energy in the relative coordinates, $\varepsilon < 0$. This behaviour is great contrast to the Cooper instability, where the pole occurs at small negative energy relative the to E_F , so the pole is at a positive energy $E_F - \xi_0$. The two electrons cannot really bind at that nereggy, since their net energy is positive. *The instability occurs because it appears to them as if they should bind, although if they tried, they would find they could not.* The role of the occupation factors in the argument of the scattering integral is what moved the apparent pole out to the Fermi energy.²

² The reason electrons must be paired with opposite momentum, P633

6.1.1 BCS Theory

The basic feature of the BCS theory is that pairing occurs between electrons in states with opposite momentum and opposite spins. The two spins are combined into a spin singlet, with $S = 0$.

7

Appendix: Complex analysis

7.1 Residue

In complex analysis, the **residue** is a complex number proportional to the contour integral of a meromorphic function along a path enclosing one of its singularities.

7.1.1 Definition

The residue of a meromorphic function f at an isolated singularity a , denoted as $\text{Res}(f, a)$, is the unique value R such that $f(z) - R/(z - a)$ has an analytic antiderivative in a punctured disk $0 < |z - a| < \delta$.

Alternatively, residues can be calculated by Laurent series expansions, and one can define the residue as the coefficient a_{-1} of a Laurent series.

7.1.2 Examples

Example.1

Computing the residue of a monomial,

$$\oint_C z^k dz$$

Since path integral computations are homotopy invariant, let C be the radius of 1, and $dz \rightarrow d(e^{i\theta}) = ie^{i\theta} d\theta$. The result is

$$\oint_C z^k dz = \int_0^{2\pi} ie^{i(k+1)\theta} d\theta = \begin{cases} 2\pi i & (k = -1) \\ 0 & (\text{otherwise}) \end{cases}$$

Example.2 Consider the contour integral, where C is some simple

closed curve about 0.

$$\begin{aligned}
 & \oint_C \frac{e^z}{z^5} dz \\
 &= \oint_C \frac{1}{z^5} \left(1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \dots\right) dz \\
 &= \oint_C \frac{1}{4!z} dz \frac{\pi i}{12}
 \end{aligned}$$

The last formula is based on the previous result.

7.1.3 Calculating residues

For residue theorem,

$$\text{Res}(f, c) = \frac{1}{2\pi i} \oint_{\gamma} f(z) dz$$

where γ traces out a circle around c in a counterclockwise manner.

Removeable singularities

If function f can be continued to a holomorphic function on the whole disk, then $\text{Res}(f, c) = 0$. The converse is not generally true.

Simple poles

At a **simple pole** c , the residue of f is given by

$$\text{Res}(f, c) = \lim_{z \rightarrow c} (z - c) f(z)$$

It may be that the function f can be expressed as a quotient of two function, $f(z) = \frac{g(z)}{h(z)}$, where g and h are **holomorphic functions** in a neighborhood of c , with $h(c) = 0$ and $h'(c) \neq 0$. In such case, **L'Hôpital's rule** can be use to simplify the formula to

$$\text{Res}(f, c) = \frac{g'(c)}{h'(c)}$$

More generally, if c is a pole of order n , the residue of f around $z = c$ can be found by the formula

$$\text{Res}(f, c) = \frac{1}{(n-1)!} \lim_{z \rightarrow c} \frac{d^{n-1}}{dz^{n-1}} [(z - c)^n f(z)]$$

In general, the residue at infinity is given by

$$\text{Res}(f(z), \infty) = -\text{Res}\left(\frac{1}{z^2} f\left(\frac{1}{z}\right), 0\right)$$

Series methods

If parts or all of a function can be expand into a Taylor series or **Laurent series**, which may be possible if the parts or the whole of the function has a standard series expansion, the calculating the residue is significantly simpler than by other methods.

Considering the integral

$$f(z) = \frac{\sin z}{z^2 - z}$$

where $z = 0$ is the removable singularity and the residue at this point is 0. The Taylor expansion gives, at point $z = 1$,

$$\begin{aligned}\sin z &= \sin 1 + \cos 1(z - 1) + \frac{-\sin 1}{2!}(z - 1)^2 + \dots \\ \frac{1}{z} &= \frac{1}{(z - 1) + 1} = 1 - (z - 1) + (z - 1)^2 - (z - 1)^3 + \dots\end{aligned}$$

Multiplying those two series and introducing $1/(z - 1)$ gives

$$\frac{\sin z}{z(z - 1)} = \frac{\sin 1}{z - 1} + (\cos 1 - \sin 1) + (z - 1)\left(-\frac{\sin 1}{2!} - \cos 1 + \sin 1\right) + \dots$$

So the residue of $f(z)$ at $z = 1$ is $\sin 1$.

7.2 Sokhotski-Plemelj theorem

Let f be a complex-valued function which is defined and continuous on the real line and let a and b be real constants with $a < 0 < b$, then

$$\lim_{\varepsilon \rightarrow 0^+} \int_a^b \frac{f(x)}{x \pm i\varepsilon} dx = \mp i\pi f(0) + \mathcal{P} \int_a^b \frac{f(x)}{x} dx,$$

where \mathcal{P} denotes the **Cauchy principal value**.

One important relation is for the Green's functions,

$$\frac{1}{\omega + E_n - E_m + i\delta} = \mathcal{P} \frac{1}{\omega + E_n - E_m} - i\pi\delta(\omega + E_n - E_m)$$

7.3 Kramers-Kronig relations

The Kramers-Kronig relations are bidirectional mathematical relations, connection the real and imaginary parts of any complex function that is analytic in the upper half-plane. The relations are often used to compute the real part from the imaginary part of response functions in physical systems, because for stable system, causality implies the condition of analyticity and conversely, analyticity implies causality of the corresponding stable physical system.

Let $\chi(\omega) = \chi_1(\omega) + i\chi_2(\omega)$ be a complex function of the complex variable ω , where χ_1 and χ_2 are real. Suppose this function is analytic in the upper half-plane of ω and vanishes like $1/|\omega|$ or faster as $|\omega| \rightarrow \infty$. The Kramers-Kronig relations are given by

$$\chi_1(\omega) = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{\chi_2(\omega')}{\omega' - \omega} d\omega'$$

and

$$\chi_2(\omega) = -\frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{\chi(\omega')}{\omega' - \omega} d\omega'$$

alternatively, we have the following formulas

$$\begin{aligned} \chi_1(\omega) &= \frac{2}{\pi} \mathcal{P} \int_0^{\infty} \frac{\omega' \chi_1(\omega')}{\omega'^2 - \omega^2} d\omega' \\ \chi_2(\omega) &= - = \frac{2\omega}{\pi} \mathcal{P} \int_0^{\infty} \frac{\chi_1(\omega')}{\omega'^2 - \omega^2} d\omega' \end{aligned}$$