MENG SUN

# NOTES ON: MANY PARTICLE PHYSICS — BY D. MAHAN

# Contents

# 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

$$[x, p_x] \quad = \quad i\hbar \tag{1.1}$$

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

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.

$$H = \frac{p^2}{2m} + \frac{K}{2}x^2 \tag{1.3}$$

Introducing the dimensionless coordinate $\xi$

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

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

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

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

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

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

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

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

For creation operators

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

with commutation relations

$$\left[a, a^\dagger\right] = 1 \tag{1.11}$$

The eigenstate of (1.8) are

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

and with

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

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

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

This suggest that

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

The time development of the position operator can be represented as

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

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

$$\begin{aligned}
H &= \frac{p^2}{2m} + \frac{K}{2}x^2 + eFx = \hbar\omega(a^\dagger a + \frac{1}{2}) + \lambda(a + a^\dagger) \tag{1.17} \\
\lambda &= eF\sqrt{\frac{\hbar}{2m\omega}} \tag{1.18}
\end{aligned}$$

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

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

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

$$
\begin{aligned}
A &= a + \frac{\lambda}{\omega} & (1.20)\\
A^{\dagger} &= a^{\dagger} + \frac{\lambda}{\omega} & (1.21)\\
\frac{\partial A}{\partial t} &= -i\omega A & (1.22)\\
A(t) &= e^{-i\omega t}A & (1.23)\\
A^{\dagger}(t) &= e^{i\omega t}A^{\dagger} & (1.24)
\end{aligned}
$$

This new operators have same properties of the Harmonic oscillator ones

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

with the eigenstate

$$
\begin{aligned}
H\,|n\rangle &= \left[\omega\left(n + \frac{1}{2}\right) - \frac{\lambda^2}{\omega}\right]|n\rangle & (1.26)\\
|n\rangle &= \frac{(A^{\dagger})^n}{\sqrt{n!}}\,|0\rangle & (1.27)
\end{aligned}
$$

The position operator for this case is

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

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

$$x_0 = \sqrt{\frac{\hbar}{2m\omega}}\,\frac{2\lambda}{\omega} = -\frac{eF}{K} \tag{1.29}$$

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

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

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

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

The classical solution is obtained by solving the equation of motion

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

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

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

The normal modes have the solution

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

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

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

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

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

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

$$[x_k, p_p] = i\delta_{kp} \tag{1.38}$$

It is easy to show that the Hamiltonian may written in wave vector space as[1]

$$H = \frac{1}{2m} \sum_k \left[p_k p_{-k} + m^2 \omega_k^2 x_k x_{-k}\right] \tag{1.39}$$

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

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

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

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

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

$$\psi = |n_1, n_2, \ldots, n_n\rangle = \Pi_k |n_k\rangle = \Pi_k \frac{(a_k^\dagger)^{n_k}}{\sqrt{n_k!}} |0\rangle \qquad (1.42)$$

with expectation value of Hamiltonian

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

In thermal equilibrium the states have an averge value of $n_k$

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

The position operator in wave vector and real space is

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

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

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

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

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 theroy is nearly identical except there are more indices. Suppose there is a potential function between atoms or ions of the form

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

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 equilibrum position

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

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

$$Q_i(t) = i \sum_{\mathbf{k},\lambda} \sqrt{\frac{\hbar}{2MN\omega_{\mathbf{k}\lambda}}} \xi_{\mathbf{k},\lambda} \left( a_{\mathbf{k},\lambda} e^{-\omega_{\mathbf{k}\lambda t}} + a^\dagger_{-\mathbf{k},\lambda} e^{i\omega_{\mathbf{k}\lambda t}} \right) e^{i\mathbf{k}\cdot R_i^0} \quad (1.51)$$

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

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

The polarization vector $\xi_{\mathbf{k},\lambda}$ are assumed to be real but change sign with $\mathbf{k}$ direction, $\xi_{-\mathbf{k}} = -\xi_{\mathbf{k}}$ 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 $\lambda$ runs over these $3L$ values of normal mode. Each mode has its own eigenfrequency. It will also have a polarization vector $\xi_{\mathbf{k},\lambda}$ which specifies the bibrational direction of the ion for each wave vector and mode $\lambda$. If there are more than one atom per unit cell, one should add further subscripts to $M$ and $\xi_{\mathbf{k},\lambda}$ to specify the values for each atom per unit cell.

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

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

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 cell[2]. 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 $\psi$ and $\psi^\dagger$ as independent variable, then the variations give

$$\frac{\partial L}{\partial \psi} = -U\psi^\dagger \tag{1.55}$$

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

$$\frac{\partial L}{\partial \dot{\psi}} = i\hbar\psi^\dagger \tag{1.57}$$

According to Euler-Lagrange equation of motion for a field[3]

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

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

$$\omega = \frac{\partial}{\partial \dot{\psi}} = i\hbar\psi^\dagger \tag{1.59}$$

The Hamiltonian density

[3] We took the covariant way from Peskin's book. Where $\mu$ is the time and space coordinate.

# 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 solved exactly. The usual approach is to set

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

where $H_0$ is the Hamiltonian can be solved exactly. The term $V$ represents all remaining parts of $H$. One tries to choose $H_0$ so that the effects $V$ 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

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

with the formal operator solution

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

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

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

or, equivalently, the equation of motion is given by

$$i\partial_t O(t) = [O(t), H] \tag{2.5}$$

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

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

### 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

$$H = H_0 + V \tag{2.7}$$

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

- The operators have a time dependence:

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

- The wavefunction have the time dependence:

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

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 relaying on the unperturbed Hamiltonian as in (2.8). For the dependence of the wavefunction is governed by

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

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

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

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

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

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

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

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

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

This expansion may be abbreviated by writing it as

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

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:

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

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

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

with the definition

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

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

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

In different representation, the wavefunction is identical at the $t = 0$, let $\psi(0)$ as the exact ground state wavefunction, and $\phi_0$ as the

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

$$\psi(0) = S(0, -\infty)\phi_0 \tag{2.20}$$

The result can be regard as the following, since

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

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

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

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

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

The important assertion is that $\hat{\psi}(-\infty) = \phi_0$. The traditional argument is that one stats in the long past with the wavefunction $\phi_0$ 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 $t \to +\infty$,

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

One possible assumption is that $\hat{\psi}(\infty)$ must be related to $\phi_0$. If they are equal except for a phase factor $L$

$$\phi_0 e^{iL} = \hat{\psi}(\infty) = S(\infty, 0)\psi(0) = S(\infty, -\infty)\phi_0 \tag{2.25}$$
$$e^{iL} = \langle\phi_0| S(\infty, -\infty) |\phi_0\rangle \tag{2.26}$$

## 2.3   Green's Function

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

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

The quantum number $\lambda$ can be anything depending on the problem[1]. At zero temperature the state $|\rangle$ must be the ground state.

In the definition of Green's function the $C_\lambda$ represent states of $H_0$, while the ground state $|\rangle$ is an eigenstate of $H$. Furthermore, (2.27) is defined in Heisenberg picture, one have 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

$$|\rangle = S(0, -\infty) |\phi_0\rangle \tag{2.28}$$

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

Next change the operators to interaction representation[2] , we have the Green's function

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

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

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

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

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

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

$$
\begin{aligned}
C_p |0\rangle &= 0 \tag{2.31} \\
a_q |0\rangle &= 0 \tag{2.32} \\
S(t, -\infty) |0\rangle &= |0\rangle \tag{2.33}
\end{aligned}
$$

Both of the ground state, $\phi_0$ and $\psi_0$ are the vacuum state $|0\rangle$. The Green's function is only possible for this time ordering

$$
G(\lambda, t - t') = -i\Theta(t - t') \langle0| \hat{C}_\lambda(t)\hat{C}_\lambda^\dagger(t) |0\rangle \tag{2.34}
$$

The unperturbed Green's function is given

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

The Fourier transform is defined as

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

The unperturbed Green's function gives[3]

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

[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 $\mu$ and all electron states with $E < \mu$ are occupied. If the unperturbed electrons, $H_0$, are characterized by energy $\varepsilon_k$, 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, $\xi_k = \varepsilon_k - \mu/$. For a spherical Fermi surface,

$$\langle\phi_0| C_k^\dagger C_k |\phi_0\rangle = \Theta(p_F - k) \tag{2.38}$$
$$\langle\phi_0| C_k C_k^\dagger |\phi_0\rangle = \Theta(k - p_F) \tag{2.39}$$

This gives the Green's function

$$G^0(k, E) = \frac{1}{E - \xi_k + i\delta\mathrm{sgn}(\xi_k)} \tag{2.40}$$

### 2.3.3   Phonons

The Green's function for phonons is defined as

$$D(\mathbf{q}, \lambda, t - t') = -i\langle| TA_{\mathbf{q}\lambda}(t)A_{-\mathbf{q}\lambda}(t') |\rangle \tag{2.41}$$
$$A_{\mathbf{q}\lambda} = a_{\mathbf{q}\lambda} + a_{-\mathbf{q}\lambda}^\dagger \tag{2.42}$$

The $\lambda$ refer to the polarization of phonons. In the interaction picture

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

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

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

and

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

For nonzero temperature, we have

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

## 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 stand method is expanding the $S(\infty, -\infty)$ matrix in (2.19).

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

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 operate 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, because[4]

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

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,
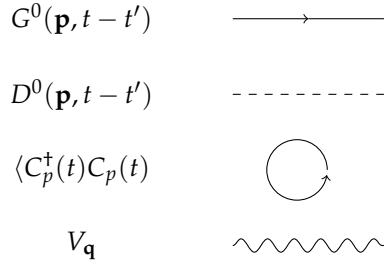
$G^0(\mathbf{p}, t - t')$         $\longrightarrow$

$D^0(\mathbf{p}, t - t')$         $- - - - - - - - -$

$\langle C_p^\dagger(t) C_p(t) \rangle$

$V_{\mathbf{q}}$         $\sim\!\sim\!\sim\!\sim$

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 another[5].

[5] The theorem is explain in    P83-P86.

## 2.7   Dyson's Equation

[6] P86-P88 in   .

The Dyson's equation is obtained by formally summing the series[6]

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

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

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

and for the electron at Fermi sea in zero temperature[7]

[7] Note the energy spectrum is different with the single electron in a band case, we have $\mu$ here.

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

The self-energy has real and imaginary parts. The switching of signs of $\text{sgn}_p$ 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

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

Similarly, we have this form,

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

The phonon self-energy term $\Pi(\mathbf{q}, \omega)$ is sometimes calleda *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

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

  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

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

  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

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

  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 $v \to \infty$, for box normalization in a finite volume the factor is

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

  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

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

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

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

  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

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

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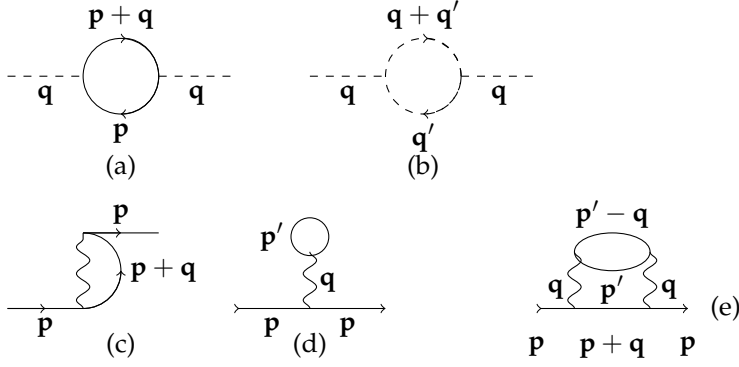
Figure 2.2: Phonon self-energies, (a) is due to electron-phonon interaction, and (b) is from lattice anharmonicity. (c) is unscreened exchange energy.

Now examine some example. For the first plot Fig. 2.2(a), we have $F = 1$, $S = \frac{1}{2}$ and $m = 1$, then[8]

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

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

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

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

The electron self-energy arising from electron-electron interaction. The self-energy term in Fig. 2.2(c) is called the *unscreened 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

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

There is a very important identity:

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

with this we have

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

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

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

with different time approach, we have

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

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 $S = \frac{1}{2}$:

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

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

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

where $N_e$ is the number of electrons. In the limit $q \to 0$ gives $v_{q=0} \to \infty$. 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

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

## 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 $\phi_0$. 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 $t \to \infty$ 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 $t \to \infty$. He proposed that the time integral in the $S$ matrix has two pieces: one goes from $(-\infty, \tau)$ while the second goes form $(\tau, -\infty)$ and let $\tau \to \infty$. 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 $\phi_0$.

Considering the time-loop expansion for the $S$ Matrix

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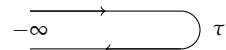


Figure 2.3: The time-loop integration path in the $S$ matrix.

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

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

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 through they are not independent. The six functions are

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

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

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

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 $\varepsilon_\lambda$. 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 operators[9]:

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

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

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

$$
\begin{aligned}
G^>(x_1, x_2) &= -i\sum_\lambda (1 - \eta_\lambda)\phi_\lambda(\mathbf{r}_1)\phi_\lambda^*(\mathbf{r}_2)e^{-i\varepsilon_\lambda t} \\
G^<(x_1, x_2) &= i\sum_\lambda \eta_\lambda\phi_\lambda(\mathbf{r}_1)\phi_\lambda^*(br_2)e^{-i\varepsilon_\lambda t} \\
G_t(x_1, x_2) &= -i\sum_\lambda [\Theta(t) - \eta_\lambda]\phi_\lambda(\mathbf{r}_1)\phi_\lambda^*(br_2)e^{-i\varepsilon_\lambda t} \\
G_{\bar{t}}(x_1, x_2) &= -i\sum_\lambda [\Theta(-t) - \eta_\lambda]\phi_\lambda(\mathbf{r}_1)\phi_\lambda^*(br_2)e^{-i\varepsilon_\lambda t} \\
G_{ret}(x_1, x_2) &= -i\Theta(t)\sum_\lambda \phi_\lambda(\mathbf{r}_1)\phi_\lambda^*(\mathbf{r}_2)e^{-i\varepsilon_\lambda t} \\
G_{adv}(x_1, x_2) &= i\Theta(-t)\sum_\lambda \phi_\lambda(\mathbf{r}_1)\phi_\lambda^*(\mathbf{r}_2)e^{-i\varepsilon_\lambda t}
\end{aligned}
\tag{2.73}
$$

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 $\lambda$ becomes the wave vector $\mathbf{k}$ and spin index $\sigma$. 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

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

with Fourier transformation and $i\delta$ infinitesimal quantity

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

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

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

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

There 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 changer 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 lowing operators. Usually, we have $A_{\mathbf{q}} = a^\dagger_{-\mathbf{q}} + a_{\mathbf{q}}$ 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 $N_{\mathbf{q}} = \langle a^\dagger_{\mathbf{q}} a_{\mathbf{q}}\rangle$. The noninteracting results are

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

### 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 opertors. 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.
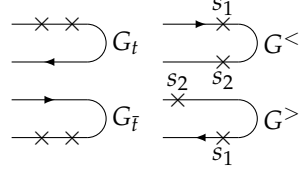


Figure 2.4: The four Green's function $G(s_1, s_2)$ depend on whether the time variable are on the outgoing or return parts of the time loop.

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

$$V = \sum_{\alpha\beta} M_{\alpha\beta} C_\alpha^\dagger C_\beta$$

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

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.

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

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

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

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

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

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

$$G = G_0 + G_0 \Sigma G \tag{2.82}$$

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

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

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

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

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

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

With the vector potential is given by expansion

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

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

where $\mathbf{k}$ is the wave vector and $\lambda$ is the polarization and $\mu$ is $x, y$ and $z$ component. The operator $a_{\mathbf{k}\lambda}$ obey boson statistics. And Each state with $\mathbf{k}$ and $\lambda$ 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,

$$v_q = \frac{4\pi e^2}{q^2} \tag{2.88}$$

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

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

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 $\epsilon$

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

For the scalar and vector potentials

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

Here the Coulomb Green's function is

$$\bar{v}_q = \frac{v_q}{\epsilon} \tag{2.92}$$

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

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

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

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

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 $\mu$, $\nu$ are the $x, y, z$ components, with vector potential in (2.87); the sum $\lambda$ is the sum over the two transverse polarizations of the light, while $\xi_\mu$ are the polarization vectors for each component. At zero temperature,

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

and with Fourier transform is

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

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.

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

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

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

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

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 $\beta$ 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

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

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

*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

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

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

Important knowledge, the expansion

$$\frac{1}{e^x - 1}$$

$$= \frac{1}{1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots - 1}$$

$$= \frac{1}{x + \frac{x^2}{2!} + \frac{x^3}{3!} + \ldots}$$

$$= \frac{1}{x(1 + \frac{x}{2!} + \frac{x^2}{3!} + \ldots)}$$

$$\approx \frac{1}{x(1 + \frac{x}{2})}$$

$$\approx \frac{1}{x}(1 - \frac{x}{2}) = \frac{1}{x} - \frac{1}{2}$$

with domain

$$-\beta \leq \tau \leq \beta \tag{3.6}$$

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

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

where

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

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

or **equivalently**. We have

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

with

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

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

### 3.1.1   Boson

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

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

Further we have

$$f(i\omega_n) = \int_0^{\beta} d\tau e^{i\omega_n \tau} f(\tau)$$

$$f(\tau) = \frac{1}{\beta} \sum_n e^{-i\omega_n \tau} f(i\omega_n) \tag{3.14}$$

$$\omega_n = 2n\pi k_B T$$

### 3.1.2   Fermion

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

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

and the result give

$$f(i\omega_n) = \int_0^{\beta} d\tau e^{i\omega_n \tau} f(\tau)$$

$$f(\tau) = \frac{1}{\beta} \sum_n e^{-i\omega_n \tau} f(i\omega_n) 3.23) \tag{3.16}$$

$$\omega_n = (2n+1)\pi k_B T$$

### 3.2   Matsubara Green's functions

The electron Green's function is defined as

$$
\begin{aligned}
\mathcal{G}(\mathbf{p}, \tau - \tau') &= -\langle T_\tau C_{\mathbf{p}\sigma}(\tau) C_{\mathbf{p}\sigma}^\dagger(\tau') \rangle && (3.17) \\
\mathcal{G}(\mathbf{p}, \tau - \tau') &= -\operatorname{Tr}\left[ e^{-\beta(H - \mu N - \Omega)} T_\tau e^{\tau(H - \mu N)} C_{\mathbf{p}\sigma} e^{-(\tau - \tau')(H - \mu N)} \right. \\
&\quad \times \left. C_{\mathbf{p}\sigma}^\dagger e^{-\tau'(H - \mu N)} \right] && (3.18) \\
e^{-\beta\Omega} &= \operatorname{Tr}\left( e^{-\beta(H - \mu N)} \right) && (3.19)
\end{aligned}
$$

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 $\mu$ 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 $i\omega_n \to E + \mu + i\delta$, 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 $i\omega_n \to E + i\delta$ and energy is measured from the chemical potential.

With some derivation[2], we have the Green's functions

$$
\begin{aligned}
\mathcal{G}(\mathbf{p}, \tau) &= -\langle T_\tau C_{\mathbf{p}\sigma}(\tau) C_{\mathbf{p}\sigma}^\dagger(0) \rangle && (3.20) \\
&= -\operatorname{Tr}\left[ e^{-\beta(K - \Omega)} T_\tau (e^{\tau K} C_{\mathbf{p}\sigma} e^{-\tau K} C_{\mathbf{p}\sigma}^\dagger) \right] && (3.21) \\
\mathcal{G}(\mathbf{p}, i\omega_n) &= \int_0^\beta d\tau\, e^{i\omega_n \tau} \mathcal{G}(\mathbf{p}, \tau) && (3.22) \\
\mathcal{G}(\mathbf{p}, \tau) &= \frac{1}{\beta} \sum_n e^{-i\omega_n \tau} \mathcal{G}(\mathbf{p}, i\omega_n) && (3.23)
\end{aligned}
$$

For noninteracting Green's function, the $\tau$ evolution of the operators is[3]

$$
\begin{aligned}
C_{\mathbf{p}\sigma}(\tau) &= e^{\tau K_0} C_{\mathbf{p}\sigma} e^{-\tau K_0} = e^{-\xi_{\mathbf{p}} \tau} C_{\mathbf{p}\sigma} && (3.24) \\
C_{\mathbf{p}\sigma}^\dagger(\tau) &= e^{\tau K_0} C_{\mathbf{p}\sigma}^\dagger e^{-\tau K_0} = e^{\xi_{\mathbf{p}} \tau} C_{\mathbf{p}\sigma}^\dagger && (3.25)
\end{aligned}
$$

[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

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

and

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

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

$$
\begin{aligned}
\mathcal{D}(\mathbf{q}, \tau - \tau') &= -\langle T_\tau \mathbf{A}(\mathbf{q}, \tau) \mathbf{A}(-\mathbf{q}, \tau') \rangle && (3.28) \\
\mathbf{A}(\mathbf{q}, \tau) &= e^{\tau H}(a_{\mathbf{q}} + a_{-\mathbf{q}}^\dagger) e^{-\tau H} && (3.29)
\end{aligned}
$$

and with the relation in (3.13), we have

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

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

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

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

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

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

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

## 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

$$
\begin{aligned}
G_{ret}(\mathbf{p}, t - t') &= G_t(\mathbf{p}, t - t') - G^<(\mathbf{p}, t - t') \tag{3.35}\\
&= -i\Theta(t - t') \langle [C_{\mathbf{p}\sigma}(t) C_{\mathbf{p}\sigma}^\dagger(t') + C_{\mathbf{p}\sigma}^\dagger(t') C_{\mathbf{p}\sigma}(t)] \rangle \\
&= -i\Theta(t - t') \operatorname{Tr}\{e^{-\beta(K-\Omega)}[C_{\mathbf{p}\sigma}(t) C_{\mathbf{p}\sigma}^\dagger(t') + C_{\mathbf{p}\sigma}^\dagger(t') C_{\mathbf{p}\sigma}(t)]\} \\
K &= H - \mu N, \quad C_{\mathbf{p}\sigma}(t) = e^{iKt} C_{\mathbf{p}\sigma} e^{-iKt} \tag{3.36}
\end{aligned}
$$

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

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

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

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

$$U = \sum_{ij} M_{ij} C_i^\dagger C_j \tag{3.38}$$

$$V = \sum_{ijk} M_{ijk} C_i^\dagger C_j C_k \tag{3.39}$$

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.

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

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

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

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

The advanced Green's function for each is defined

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

$$D_{adv}(\mathbf{q}, t-t') = i\Theta(t-t')\langle A(\mathbf{q}, t)A(-\mathbf{q}, t') $$
$$ - A(-\mathbf{q}, t')A(\mathbf{q}, t)\rangle \tag{3.44}$$

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.

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

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

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

This step is called an analytic continuation. The advanced Green's
function can be changed by $i\omega_n \to \omega - i\delta$, 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:

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

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

$$U_{ret}(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\omega')}{\omega - \omega' + i\delta}$$

$$\mathcal{U}(i\omega_n) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\omega')}{i\omega_n - \omega'} \quad (3.48)$$

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 may 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 $bp$ 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]

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

check the definition of delta function in link

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

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

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

Define the retarded self-energies according to (3.46)

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

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

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

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

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

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,

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

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

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

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

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

and for advanced

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

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

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

[5] To get this relation

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

and also implies that

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

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

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

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

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

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 $\text{Im} \to 0$ and obtain

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

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

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

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

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

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

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

$$\zeta_{\mathbf{p}} = \frac{p^2}{2m} - \mu = \varepsilon_{\mathbf{p}} - \mu \tag{3.72}$$

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

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

The proportionality constant is the inverse effective mass $m^*$

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

from the definition of (3.69), we get

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

With (3.74), the final term is arrived

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

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:

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

$$e^{-\beta \Omega} = \operatorname{Tr} \left( e^{-\beta K} \right) \tag{3.78}$$

where we consider the general case

$$K = K_0 + V = H_0 - \mu N + V \tag{3.79}$$

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

$$[H_0, N] = [H, N] = 0 \tag{3.80}$$

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

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

ant the time dependence of operators

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

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

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

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

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

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

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

Next consider the definition

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

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

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

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

$$\langle T_{\tau} S(\beta) \hat{C}_{\mathbf{p}}(\tau) \hat{C}_{\mathbf{p}}^{\dagger} \rangle_0 \tag{3.88}$$

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

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

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

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

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

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

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

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

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.

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

$$+ \frac{N_\mathbf{q} + 1 - \eta_F(\xi_\mathbf{p})}{ip_n - \xi_\mathbf{p} - \omega_\mathbf{q}} \qquad (3.93)$$

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

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

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

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

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

Denote this equation as

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

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[6],

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

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

[6] This gives $I = \lim_{R\to\infty} \oint \frac{dz}{2\pi i} f(z)\eta_B(z) = 0$ if $f(z)$ decay faster than $z^{-1}$.

The function $f(z)$ is

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

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

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

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

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

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

$$S = \sum_J r_j \eta_B(z_j) \qquad (3.103)$$

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

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

The minus sign in font occurs because the residue of the fermion $\eta_F$ is $-\frac{1}{\beta}$ and is $\frac{1}{\beta}$ for boson $\eta_B$. [7]

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 $\tau \to 0$. This limit is ambiguous, since a different result is obtained if $\tau = 0$ is approached from the positive or negative direction

$$
\begin{aligned}
\mathcal{G}^0(\mathbf{p}, \tau = 0^+) &= -\left[1 - \eta_F(\xi_{\mathbf{p}})\right] \qquad (3.105) \\
\mathcal{G}^0(\mathbf{p}, \tau = 0^-) &= \eta_F(\xi_{\mathbf{p}}) \qquad (3.106)
\end{aligned}
$$

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

[7]

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

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

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

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

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

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

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

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

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 $\Omega$. 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

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

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

$$-\frac{\partial\Omega}{\beta\partial\mu} = \langle N_e\rangle \tag{3.112}$$

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

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

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

For an interacting system

$$K = K_0 + V \tag{3.115}$$

For a system of electrons and phonons,

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

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

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

The logarithm of both sides of this equation

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

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 $\Omega_0$ which changes it into $\Omega$. The method of evaluating this correlation function is by the $S$-matrix expansion

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

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 $\lambda$, 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

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

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

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

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

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

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

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

**The basic theorem is that the thermodynamic potential is the summation of the different connected diagrams.** With some discussion discussed in the book[8], we have the identity

[8] P144, Mahan

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

In terms of the Green's functions, we have

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

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

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

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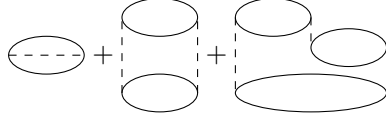
is shown here in Fig.3.1 for the electron-phonon interaction. They can be summed to give an approximate simple answer. The rules for constructing diagrams for the terms in the thermodynamic potential are similar to those in Sec 3.4. One follows all those rules and then multiplies the result by $\frac{\beta}{l}$.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

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

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

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

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

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

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

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

It is simple to sum the series

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

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 the 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

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

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

Then for $\lambda = 1$

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

The logarithm has been eliminated, but now the right-hand side must be evaluated for each value of $\eta$ and then the integral is taken over $\eta$. *Since $\eta$ 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

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

where the coupling constant $\eta$ 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

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

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

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

This expression is an approximation to $\Omega$ since it employs an approximate self-energy $\pi^{(1)}$. According the [9], the exact correction to the themodynamic potential from electron-phonon interactions is

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

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 withe excat self-energy.



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 then on phonon line.

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

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 twices. The two electron vertives 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 twices. The two electron vertives can be connected by a single Coulomb line or a single phonon line. The sum of these contributions is

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

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

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

with the Dyson equation

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

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

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

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

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

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

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

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

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

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

$$\lim_{T \to 0} \beta eta_F(\xi_{\mathbf{p}}) \left[ 1 - \eta_F(\xi_{\mathbf{q}}) \right] = \lim_{T \to 0} \frac{d}{d\xi_{\mathbf{p}}} \left[ -\eta_F(\xi_{\mathbf{p}}) \right] = \delta(\xi_{\mathbf{p}}) \tag{3.147}$$

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

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

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

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

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 $\eta$ enters as just a mulitplicative factor, as shown in (3.149). If further self-energy diagrams are needed to get a good phonon $\pi$, then $\eta$ 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

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

Introduce the frequency

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

The summation over Matsubara frequencies can be done easily since,

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

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

$$\Omega - \Omega_0 = \frac{1}{2}\sum_{\mathbf{q}}(\Omega_{\mathbf{q}}^2 - \omega_{\mathbf{q}}^2)\int_0^1\frac{d\eta}{2\Omega_\eta}\left(1 + \frac{2}{e^{\beta\Omega_\eta} - 1}\right)$$

$$= \frac{1}{2}\sum_{\mathbf{q}}\left[\Omega_\eta + \frac{2}{\beta}\ln\left(1 - e^{-\beta\Omega_\eta}\right)\right]_{\eta=0}^{\eta=1}$$

$$= \sum_{\mathbf{q}}\left[\frac{1}{2}\left(\Omega_{\mathbf{q}} - \omega_{\mathbf{q}}\right) + \frac{1}{\beta}\ln\left(\frac{1 - \exp(-\beta\Omega_{\mathbf{q}})}{1 - \exp(-\beta\omega_{\mathbf{q}})}\right)\right] \quad (3.153)$$

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 $\Omega_0$, the terms with $\omega_{\mathbf{q}}$ all cancel. THe final answer is

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

$$(3.154)$$

## 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 $\langle\ldots\rangle$ have different meanings, depending on the circumstance:

- At zero temperature, and in equilibrium, $\langle\ldots\rangle$ 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 constrains 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 have[10]

$$
\begin{aligned}
\mathcal{G}^<(\mathbf{p},\omega) &= i\eta_F(\omega)A(\mathbf{p},\omega) & (3.156)\\
\mathcal{G}^>(\mathbf{p},\omega) &= -i\left[1-\eta_F(\omega)\right]A(\mathbf{p},\omega) & (3.157)\\
\mathcal{G}_t(\mathbf{p},\omega) &= \left[1-\eta_F(\omega)\right]\mathcal{G}_{ret}(\mathbf{p},\omega)+\eta_F(\omega)\mathcal{G}_{adv}(\mathbf{p},\omega) & (3.158)\\
\mathcal{G}_{\bar{t}}(\mathbf{p},\omega) &= -\left[1-\eta_F(\omega)\right]\mathcal{G}_{adv}(\mathbf{p},\omega)-\eta_F(\omega)\mathcal{G}_{ret}(\mathbf{p},\omega) & (3.159)
\end{aligned}
$$

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 $\tau$ as a complex variable, on can deform the contour of integration, and end up with (2.81) [11]. 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)

$$
\begin{aligned}
\left(i\frac{\partial}{\partial t}-\varepsilon_{\mathbf{k}}\right)\tilde{G}_0(\mathbf{k},t) &= \delta(t)\tilde{I} & (3.160)\\
\left(i\frac{\partial}{\partial t}-H_0(x)\right)\tilde{G}_0(x) &= \delta^4(x)\tilde{I} & (3.161)
\end{aligned}
$$

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

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.

[11]

which the above result is used to find

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

(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

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

(3.163)

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

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

(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

$$
(\mathbf{R}, T) = \frac{1}{2}(x_1 + x_2) \tag{3.165}
$$
$$
(\mathbf{r}, t) = x_1 - x_2 \tag{3.166}
$$

with this notation

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

with Fourier transformation

$$f(\mathbf{k}, \omega; \mathbf{R}, T) = -iG^<(\mathbf{k}, \omega; \mathbf{R}, T) \qquad (3.168)$$

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

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

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

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

$$= i\left[\frac{\partial}{\partial t}\langle\psi^\dagger(\mathbf{R}, T - \frac{1}{2}t)\psi(\mathbf{R}, T + \frac{1}{2}t)\rangle\right]_{t=0}$$

$$= \langle\psi^\dagger(\mathbf{R}, T)H\psi(\mathbf{R}, T)\rangle \qquad (3.171)$$

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.[12]

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

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

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.[13]

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

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

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

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

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

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

[13] 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

$$
\begin{aligned}
f(x,\omega;X) &= \eta_F(\omega)A(x,\omega;X) & (3.176) \\
A(x,\omega;X) &= \frac{2\pi}{L}\sum_n [\cos(k_n x) - \cos(2k_n X)]\,\delta(\omega - \varepsilon n^2) & (3.177)
\end{aligned}
$$

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 $E_\alpha^{ext}$ 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 $\sigma$ is the one which responds tot he actual electric field in solid

$$
\begin{aligned}
J_\alpha(\mathbf{r},t) &= \sum_\beta \sigma_{\alpha\beta}(\mathbf{q},\omega)E_\beta(\mathbf{r},t) & (3.178) \\
E_\alpha(\mathbf{r},t) &= \Xi_\alpha \exp[i(\mathbf{q}\mathbf{r} - \omega t)] & (3.179)
\end{aligned}
$$

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

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

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 $\mathbf{q} \to 0$ and $\omega \to 0$ 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

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

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

with the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$, also the electric and vector potential are taken to be transverse, so the scalar potential $\phi$ is set equal to zero. The terms in (2.85) with $A^2$ are dropped, since their effects are nonlinear in the electric field. [14] 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.

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

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

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

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

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

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

where $\lambda, \delta$ are the states associated with some unperturbed Hamiltonian $H_0$ which is chosen as the basis for the perturbation expansion. A distinction is make between the current operator $j_\alpha$ in (3.185) and the induced current $J_\alpha$ in (3.178). The operator $j_\alpha$ is used in the Hamiltonian, while $J_\alpha$ 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

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

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

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

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

[14] 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

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

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

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

$$\mathbf{J}^{(1)} = \frac{i n_0 e^2}{m\omega} \mathbf{E}(\mathbf{r}, t) \tag{3.192}$$

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

### 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

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

The **Heisenberg representation** is used here, as explained in 2.2. Next go to the interaction representation, where $H'$ is treated as the perturbation.

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

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

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

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

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

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

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)

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

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

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

The expectation value of the current is

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

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

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

From (3.202), we have the expectation value of the current operator. The first term is assumed to vanish

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

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

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

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

$$\left[j_\alpha(\mathbf{r},t),H'(t')\right] = \frac{i}{\omega}\Xi_\beta e^{-i\omega t'} \left[j_\alpha(\mathbf{r},t),j_\beta(\mathbf{q},t')\right] \tag{3.206}$$

$$= \frac{i}{\omega}E_\beta(\mathbf{r},t)e^{-i\mathbf{q}\mathbf{r}}e^{i\omega(t-t')} \left[j_\alpha(\mathbf{r},t),j_\beta(\mathbf{q},t')\right]$$

Comparing the result with (3.178) shows that

$$\sigma_{\alpha\beta} = \frac{1}{\omega}e^{-i\mathbf{q}\mathbf{r}}\int_{-\infty}^t dt'e^{i\omega(t-t')} \langle\psi| \left[j_\alpha(\mathbf{r},t),j_\beta(\mathbf{q},t')\right] |\psi\rangle + i\frac{n_0e^2}{m\omega}\delta_{\alpha\beta} \tag{3.207}$$

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 expression[15]

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

Then by change the notation of $t$, the Kubo formula

$$\sigma_{\alpha\beta}(\mathbf{q},\omega) = \frac{1}{\omega V}\int_0^\infty dt e^{i\omega t} \langle\psi| \left[j_\alpha^\dagger(\mathbf{q},t),j_\beta(\mathbf{q},0)\right] |\psi\rangle + i\frac{n_0e^2}{m\omega}\delta_{\alpha\beta} \tag{3.209}$$

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

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

[15] Not Fourier transformation, check (3.183) and (3.185).

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)

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

With Fourier transformation,

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

we have

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

The conductivity is the **retarded correlation function** of the current multiplied by $i$ and divided by $\omega$. 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 $\mathbf{q} \to 0$ and then the limit $\omega \to 0$. Be careful that wrong answer may be obtained if the order of these limits is reversed.

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

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

$$\text{Re}\,\sigma_{\alpha\beta} = -\lim_{\omega\to 0}\frac{1}{\omega}\text{Im}\left[\Pi_{\alpha\beta}(\omega)\right] \qquad (3.215)$$

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,and 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

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

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

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

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 $\rho_0 = \exp\left[\beta(\Omega - H + \mu N)\right]$ 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, $t \to -\infty$. 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

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

$$J_\alpha^{(2)} = \mathrm{Tr}\left[\rho(t) j_\alpha\right] \tag{3.219}$$

Kubo's staring 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 $\rho_0$ is the density matrix in the absence of $H'$. The equilibrium density matrix $\rho_0$ is time independent,

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

$$[H, \rho_0] = 0 \tag{3.221}$$

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

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

The linear differential equation may be integrated to give

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

Then the evaluation of (3.219) is [16]

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

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

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

[16] The derivation in P169 is not so clear to me still

# 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

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

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

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

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

The Hamiltonian is expressed (without spin index) [1]

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

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

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

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

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

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

This form of the integral equation is valid for the free-particle states with energy $\varepsilon_k$. For bound states, the energy is changed to the binding energy $\varepsilon_k \to -\varepsilon_B$ 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 $H_0 - \varepsilon_k$,

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

this gives

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

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

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

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

Then we have the desired answer

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

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

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

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

The integral is standard and gives

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

Where the density of stats of the particles

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

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

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

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

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

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

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

for the actual wave function

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

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

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

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

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

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

$$
\begin{aligned}
R_l(kr) &= j_l(kr) + 4\pi^2 \rho(k) \int_0^\infty r'^2 dr' j_l(kr_<) \eta_l(kr_>) V(r') R_l(kr') \\
&= j_l(kr) + 4\pi^2 \rho(k) \left[ \eta_l(kr) \int_0^r r'^2 dr' j_l(kr') V(r') R_l(kr') \right. \\
&\quad \left. + j_l(kr) \int_r^\infty r'^2 dr' \eta_l(kr') V(r') R_l(kr') \right]
\end{aligned}
\tag{4.23}
$$

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 $kr \to \infty$. From (4.21) it can be shown that the radial wave function must asymptotically approach the value

$$
\lim_{kr \to \infty} R_l(kr) \to \frac{C_l(k)}{kr} \sin\left[ kr + \delta_l(k) - \frac{l\pi}{2} \right]
\tag{4.24}
$$

The prefactor $C_l$ is determined below. The asymptotic limit of the integral equation (4.23) is

$$
\lim R_l(kr) \to j_l(kr) + D_l(k) \eta_l(kr) \to \frac{\sin(kr - l\pi/2)}{kr} - D_l \frac{\cos(kr - l\pi/2)}{kr}
\tag{4.25}
$$

where

$$
D_l(k) = 4\pi^2 \rho(k) \int_0^\infty r^2 dr j_l(kr) V(r) R_l(kr)
\tag{4.26}
$$

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

$$
D_l = -\tan(\delta_l) = 4\pi^2 \rho(k) \int_0^\infty r^2 dr j_l(kr) V(r) R_l(kr)
\tag{4.27}
$$

The complicated integral just defines the tangent of the phase shift. Then (4.25) becomes

$$
\lim_{kr \to \infty} R_l(kr) \to \frac{1}{kr \cos(\delta)} \left[ \cos(\delta) \sin(kr - l\pi/2) + \sin(\delta) \cos(kr - l\pi/2) \right] = \frac{\sin(kr + \delta_l l\pi/2)}{kr \cos(\delta_l)}
\tag{4.28}
$$

The normalization coefficient in (4.24) is

$$
C_l = \frac{1}{\cos(\delta_l)}
\tag{4.29}
$$

When solving the radial wave function (4.21), the solution is obtained which is will 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

$$R_{\mathbf{k'k}} = \int d^3 \phi_{\mathbf{k'}}^*(\mathbf{r}) V(r) \psi_{\mathbf{k}}(\mathbf{r}) \tag{4.30}$$

Expanding in angular momentum state by using the expansions for the wave function and the plane wave, the angular integrals give

$$R_{\mathbf{k'k}} = 4\pi \sum_l (2l+1) P_l(\hat{k} \cdot \hat{k}') R_l(k', k) \tag{4.31}$$

where the radial integral is

$$R_l(k', k) = \int_0^\infty r^2 dr \, j_l(k'r) V(r) R_l(kr) \tag{4.32}$$

It is defined for the general case where $k' \neq k$. And if they are equal, the answer is just (4.27)

$$R_l(k, k) = -\frac{\hbar^2 \tan(\delta_l)}{2mk} \tag{4.33}$$

The reaction matrix obeys an integral equation which is deduced by putting (4.30) into the integral equation (4.5) for $\psi_{\mathbf{k}}(\mathbf{r})$

$$R_{\mathbf{k'k}} = V_{\mathbf{k'k}} + P \sum_{\mathbf{k_1}} \frac{V_{\mathbf{k'k_1}} R_{\mathbf{k_1 k}}}{\varepsilon_k - \varepsilon_{k_1}} \tag{4.34}$$

# 5
# *Homogeneous Electron Gas*

## 5.1   *Exchange and Correlation*

The homogeneous electron gas is describe by the Hamiltonian

$$H = \sum_{\mathbf{p}\sigma} \varepsilon_\mathbf{p} C^\dagger_{\mathbf{p}\sigma} C_{\mathbf{p}\sigma} + \frac{1}{2V} \sum_{\mathbf{k}\mathbf{k'}\sigma\sigma'} \sum_{\mathbf{q}\neq 0} v_q C^\dagger_{\mathbf{k}+\mathbf{q}\sigma} C^\dagger_{\mathbf{k'}-\mathbf{q}\sigma'} C_{\mathbf{k'}\sigma'} C_{\mathbf{k}\sigma} \quad (5.1)$$

$$\varepsilon_p = \frac{p^2}{2m}$$

$$v_q = \frac{4\pi e^2}{q^2} \quad (5.2)$$

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 homoge-
neous 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 $r_s$,

$$k_F a_0 = \frac{1.9192}{r_s}$$

$$E_F = \frac{3.6832}{r_s^2} E_{ry}, \quad E_{ry} = 13.60 eV \quad (5.5)$$

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 hight, $r_s$ 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

$$
\begin{aligned}
E & = \sum_{\mathbf{p}\sigma} \varepsilon_p n_p = 2V \int \frac{d^3 p}{(2\pi)^3} \frac{p^2}{2m} \eta_p = \left( \frac{N_e}{n_0} \right) \frac{1}{2\pi^2 m} \int_0^{k_F} p^4 dp \\
& = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} N_e = \frac{3}{5} E_F N_e = \frac{2.2099}{r_s^2} E_{ry} N_e
\end{aligned} \tag{5.7}
$$

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

$$
N_e E_0 = \frac{e^2}{2} \int \frac{d^3 r_1 d^3 r_2}{|\mathbf{r}_1 - \mathbf{r}_2|} \left[ \rho_e(\mathbf{r}_1) - \rho_i(\mathbf{r}_1) \right] \left[ \rho_e(\mathbf{r}_2) - \rho_i(\mathbf{r}_2) \right] \tag{5.8}
$$

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

$$
\sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'} \langle C_{\mathbf{k}+\mathbf{q},\sigma}^\dagger C_{\mathbf{k}'-\mathbf{q},\sigma'}^\dagger C_{\mathbf{k}',\sigma'} C_{\mathbf{k},\sigma} \rangle \approx \delta_{\mathbf{q}=0} \sum_{\mathbf{k}\sigma} \langle C_{\mathbf{k},\sigma}^\dagger C_{\mathbf{k},\sigma} \rangle \sum_{\mathbf{k}'\sigma'} \langle C_{\mathbf{k}',\sigma'}^\dagger C_{\mathbf{k}',\sigma'} \rangle
$$

$$
\tag{5.9}
$$

Another way to pair the same operator gives

$$\approx - \sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'} \langle C^\dagger_{\mathbf{k}+\mathbf{q},\sigma} C_{\mathbf{k}',\sigma'} \rangle \langle C^\dagger_{\mathbf{k}'-\mathbf{q},\sigma'} C_{\mathbf{k},\sigma'} \rangle = - \sum_{\mathbf{k}\sigma} n_{\mathbf{k}+\mathbf{q}} n_{\mathbf{k}} \tag{5.10}$$

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**,

$$\Sigma_x(k) = -\frac{1}{V} \sum_{\mathbf{q}} v_q n_{\mathbf{k}+\mathbf{q}} \tag{5.11}$$

$$E_{gx} = - \sum_{\mathbf{k}\mathbf{q}\sigma} \frac{v_q}{2V} n_{\mathbf{k}+\mathbf{q}} n_{\mathbf{k}} = \frac{1}{2N_e} \sum_{\mathbf{k}\sigma} n_{\mathbf{k}} \Sigma_x(k) \tag{5.12}$$

The self-energy $\Sigma_x(k)$ depends only on the magnitude of the wave vector $k$ of the particle and gives

$$
\begin{aligned}
\Sigma_x(k) &= - \int \frac{d^3p}{(2\pi)^3} \frac{4\pi e^2}{|\mathbf{p}-\mathbf{k}|^2} n_p \\
&= -\frac{e^2}{\pi} \int_0^{k_F} p^2 dp \int_{-1}^1 \frac{d\cos\theta}{k^2 + p^2 - 2pk\cos\theta} \\
&= -\frac{e^2 k_F}{\pi} \left( 1 + \frac{1-y^2}{2y} \ln\left|\frac{1+y}{1-y}\right| \right) \tag{5.13} \\
y &= \frac{k}{k_F} \tag{5.14}
\end{aligned}
$$

A particle at the Fermi energy $k = k_F$ has

$$\Sigma_x(k_F) = -\frac{e^2 k_F}{\pi} \tag{5.15}$$

It is convenient to write

$$
\begin{aligned}
\Sigma_x(k) &= \frac{e^2 k_F}{\pi} S(y) \tag{5.16} \\
S(y) &= -\left( 1 + \frac{1-y^2}{2y} \ln\left|\frac{1+y}{1-y}\right| \right) \tag{5.17}
\end{aligned}
$$

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 $y \to 1$. 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

$$\left(\frac{m}{m^*}\right) = 1 + \partial_{\varepsilon_k} \Sigma_x(k) = \frac{e^2 m}{2\pi k_F} \frac{1}{y^2} \left( \frac{1+y^2}{y} \ln\left|\frac{1+y}{1-y}\right| - 1 \right) \tag{5.18}$$
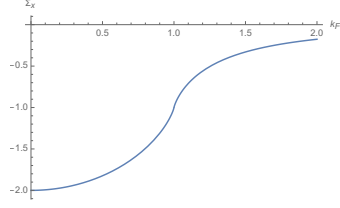
which diverges at Fermi energy $y \rightarrow 1$. If the inverse effective mass really diverged at the Fermi surface, it would have several observable consequences. The electron gas would be unstable at low temperatures, and the specific heat would diverge. Further terms in the perturbation theory produces 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

$$
\begin{aligned}
E_{gx} &= \frac{1}{N_e} \sum_{\mathbf{k}} n_{\mathbf{k}} \Sigma_x(k) = \frac{1}{n_0} \int \frac{d^3k}{(2\pi)^3} n_k \Sigma_x(k) \\
&= -\frac{3}{4} \frac{e^2 k_F}{\pi}
\end{aligned}
\tag{5.19}
$$

The average exchange energy per electron is $\frac{3}{2}$ of the value ate the Fermi energy. In therms of the parameter $r_s$, the total ground state exchange energy per electron is

$$
E_{gx} = -\frac{3}{2\pi}(k_F a_0) \left( \frac{e^2}{2a_0} \right) = -\frac{0.9163}{r_s}
\tag{5.20}
$$

So far two terms have been found for the energy of the particle,

$$
E(k) = \frac{\hbar^2 k^2}{2m} + \Sigma_x(k) + \dots
\tag{5.21}
$$

The corresponding two terms for the ground state energy per particle are,

$$
E_g = \frac{2.2099}{r_s^2} - \frac{0.9163}{r_s} + \dots
\tag{5.22}
$$

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

$$
E_g = \frac{2.2099}{r_s^2} - \frac{0.9163}{r_s} - 0.094 + 0.0622 \ln(r_s) + \dots
\tag{5.23}
$$

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,

$$E_g = \frac{2.2099}{r_s^2} - \frac{0.9163}{r_s} + E_c \qquad (5.24)$$

where the correlation energy $E_c$ needs to be determined. The result

$$E_c = -0.094 + 0.0622 \ln(r_s) + O(r_s) \qquad (5.25)$$

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 $k_F$

$$\mu = \frac{\hbar^2 k_F^2}{2m} + \Sigma_x(k_F) + \mathrm{Re}\,\Sigma_c(k_f, 0) \qquad (5.26)$$

where $ik_n = 0$ is the chemical potential. The chemical potential $\mu$ is
only a function of the electron $n_0$. The theorem of Seitz is

$$\mu(n_0) = \frac{d}{dn_0}\left[n_0 E_g(n_0)\right] = E_g + n_0 \frac{dE_g}{dn_0} \qquad (5.27)$$

The proof, by definition of chemical potential

$$\mu = E_T(N_e + 1) - E_T(N_e) \qquad (5.28)$$

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,

$$
\begin{aligned}
E_T(N_e + 1) &= (N_e + 1)E_g(n_0 + 1/V) = (N_e + 1)\left(E_g(n_0) + \frac{1}{V}\frac{dE_g}{dn_0}\right) \\
&= N_e E_g + E_g(n_0) + n_0 \frac{dE_g}{n_0} + O(\frac{1}{V}) \qquad (5.29)
\end{aligned}
$$

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 im-
balance, 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 form 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.

$$E_T = N_e E_g + A E_S \tag{5.30}$$

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, $\mu$ 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 $\mu_B$. In Hartree-Fock approximation the chemical potential gives for the bulk contribution,

$$\mu_{B,HF} = \frac{d}{dn_0} \left( n_0 E_{g,HF} \right) = E_F - \frac{e^2 k_F}{\pi} \tag{5.31}$$

### 5.1.5   $\Sigma^{2a}$

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.
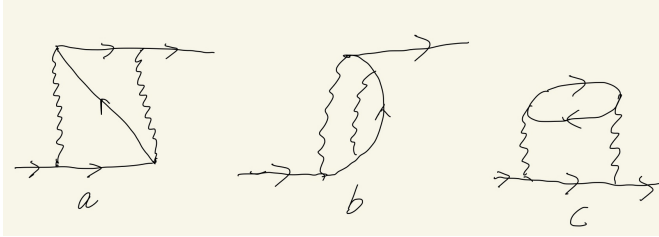


Figure 5.2: Diagrame

For Figure 5.2a, the self-energy contribution is

$$\Sigma^{2a}(k) = \frac{1}{V^2 \beta^2} \sum_{\mathbf{qq'}} v_q v_{q'} \sum_{iq_n, iq_{n'}} \mathcal{G}^0(k+q) \mathcal{G}^0(k+q') \mathcal{G}^0(k+q+q') \tag{5.32}$$

according (3.94) and calculation, we have

$$
\begin{aligned}
\Sigma^{2a}(k) &= -\frac{1}{V^2} \sum_{\mathbf{qq'}} \frac{v_q v_{q'}}{ik_n + \xi_{\mathbf{k+q+q'}} - \xi_{\mathbf{k+q'}} - \xi_{\mathbf{k+q}}} \\
&= \left[ \eta_F(\xi_{\mathbf{k+q'}}) \left( \eta_F(\xi_{\mathbf{k+q}}) - \eta_F(\xi_{\mathbf{k+q+q'}}) \right) \right. \\
&\quad + \left. \eta_F(\xi_{\mathbf{k+q+q'}}) \left( 1 - \eta_F(\xi_{\mathbf{k+q}}) \right) \right]
\end{aligned}
\tag{5.33}
$$

The self-energy of a particle is needed on the Fermi surface. Set $k = k_F$ and $ik_n = \tilde{\xi}_{k_F} = k_F^2/2m - \mu = 0$. The terms in the energy denominator largely cancel,

$$\xi_{\mathbf{k}} + \xi_{\mathbf{k+q+q'}} - \xi_{\mathbf{k+q}} - \xi_{\mathbf{k+q'}} = \frac{\mathbf{q} \cdot \mathbf{q}'}{m} \tag{5.34}$$

The self-energy is

$$
\begin{aligned}
\Sigma^{2a}(k_F, 0) &= -\frac{(4\pi e^2)^2 m}{(2\pi)^6} \int \frac{d^3 q}{q^2} \int \frac{d^3 q'}{(q')^2} \frac{1}{\mathbf{q} \cdot \mathbf{q}'} \\
&\times \left\{ \eta_F(\xi_{\mathbf{k}+\mathbf{q}'}) \left[ \eta_F(\xi_{\mathbf{k}+\mathbf{q}}) - \eta_F(\xi_{\mathbf{k}+\mathbf{q}+\mathbf{q}'}) \right] + \dots \right\} (5.35)
\end{aligned}
$$

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

$$
\Sigma^{2a} = \frac{1}{3} \ln(2) - \frac{3}{2\pi^2} \zeta(3) = 0.0436 \tag{5.36}
$$

### 5.1.6   $\Sigma^{2b}$

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

$$
\Sigma'_x(k) = -\frac{1}{V\beta} \sum_{\mathbf{q}, ik_n} v_q \mathcal{G}(\mathbf{k} + \mathbf{q}, ik_n) \tag{5.37}
$$

$$
\mathcal{G}(\mathbf{k} + \mathbf{q}, ik_n) = \frac{1}{ik_n - \xi_{\mathbf{k}+\mathbf{q}} - \Sigma_x(\mathbf{k} + \mathbf{q})} \tag{5.38}
$$

where the Green's function has a self-energy due to exchange. Since the self-energy $\Sigma_x(k)$ does not depend on frequency, the frequency summation of the Green's function yields the simple number operator as in (3.96)

$$
\frac{1}{\beta} \sum_{ik_n} \mathcal{G}(\mathbf{k} + \mathbf{q}, ik_n) = \eta_F \left[ \xi_{\mathbf{k}+\mathbf{q}} + \Sigma_x(\mathbf{k} + \mathbf{q}) \right] = \frac{1}{e^{\beta(\xi + \Sigma)} + 1} \tag{5.39}
$$

and the self-energy of (5.37) is

$$
\Sigma'_x(k) = -\frac{1}{V} \sum_{\mathbf{p}} v_{\mathbf{p}-\mathbf{k}} \eta_F \left[ \xi_{\mathbf{p}} + \Sigma_x(\mathbf{p}) \right] \tag{5.40}
$$

At zero temperature the electron distribution function is a step function. **This step function must also be normalized so that the electron density is still $n_0$,** as

$$
n_0 = 2 \int \frac{d^3 p}{(2\pi)^3} \eta_F \left[ \xi_p + \Sigma_x(p) \right] \tag{5.41}
$$

The effect of the exchange energy $\Sigma_x(p)$ in the argument of $\eta_F$ is to change the chemical potential. **However, the Fermi wave vector $k_F$ is**

**the same, even after the exchange energy has been included in the occupation function**. Since the Fermi wave vector determines by the density $n_0$. Thus the addition of the exchange energy must be canceled by an equal change in chemical potential, at zero temperature

$$\lim_{T \to 0} \eta_F \left[ \tilde{\xi}_k + \Sigma_x(k) \right] = \Theta(k_F - k) \tag{5.42}$$

The exchange energy $\Sigma_x'(k)$ in (5.40) is exactly equal to the one calculated earlier. Thus the summation of all terms just yields the value of the first term alone. All of the subsequent terms in that series sum to zero, because of a shift in the chemical potential.

The exchange self-energy has a remarkable effect upon the zero temperature electron distribution. It leaves $k_F$ unchanged. This simple result is a consequence of the feature that $\Sigma_x(k)$ is independent of frequency.

### 5.1.7  $\Sigma^{2c}$

The third self-energy with two Coulomb lines is written as

$$\Sigma^{2c}(k) = -\frac{1}{V\beta} \sum_{\mathbf{q}, iq_m} v_q^2 \mathcal{P}^{(1)}(\mathbf{q}, iq_m) \mathcal{G}^0(\mathbf{k} + \mathbf{q}, ik_n + iq_m) \tag{5.43}$$

The closed fermion loop gives the polarization diagram $\mathcal{P}^{(1)}(\mathbf{q}, iq_m)$ [1]. This diagram has one drawback. The wave vector integral appears to diverge at small values of $q$, because of the factor $v_q^2$,

[1] Eq.3.214 in the book

$$\int \frac{d^3q}{q^4} \implies \int_0 \frac{dq}{q^2} \to \infty \tag{5.44}$$

So this self-energy term is infinite. The divergence is removed by summing a series of self-energy diagram, as shown Fig. 5.3. Each



Figure 5.3: Summation of diagram.

term has one more polarization bubble and one more Coulomb line–hence an additional factor of $v_q \mathcal{P}^{(1)}$. The summation of these terms gives the simple series

$$\begin{aligned}
\Sigma^c(k) &= -\frac{1}{V\beta} \sum_q v_q \mathcal{G}^{(0)}(k+q) \\
&\quad \times \left\{ v_q \mathcal{P}^{(1)}(q) + \left[ v_q \mathcal{P}^{(1)}(q) \right]^2 + \left[ v_q \mathcal{P}^{(1)}(q) \right]^3 + \dots \right\} \\
&= -\frac{1}{V\beta} \sum_q v_q \mathcal{G}^{(0)}(k+q) \frac{v_q \mathcal{P}^{(1)}(q)}{1 - v_q \mathcal{P}^{(1)}(q)} \tag{5.45}
\end{aligned}$$

The summation of terms shown in Fig. 5.3 is called the **random phase approximation (RPA)**. The approximation in RPA is that this series of terms is used to represent the entire answer. RPA ignores other terms, such as (5.35), which was found from the diagram in Fig. 5.2(a). RPA ignores many more terms in each higher order of perturbation series.

The denominator in (5.45) is a very important quantity because it is very often used in calculations. It is the RPA approximation to the dielectric function and is defined as

$$\varepsilon_{RPA}(q) = 1 - v_q \mathcal{P}^{(1)}(q) \qquad (5.46)$$

Then the self-energy series may be written as

$$\Sigma^c(k) = -\frac{1}{V\beta} \sum_q v_q \mathcal{G}^{(0)}(k+q) \left[ \frac{1}{\varepsilon_{RPA}(q)} - 1 \right] \qquad (5.47)$$

Remember the exchange energy term in (5.37), which is exactly the $-1$ term. Then adding the exchange energy to the above result gives a term containning the *RPA* dielectric function

$$\Sigma_{RPA}(k) = \Sigma^c(k) + \Sigma_x(k) = -\frac{1}{V\beta} \sum_q v_q \frac{\mathcal{G}^{(0)}(k+q)}{\varepsilon_{RPA}(q)} \qquad (5.48)$$

The summation of these two terms is define as the **RPA self-energy** or called **screened exchange energy**. With this correction, the inverse effective mass no longer diverges at the Fermi surface as will shown later.

### 5.1.8  Hight=Density Limit

In RPA the correlation energy is

$$E_{c,RPA} = -0.142 + 0.0622 \ln r_s + O(r_s, r_s \ln(r_s)) \qquad (5.49)$$

Adding the Onsager result, for the second-order diagram $\Sigma^{(2a)}$ in (5.35), gives the result of Gell-Mann and Bruckner

$$E_c = -0.094 + 0.0622 \ln r_s + \dots \qquad (5.50)$$

Another term is obtained by Carr and Maradudin

$$E_c = -0.094 + 0.0622 \ln r_s + 0.018 r_s \ln r_s + a r_s + O(r_s^2) \qquad (5.51)$$

In high density limit, $r_s \to 0$, the energy in (5.51) is not analytic, but the series is accurate in this limit. For metallic the density is around $1.8 < r_s < 56$, in this region the perturbation formula for $E_c$ is not valid, because the correlation energy must be negative.

### 5.1.9   Pair Distribution Function

The correlation energy is the improvement in the ground state energy beyond the Hartree-Fock approximation. It is useful to examine an important property of the Hartree-Fock theory, the pair distribution function $g(r)$, to understand the correlation energy. The pair distribution function $g(r)$ is the probability per unit volume that an election is at $\mathbf{r}$ is there is already one at $\mathbf{r} = 0$. There are two different pair distribution functions in an unmagnetized electron gas: $g_{\uparrow\uparrow}(\mathbf{r}) = g_{\downarrow\downarrow}(\mathbf{r})$ and $g_{\uparrow\downarrow}(\mathbf{r}) = g_{\downarrow\uparrow}(\mathbf{r})$ [2]. Of course, the electrons are not fixed, and they are usually moving rapidly. Then these pair distribution functions are averages for the moving particles. Even the electron at $\mathbf{r} = 0$ is not fixed, so that this reference point moves with the electron.

The N-particle wave function is a Slater determinant,

$$\Psi_{\lambda_1,\lambda_2,\dots\lambda_N}(\mathbf{r}_1\dots\mathbf{r}_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \phi_{\lambda_1}(\mathbf{r}_1) & \phi_{\lambda_1}(\mathbf{r}_2) & \cdots & \phi_{\lambda_1}(\mathbf{r}_N) \\ \phi_{\lambda_2}(\mathbf{r}_1) & \phi_{\lambda_2}(\mathbf{r}_2) & \cdots & \phi_{\lambda_2}(\mathbf{r}_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{\lambda_N}(\mathbf{r}_1) & \phi_{\lambda_N}(\mathbf{r}_2) & \cdots & \phi_{\lambda_N}(\mathbf{r}_N) \end{vmatrix}$$
(5.52)

where the $\lambda_j$ are the quantum numbers which describe the states, and there is one wave function for every occupied electron state. The pair distribution function is given by the two-particle density matrix, by integrating the N-particle density wave function

$$g_{ss'}(\mathbf{r}_1,\mathbf{r}_2) = V^2 \int d\mathbf{r}_3 d\mathbf{r}_4\dots d\mathbf{r}_N \left|\Psi_{\lambda_1\lambda_2\dots\lambda_N}(\mathbf{r}_1\dots\mathbf{r}_N)\right|^2$$
(5.53)

If the one-electron orbital $\phi_{\lambda_j}(\mathbf{r})$ are assumed orthogonal, then this integration just yield the sum over all possible pair wave function,

$$g_{ss'}(\mathbf{r}_1,\mathbf{r}_2) = \frac{V^2}{N(N-1)}\sum_{\lambda_i,\lambda_j}\begin{bmatrix} \phi_{\lambda_i}(\mathbf{r}_1) & \phi_{\lambda_i}(\mathbf{r}_2) \\ \phi_{\lambda_j}(\mathbf{r}_1) & \phi_{\lambda_j}(\mathbf{r}_2) \end{bmatrix}^2$$
(5.54)

The sum over $\lambda_i$, $\lambda_j$ is over all occupied state, so each pair is summed twice. For the homogeneous electron gas, the orbitals must describe plane wave,

$$\phi_\lambda(\mathbf{r}) = \frac{\chi_s}{\sqrt{V}}e^{i\mathbf{k}\cdot\mathbf{r}}$$
(5.55)

where the $\chi_s$ are the sin functions. Due to the orthogonal and normalize condition, the spin averages are $\langle\chi_\uparrow\chi_\uparrow\rangle = 1$, $\langle\chi_\uparrow\chi_\downarrow\rangle = 0$. The

[2] The first is the spin for $\mathbf{r} = 0$.

two pair distribution functions are

$$
g_{\uparrow\downarrow}(\mathbf{r}_1 - \mathbf{r}_2) = \frac{1}{N(N-1)} \sum_{\mathbf{k}_1 \mathbf{k}_2} \left( \left| e^{i\mathbf{k}_1 \cdot \mathbf{r}_1 + i\mathbf{k}_2 \cdot \mathbf{r}_2} \right|^2 + \left| e^{i\mathbf{k}_1 \cdot \mathbf{r}_2 + i\mathbf{k}_2 \cdot \mathbf{r}_1} \right|^2 \right)
$$

$$
= \frac{2}{N(N-1)} \left( \frac{N}{2} \right)^2 = \frac{1}{2} \tag{5.56}
$$

$$
g_{\uparrow\uparrow}(\mathbf{r}_1 - \mathbf{r}_2) = \frac{1}{N(N-1)} \sum_{\mathbf{k}_1 \mathbf{k}_2} \left| e^{i\mathbf{k}_1 \cdot \mathbf{r}_1 + i\mathbf{k}_2 \cdot \mathbf{r}_2} - e^{i\mathbf{k}_1 \cdot \mathbf{r}_2 + i\mathbf{k}_2 \cdot \mathbf{r}_1} \right|^2
$$

$$
= \frac{1}{2} \left[ 1 - \Lambda(\mathbf{r}_1 - \mathbf{r}_2)^2 \right] \tag{5.57}
$$

$$
\Lambda(\mathbf{r}) = \frac{2}{N} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} \tag{5.58}
$$

The summation over $\mathbf{k}$ runs only over occupied states. The antiparallel spin distribution function $g_{\uparrow\downarrow} = g_{\downarrow\uparrow} = 1/2$ in the Hartree-Fock approximation. The cross term which results from the determinant is zero because of the orthogonality of the two spin functions. There is no correlation in the position of electrons of opposite spin. The parallel spin $g_{\uparrow\uparrow} = g_{\downarrow\downarrow}$ has a definite spatial dependence, which comes from the cross term which is retained since the spins are parallel and the spin averages are unity. The function $\Lambda(\mathbf{r})$ is calculated

$$
\Lambda(\mathbf{r}) = \frac{2}{n_0} \int \frac{d^3k}{(2\pi)^3} \eta_k e^{i\mathbf{k} \cdot \mathbf{r}} = \frac{3}{rk_F^3} \int_0^{k_F} k \, dk \sin(kr) = \frac{3}{rk_F} j_1(rk_F) \tag{5.59}
$$

where $j_1(x)$ is spherical Bessel function. This gives the parallel spin $g_{\uparrow\uparrow}(r)$ vanish as $r = 0$ and approaches $\frac{1}{2}$ at large distance.

The total pair distribution function for a particle is the combination of the result for parallel and antiparallel spin distributions,

$$
g(r) = g_{\uparrow\uparrow}(r) + g_{\uparrow\downarrow}(r) \tag{5.60}
$$

In a nonmagnetic system, the same result is obtained if the central particle has spin down.

The pair distribution function has two features which are important for later discussion. First, there is the normalization integral,

$$
n_0 \int d\mathbf{r} \left[ g(\mathbf{r}) - 1 \right] = -1 \tag{5.61}
$$

The second is a statement about the ground state energy of the electron gas. It has kinetic energy plus Coulomb parts. The Coulomb energy around the hole in the Hartree-Fock approximation is

$$
E_{Coul} = \frac{e^2 n_0}{2} \int d\mathbf{r} \frac{g(\mathbf{r}) - 1}{r} \tag{5.62}
$$

The integral $E_{Coul}$ is related to the exchange energy which is discussed later in ??. The above two relations for $g(\mathbf{r})$ can be checked in

the Hartree-Fock approximation. In the case of $g(\mathbf{r}) = 1/2 + g_{\uparrow\uparrow}(\mathbf{r})$, the normalization integral yields ($x = rk_F$).

$$n_0 \int d\mathbf{r} \left[ g_{\uparrow\uparrow}(\mathbf{r}) - \frac{1}{2} \right] = -\frac{n_0}{2} \int d^3r \Lambda(r)^2 = -\frac{6}{\pi} \int_0^\infty dx j_1(x)^2 = -1$$

and the Coulomb integral yields

$$E_{Coul} = -\frac{3e^2 k_F}{4\pi} \tag{5.63}$$

These result are correct for Hartree-Fock. It is the same exchange energy per particle which was derived by diagrammatic means.

The pair distribution function $g(\mathbf{r})$ is the distribution of electrons, on the average, about any electron. It goes to unity at large distance, which is a result of the uniform distribution $n_0$ of electron charge. That is, the electron charge density is $-en_0 g(\mathbf{r})$. Since $g(\mathbf{r})$ is less than unity near $\mathbf{r} \to 0$, the electron charge is depleted in the vicinity of electron. This reduction may be viewed as a hole in the electron density. Wigner suggested the name **exchange and correlation hole**. The hole moves with the electron.

According to the normalization (5.61), the total charge missing from this hole is one electron charge. The factor $-n_0(g - 1)$ is the density of hole charge, which integrates to 1. The homogeneous electron gas has a uniform charge density only on the average. To a particular electron, the system is not uniform at all, since other electrons are not as likely to venture near to it as they are to other points.

The Coulomb integral (5.63) gives the potential energy of the system. The electron interacts with its own hole charge. It is not influenced by the electrons or uniform charge density farther away,since they cancel on the average. Near the electron the positive background charge is not canceled by the other electrons, since the other electrons are not as likely to be nearby. In the Hartree-Fock approximation, only electrons of parallel spin make the exchange and correlation hole. Since $g_{\uparrow\downarrow} = 1/2$, the antiparallel spin are not affected.

It is possible to arrange $g(r)$ so that the sum rule (5.61) is still obeyed, yet the potential energy is lower than found in Hartree-Fock. This lowering is done by permitting $g_{\uparrow\downarrow} = 1/2$ to become less than $1/2$ near the point $\mathbf{r} \to 0$. It is these charges which give rise to the correlation energy. Charges in $g_{\uparrow\downarrow}$ and $g_{\uparrow\uparrow}$ will usually cost some kinetic energy, so that one cannot just adjust $g_{ss'}$ to maximize the potential energy alone. The system will seek the lowest energy stat at $T = 0$, which is the state with some "correlation" between the motion of electrons with antiparallel spins. This "correlation" between the motion of pairs of electrons is what gives rise to the "correlation energy".

## 5.2   Wigner Lattice

Actual electron systems exist over a range of densities. For metals
usually we have $1.8 < r_s < 6$. The correlation energy in the high
density limit, $r_s \to 0$, have been discussed in previous section. For
low-density limit and final formulas for intermediate rages was given
by Wigner

$$E_c = \frac{0.88}{r_s + 7.8} E_{ry} \tag{5.64}$$

and still widely used. At low densities, Wigner speculated that the
electrons would become localized and form a regular lattice. With the
jellium model where the positive charge is uniformly spread through
the system. The electron lattice would presumably be a close-packed
structure such as bcc, fcc or hcp, in which electrons would vibrate
around their equilibrium positions. The localization cannot occur
until the zero point energy is less than the potential energy.

Consider the Wigner-Seitz model for the unit cell of the lattice.
With a sphere of radius $r_s a_0$ a electron locate at the center. *Each sphere
has overall neutrality, since the one-electron charge at the center is canceled
by the positive charge inside the volume of the sphere.* Outside of each
sphere, the electric field is zero. If all unit cells are neutral spheres,
then they exert no electric fields on each other. The electric fields in-
side a sphere arise only from the electron and positive charge within
that sphere. This approximation made by Wigner-Seitz assumption is
remarkably small.

The first term is the potential energy between the electron and the
*uniform* positive background. This give

$$
\begin{aligned}
E_{ep} &= \int d^3 \left( -\frac{e^2}{r} \right) n_0 = -\frac{3e^2}{r_s^3 a_0^3} \int_0^{r_s a_0} r \, dr \\
&= -\frac{3e^2}{2a_0 r_s} = -\frac{3}{r_s} \left( \frac{e^2}{2a_0} \right)
\end{aligned} \tag{5.65}
$$

where $-e^2/r$ is the potential energy and $n_0 = 3/(4\pi r_s^3 a_0^3)$ is the
density of positive charge at each distance $r$.

The second term in the potential energy is the interaction of the
positive charge with itself. The potential energy $V(r)$ from the posi-
tive charge at a distance $r$ form the center is obtained by solving first
for its equivalent electric field,

$$-\frac{dV}{dr} = eE(r) = \frac{e^2}{r^2} n_0 \left( \frac{4\pi r^3}{3} \right) = \frac{e^2 r}{r_s^3 a_0^3} \tag{5.66}$$

which is $e^2/r^2$ times the total charge within the sphere of radius $r$.
Integrating this equation to obtain $V(r)$, there is a constant of integra-
tion. It is determined by the condition that the total potential, from

electron and positive charge, must vanish at the surface of the sphere. The constant is chosen to make $V(r)$ be $e^2/r_s a_0$ at the surface. The result is

$$V(r) = \frac{e^2}{2r_s a_0}\left[3 - \left(\frac{r}{r_s a_0}\right)^2\right] = \frac{1}{r_s}\left[3 - \left(\frac{r}{r_s a_0}\right)^2\right]E_{ry} \qquad (5.67)$$

The potential energy of the positive charge interacting with itself is found using

$$
\begin{aligned}
E_{pp} &= \frac{1}{2}\int d^3 r V(r)n_0 = \frac{3}{4}\frac{e^2}{(r_s a_0)^4}\int_0^{r_s a_0} r^2 dr \left[3 - \left(\frac{r}{r_s a_0}\right)^2\right] \\
&= \frac{3}{5}\frac{e^2}{r_s a_0} = \frac{6}{5r_s}E_{ry} \qquad (5.68)
\end{aligned}
$$

The result is multiplied by $1/2$ because it is a self-energy. There are only two potential energy terms. The interaction of the electron with itself is not included. Aside form the fact that it is infinity, it does not change the metal and so does not contribute to the cohesive energy of the system.

The sum of these two terms is the total potential energy in the Wigner lattice in the Wigner-Seitz approximation. It is a large term , it has a larger coefficient than the exchange and correlation energies which is found for the free-particle system. The system apparently has gained energy by the localization of the electrons.

The Wigner lattice is stable in the large value of $r_s$.

## 5.3   Metallic Hydrogen

Skip

## 5.4   Linear Screening

Screening is one of the most important concepts in many-body theory. Charges, which are able, will move in response to an electric field. This charge movement will stabilize into a new distribution of charge around the electric field and this new distribution is just the right amount of charge to cancel the electric field at large distance. If the electric field is caused by an impurity charge distribution $\rho_i$ with net charge $Q_i$, the amount of mobile charge attached to the surrounding is exactly $-Q_i$. The name screening charge is applied to the mobile charge attached by the impurity electric field with own distribution in space $\rho_s$. The screened potential from the impurity charge and the screening charge is given by

$$\phi(\mathbf{r}) = \int d\mathbf{r}'\frac{\rho_i(\mathbf{r}') + \rho_s(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \qquad (5.69)$$

The screening charge is not necessarily in bound states due to the electric field from the impurity[3]. But quite often the screening charge is from the unbound conduction electrons of the metal or semiconductor. In their motion through the crystal, they spend a little more time near the impurity potential, if it is attractive, than they do elsewhere in the solid. When this motions are averaged, there is more electron density near the impurity than elsewhere, which is the screening charge. For repulsive interaction the screening charge is similar but with positive charge since it reduce the average density of electrons.

The classical macroscopic theory give the electric field and displacement as

$$\nabla \cdot \mathbf{D}(\mathbf{r}) \;=\; 4\pi \rho_i(\mathbf{r}) \tag{5.70}$$

$$\nabla \cdot \mathbf{E}(\mathbf{r}) \;=\; 4\pi[\rho_i(\mathbf{r}) + \rho_s(\mathbf{r})] \tag{5.71}$$

with Fourier-transformation

$$i\mathbf{q} \cdot \mathbf{D}(\mathbf{q}) \;=\; 4\pi \rho_i(\mathbf{q}) \tag{5.72}$$

$$i\mathbf{q} \cdot \mathbf{E}(\mathbf{q}) \;=\; 4\pi[\rho_i(\mathbf{q}) + \rho_s(\mathbf{q})] \tag{5.73}$$

For the components that along the direction $\mathbf{q}$ are the longitudinal fields $D_l$ and $E_l$. The longitudinal electric field is related to the scalar potential,

$$E_l(\mathbf{r}) \;=\; -\nabla\phi(\mathbf{r}) \tag{5.74}$$

$$\phi(\mathbf{q}) \;=\; i\frac{E_l(\mathbf{q})}{q} \tag{5.75}$$

These gives us the result

$$D_l(\mathbf{q}) \;=\; \frac{4\pi}{iq}\rho_i(\mathbf{q}) \tag{5.76}$$

$$E_l(\mathbf{q}) \;=\; \frac{4\pi}{iq}[\rho_i(\mathbf{q}) + \rho_s(\mathbf{q})] \tag{5.77}$$

$$\phi(\mathbf{q}) \;=\; \frac{4\pi}{q^2}[\rho_i(\mathbf{q}) + \rho_s(\mathbf{q})] \tag{5.78}$$

The **dielectric response function** is defined as the ration of $\frac{D_l(\mathbf{q})}{E_l(\mathbf{q})}$ int he limit where $\rho_i \to 0$

$$\varepsilon(\mathbf{q}) = \lim_{\rho_i \to 0} \frac{D_l(\mathbf{q})}{E_l(\mathbf{q})} = \lim_{\rho_i \to 0} \left[\frac{\rho_i(\mathbf{q})}{\rho_i(\mathbf{q}) + \rho_s(\mathbf{q})}\right] \tag{5.79}$$

In this limit $\varepsilon(\mathbf{q})$ becomes a property of the material and is independent of the charge distribution.

To calculate the dielectric function. The linear screening model assumes this definition of (5.79) is true for nonzero $\rho_i(\mathbf{q})$, which gives

[3] That could happen if the electric field from the impurity is strong enough.

for the potential

$$\phi'(\mathbf{q}) = \frac{4\pi}{q^2} \frac{\rho_i(\mathbf{q})}{\varepsilon(\mathbf{q})} \tag{5.80}$$

$$\phi'(\mathbf{r}) = \int \frac{d^3q}{(2\pi)^3} \frac{4\pi}{q^2} \frac{\rho_i(\mathbf{q})}{\varepsilon(\mathbf{q})} e^{i\mathbf{q}\cdot\mathbf{r}} \tag{5.81}$$

The potential $\phi'$ is the total potential from screening charge and impurity charge. The potential $\phi'$ should be similar to the exact screened potential $\phi$ in (5.69) and they are identical in the limit where $\rho_i$ is small. The linear screening approximation is to calculate $\phi'$ in place of $\phi$. Another feature of the linear screening model is that the screening charge $\rho_s(\mathbf{q})$ density is proportional, in $\mathbf{q}$ space, to the impurity charge density $\rho_i(\mathbf{q})$. Linear screening model assume that

$$\varepsilon(\mathbf{q}) = \frac{\rho_i(\mathbf{q})}{\rho_i(\mathbf{q}) + \rho_s(\mathbf{q})} \tag{5.82}$$

$$\frac{\rho_s(\mathbf{q})}{\rho_i(\mathbf{q})} = \frac{1}{\varepsilon(\mathbf{q})} - 1 \tag{5.83}$$

are valid for finite values of $\rho_i$, rather than infinitesimal ones.[4]

The macroscopic theory defined the dielectric function $\varepsilon(\mathbf{q})$. To calculate it one needs the microscopic theory. The derivation of the exact equation for $\varepsilon(\mathbf{q})$ starts by considering the interaction between two impurity charges $Z_1 e$ and $Z_2 e$ in the homogeneous electron gas. In linear screen model, the interaction potential between these charge is proportional to the product $Z_1 Z_2$. The ground state energy of the system is evaluated, and all energy terms are extracted which are proportional to $Z_1 Z_2$. The summation of there terms is defined as the interaction potential between the two charges. Of course, there will also be terms proportional to $Z_1^n$ or $Z_2^n$, which are the energies needed to put each separate charge in by itself. These terms are contributions to the nonlinear interaction. All other terms are ignored except $Z_1 Z_2$, since the immediate interest is the derivation of linear screening.

The Hamiltonian of the homogeneous electron gas, with two impurity charges $Z_1 e$ and $Z_2 e$ at $\mathbf{R}_1$ and $\mathbf{R}_2$ is written as

$$H = H_0 + \frac{Z_1 Z_2 e^2}{|\mathbf{R}_1 - \mathbf{R}_2|} - \frac{1}{V} \sum_{\mathbf{q}\neq 0} v_q \rho(\mathbf{q}) \sum_{j=1}^{2} Z_j e^{i\mathbf{q}\cdot\mathbf{R}_j} \tag{5.84}$$

$$\rho(\mathbf{q}) = \sum_{\mathbf{p}\sigma} C^\dagger_{\mathbf{p}+\mathbf{q},\sigma} C_{\mathbf{p}\sigma} \tag{5.85}$$

The $H_0$ is the Hamiltonian for the homogeneous electron gas (5.1). The second term is the direct interaction between the two charges. The last term is the interaction potential between each impurity

[4] The validity is discussed in P318.

charge and the electrons of the homogeneous electron gas. They are represented by the density operator $\rho(\mathbf{q})$.

The ground state energy is calculated from the thermodynamic potential, which is found from the linked cluster theorems of (3.122)–(3.124)

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

$$
U_l = \frac{(-1)^l}{l}\int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_l \langle T_\tau V_1 \ldots V_l\rangle_{different connected}
$$

where $U_l$ are the different connected diagrams. Only the terms in this series will be evaluated which are proportional to $Z_1 Z_2$. The noninteracting potential $\Omega_0$ comes from $H_0$. The last two terms in (5.84) are the interaction potential $V$ which enters the perturbation expansion for the thermodynamic potential.

The term $U_1$ in the expansion has only one power of $V$. In this order, the only contribution proportional to $Z_1 Z_2$ is from the direct interaction

$$
U_1 = -\beta\frac{Z_1 Z_2 e^2}{|\mathbf{R}_1 - \mathbf{R}_2|} \equiv -\beta Z_1 Z_2 \int \frac{d^3 q}{(2\pi)^3} v_q e^{i\mathbf{q}\cdot(\mathbf{R}_1 - \mathbf{R}_2)}  \qquad (5.86)
$$

**The other first-order term is zero, since the average of $\rho(\mathbf{q})$ is zero in the electron gas unless $\mathbf{q} = 0$.**

The term $U_2$ have two powers of $V$. This gives

$$
U_2 = \frac{1}{2V^2}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_{\mathbf{q}\mathbf{q}'} v_q v_{q'} \langle T_\tau \rho(\mathbf{q}, \tau_1)\rho(\mathbf{q}', \tau_2)\rangle
$$

$$
\times \left(Z_1 e^{i\mathbf{q}\cdot\mathbf{R}_1} + Z_2 e^{i\mathbf{q}\cdot\mathbf{R}_2}\right)\left(Z_1 e^{i\mathbf{q}'\cdot\mathbf{R}_1} + Z_2 e^{i\mathbf{q}'\cdot\mathbf{R}_2}\right) \qquad (5.87)
$$

This term is the only one in $U_2$. The higher linked cluster terms $U_l$ have only higher power of the charges. **The $U_2$ term is simplified by the fact that in a homogeneous system it is nonzero only when $\mathbf{q} + \mathbf{q}' = 0$, since the density–density correlation function of the electron operators is nonzero only in this circumstance**

$$
\Delta\Omega = Z_1 Z_2 \int \frac{d^3 q}{(2\pi)^3} v_q e^{i\mathbf{q}\cdot(\mathbf{R}_1 - \mathbf{R}_2)}
$$

$$
\times \left[1 - \frac{v_q}{V\beta}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \langle T_\tau \rho(\mathbf{q}, \tau_1)\rho(\mathbf{q}', \tau_2)\rangle\right] \qquad (5.88)
$$

This formula is compared with the linear screening model (5.81) for the potential from a charge distribution. One charge, say $Z_1$, is the impurity $\rho_i(\mathbf{q}) = Z_1$. The other charge $Z_2$ is the test charge which measure the strength of the screened potential. The net interaction between the charge can be written as a screened coulomb interaction

of the form

$$V_s(\mathbf{R}_1 - \mathbf{R}_2) = \Delta\Omega = Z_1 Z_2 \int \frac{d^3 q}{(2\pi)^3} \frac{v_q}{\varepsilon(\mathbf{q})} e^{i\mathbf{q}\cdot(\mathbf{R}_1 - \mathbf{R}_2)} \tag{5.89}$$

which provides a rigorous definition of the dielectric function

$$\frac{1}{\varepsilon(\mathbf{q})} = 1 - \frac{v_q}{V\beta} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \langle T_\tau \rho(\mathbf{q}, \tau_1)\rho(-\mathbf{q}, \tau_2)\rangle \tag{5.90}$$

The correlation term can be further simplified. Along with the periodicity (3.13) of the argument, permit one of the $\tau$ integrals to be eliminated to give

$$\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \langle T_\tau \rho(\mathbf{q}, \tau_1)\rho(-\mathbf{q}, \tau_2)\rangle = \beta \int_0^\beta d\tau \langle T_\tau \rho(\mathbf{q}, \tau)\rho(-\mathbf{q}, 0)\rangle \tag{5.91}$$

so the inverse dielectric function is

$$\frac{1}{\varepsilon(\mathbf{q})} = 1 - \frac{v_q}{V} \int_0^\beta d\tau \langle T_\tau \rho(\mathbf{q}, \tau)\rho(-\mathbf{q}, 0)\rangle \tag{5.92}$$

It relates the dielectric function to the density–density correlation function. The time variation of the operator $\rho(\mathbf{q}, \tau) = e^{\tau H_0}\rho(\mathbf{q})e^{-\tau H_0}$ is governed by $H_0$ which is the full Hamiltonian for the homogeneous electron gas without the potential of the impurities.

The static density–density correlation function is related to the static structure factor $S(\mathbf{q})$, for a system of $N_e$ electrons

$$\frac{1}{N_e}\langle \rho(\mathbf{q})\rho(-\mathbf{q})\rangle = N_e \delta_{\mathbf{q}=0} + S(\mathbf{q}) \tag{5.93}$$

Further, generalize (5.92) to nonzero value of frequency

$$\frac{1}{\varepsilon(\mathbf{q}, i\omega_n)} = 1 - \frac{v_q}{V} \int_0^\beta d\tau e^{i\omega_n \tau} \langle T_\tau \rho(\mathbf{q}, \tau)\rho(-\mathbf{q}, 0)\rangle \tag{5.94}$$

Equation (5.94) is used to prove the following important theorem

$$N_e \delta_{\mathbf{q}=0} + S(\mathbf{q}) = -\frac{1}{n_0 v_q} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{1 - e^{-\beta\omega}} \operatorname{Im}\left[\frac{1}{\varepsilon(\mathbf{q}, \omega)}\right] \tag{5.95}$$

The function $\varepsilon(\mathbf{q}, \omega)$ is the retarded function obtained from $\varepsilon(\mathbf{q}, i\omega_n)$, the factor $n_0 = k_F^3/3\pi^2$ is the particle density and $v_q = 4\pi e^2/q^2$. At zero temperature, the above formula becomes ($\mathbf{q} \neq 0$)

$$S(\mathbf{q}) = -\frac{1}{n_0 v_q} \int_0^\infty \frac{d\omega}{\pi} \operatorname{Im}\left[\frac{1}{\varepsilon(\mathbf{q}, \omega)}\right] \tag{5.96}$$

which is the way it is often written. The pair distribution function $g(\mathbf{r})$ or the static structure factor $S(\mathbf{q})$ is obtained from a knowledge of the frequency-dependent dielectric function $\varepsilon(\mathbf{q}, \omega)$. The latter formula is not dependent on any assumptions regarding linear screening. It is exact. It arises because both $S(\mathbf{q})$ and $\varepsilon(\mathbf{q}, \omega)$ are related to

the density–density correlation function. The assumption of the linear screening is merely using (5.81) to calculate the screened potential from the impurity charge distribution $\rho_i(\mathbf{q})$.

The density–density correlation function

$$-\int_0^\beta d\tau e^{i\omega_n\tau} \langle T_\tau \rho(\mathbf{q},\tau)\rho(-\mathbf{q},0)\rangle \tag{5.97}$$

has the appearance of a Green's function in the Matsubara representation. Since the operator is the density, the Green's function provides the response of the system to a density fluctuation. To develop the analogy further, the function

$$S(\mathbf{q},\omega) = -\frac{1}{n_0 v_q} \text{Im}\left[\frac{1}{\varepsilon(\mathbf{q},\omega)}\right] \tag{5.98}$$

is the spectral function of this operator, since it is proportional to the imaginary part of the retarded Green's functions associated with this correlation function. This observation is important, since the spectral functions provide direct physical information. For the electron or the phonon, peaks in their spectral functions are interpreted as excitations of these operators. In a similar way, the peaks in $S(\mathbf{q},\omega)$ are interpreted as longitudinal excitations of the electron gas. These are two–particle excitations, since the density operator itself contains two operators.

The density operator has boson properties, so $S(\mathbf{q},\omega)$ is a spectral function for boson operators. Consequently, it has many features in common with other spectral function for bosons; compare (5.95) with the similar phonon result (3.53):

$$2N_\mathbf{q} + 1 = \int_{-\infty}^\infty \frac{d\omega}{2\pi} \eta_B(\omega)\mathbf{B}(\mathbf{q},\omega) \tag{5.99}$$

Another feature of $S(\mathbf{q},\omega)$ is that it is positive for $\omega > 0$ and negative for $\omega < 0$ with $S(\mathbf{q},-\omega) = -S(\mathbf{q},\omega)$.

The dielectric function has been defined in terms of the interaction between two fixed impurity charges. The assumption has been that the impurity charges are **classical** objects. There remains the question of the effective interaction between two electrons, which are surely not classical objects. The present theory suggests that there is an additional factor in the effective interaction between two electrons, which is a vertex correction

$$W(q) = \frac{v_q}{\varepsilon(q)}\Gamma(q) \tag{5.100}$$

The main contribution to the vertex correction $\Gamma(q)$ arises from the ladder diagrams at the end points of the interaction.

## 5.5    Model Dielectric Functions

The exact dielectric function of the homogeneous electron gas is not derived. Instead of the approximate solutions (5.92), there are some other model.

### 5.5.1    Thomas–Fermi

Thomas–Fermi theory begins with the exact equation for the screened potential energy from tan impurity charge distribution $\rho_i(\mathbf{r})$,

$$\nabla^2 V(\mathbf{r}) = 4\pi e \left[ \rho_i(\mathbf{r}) + \rho_s(\mathbf{r}) \right] \tag{5.101}$$

where $\rho_s(\mathbf{r})$ is the screening charge, $n(\mathbf{r})$ for particle density and $\rho(\mathbf{q})$ for density operator. *In Thomas–Fermi theory, electron density $n(\mathbf{r})$ is represented locally as a free-particle system.* Write the screening charge as the difference between $n(\mathbf{r})$ and the equilibrium charge density $n_0$

$$\rho_s(\mathbf{r}) = -e \left[ n(\mathbf{r}) - n_0 \right] \tag{5.102}$$

For a free–particle system, the local density is $n(\mathbf{r}) = \frac{k_F^3(\mathbf{r})}{3\pi^2}$, where the Fermi wave vector is a local quantity and it is determined by the condition that the chemical potential $\mu$ is independent of position

$$\frac{k_F^2(\mathbf{r})}{2m} = E_F(\mathbf{r}) = \nu - V(\mathbf{r}) \tag{5.103}$$

Assume the potential is slowly varying in space. If the absolute Fermi level is at $\mu$, then the effective Fermi level is modified by the local potential. If these approximations are collected, there results the equation

$$\nabla^2 V(\mathbf{r}) = 4\pi e \left( \rho_i(\mathbf{r}) + e n_0 - e n_0 \left[ 1 - \frac{V(\mathbf{r})}{E_F} \right]^{3/2} \right) \tag{5.104}$$

For atoms, this approximate equation is solved exactly with $E_F = 0$ and $\rho_i = Z\delta^3(\mathbf{r})$ to give a good description of atomic potentials and charge distributions. The assumption that $V(\mathbf{r})$ is slowly varying does not seem unduly restrictive. To get a linear screening model, and hence a dielectric function, a further assumption is needed. It is assumed that $\frac{V}{E_F} \ll 1$, so $(1 - V/E_F)^{3/2} \approx 1 - 3V/2E_F$ to obtain the equation

$$\nabla^2 V = 4\pi e \rho_i(\mathbf{r}) + \frac{6\pi e^2 n_0}{E_F} V(\mathbf{r}) \tag{5.105}$$

Defining the Thomas–Fermi screening wave vector $q_{TF}$, (5.105) reads

$$\left( \nabla^2 - q_{TF}^2 \right) V(\mathbf{r}) = 4\pi e \rho_i(\mathbf{r}) \tag{5.106}$$

$$q_{TF}^2 = \frac{6\pi e^2 n_0}{E_F} \tag{5.107}$$

Solving this in Fourier transform space we get

$$V(\mathbf{r}) = -4\pi e \int \frac{d^3 q}{(2\pi)^3} \frac{\rho_i(\mathbf{q})}{q^2 + q_{TF}^2} e^{i\mathbf{q}\cdot\mathbf{r}} \tag{5.108}$$

Compare this equation with (5.80), and conclude that the Thomas–Fermi dielectric function is

$$\varepsilon(q) = 1 + \frac{q_{TF}^2}{q^2} \tag{5.109}$$

It has a simple form, which makes it easy to use in a variety of calculations.

For example, an analytical result can be obtained when the impurity is a point charge $\rho_i(\mathbf{q}) = Q_i$. The integrals to evaluate are $(v = \cos\theta)$

$$
\begin{aligned}
V(\mathbf{r}) &= -\frac{eQ_i}{\pi} \int_0^\infty \frac{q^2 dq}{q^2 + q_{TF}^2} \int_{-1}^1 dv e^{iqrv} \\
&= -\frac{eQ_i}{r} e^{-q_{TF}r} \tag{5.110}
\end{aligned}
$$

The screened interaction has the form of a Yukawa potential. In metals, the Thomas–Fermi wave vector has a typical value of $\text{Å}^{-1}$. The screened Coulomb potential declines rapidly on the scale of a unit cell. The screening wave vector may be expressed in the atomic unit as

$$a_0 q_{TF} = \sqrt{\frac{4}{\pi} k_F a_0} = \frac{1.5632}{\sqrt{r_s}} \tag{5.111}$$

Thomas–Fermi theory provides only a static model for $\varepsilon(q)$. It is not usually used to describe the dynamic response $\varepsilon(\mathbf{q}, \omega)$.

### 5.5.2 Lindhard, or RPA

The Lindhard dielectric function is more commonly called the RPA, for random phase approximation. It is a model for a static $\varepsilon(q)$ or dynamic $\varepsilon(\mathbf{q}, \omega)$ dielectric function.

The derivation by equations of motion is also called the method of **self-consistent field**. Define the total, impurity and screened variable as

$$V(\mathbf{q}, \omega) = V_i(\mathbf{q}, \omega) + V_s(\mathbf{q}, \omega) \tag{5.112}$$

$$\nabla^2 V_s(\mathbf{r}, t) = 4\pi e \rho_s(\mathbf{r}, t), \quad V_s(\mathbf{q}, \omega) = -\frac{4\pi e}{q^2} \rho_s(\mathbf{q}, \omega) \tag{5.113}$$

$$\nabla^2 V_i(\mathbf{r}, t) = 4\pi e \rho_i(\mathbf{r}, t), \quad V_i(\mathbf{q}, \omega) = -\frac{4\pi e}{q^2} \rho_i(\mathbf{q}, \omega) \tag{5.114}$$

The major assumption in the derivation is that the electrons respond to the total energy $V$ and in the linear screening model gives

$$\varepsilon(\mathbf{q}, \omega) = \frac{V_i(\mathbf{q}, \omega)}{V(\mathbf{q}, \omega)} \tag{5.115}$$

In the method of self–consistent field, it is assumed that the electrons respond to $V$; then try to determine this function self–consistently. The effective Hamiltonian for the electrons as

$$H = \sum_{\mathbf{q}\sigma} \varepsilon_p C_{\mathbf{p}\sigma}^\dagger C_{\mathbf{p}\sigma} + \frac{1}{V} \sum_{\mathbf{q}} V(\mathbf{q}, t)\rho(\mathbf{q}) \tag{5.116}$$

The time dependence $V(\mathbf{q}, t)$ is put directly into the Hamiltonian (5.116). The impurity charge is regarded as a classical system which is oscillating. The goal is to find the quantum response of the electron gas to this classical oscillation. Furthermore, the impurity is assumed to oscillate at a single frequency: $\rho_i(\mathbf{r}, t) = \rho_i(\mathbf{r})e^{-i\omega t}$ and $V_i(\mathbf{r}, t) = V_i(\mathbf{r})e^{-i\omega t}$. The average response of the system will depend on $\omega$, so write the average of $\rho(\mathbf{q}, t)$ as $\langle \rho(\mathbf{q}, t) \rangle = \rho(\mathbf{q}, \omega)e^{-i\omega t}$. For the homogeneous electron gas, the density operator $\rho(\mathbf{q})$ has an expectation value of zero for $\mathbf{q} \neq 0$. When the impurity is present, the expectation value is nonzero and is proportional to the average for the screening charge

$$\langle \rho_s(\mathbf{q}, t) \rangle = -e\langle \rho(\mathbf{q}, t) \rangle = -e \sum_{\mathbf{q}\sigma} \langle C_{\mathbf{p}+\mathbf{q},\sigma}^\dagger C_{\mathbf{p}\sigma} \rangle = -e\rho(\mathbf{q}, \omega)e^{-i\omega t}$$

$$\tag{5.117}$$

Since the averages for $\rho_s$ and $\rho$ are proportional, it simplifies the use only one symbol, choose to be $\rho$. For example, in terms of the average $\langle \rho_s \rangle = -e\langle \rho \rangle$, then (5.113) reads

$$V_s(\mathbf{q}, \omega) = \frac{4\pi e^2}{q^2}\rho(\mathbf{q}, \omega) \tag{5.118}$$

The dielectric response function is defined as the ration (5.115). The first term in (5.116) is the kinetic energy of electrons, and the second is their interaction with the self–consistent potential $V(\mathbf{q}, t)$. **Note** that there are no explicit electron–electron interactions. They are included, indirectly, in the interaction term: the part of $V(\mathbf{q}, t)$ from the screening $V_s(\mathbf{q}, t)$ is caused by electron–electron interactions. *It is a rather crude way to include these interactions, since it includes screening but neglects all other effects of correlation and exchange.*

To obtain the screened potential $V_s$ in (5.113), an expression is derived for the screening particle density $\rho_s(\mathbf{q}, t)$. It is obtained by writing an equation of motion for this operator and then solving it approximately. *A perturbation on the system of $(\mathbf{q}, \omega)$ will cause polarization of the electron system, so that the average $\langle \rho(\mathbf{q}, t) \rangle$ will now have a nonzero value.* In the linear screening model, this average is assumed to be proportional to the potential causing the perturbation, $\langle \rho(\mathbf{q}, t) \rangle \propto \langle V(\mathbf{q}, t) \rangle$. The goal is to determine the constant of proportionality.

The equation of motion of the density operator comes from

$$i\frac{d}{dt}\rho(\mathbf{q}, t) = [H, \rho(\mathbf{q}, t)] \tag{5.119}$$

To be more convenient

$$i\frac{d}{dt}C^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}C_{\mathbf{p}\sigma} = \left[H, C^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}C_{\mathbf{p}\sigma}\right] \tag{5.120}$$

The impurity potential $V(\mathbf{q}, t)$ is assumed to be oscillating at at a single frequency $\exp[-i\omega t]$ so that the time derivative on the left of (5.119) gives $-i\omega C^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}C_{\mathbf{p}\sigma}$. The commutators on the right are evaluated for Hamiltonian (5.116)

$$\sum_{\mathbf{k},s}\varepsilon_k\left[C^{\dagger}_{\mathbf{k}s}C_{\mathbf{k}s}, C_{\mathbf{p}+\mathbf{q},\sigma}C_{\mathbf{p}\sigma}\right] = \left(\varepsilon_{\mathbf{p}+\mathbf{q}} - \varepsilon_{\mathbf{p}}\right)C^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}C_{\mathbf{p}\sigma} \tag{5.121}$$

and

$$\frac{1}{V}\sum_{\mathbf{q}'\mathbf{k},s}V(\mathbf{q}',t)\left[C^{\dagger}_{\mathbf{k}+\mathbf{q}',s}C_{\mathbf{k}s}, C^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}C_{\mathbf{p}\sigma}\right]$$

$$= \frac{1}{V}\sum_{\mathbf{q}'}V(\mathbf{q}',t)\left(C^{\dagger}_{\mathbf{p}+\mathbf{q}+\mathbf{q}',\sigma}C_{\mathbf{p}\sigma} - C^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}C_{\mathbf{p}-\mathbf{q}',\sigma}\right) \tag{5.122}$$

which gives the equation (5.119) as

$$\left(\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}+\mathbf{q}} + \omega\right)C^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}C_{\mathbf{p}\sigma} = \frac{1}{V}\sum_{\mathbf{q}'}V(\mathbf{q}',t)\left(C^{\dagger}_{\mathbf{p}+\mathbf{q}+\mathbf{q}',\sigma}C_{\mathbf{p}\sigma} - C^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}C_{\mathbf{p}-\mathbf{q}',\sigma}\right)$$

$$\approx \frac{1}{V}V(\mathbf{q},t)\left(C^{\dagger}_{\mathbf{p}\sigma}C_{\mathbf{p}\sigma} - C^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}C_{\mathbf{p}+\mathbf{q}\sigma}\right) \tag{5.123}$$

The approximation is taken by only count the case $\mathbf{q}' = -\mathbf{q}$. The terms with other values of $\mathbf{q}'$ are neglected. **It is assumed they average out to zero by the meant of random phase approximation**. The approximate equation can be solved

$$C^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}C_{\mathbf{p}\sigma} = \frac{V(\mathbf{q},t)}{V}\left(\frac{C^{\dagger}_{\mathbf{p}\sigma}C_{\mathbf{p}\sigma} - C^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}C_{\mathbf{p}+\mathbf{q},\sigma}}{\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}+\mathbf{q}} + \omega}\right) \tag{5.124}$$

The above equation is summed over $\mathbf{p}\sigma$ to give

$$\rho(\mathbf{q},t) = \sum_{\mathbf{p}\sigma}C^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}C_{\mathbf{p}\sigma} = \frac{V(\mathbf{q},t)}{V}\sum_{\mathbf{p},\sigma}\left(\frac{C^{\dagger}_{\mathbf{p}\sigma}C_{\mathbf{p}\sigma} - C^{\dagger}_{\mathbf{p}+\mathbf{q},\sigma}C_{\mathbf{p}+\mathbf{q}\sigma}}{\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}+\mathbf{q}} + \omega}\right) \tag{5.125}$$

This equation shows that the operator on the left, $\rho(\mathbf{q}, t)$, is proportional to the operator on the right, $V(\mathbf{q}, t)$. The average is taken of this equations, so that $\langle\rho\rangle$ and $\langle V\rangle$ are replaced by $\rho(\mathbf{q},\omega)e^{i\omega t}$ and $V(\mathbf{q},\omega)e^{-i\omega t}$ based on (5.117). In addition, the number operators are replaced by their averages. These steps give an equation which relates the average of these operators

$$\rho(\mathbf{q},\omega) = \frac{V(\mathbf{q},\omega)}{V}\sum_{\mathbf{p}\sigma}\frac{\eta_F(\xi_{\mathbf{p}}) - \eta_F(\xi_{\mathbf{p}+\mathbf{q}})}{\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}+\mathbf{q}} + \omega} = V(\mathbf{q},\omega)\mathbf{P}^{(1)}(\mathbf{q},\omega) \tag{5.126}$$

which can now be used in (5.118)

$$V_s(\mathbf{q}, \omega) = \frac{4\pi e^2}{q^2} \rho(\mathbf{q}, \omega) = V(\mathbf{q}, \omega) v_q \mathbf{P}^{(1)}(\mathbf{q}, \omega) \qquad (5.127)$$

The result has the screening particle density $\rho(\mathbf{q}, \omega)$ proportional to the self–consistent potential $V(\mathbf{q}, \omega)$. The constant $\mathbf{P}^{(1)}$ is evaluated below.

The equations may now be solved to obtain the dielectric function, in the equation for $V(\mathbf{q}, \omega)$,

$$V(\mathbf{q}, \omega) = \frac{V_i(\mathbf{q}, \omega)}{1 - v_q \mathbf{P}^{(1)}(\mathbf{q}, \omega)} \qquad (5.128)$$

where we have

$$\varepsilon_{RPA}(\mathbf{q}, \omega) = 1 - v_q \mathbf{P}^{(1)}(\mathbf{q}, \omega) \qquad (5.129)$$

$$\mathbf{P}^{(1)}(\mathbf{q}, \omega) = \frac{1}{V} \sum_{\mathbf{p}\sigma} \frac{\eta_F(\xi_\mathbf{p}) - \eta_F(\xi_{\mathbf{p}+\mathbf{q}})}{\varepsilon_\mathbf{p} - \varepsilon_{\mathbf{p}+\mathbf{q}} + \omega + i\delta} \qquad (5.130)$$

The second method of the derivation is based on the diagrammatic analysis using Green's functions. The basic definition of $1/varepsilon$ in (5.94) is rewritten in the interaction representation

$$\frac{1}{\varepsilon(\mathbf{q}, i\omega)} = 1 - \frac{v_q}{V} \int_0^\beta d\tau e^{i\omega_n \tau} \frac{\langle T_\tau \hat{S}(\beta) \hat{\rho}(\mathbf{q}, \tau) \hat{\rho}(-\mathbf{q}, 0) \rangle}{\langle \hat{S}(\beta) \rangle} \qquad (5.131)$$

$$V = \frac{1}{V} \sum_{\mathbf{q}\mathbf{k}\mathbf{p}} \sum_{\sigma\sigma'} v_q C^\dagger_{\mathbf{p}+\mathbf{q},\sigma} C^\dagger_{\mathbf{k}-\mathbf{q},\sigma'} C_{\mathbf{k}\sigma'} C_{\mathbf{p}\sigma} \qquad (5.132)$$

where $H_0$ is the kinetic energy term in the homogeneous electron gas and $V$ is the electron–electron interaction. The operator $\hat{\rho}$ has its time dependence determined by $H_0$ in the interaction representation. The $S$ matrix will be expanded term by term, and one particular subset of these terms will be summed and will yield the RPA.

The first term in the expansion for the $S$ matrix is just

$$\mathbf{P}^{(1)}(\mathbf{q}, i\omega) = -\frac{1}{V} \int_0^\beta d\tau e^{i\omega_n \tau} \langle T_\tau \hat{\rho}(\mathbf{q}, \tau) \hat{\rho}(-\mathbf{q}, 0) \rangle$$

$$= \frac{1}{V} \sum_{\mathbf{p}\sigma} \frac{\eta_F(\xi_\mathbf{p}) - \eta_F(\xi_{\mathbf{p}+\mathbf{q}})}{\varepsilon_\mathbf{p} - \varepsilon_{\mathbf{p}+\mathbf{q}} + i\omega_n} \qquad (5.133)$$

The Feynman diagram is shown as a single–fermion closed loop Figure 5.4. The wiggly lines at each end are just added to define the two vertices of the polarization diagram. They could indicate that the polarization term is in response to an excitation with wave vector $\mathbf{q}$ and frequency $i\omega_n$. The calculation for $\varepsilon_{RPA}$ is not terminated here, sin the terms so far are $\frac{1}{\varepsilon} = 1 + v_q \mathbf{P}^{(1)} + \ldots$ rather that $\varepsilon_{RPA} = 1 - v_q \mathbf{P}^{(1)}$. Obviously, more terms are needed to get RPA.
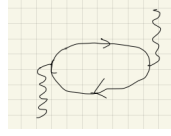
The next term in the S-matrix expansion is

$$\frac{1}{V}\sum_{\mathbf{pkq'}}\sum_{\sigma\sigma'}\int_0^\beta d\tau e^{i\omega_n\tau}\int_0^\beta d\tau_1 v_{q'}\langle T_\tau\hat{\rho}(\mathbf{q},\tau)\hat{C}^\dagger_{\mathbf{p+q'},\sigma}(\tau_1)\hat{C}^\dagger_{\mathbf{k-q'},\sigma'}(\tau_1)\hat{C}_{\mathbf{k}\sigma'}(\tau_1)\hat{C}_{\mathbf{p}\sigma}(\tau_1)\hat{\rho}(-\mathbf{q},0)\rangle$$

$$(5.134)$$

There are four terms which result when Wick's theorem is applied
to this correlation function. All contributions have four electron
Green's functions and one Coulomb interaction $v_{q'}$. Their diagrms
are shown in Figure 5.5. The first one is a vertex correction to the ba-
sic bubble diagram. The next two are exchange energy diagrams for
the Green's functions in the bubble; they contribute the self–energy
of these Green's functions. The last diagram contains two bubbles
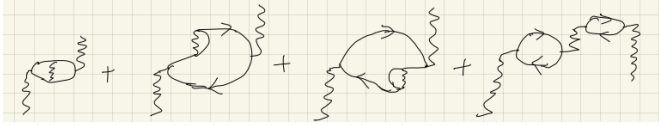which are connected by the Coulomb line $v_q$.

Earlier it was remarked that the density–denisty correlation func-
tion had the appearance of a Green's function. It also has a Dyson
equation. The exact evaluation of the correlation functino may be
written as[5]

$$-\frac{1}{V}\int_0^\beta d\tau e^{i\omega_n\tau}\langle T_\tau\rho(\mathbf{q},\tau)\rho(-\mathbf{q},0)\rangle = \frac{\mathbf{P}(\mathbf{q},i\omega)}{1-v_q\mathbf{P}(\mathbf{q},\omega)}\qquad(5.135)$$

There the density operators have the $\tau$ dependence governed by
$H = H_0 + V$, instead of only $H_0$ as in $\mathbf{P^{(1)}}$. The polarization diagram
$\mathbf{P}(\mathbf{q},i\omega_n)$ is the summation of all **different** polarization terms. Polar-
ization diagrams are not "different" if any of their parts are linked by
a single Coulomb line $v_q$. For example teh last diagrme in Figure 5.5
is not a different polarization diagram. This term arises from the
expansion of geometric series

$$\frac{P^{(1)}+P^{(2)}+\cdots}{1-v_q\left(P^{(1)}+\cdots\right)} = \left(P^{(1)}+\cdots\right)\left[1+v_q\left(P^{(1)}+\cdots\right)+\cdots\right] = P^{(1)}+v_q\left(P^{(1)}\right)^2+\cdots$$

$$(5.136)$$

where it is the term $v_q\left(P^{(1)}\right)^2$. There are terms in $\mathbf{P}(\mathbf{q},i\omega_n)$ which
have more than one bubble, but they must be connected by more
than one Coulomb line.

The random phase approximation is approximating the exact po-
larization diagram $\mathbf{P}(\mathbf{q}, i\omega)$ by its first term, which is $\mathbf{P}^{(1)}(\mathbf{q}, i\omega)$. The
RPA is found from the summation of all single bubble polarization
diagrams

$$\frac{1}{\varepsilon_{RPA}} = 1 + \frac{v_q P^{(1)}}{1 - v_q P^{(1)}} = \frac{1}{1 - v_q P^{(1)}} \tag{5.137}$$

which does give $\varepsilon_{RPA} = 1 - v_q P^{(1)}(\mathbf{q}, i\omega)$. The eact dielectric function
is easily shown to be

$$\varepsilon(\mathbf{q}, i\omega) = 1 - v_q \mathbf{P}(\mathbf{q}, i\omega) \tag{5.138}$$

Obviously, to improve the directiic function is to include more terms
in the summation of polarization contribution but it is very hard.
In fact, most progress has been made by nondiagramic means, as
discussed below.

Using the analytical continuation, the retarded dielectric function
is complex

$$\varepsilon_{RPA} = \varepsilon_1(\mathbf{q}, \omega) + i\varepsilon_2(\mathbf{q}, \omega) \tag{5.139}$$

The real part $\varepsilon_1$ always approach 1 at large $\omega$. At $\omega \to 0$ then
$\omega_2 \to 0$, and the static $\varepsilon_{RPA}$ is just $\varepsilon(\mathbf{q}, 0)$. Using the notation $x = q/2k_F$,

$$\varepsilon(\mathbf{q}, 0) = 1 + \frac{q_{TF}^2}{2q^2} \left[ 1 + \frac{1}{2x} \left( 1 - x^2 \right) \ln \left| \frac{1+x}{1-x} \right| \right] \tag{5.140}$$

which is always positive. For values $q < k_F$, then $\varepsilon_1(q, \omega)$ becomes
negative for intermediate values of $\omega$. This requres two crossings of
the $\varepsilon_1 = 0$ axis. The low–frequency crossing always happens when
$\varepsilon_2$ is large, so that $-\text{Im}(1/\varepsilon) = \varepsilon_2/(\varepsilon_1^2 + \varepsilon_2^2)$ is well behaved when
$\varepsilon \approx 0$. However, the high-frequency point where $\varepsilon_1 = 0$ has $\varepsilon_2 = 0$,
in that case $-\text{Im}(1/varepsilon) = \pi\delta(\varepsilon_1)$, so that a delta function is
obtained. This delta function is the plasmon peak which is the sharp
singularity on the right of the graph. Remember that peaks in $S(q, \omega)$
are interpreted as excitations of the system

$$S(\mathbf{q}, \omega) = -\frac{1}{n_0 v_q} \text{Im} \left[ \frac{1}{\varepsilon(\mathbf{q}, \omega)} \right] = \frac{1}{n_0 v_q} \frac{\varepsilon_2}{\varepsilon_1^2 + \varepsilon_2^2} \tag{5.141}$$

Plasmons are excitations which exist in real metals and in any elec-
tron gas with frequency $\omega_0^2 = \frac{4\pi e^2 n_0}{m}$.

The disscussion abuot the dielectric function is not included in this
manuscript.

### 5.5.3  Hubbard

Hubbard (1957) introduced a correction factor to the RPA of the form

$$\varepsilon_H(\mathbf{q}, \omega) = 1 - \frac{v_q \mathbf{P}^{(1)}(\mathbf{q}, \omega)}{1 + v_q G_H(q) \mathbf{P}^{(1)}(\mathbf{q}, \omega)} \qquad (5.142)$$

$$G_H(q) = \frac{1}{2} \frac{q^2}{q^2 + k_F^2} \qquad (5.143)$$

The factor $G_H(q)$ is a local field correction. There is an analogy with the Lorenz–Lorenz dielectric function, which has the form in cubic insulators

$$\varepsilon = 1 + \frac{4\pi\alpha}{1 - \frac{4\pi\alpha}{3}} \qquad (5.144)$$

The two formulas have the same structure if we associate $-v_q \mathbf{P}^{(1)} \to 4\pi\alpha$ and $G_H \to \frac{1}{3}$. The factor of $\frac{4\pi\alpha}{3}$ cones from summing the local dipoles in the lattice. It is called a " local field correction". Similarly, $G_H(q)$ in the Hubbard dielectric function cones from summing over the surrounding structure of the dielectric, which in this case is the exchange–correlation hole.

The factor $G_H(q)$ is introduced to account for the existence of the exchange and correlation hole around the electron. The dielectric function describes how the conduction electrons of the metal rearrange their positions to screen the Coulomb potential. Because of the exchange and correlation hole around each electron, when one electron is participating in the dielectric screening, others are less likely to be found nearby. The exchange–correlation hole should have some affect upon the nature of the dielectric screening.

The Hubbard local field comes from the vertex corrections in the polarization function $\mathbf{P}(\mathbf{q}, \omega)$. The most important vortex corrections are the ladder diagrams Figure 5.6. They can be evaluated by
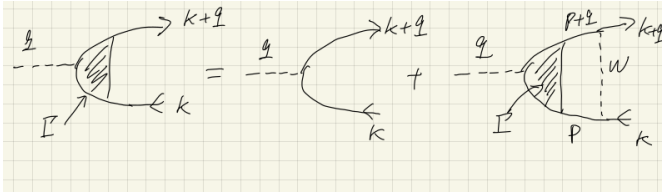


Figure 5.6: Ladder diagrams of the polarization bubble.

introducing a vortex function $\Gamma(k, k + q)$ in a four vector notation $k \equiv (\mathbf{k}, ik_n)$. This approximation to the polarization diagrams is denoted $P_L$ where $L$ denotes ladder

$$P_L(\mathbf{q}, \omega) = \frac{2}{\beta V} \sum_k \mathcal{G}^0(k) \mathcal{G}^{(0)}(k + q) \Gamma(k, k + q) \qquad (5.145)$$

$$\Gamma(k, k + q) = 1 - \frac{1}{\beta V} \sum_p W(k - p) \mathcal{G}^{(0)}(p) \mathcal{G}^{(0)}(p + q) \Gamma(p, p + q)$$

The above expression is rather difficult to evaluate exactly. The degree of complexity depends upon the choice for the effective interaction $W(k-p)$ which are the ladders.

Consider the screened interaction $W(q) = v_q/\varepsilon(q)$. Assuming that $\Gamma(k, k+q) \approx \Gamma(q)$ and $k$ dependence is ignored. Then we have

$$P_L(q) = \Gamma(q)P^{(1)}(q) \tag{5.146}$$

$$\Gamma(q) = 1 - \Gamma(q)\Lambda(q) = \frac{1}{1+\Lambda(q)} \tag{5.147}$$

$$\Lambda(q) = \frac{1}{\beta V}\sum_p W(k-p)\mathcal{G}^{(0)}(p)\mathcal{G}^{(0)}(p+q) \tag{5.148}$$

Since the approximation require $\Gamma$ is independent on $k$, so it also requires that $\Lambda$ and $W$ is independent on $k$. With Hubbard approximation, one have the following replacement

$$W(k-p) \rightarrow \frac{4\pi e^2}{q^2 + q_{TF}^2} \tag{5.149}$$

$$\Lambda(q) = \frac{2\pi e^2}{q^2 + q_{TF}^2}P^{(1)}(q) = v_q G_H(q)P^{(1)}(q) \tag{5.150}$$

$$G_H(q) = \frac{1}{2}\frac{q^2}{q^2 + q_{TF}^2} \tag{5.151}$$

The factor of $\frac{1}{2}$ comes because $P^{P(1)}$ contains a summation over spins which multiplies the result by two. The ladder terms do not have a summation over spin states. Each electron line in the polarization bubble diagram has the same spin configuration. So the result is multiplied by 1/2 to account of the factor of 2 in the $P^{(1)}$.

# 6

# *Optical Properties of Solids*

## *6.1 Wannier Excitons*

### *6.1.1 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 valenec band hole*.
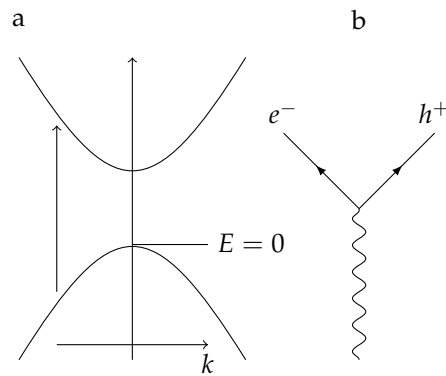
a                                          b



Figure 6.1: Optical transition in a semi-conductor 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.6.1(a), the interband transition is direct. The valance 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.6.1(a) is a single-particle picture of the transition process*. The transition rate for the absorption of photons is given by

golden rule

$$
A(\omega) \quad = \quad \frac{2\pi}{\hbar V} \sum_{\mathbf{k}\mathbf{k}'} \left|\langle c, \mathbf{k}'| \, \hat{\varepsilon} \cdot \mathbf{p} \, |v, \mathbf{k}\rangle\right|^2 \delta\left[\varepsilon_v(\mathbf{k}) + \hbar\omega - \varepsilon_c(\mathbf{k}')\right] \quad (6.1)
$$

$$
\varepsilon_v(\mathbf{k}) \quad = \quad -\frac{k^2}{2m_v}, \quad \varepsilon_c(\mathbf{k}) = E_g + \frac{k^2}{2m_c} \quad\quad\quad (6.2)
$$

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 $u_{\mathbf{k}}(\mathbf{r}) \otimes \exp(i\mathbf{kr})$. For discussion reason assume the cell-periodic parts as independent of wave vector $\mathbf{k}$, and assumed that the valance 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

$$
|v, \mathbf{k}\rangle \quad = \quad u_v(\mathbf{r}) \frac{e^{i\mathbf{kr}}}{\sqrt{V}} \quad\quad\quad (6.3)
$$

$$
|c, \mathbf{k}'\rangle \quad = \quad u_v(\mathbf{r}) \frac{e^{i\mathbf{k}'\mathbf{r}}}{\sqrt{V}} \quad\quad\quad (6.4)
$$

$$
\langle c, \mathbf{k}'| \, \hat{\varepsilon}\mathbf{p} \, |v, \mathbf{k}\rangle \quad \equiv \quad \hat{\varepsilon}\mathbf{p}_{cv}\delta_{\mathbf{k}\mathbf{k}'} \quad\quad\quad (6.5)
$$

$$
\hat{\varepsilon}\mathbf{p} \quad = \quad \frac{1}{V} \int_{cell} d^3r\, u_c^* \hat{\varepsilon}\mathbf{p} u_v \quad\quad\quad (6.6)
$$

neglect the wave vector $\mathbf{q}$ for photons since it is in the optical frequencies.

$$
A(\omega) = |\hat{\varepsilon}\mathbf{p}_{cv}|^2 \frac{(2\mu)^{3/2}}{2\pi} \sqrt{\hbar\omega - E_g}\,\Theta(\hbar\omega - E_g) \quad\quad\quad (6.7)
$$

with $\mu^{-1} = m_c^{-1} + m_v^{-1}$. Equation (6.7) 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.6.1(b). In this new picture, the electron and hole are particles with charges of opposite sign, so that there is a Coulomb attraction $-\frac{2}{\varepsilon_0 r}$ between them, where $\varepsilon_0$ 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

[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 **??**

Schödinger equation

$$\Psi(\mathbf{r}_e, \mathbf{r}_h) = u_c(\mathbf{r}_e)u_v(\mathbf{r}_h)\Phi(\mathbf{r}_e, \mathbf{r}_h) \tag{6.8}$$

$$0 = \left[ -\frac{\hbar^2\nabla_e^2}{2m_c} - \frac{\hbar^2\nabla_h^2}{2m_v} - \frac{e^2}{\varepsilon_0|\mathbf{r}_e - \mathbf{r}_h|} - E \right] \Phi(\mathbf{r}_e, \mathbf{r}_h) \tag{6.9}$$

$\Phi(\mathbf{r}_e, \mathbf{r}_h)$ 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

$$\mathbf{R} = \frac{m_c\mathbf{r}_e + m_v\mathbf{r}_h}{M} \tag{6.10}$$

$$\Phi(\mathbf{r}_e, \mathbf{r}_h) = \frac{e^{i\mathbf{PR}}}{\sqrt{V}}\phi(\mathbf{r}) \tag{6.11}$$

$$0 = \left( -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{e^2}{\varepsilon_0\mathbf{r}} - \varepsilon_r \right)\phi(\mathbf{r}) \tag{6.12}$$

$$E = E_g + \varepsilon_r + \frac{P^2}{2M} \tag{6.13}$$

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 (6.7), the transition rate is

$$A(\omega) = \frac{2\pi}{\hbar}|\hat{\varepsilon}\mathbf{p}_{cv}|^2 \sum_j |\phi_j(0)|^2 \delta(\hbar\omega - E_g - \varepsilon_j) \tag{6.14}$$

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 $a_0$,

$$\phi_n(0) = \frac{1}{\sqrt{\pi a_0^3 n^3}} \tag{6.15}$$

For continuum states, with energy $\varepsilon_k = \frac{k^2}{2\mu}$, the relative wave function at the origin is

$$\psi_{k,l=0}(0) = \frac{2\pi\eta}{V\left[2 - e^{-2\pi\eta}\right]} \tag{6.16}$$

where $\eta^{-1} = ka_0$. Then (6.15) 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 $\hbar\omega = E_g$.

### 6.1.2   Solution by Green's Functions

# 7
# *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 $\lambda$ 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.

## 7.1   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.

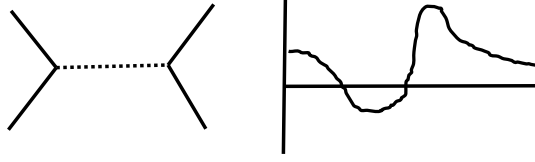The scattering process as shown 7.1. The screened interaction

between two electrons was derived before as

$$V_s(\mathbf{q}, \omega) = \frac{v_q}{\varepsilon(\mathbf{q}, \omega)} + \frac{2\omega \lambda M_{\mathbf{q}}^2}{\varepsilon(\mathbf{q})^2 \left[\omega^2 - \omega_\lambda(\mathbf{q})^2\right]} \qquad (7.1)$$

The first is the screened Coulomb interaction. The theory of super-conductivity 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 (7.1) 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 (7.1) use a interaction model

$$V_s(\mathbf{q}, \omega) = \begin{cases} -V_0 & |\xi_q| < \omega_D \\ 0 & |\xi_q| > \omega_D \end{cases} \qquad (7.2)$$

This potential is constant and attractive up to a cutoff energy which is of the order of the Debye energy $\omega_D$ 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 (7.2). 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 occur[1]. The interaction poten-

[1] P298 Hatree fock approximation

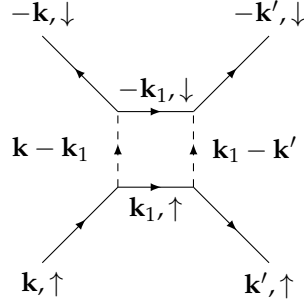tial does not flip the electron spin and the spin states are preserved in the scattering process.

In Figure 7.2 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 firs Born approximation is shown in Fig.7.1. The effective scattering in the first and second Born approximation is

$$V_{eff}(\mathbf{k}-\mathbf{k}') = V(\mathbf{k}-\mathbf{k}') + \int \frac{d^3 k_1}{(2\pi)^3} \frac{V(\mathbf{k}-\mathbf{k}_1)V(\mathbf{k}_1-\mathbf{k}')}{2\xi_{\mathbf{k}} - 2\xi_{\mathbf{k}_1}} \left( \left[1 - \eta_F(\xi_{\mathbf{k}_1})\right]\left[1 - \eta_F(\xi_{\mathbf{k}_1})\right] - \eta_F(\xi_{\mathbf{k}_1})^2 \right)$$

$$(7.3)$$

The second term on the right is the contribution of Fig.7.2. The denominator contains the initial state energy minus the intermediate state energy. The factors $\left[1 - \eta_f(\xi_{k_1})\right]^2 - \eta_F(\xi_{\mathbf{k}_1})^2 = 1 - 2\eta_F(\xi_{\mathbf{k}_1})$, which occur because the two particle can scatter into the state when they are not occupied. The term $\eta_F(\xi_{\mathbf{k}_1})^2$ represents the scattering back into this state, $|\mathbf{k}_1, \uparrow\rangle \to |\mathbf{k}, \uparrow\rangle$, since the result depends upon the net scattering. What is left are the remaining factors $1 - 2\eta_F(\xi_{\mathbf{k}_1})$, these occupation factors play a crucial role in the theory and are the cause of instability.

The integral in (7.3) 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

$$\int \frac{d^3 k_1}{(2\pi)^3} = \int d\xi_1 N(\xi_1) \qquad (7.4)$$

and treat $N(\xi \approx 0) \equiv N_F$ as an constant. At zero temperature the result is ($\xi_{\mathbf{k}_1} = \xi_1$)

$$V_{eff}(\mathbf{k}-\mathbf{k}') = V(\mathbf{k}-\mathbf{k}') + N_F V_0^2 \int_{-\omega_D}^{\omega_D} d\xi_1 \frac{\frac{1}{2} - \eta_F(\xi_1)}{\xi - \xi_1} \qquad (7.5)$$

The factor $1/2$ does not cause any singularity and may be ignored,

To under the (7.3), 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





The Green function of election gives the different combination of distribution function.

then in zero temperature

$$\int_{-\omega_D}^{\omega_D} d\xi_1 \frac{\eta_F(\xi_1)}{\xi - \xi_1} = -\ln\left(\frac{\xi}{\omega_D}\right) \tag{7.6}$$

and

$$V_{eff} = -V_0 \left[1 - N_F V_0 \ln\left(\frac{\xi}{\omega_D}\right)\right] \tag{7.7}$$

The term $-N_F V_0 \ln(\xi/\omega_D)$ 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

$$-V_0 \left[-N_F V_0 \ln\left(\frac{\xi}{\omega_D}\right)\right]^n \tag{7.8}$$

The summation of these terms produces the series

$$\begin{aligned}
V_{eff} &= -V_0 \sum_{N=0}^{\infty} \left[-N_F V_0 \ln\left(\frac{\xi}{\omega_D}\right)\right]^n \\
&= -\frac{V_0}{1 + N_F V_0 \ln\left(\xi/\omega_D\right)} \tag{7.9}
\end{aligned}$$

The denominator equals zero at $(V_{eff} = 0)$

$$\xi_0 = \omega_D \exp\left[-\frac{1}{N_F V_0}\right] \tag{7.10}$$

This $\xi_0$ gives a pole in (7.9). In the vicinity of $\xi_0$ can be approximated by using $\xi = \xi_0 + (\xi - \xi_0)$ and the scattering has a pole

$$\begin{aligned}
V_{eff} &= -\frac{1}{N_F} \frac{1}{\ln(\xi/\xi_0)} = -\frac{1}{N_F} \frac{1}{\ln\left[1 + (\xi - \xi_0)/\xi_0\right]} \\
&\approx -\frac{\xi_0}{N_F(\xi - \xi_0)} \tag{7.11}
\end{aligned}$$

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 pairs 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 whether this sharp distribution still exits. A theory of superconductivity must self-consistently determine the properties of bound electron pairs.
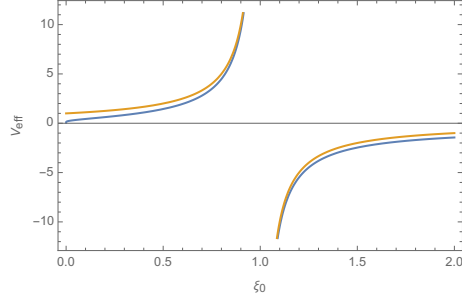
Figure 7.3: The behaviour of $V_{eff}$ as the function of $\xi_0$. The yellow line is the approximation one.

Another way to describe the instability is as a function of temperature. It enters into the electron distribution $\eta_F$ by changing the step function into a smooth function with an energy width of several $k_B T$. By expressing the (7.6) as

$$\int_{-\omega_D}^{\omega_D} d\xi_1 \frac{\eta_F(\xi_1)}{\xi - \xi_1} \approx -\frac{1}{2} \ln \left[ \frac{\xi^2 + (k_B T)^2}{\omega_D^2} \right] \tag{7.12}$$

Summation of all the ladder diagrams and the effective potential have the form

$$V_{eff} = -\frac{V_0}{1 + N_F V_0 \ln \left[ \sqrt{\xi^2 + (k_B T)^2}/\omega_D \right]} \tag{7.13}$$

At zero energy, $\xi = 0$, $V_{eff}$ becomes singular when the temperature is lower to the critical temperature $T_c$

$$k_B T_c = \omega_D \exp \left[ -\frac{1}{N_F V_0} \right] \tag{7.14}$$

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 6.1, the multiple scattering theory may be described by a vertex function

$$\Gamma(\mathbf{k}, \mathbf{k}') = V(\mathbf{k} - \mathbf{k}') + \int \frac{d^3 k_1}{(2\pi)^3} \frac{V(\mathbf{k} - \mathbf{k}_1)\Gamma(\mathbf{k}_1, \mathbf{k}')}{2\xi_{\mathbf{k}} - 2\xi_{\mathbf{k}_1}} \tag{7.15}$$

The solution to this vertex function is equivalent to solving the two-particle Schrödinger equation in relative coordinates

$$\left[ -\frac{1}{2m} \left( \nabla_1^2 + \nabla_2^2 \right) + V(\mathbf{r}_1 - \mathbf{r}_2) - E \right] \psi(\mathbf{r}_1, \mathbf{r}_2) = 0 \tag{7.16}$$

The problem is factored into the relative and center of mass motions

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \quad \psi(\mathbf{r}_1, \mathbf{r}_2) = e^{i\mathbf{p}\cdot\mathbf{R}}\phi(\mathbf{r}) \tag{7.17}$$

$$\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2), \quad E = \frac{p^2}{2m} + \varepsilon \tag{7.18}$$

$$\left[-\frac{\nabla^2}{m} + V(\mathbf{r}) - \varepsilon\right]\phi(\mathbf{r}) = 0 \tag{7.19}$$

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 $E_F - \zeta_0$. The two electrons cannot really bind at that energy, 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

### 7.1.1    BCS Theory

The basic feature of the BCS theory is that pairing occurs between electrons in states with opposite momentum ans opposite spins. The two spins are combined into a spin singlet, with $S = 0$. We will assume this spin arrangement during the discussion.

The pairing of electrons in the BEC theory mus cause correlations in the relative motion. The pairing is describe by introducing a new correlation function, similar to Green's function, for particles of opposite spin. They are

$$\begin{aligned}
\mathcal{G}(\mathbf{p}, \tau - \tau') &= -\langle T_\tau C_{\mathbf{p}\sigma}(\tau) C_{\mathbf{p}\sigma}^\dagger(\tau')\rangle \\
\mathcal{F}(\mathbf{p}, \tau - \tau') &= \langle T_\tau C_{-\mathbf{p}\downarrow}(\tau) C_{\mathbf{p}\uparrow}(\tau')\rangle \\
\mathcal{F}^\dagger(\mathbf{p}, \tau - \tau') &= \langle T_\tau C_{\mathbf{p}\uparrow}^\dagger(\tau) C_{-\mathbf{p}\downarrow}^\dagger(\tau')\rangle
\end{aligned} \tag{7.20}$$

The Green's function $\mathcal{G}$ has the same definition as usual, although it has a different algebraic form in the superconducting state. The $\mathcal{F}$ functions are identically zero in the normal state. A basic feature of the BCS ground state wave function is that it is composed of a superposition of electronic states containing a different number of electrons. One need to find a self–consistent equation for the correlation function and its conjugate.

To provide the simplest possible model of BCS theory, assume a

Hamiltonian of the form

$$H = \sum_{\mathbf{p}\sigma} \xi_\mathbf{p} C_{\mathbf{p}\sigma}^\dagger C_{\mathbf{p}\sigma} + \frac{1}{2V} \sum_{\mathbf{q}\mathbf{p}\mathbf{p}'ss'} V(q) C_{\mathbf{p}+\mathbf{q},s}^\dagger C_{\mathbf{p}'-\mathbf{q},s'}^\dagger C_{\mathbf{p}'s'} C_{\mathbf{p}s} \qquad (7.21)$$

The interaction potential $V(q)$ between electrons is taken to have the form in (7.2), which is an attractive constant $V(q) = -V_0$ over a range of energies within a Debye energy of the Fermi surface. With this Hamiltonian, a set of self–consistent equations will be derived for the Green's functions $\mathcal{G}$, $\mathcal{F}$ and $\mathcal{F}^\dagger$. Using the equation of the motion

$$\frac{d}{d\tau} C_{\mathbf{p}\sigma}(\tau) = [H, C_{\mathbf{p}\sigma}] = -\xi_\mathbf{p} C_{\mathbf{p}\sigma} - \frac{1}{V} \sum_{\mathbf{q}\mathbf{p}'s'} V(q) C_{\mathbf{p}'-\mathbf{q},s'}^\dagger C_{\mathbf{p}'s'} C_{\mathbf{p}-\mathbf{q},\sigma}$$

$$(7.22)$$

From the definition of the $\tau$–order product, the first derivative of the equation for the Green's function is

$$\frac{\partial}{\partial\tau} \mathcal{G}(\mathbf{q}, \tau - \tau') = -\delta(\tau - \tau') - \langle T_\tau \left[ \frac{\partial}{\partial\tau} C_{\mathbf{p}\sigma}(\tau) \right] C_{\mathbf{p}\sigma}^\dagger(\tau') \rangle \qquad (7.23)$$

Using the result (7.22) for the derivative gives

$$\left( -\frac{\partial}{\partial\tau} - \xi_p \right) \mathcal{G}(\mathbf{q}, \tau - \tau') + \frac{1}{V} \sum_{\mathbf{q}\mathbf{p}'s} V(q)$$

$$\times \langle T_\tau C_{\mathbf{p}'-\mathbf{q},s'}^\dagger C_{\mathbf{p}'s'}(\tau) C_{\mathbf{p}-\mathbf{q},\sigma}(\tau) C_{\mathbf{p}\sigma}^\dagger(\tau') \rangle = \delta(\tau - \tau') \quad (7.24)$$

There are many ways of doing the pairing. One simplification is to assume that long–wavelength phonons give a zero potential, so that $V(\mathbf{q} = 0) = 0$. For a normal metal, there would only remain the pairing $\delta_{\mathbf{p}\mathbf{p}'}\delta_{s'\sigma}\eta_{\mathbf{p}-\mathbf{q}}\mathcal{G}(\mathbf{p}, \tau - \tau')$ which gives the exchange energy. This pairing occurs in the superconductor as well but is not the only term. The pairing which include the $\mathcal{F}$ function must pay attention to the spin variables. The combination $\sigma = -s' =\uparrow$ gives

$$\langle T_\tau C_{\mathbf{p}'-\mathbf{q},s'}^\dagger C_{\mathbf{p}'s'}(\tau) C_{\mathbf{p}-\mathbf{q},\sigma}(\tau) C_{\mathbf{p}\sigma}^\dagger(\tau') \rangle = -\delta_{\sigma,-s'}\delta_{\mathbf{p}',-\mathbf{p}+\mathbf{q}}\mathcal{F}(\mathbf{p}-\mathbf{q}, 0)\mathcal{F}^\dagger(\mathbf{p}, \tau' - \tau)$$

$$(7.25)$$

where the sign change result from an odd number of operator rearrangements. Similarly, the choice $\sigma = -s' =\downarrow$ gives

$$\langle T_\tau C_{\mathbf{p}'-\mathbf{q},s'}^\dagger C_{\mathbf{p}'s'}(\tau) C_{\mathbf{p}-\mathbf{q},\sigma}(\tau) C_{\mathbf{p}\sigma}^\dagger(\tau') \rangle = -\delta_{\sigma,-s'}\delta_{\mathbf{p}',-\mathbf{p}+\mathbf{q}}\mathcal{F}(-\mathbf{p}+\mathbf{q}, 0)\mathcal{F}^\dagger(-\mathbf{p}, \tau - \tau')$$

$$(7.26)$$

*These two results are identical, since later it is shown that $\mathcal{F}$ and $\mathcal{F}^\dagger$ do not depend on the sign of the arguments either momentum or $\tau$.* The last term in (7.24) gives the expression

$$\frac{1}{V} \sum_{\mathbf{q}\mathbf{p}'s} V(q) \langle T_\tau C_{\mathbf{p}'-\mathbf{q},s'}^\dagger C_{\mathbf{p}'s'}(\tau) C_{\mathbf{p}-\mathbf{q},\sigma}(\tau) C_{\mathbf{p}\sigma}^\dagger(\tau') \rangle \qquad (7.27)$$

$$= \frac{1}{V} \sum_{\mathbf{q}} V(q) \left[ \mathcal{G}(\mathbf{p}, \tau - \tau')\eta_{\mathbf{p}-\mathbf{q}} - \mathcal{F}(\mathbf{p}-\mathbf{q}, 0)\mathcal{F}^\dagger(\mathbf{p}, \tau - \tau') \right]$$

The first term is the exchange self–energy of the electron due to the phonon induced interaction between electrons. A careful investigation shows that this self–energy does not change much between the normal and superconducting states. The self–energy of the electrons, from phonons, causes a change in the electron effective mass given by the parameter $\lambda$. This effect is not large in weak superconductors, so it may be **ignored**. In metals where $\lambda$ is large, the superconducting state can be expected to significantly alter the properties of electrons near the Fermi surface where strong coupling theory is needed.

In the second term of (7.27) there arises the combination of factors which are defined as

$$\Delta(\mathbf{p}) = -\frac{1}{V}\sum_{\mathbf{q}} V(q)\mathcal{F}(\mathbf{p}-\mathbf{q}, \tau = 0) \tag{7.28}$$

The quantity $\Delta(\mathbf{p})$ is the gap function in the BCS theory. This quantity is defined to be positive, since the right–hand side of the definition is positive, with an attractive potential $V(q) < 0$. So the (7.24) gives

$$\left(-\frac{\partial}{\partial\tau} - \xi_p\right)\mathcal{G}(\mathbf{p}, \tau - \tau') + \Delta(\mathbf{p})\mathcal{F}^\dagger(\mathbf{p}, \tau - \tau') = \delta(\tau - \tau') \tag{7.29}$$

Similarly, consider the equation of motion for the $\mathcal{F}^\dagger$ function

$$\frac{\partial}{\partial}\mathcal{F}^\dagger(\mathbf{p}, \tau - \tau') = \langle T_\tau \left[\frac{\partial}{\partial\tau}C_{\mathbf{p}\uparrow}^\dagger(\tau)\right] C_{-\mathbf{p}\downarrow}^\dagger(\tau')\rangle \tag{7.30}$$

Calculate the time development of the $\mathcal{F}^\dagger$ operator, notice that $C_{\mathbf{p}\sigma}^\dagger(\tau)$ is not the Hermitian conjugate of $C_{\mathbf{p}\sigma}(\tau)$, the for $\frac{\partial\mathcal{F}^\dagger}{\partial\tau}$ gives

$$\left(-\frac{\partial}{\partial\tau} + \xi_p\right)\mathcal{F}^\dagger(\mathbf{p}, \tau - \tau') + \frac{1}{V}\sum_{\mathbf{q}\mathbf{p}'s} V(q)$$

$$\times \quad \langle T_\tau C_{\mathbf{p}-\mathbf{q},\uparrow}^\dagger(\tau)C_{\mathbf{p}'+\mathbf{q},s'}^\dagger(\tau)C_{\mathbf{p}'s'}(\tau)C_{-\mathbf{p}\downarrow}^\dagger(\tau')\rangle = 0 \tag{7.31}$$

Neglect the exchange potential, we have

$$\left(-\frac{\partial}{\partial\tau} + \xi_p\right)\mathcal{F}^\dagger(\mathbf{p}, \tau - \tau') + \Delta^\dagger(\mathbf{p})\mathcal{G}(\mathbf{p}, \tau - \tau') = 0 \tag{7.32}$$

The gap function is assumed real, $\Delta^\dagger = \Delta$, which is verified later.

After Fourier transform, the two equations (7.29) and (7.32) are

$$(ip_n - \xi_p)\mathcal{G}(\mathbf{p}, ip_n) + \Delta(\mathbf{p})\mathcal{F}^\dagger(\mathbf{p}, ip_n) = 1 \tag{7.33}$$

$$(ip_n + \xi_p)\mathcal{F}^\dagger(\mathbf{p}, ip_n) + \Delta(\mathbf{p})\mathcal{G}(\mathbf{p}, ip_n) = 0 \tag{7.34}$$

These algebraic equations are solved

$$\mathcal{G}(\mathbf{p}, ip_n) = -\frac{ip_n + \xi_p}{p_n^2 + \xi_p^2 + \Delta^2(\mathbf{p})} \tag{7.35}$$

$$\mathcal{F}(\mathbf{p}, ip_n) = \mathcal{F}^\dagger(\mathbf{p}, ip_n) = \frac{\Delta(\mathbf{p})}{p_n^2 + \xi_p^2 + \Delta^2(\mathbf{p})} \tag{7.36}$$

The equivalence of $\mathcal{F}$ and $\mathcal{F}^\dagger$ can be shown by deriving similar equation for $\mathcal{F}$.

There are some properties, for Fourier transformation, by changing the sign of the dummy variable of summation $n$ gives

$$\mathcal{F}(\mathbf{p}, -\tau) = \frac{1}{\beta} \sum_n e^{-i\tau p_n} \mathcal{F}(\mathbf{p}, -ip_n) = \mathcal{F}(\mathbf{p}, tau) \qquad (7.37)$$

This relation causes the energy gap equation to be real

$$\Delta(\mathbf{p}) = -\frac{1}{V} \sum_\mathbf{q} V(q) \mathcal{F}(\mathbf{p} - \mathbf{q}, 0) = -\frac{1}{V} \sum_\mathbf{q} V(q) \mathcal{F}^\dagger(\mathbf{p} - \mathbf{q}, 0) = \Delta^\dagger(\mathbf{p})$$

$$(7.38)$$

If the energy gap $\Delta$ is set equal to zero, there is fond the usual form for the normal state Green's function and zero for the others. It must still be shown that there is a self–consistent solution to the equations for $\Delta \neq 0$.

The Green's function $\mathcal{G}$, $\mathcal{F}$ and $\mathcal{F}^\dagger$ have poles at the points $\pm E_p = \pm\sqrt{\xi_p^2 + \Delta^2(\mathbf{p})}$. The $E_p$ is called the **excitation energy** of the super-conductor. In BCS theory the gap function $\Delta(\mathbf{p})$ for s–wave superconductors is not dependent on momentum $\mathbf{p}$ and treated as a constant for each temperature. The excitation energy $E_p$ depends on $\xi_p^2 > 0$. The minimum excitation energy is $\Delta$, and $E_p \geq \Delta$. An important feature of the BCS theory is that the particles are paired, and it is not possible to excite just one quasiparticle with excitation energy $E_p$. Instead, one must break a pair of particles and excite them both to the band of excitations.

It is conventional to introduce the following coherence factors

$$\begin{aligned}
u_p^2 &= \frac{1}{2}\left(1 + \frac{\xi_p}{E_p}\right) \\
v_p^2 &= \frac{1}{2}\left(1 - \frac{\xi_p}{E_p}\right) \\
2u_p v_p &= \sqrt{1 - \frac{\xi_p^2}{E_p^2}} = \frac{\Delta}{E_p} \qquad (7.39) \\
u_p^2 + v_p^2 &= 1
\end{aligned}$$

They are useful the show the residues of the poles of the Green's functions.

$$\mathcal{G}(\mathbf{p}, ip) = \frac{u_p^2}{ip - E_p} + \frac{v_p^2}{ip + E_p} \qquad (7.40)$$

$$\mathcal{F}(\mathbf{p}, ip) = \mathcal{F}^\dagger(\mathbf{p}, ip) = -u_p v_p \left(\frac{1}{ip - E_p} - \frac{1}{ip + E_p}\right) \qquad (7.41)$$

The spectral function for the Green's function is

$$A(p, \varepsilon) = -2\,\mathrm{Im}\left[G_{ret}(\mathbf{p}, \varepsilon)\right] = 2\pi\left[u_p^2 \delta(\varepsilon - E_p) + v_p^2 \delta(\varepsilon + E_p)\right] \qquad (7.42)$$

To evaluate the $\Delta$, consider the definition of the gap function in (7.28),

$$\mathcal{F}(\mathbf{p}, \tau = 0) = \frac{1}{\beta} \sum_{p_n} \frac{\Delta}{p_n^2 + E_p^2} = \frac{\Delta}{2E_p} \tanh\left(\frac{\beta E_p}{2}\right) \tag{7.43}$$

The summation is evaluated in the contour integral

$$\oint \frac{dz}{2\pi i} \eta_F(z) \frac{\Delta}{z^2 - E_p^2} = 0 \tag{7.44}$$

# 8
# *Appendix: Complex analysis*

## *8.1   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.

### *8.1.1   Definition*

The residue of a meromorphic function $f$ at an isolated singularity $a$, denoted as $\mathrm{Res}(f,a)$, is the unique value $R$ such tat $f(z) - R/(z-a)$ 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.

### *8.1.2   Examples*

**Eaxmple.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 $dz \to d(e^{i\theta}) = ie^{i\theta}d\theta$. 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.

$$\oint_C \frac{e^z}{z^5} dz$$
$$= \oint_C \frac{1}{z^5}(1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \dots)dz$$
$$= \oint_C \frac{1}{4!z} dz \frac{\pi i}{12}$$

The last formula is based on the previous result.

### 8.1.3   Calculating residues

For residue theorem,

$$\text{Res}(f,c) = \frac{1}{2\pi i} \oint_\gamma f(z)dz$$

where $\gamma$ 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

$$\text{Res}(f,c) = \lim_{z \to c}(z - c)f(z)$$

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

$$\text{Res}(f,c) = \frac{1}{(n-1)!} \lim_{z \to c} \frac{d^{n-1}}{dz^{n-1}} \left[(z - c)^n f(z)\right]$$

In general, the residue at infinity is given by

$$\text{Res}(f(z), \infty) = -\text{Res}\left(\frac{1}{z^2}f(\frac{1}{z}), 0\right)$$

**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

$$\frac{\sin z}{z(z-1)} = \frac{\sin 1}{z-1} + (\cos 1 - \sin 1) + (z-1)(-\frac{\sin 1}{2!} - \cos 1 + \sin 1) + \dots$$

So the residue of $f(z)$ at $z = 1$ is $\sin 1$.

## 8.2 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

$$\lim_{\varepsilon \to 0^+} \int_a^b \frac{f(x)}{x \pm i\varepsilon} dx = \mp i\pi f(0) + \mathcal{P} \int_a^b \frac{f(x)}{x} dx,$$

where $\mathcal{P}$ denotes the Cauchy principal value.

One important relation is for the Green's functions,

$$\frac{1}{\omega + E_n - E_m + i\delta} = \mathcal{P} \frac{1}{\omega + E_n - E_m} - i\pi\delta(\omega + E_n - E_m)$$

## 8.3 Kramers-Kronig relations

The Kramers-Kronig relations are bidirectional mathematical relations, connection the real and imaginary parts of any complex funtion 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 $\omega$, where $\chi_1$ and $\chi_2$ are real. Suppose this function is analytic in the upper half-plane of $\omega$ and vanishes like $1/|\omega|$ or faster as $|\omega| \to \infty$. 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

$$\chi_1(\omega) \quad = \quad \frac{2}{\pi} \mathcal{P} \int_0^{\infty} \frac{\omega' \chi_1(\omega')}{\omega'^2 - \omega^2} d\omega'$$

$$\chi_2(\omega) \quad = \quad - = \frac{2\omega}{\pi} \mathcal{P} \int_0^{\infty} \frac{\chi_1(\omega')}{\omega'^2 - \omega^2} d\omega'$$