MENG SUN

NOTES ON: MANY PAR-TICLE PHYSICS —BY D. MAHAN

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1
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

$$H = H_0 + V \qquad (1.1)$$

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.

1.1 Interaction representation

1.1.1 Schrödinger

In Schrödinger representation

$$i\partial_t \psi(t) = H\psi(t) \qquad (1.2)$$

with the formal operator solution

$$\psi(t) = e^{-iHt}\psi(0) \qquad (1.3)$$

The use of this formula requires:

- The wavefunction is time dependent.

- Operators such as the Hamiltonian H are taken to be independent of time.

1.1.2 Heisenberg

The Heisenberg representation has the following properties:

- The wavefunction is independent of the time

- The operators are time dependent and given by

$$O(t) = e^{iHt}O(0)e^{-iHt} \tag{1.4}$$

or, equivalently, the equation of motion is given by

$$i\partial_t O(t) = [O(t), H] \tag{1.5}$$

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

$$\langle \psi_1^\dagger(t)O\psi_2(t)\rangle_S = \langle \psi_1^\dagger O(t)\psi_2\rangle_H = \langle \psi_1^\dagger(0)e^{iHt}O(0)e^{-iHt}\psi_2(0)\rangle \tag{1.6}$$

1.1.3   Interaction

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

$$H = H_0 + V \tag{1.7}$$

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:

$$\hat{O}(t) = e^{iH_0t}O_S e^{-iH_0t} \quad i\partial_t\hat{O}(t) = [\hat{O}(t), H_0] \tag{1.8}$$

- The wavefunction have the time dependence:

$$\hat{\psi}(t) = e^{iH_0t}e^{-iHt}\psi(0) \tag{1.9}$$

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 (1.8). For the dependence of the wavefunction is governed by

$$\partial_t\hat{\psi}(t) = -i\hat{V}(t)\hat{\psi}(t) \tag{1.10}$$

As operator was introduced into (1.9), which can be defined as

$$U(t) = e^{iH_0t}e^{-iHt} \tag{1.11}$$

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

$$\partial_t U(t) = -i\hat{V}(t)U(t) \tag{1.12}$$

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

$$U(t) = 1 - i \int_0^t dt_1 \hat{V}(t_1) U(t_1) \tag{1.13}$$

$$= \sum_{n=0}^{\infty} (-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \hat{V}(t_1) \hat{V}(t_2) \dots \hat{V}(t_n)$$

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

$$U(t) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_0^t dt_1 \cdots \int_0^{t_{n-1}} dt_n T[\hat{V}(t_1) \dots \hat{V}(t_n)] \tag{1.14}$$

This expansion may be abbreviated by writing it as

$$U(t) = T \exp\left[-i \int_0^t dt_1 \hat{V}(t_1) \right] \tag{1.15}$$

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

1.2 S Matrix

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

$$\hat{\psi}(t) = U(t) \hat{\psi}(0) \tag{1.16}$$

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

$$\hat{\psi}(t) = S(t, t') \hat{\psi}(t') \tag{1.17}$$

with the definition

$$S(t, t') = U(t) U^\dagger(t') \tag{1.18}$$

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

$$S(t, t') = T \exp\left[-i \int_{t'}^t dt_1 \hat{V}(t_1) \right] \tag{1.19}$$

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

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

$$\psi(0) = S(0, -\infty)\phi_0 \tag{1.20}$$

The result can be regard as the following, since

$$\hat{\psi}(t) = S(t, 0)\psi(0) \tag{1.21}$$

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

$$\psi(0) = S(0, t)\hat{\psi}(t) \tag{1.22}$$

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

$$\psi(0) = S(0, -\infty)\hat{\psi}(-\infty) \tag{1.23}$$

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

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

$$\hat{\psi}(\infty) = S(\infty, 0)\psi(0) \tag{1.24}$$

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

$$\phi_0 e^{iL} = \hat{\psi}(\infty) = S(\infty, 0)\psi(0) = S(\infty, -\infty)\phi_0 \tag{1.25}$$

$$e^{iL} = \langle\phi_0| S(\infty, -\infty) |\phi_0\rangle \tag{1.26}$$

1.3   Green's Function

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

$$G(\lambda, t - t') = -i \langle| TC_\lambda(t)C_\lambda^\dagger(t') |\rangle \tag{1.27}$$

The quantum number λ 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_λ represent states of H_0, while the ground state $|\rangle$ is an eigenstate of H. Furthermore, (1.27) is defined in Heisenberg picture, one have the usual dependence of time on operators (1.4).

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

$$|\rangle = S(0, -\infty) |\phi_0\rangle \tag{1.28}$$

[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 (1.25) and (1.26)

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

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

$$
G(\lambda, t - t') = -i \frac{\langle \phi_0 | \, T \hat{C}_\lambda(t) \hat{C}_\lambda^\dagger(t') S(\infty, -\infty) \, | \phi_0 \rangle}{\langle \phi_0 | \, T S(\infty, -\infty) \, | \phi_0 \rangle} \tag{1.29}
$$

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

$$
G^0(\lambda, t - t') = -i \langle \phi_0 | \, T \hat{C}_\lambda(t) \hat{C}_\lambda^\dagger(t') \, | \phi_0 \rangle \tag{1.30}
$$

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.

1.3.1   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

$$
\begin{aligned}
C_p \, |0\rangle &= 0 & (1.31) \\
a_q \, |0\rangle &= 0 & (1.32) \\
S(t, -\infty) \, |0\rangle &= |0\rangle & (1.33)
\end{aligned}
$$

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

$$
G(\lambda, t - t') = -i\Theta(t - t') \langle 0 | \, \hat{C}_\lambda(t) \hat{C}_\lambda^\dagger(t) \, |0\rangle \tag{1.34}
$$

The unperturbed Green's function is given

$$G^0(\lambda, t - t') = -i\Theta(t - t')e^{-i\varepsilon_\lambda(t-t')} \tag{1.35}$$

The Fourier transform is defined as

$$G(\lambda, E) = \int_{-\infty}^{\infty} dt e^{iEt} G(\lambda, t) \tag{1.36}$$

The unperturbed Green's function gives[3]

$$G^0(\lambda, E) = \frac{1}{E - \varepsilon_\lambda + i\delta} \tag{1.37}$$

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

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

1.3.2 A degenerate electron gas

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

$$\langle\phi_0| C_k^\dagger C_k |\phi_0\rangle = \Theta(p_F - k) \tag{1.38}$$
$$\langle\phi_0| C_k C_k^\dagger |\phi_0\rangle = \Theta(k - p_F) \tag{1.39}$$

This gives the Green's function

$$G^0(k, E) = \frac{1}{E - \xi_k + i\delta\text{sgn}(\xi_k)} \tag{1.40}$$

1.3.3 Phonons

The Green's function for phonons is defined as

$$D(\mathbf{q}, \lambda, t - t') = -i\langle| T A_{\mathbf{q}\lambda}(t) A_{-\mathbf{q}\lambda}(t') |\rangle \tag{1.41}$$
$$A_{\mathbf{q}\lambda} = a_{\mathbf{q}\lambda} + a_{-\mathbf{q}\lambda}^\dagger \tag{1.42}$$

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

$$D(q, t - t') = -i\frac{\langle\phi_0| T\hat{A}_{-q}(t)\hat{A}_{-q}(t')S(\infty, -\infty) |\phi_0\rangle}{\langle\phi_0| S(\infty, -\infty) |\phi_0\rangle} \tag{1.43}$$

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

$$D^0(\mathbf{q}, t - t') = -i\left[\Theta(t - t')e^{-i\omega_q(t-t')} + \Theta(t' - t)e^{i\omega_q(t-t')}\right] \tag{1.44}$$

and

$$D^0(\mathbf{q}, \omega) = \frac{2\omega_\mathbf{q}}{\omega^2 - \omega_\mathbf{q}^2 + i\delta} \qquad (1.45)$$

For nonzero temperature, we have

$$D^0(\mathbf{q}, t - t') = -i \left[(N_\mathbf{q} + 1)e^{-i\omega_\mathbf{q}|t-t'|} + N_\mathbf{q}e^{i\omega_\mathbf{q}|t-t'|} \right] \qquad (1.46)$$

1.4   Wick's Theorem

For Green's function as defined in interaction picture such as (1.29) and (1.43). To evaluate these, the stand method is expanding the $S(\infty, -\infty)$ matrix in (1.19).

$$G(p, t - t') = \sum_{n=0}^{\infty} \frac{(-i)^{n+1}}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \frac{{}_0\langle|T\hat{C}_p(t)\hat{V}(t_1)\dots\hat{V}(t_n)\hat{C}_p^\dagger(t')|\rangle_0}{{}_0\langle|S(\infty, -\infty)|\rangle_0}$$
$$(1.47)$$

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.

1.5   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]

$$D^0(\mathbf{q}, t - t') = D^0(-\mathbf{q}, t' - t) \tag{1.48}$$

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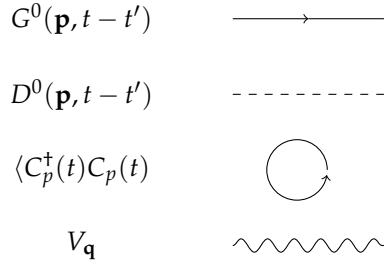
$G^0(\mathbf{p}, t - t')$

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

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

$V_\mathbf{q}$

Figure 1.1: Elements of Feynman diagram.

1.6   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].

1.7   Dyson's Equation

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

$$G(\mathbf{p}, E) = \frac{G^0(\mathbf{p}, E)}{1 - G^0(\mathbf{p}, E)\Sigma(\mathbf{p}, E)} \tag{1.49}$$

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

$$G(\mathbf{p}, E) = \frac{1}{E - \varepsilon_\mathbf{p} + i\delta - \Sigma(\mathbf{p}, E)} \tag{1.50}$$

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

$$G(\mathbf{p}, E) = \frac{1}{E - \xi_\mathbf{p} + i\delta \mathrm{sgn}(p) - \Sigma(\mathbf{p}, E)} \tag{1.51}$$

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

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

$$D(\mathbf{q}, \omega) = \frac{D^0(\mathbf{q}, \omega)}{1 - D^0(\mathbf{q}, \omega)\Pi(\mathbf{q}, \omega)} \tag{1.52}$$

Similarly, we have this form,

$$D(\mathbf{q}, \omega) = \frac{2\omega_\mathbf{q}}{\omega^2 - \omega_\mathbf{q}^2 + i\delta - 2\omega_\mathbf{q}\Pi(\mathbf{q}, \omega)} \tag{1.53}$$

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.

1.8   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

$$G^0_{\alpha\beta}(\mathbf{p}, E) = \frac{\delta_{\alpha\beta}}{E - \varepsilon_\mathbf{p} + i\delta_\mathbf{p}} \tag{1.54}$$

  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

$$D^0(\mathbf{q}, \omega_\omega) = \frac{2\omega_\mathbf{q}}{\omega^2 - \omega_\mathbf{q}^2 + i\delta} \tag{1.55}$$

  Also add a factor of $\left|M_\mathbf{q}\right|^2$ 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

$$\frac{i^m}{(2\pi)^{4m}}(-1)^F(2S+1)^F \tag{1.56}$$

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

$$\frac{i^m}{(2\pi v)^m}(-1)^F(2S+1)^F \tag{1.57}$$

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

$$\frac{e}{c}\sum_i \mathbf{j}(\mathbf{r}_i) \cdot \mathbf{A}(\mathbf{r}_i) = \frac{e}{c}\sum_{\mathbf{q}\mu} j_\mu(\mathbf{q})A_\mu(\mathbf{q}) = \frac{e}{mc}\sum_{\mathbf{q}\mu} A_\mu(\mathbf{q})\sum_{\mathbf{k}\sigma}(\mathbf{k}+\tfrac{1}{2}\mathbf{q})_\mu C^\dagger_{\mathbf{k}+\mathbf{q},\sigma}C_{\mathbf{k},\sigma} \tag{1.58}$$

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

$$\frac{e^2}{m^2}\sum_{\mu\nu}(\mathbf{k}+\tfrac{1}{2}\mathbf{q})_\mu D_{\mu\nu}(\mathbf{q},\omega)(\mathbf{k}'+\tfrac{1}{2}\mathbf{q})_\nu \tag{1.59}$$

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.
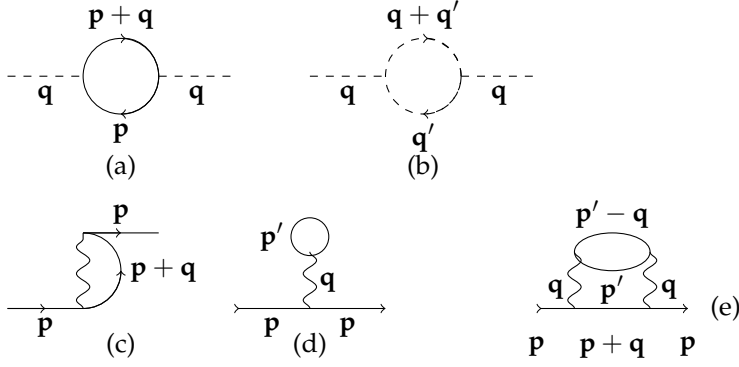
Figure 1.2: Phonon self-energies, (a) is due to electron-phonon interaction, and (b) is from lattice anharmonicity. (c) is unscreened exchange energy.

Now examine some example. For the first plot Fig. 1.2(a), we have $F = 1$, $S = \frac{1}{2}$ and $m = 1$, then[8]

$$\Pi(\mathbf{q}, \omega) = |M_{\mathbf{q}}|^2 P^1(\mathbf{q}, \omega) \tag{1.60}$$

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

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

$$\Pi^1(\mathbf{q}, \omega) = \frac{i}{(2\pi)^4} \int d\omega' \int d\mathbf{q}' \left|M_{\mathbf{q},\mathbf{q}'}\right|^2 D^0(\mathbf{q}', \omega') D^0(\mathbf{q} + \mathbf{q}', \omega + \omega') \tag{1.61}$$

The electron self-energy arising from electron-electron interaction. The self-energy term in Fig. 1.2(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

$$\Sigma_x(\mathbf{p}, E) = \frac{i}{(2\pi)^4}(-1)^0 (2)^0 \int d\omega \int d\mathbf{q} v_q G^0(\mathbf{p} + \mathbf{q}, E + \omega) \tag{1.62}$$

There is a very important identity:

$$i \int \frac{d\omega}{2\pi} G^0(\mathbf{p} + \mathbf{q}, E + \omega) = -\eta_F(\xi_{\mathbf{p}+\mathbf{q}}) \tag{1.63}$$

with this we have

$$\Sigma_x(\mathbf{p}) = -\frac{1}{v} \sum_{\mathbf{q}} v_q \eta_F(\xi_{\mathbf{p}+\mathbf{q}}) = -\int \frac{d^3 q}{(2\pi)^3} v_q \eta_F(\xi_{\mathbf{p}+\mathbf{q}}) \tag{1.64}$$

where subscript x denotes exchange.

Important identity: By Fourier transformation

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

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

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

with different time approach, we have

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

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. 1.2(d). With $F = 1$, $m = 1$ and $S = \frac{1}{2}$:

$$\Sigma_H(\mathbf{p}, E) = -\frac{2i}{(2\pi)^4} \int dE' \int d\mathbf{p}' v_{\mathbf{q}=0} G^0(\mathbf{q}', E') \qquad (1.65)$$

where the subscript "H" denotes "Hartree" approximation. This self-energy depends on neither $\mathbf{p}$ nor E. The identity (1.63) man be used again to produce

$$\Sigma_H = 2v_{\mathbf{q}=0} \sum_{\mathbf{p}'} \eta_F(\xi_{\mathbf{p}'}) = v_{\mathbf{q}=0} N_e \qquad (1.66)$$

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. 1.2(e). Its evaluation yields

$$\Sigma(\mathbf{p}, E) = \frac{1}{(2\pi)^4} \int d\omega \int d\mathbf{q} v_{\mathbf{q}}^2 P^1(\mathbf{q}, \omega) G^0(\mathbf{p} + \mathbf{q}, E + \omega) \qquad (1.67)$$

1.9   Time-loop S Matrix

The S matrix is defined in Sec. 1.2. As time in (1.25) is taken over the whole interval. The state at $t = -\infty$ is well defined as the ground state of the noninteracting system ϕ_0. The interaction are turned on slowly. At $t \approx 0$ the fully interacting ground state is $\psi(0) = S(0, -\infty)\phi_0$. In condensed matter physics the state at $t \to \infty$ 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 ϕ_0.

Considering the time-loop expansion for the S Matrix

$$S(-\infty, -\infty) = T_s \exp\left[-i \int_{loop} ds_1 \hat{V}(s_1)\right] \qquad (1.68)$$
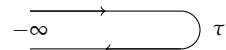

Figure 1.3: The time-loop integration path in the S matrix.

The integration path is the time loop in Fig. 1.3. 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

$$G(\lambda, s_1 - s_2) = -i \langle \phi_0 | T_s C_\lambda(s_1) C_\lambda^\dagger(s_2) | \phi_0 \rangle \qquad (1.69)$$

where s_1 and s_2 can be in different place of Fig.1.3.

1.9.1 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

$$
\begin{aligned}
G^>(x_1, x_2) &= -i\langle \psi(x_1)\psi^\dagger(x_2)\rangle \\
G^<(x_1, x_2) &= i\langle \psi^\dagger(x_2)\psi(x_1)\rangle \\
G_t(x_1, x_2) &= \Theta(t_1 - t_2)G^>(x_1, x_2) + \Theta(t_2 - t_1)G^<(x_1, x_2) \\
G_{\bar{t}}(x_1, x_2) &= \Theta(t_2 - t_1)G^>(x_1, x_2) + \Theta(t_1 - t_2)G^<(x_1, x_2) \\
G_{ret}(x_1, x_2) &= G_t - G^< = G^> - G_{\bar{t}} \\
G_{adv}(x_1, x_2) &= G_t - G^> = G^< - G_{\bar{t}} \qquad (1.70)
\end{aligned}
$$

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

$$G(\mathbf{k}, E) = \int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} \int dt e^{-iEt} G(\mathbf{r}, t) \qquad (1.71)$$

where G represents any of the six functions.

Often the Hamiltonian H can be solved exactly in terms of eigenfunctions $\phi_\lambda(\mathbf{r})$ and eigenvalues ε_λ. Two example are the electron in a magnetic field or a free particle. It is useful to have the expressions for the Green's function in terms of these eigenfunctions. They are derived by expanding the field operators in terms of eigenfunctions and creation and destruction operators[9]:

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

$$
\begin{aligned}
\phi(x_1) &= \sum_\lambda C_\lambda \phi_\lambda(\mathbf{r}_1) e^{-i\varepsilon_\lambda t} \\
\phi^\dagger(x_1) &= \sum_\lambda C_\lambda^\dagger \phi_\lambda^*(\mathbf{r}_1) e^{i\varepsilon_\lambda t} \qquad (1.72)
\end{aligned}
$$

Then the Green's function in (1.70) are evaluated with the occupation

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

$$
\begin{aligned}
G^>(x_1, x_2) &= -i \sum_\lambda (1 - \eta_\lambda) \phi_\lambda(\mathbf{r}_1) \phi_\lambda^*(\mathbf{r}_2) e^{-i\varepsilon_\lambda t} \\
G^<(x_1, x_2) &= i \sum_\lambda \eta_\lambda \phi_\lambda(\mathbf{r}_1) \phi_\lambda^*(br_2) e^{-i\varepsilon_\lambda t} \\
G_t(x_1, x_2) &= -i \sum_\lambda [\Theta(t) - \eta_\lambda] \phi_\lambda(\mathbf{r}_1) \phi_\lambda^*(br_2) e^{-i\varepsilon_\lambda t} \\
G_{\bar{t}}(x_1, x_2) &= -i \sum_\lambda [\Theta(-t) - \eta_\lambda] \phi_\lambda(\mathbf{r}_1) \phi_\lambda^*(br_2) e^{-i\varepsilon_\lambda t} \\
G_{ret}(x_1, x_2) &= -i\Theta(t) \sum_\lambda \phi_\lambda(\mathbf{r}_1) \phi_\lambda^*(\mathbf{r}_2) e^{-i\varepsilon_\lambda t} \\
G_{adv}(x_1, x_2) &= i\Theta(-t) \sum_\lambda \phi_\lambda(\mathbf{r}_1) \phi_\lambda^*(\mathbf{r}_2) e^{-i\varepsilon_\lambda t} \quad (1.73)
\end{aligned}
$$

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

The starting point for any calculation, is the behavior of the Green's functions for system without interaction. Then the quantum number λ becomes the wave vector $\mathbf{k}$ and spin index σ. The eigenvalue combination is $\phi_\lambda(\mathbf{r}_1) \phi_\lambda^*(\mathbf{r}_2) = \exp[i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}_2)]/v$. In noninteracting system in equilibrium, for (1.71), with Fourier transformation give the free-particle Green's functions

$$
\begin{aligned}
G_0^>(\mathbf{k}, t) &= -i[1 - \eta_\mathbf{k}] e^{i\varepsilon_\mathbf{k} t} \\
G_0^<(\mathbf{k}, t) &= i\eta_\mathbf{k} e^{-i\varepsilon_\mathbf{k} t} \\
G_t^0(\mathbf{k}, t) &= -i[\Theta(t) - \eta_\mathbf{k}] e^{-i\varepsilon_\mathbf{k} t} \\
G_{\bar{t}}^0(\mathbf{k}, t) &= -i[\Theta(-t) - \eta_\mathbf{k}] e^{-i\varepsilon_\mathbf{k} t} \\
G_{ret}^0(\mathbf{k}, t) &= -i\Theta(t) e^{-i\varepsilon_\mathbf{k} t} \\
G_{adv}^0(\mathbf{k}, t) &= i\Theta(-t) e^{-i\varepsilon_\mathbf{k} t} \quad (1.74)
\end{aligned}
$$

with Fourier transformation and $i\delta$ infinitesimal quantity

$$
\begin{aligned}
G_0^>(\mathbf{k}, E) &= -2\pi i[1 - \eta_\mathbf{k}] \delta(E - \varepsilon_\mathbf{k}) \\
G_0^<(\mathbf{k}, E) &= 2\pi i \eta_\mathbf{k} \delta(E - \varepsilon_\mathbf{k}) \\
G_{ret}^0(\mathbf{k}, E) &= \frac{1}{E - \varepsilon_\mathbf{k} + i\delta} \\
G_{adv}^0(\mathbf{k}, E) &= \frac{1}{E - \varepsilon_\mathbf{k} - i\delta} \\
G_t^0(\mathbf{k}, E) &= G_{ret}^0 + G_0^< = \frac{1}{E - \varepsilon_\mathbf{k} + i\delta_\mathbf{k}} \\
G_{\bar{t}}^0(\mathbf{k}, E) &= G_0^< - G_{adv}^0 = \frac{-1}{E - \varepsilon_\mathbf{k} - i\delta_\mathbf{k}} \quad (1.75)
\end{aligned}
$$

The time-order function G_t^0 is exactly the same on in (1.40). Note the two kinds of infinitesimal delta, where $\delta_\mathbf{k} \equiv \delta \text{sign}(\mathbf{k} - \mathbf{k}_F)$.

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

$$
\begin{aligned}
D^>(x_1, x_2) &= -i\langle Q(x_1)Q(x_2)\rangle \\
D^<(x_1, x_2) &= -i\langle Q(x_2)Q(x_1)\rangle \\
D_t(x_1, x_2) &= \Theta(t_1 - t_2)D^>(x_1, x_2) + \Theta(t_2 - t_1)D^<(x_1, x_2) \\
D_{\bar{t}}(x_1, x_2) &= \Theta(t_2 - t_1)D^>(x_1, x_2) + \Theta(t_1 - t_2)D^<(x_1, x_2) \\
D_{ret} &= D_t - D^< = \Theta(t_1 - t_2)[D^> - D^<] \\
D_{adv} &= D_t - D^> = -\Theta(t_2 - t_1)[D^> - D^<] \qquad (1.76)
\end{aligned}
$$

There expressions are rather similar to those in (1.70) 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

$$
\begin{aligned}
D^>(\mathbf{q}, t) &= -i[(N_\mathbf{q} + 1)e^{-i\omega_\mathbf{q} t} + N_\mathbf{q} e^{i\omega_\mathbf{q} t}] \\
D^<(\mathbf{q}, t) &= -i[(N_\mathbf{q} + 1)e^{i\omega_\mathbf{q} t} + N_\mathbf{q} e^{-i\omega_\mathbf{q} t}] \\
D_{ret}(\mathbf{q}, t) &= -2\Theta(t)\sin(\omega_\mathbf{q} t) \\
D_{adv}(\mathbf{q}, t) &= -2\Theta(-t)\sin(\omega_\mathbf{q} t) \qquad\qquad (1.77) \\
D_t(\mathbf{q}, t) &= -i\{(N_\mathbf{q} + \Theta(-t))e^{i\omega_\mathbf{q} t} + [N_\mathbf{q} + \Theta(t)]e^{-i\omega_\mathbf{q} t}\} \\
D_{\bar{t}}(\mathbf{q}, t) &= -i\{(N_\mathbf{q} + \Theta(t))e^{i\omega_\mathbf{q} t} + [N_\mathbf{q} + \Theta(-t)]e^{-i\omega_\mathbf{q} t}\}
\end{aligned}
$$

1.9.2   Dyson's Equation

Each of the six Green's functions can be evaluated for an interacting system in terms of the S matrix in (1.68).

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. 1.4. The nth 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. 1.4.
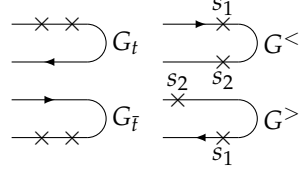
Considering an example. Below is given a potential term V of the type found for *electrons scattering from impurities*. The first term in the S-matrix expansion for $G^<$ with this interaction is

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

$$G^<(\lambda, t_1 - t_2) = G_0^<(\lambda, t_1 - t_2) \tag{1.78}$$
$$+ \sum_{\alpha\beta} M_{\alpha\beta} \int ds \, \langle\phi_0| TC_\lambda^\dagger(t_2)C_\beta(s) |\phi_0\rangle \langle\phi_0| TC_\alpha^\dagger(s)C_\lambda(t_1) |\phi_0\rangle$$

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.

$$G^<(\lambda, t_1 - t_2) = G_0^<(\lambda, t_1 - t_2) + M_{\lambda\lambda} \int_{-\infty}^{\infty} ds [G_t^0(\lambda, t_1 - s)G_0^<(\lambda, s - t_2) - G_0^<(\lambda, t_1 - s)G_{\bar{t}}^0(s - t_2)]$$
$$\tag{1.79}$$

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 nth term in the S-matrix expansion produce 2^n arrangements. All of there terms can be managed by using a matrix formulation

$$G = \begin{bmatrix} G_t & -G^< \\ G^> & -G_{\bar{t}} \end{bmatrix} \quad \Sigma = \begin{bmatrix} \Sigma_t & -\Sigma^< \\ \Sigma^> & -\Sigma_{\bar{t}} \end{bmatrix} \tag{1.80}$$

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

$$G(x_1, x_2) = G_0(x_1 - x_2) + \int_{-\infty}^{\infty} dx_3 \int_{-\infty}^{\infty} dx_4 G_0(x_1 - x_3)$$
$$\times \quad \Sigma(x_3, x_4)G(x_4, x_2) \tag{1.81}$$

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

$$G = G_0 + G_0 \Sigma G \qquad (1.82)$$

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

$$
\begin{aligned}
G_{ret} &= G^0_{ret}[1 + \Sigma_{ret} G_{ret}] \\
G_{adv} &= G^0_{adv}[1 + \Sigma_{adv} G_{adv}] \\
G^> &= [1 + G_{ret}\Sigma_{ret}]G_0^>[1 + \Sigma_{adv}G_{adv}] + G_{ret}\Sigma^> G_{adv} \\
G^< &= [1 + G_{ret}\Sigma_{ret}]G_0^<[1 + \Sigma_{adv}G_{adv}] + G_{ret}\Sigma^< G_{adv} \\
G_t &= [1 + G_{ret}\Sigma_{ret}]G_t^0[1 + \Sigma_{adv}G_{adv}] + G_{ret}\Sigma_{\bar{t}} G_{adv} \\
G_{\bar{t}} &= [1 + G_{ret}\Sigma_{ret}]G_{\bar{t}}^0[1 + \Sigma_{adv}G_{adv}] + G_{ret}\Sigma_t G_{adv} \qquad (1.83)
\end{aligned}
$$

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

$$
\begin{aligned}
G_{ret}(k, \omega) &= \frac{1}{\omega - \varepsilon_k - \Sigma_{ret}}, \quad \sigma = \omega - \varepsilon_k - Re[\Sigma_{ret}] \\
G_{adv}(k, \omega) &= \frac{1}{\omega - \varepsilon_k - \Sigma_{adv}}, \quad \Sigma_{adv} = \Sigma_{ret}^* \\
A(k, \omega) &= -2Im[G_{ret}(k, \omega)] = \frac{2\Gamma}{\sigma^2 + \Gamma^2}, \quad \Gamma = -Im[\Sigma_{ret}] > 0 \\
\Sigma^< &= 2i\eta_F(\omega)\Gamma(k, \omega), \quad G^< = i\eta_F(\omega)A(k, \omega) \\
\Sigma^> &= -2i(1 - \eta_F)\Gamma, \quad G^> = -i(1 - \eta_F)A \qquad (1.84)
\end{aligned}
$$

More will discussed in next chapter.

1.10 Photon Green's Functions

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

$$H = \sum_i \frac{1}{2m}[\mathbf{p}_i - \frac{e}{c}\mathbf{A}(\mathbf{r}_i)]^2 + \frac{1}{2}\sum_{i \neq j}\frac{e_i e_j}{r_{ij}} + \sum_{\mathbf{k}\lambda}\omega_{\mathbf{k}\lambda}a^\dagger_{\mathbf{k}\lambda}a_{\mathbf{k}\lambda} \qquad (1.85)$$

With the vector potential is given by expansion

$$\frac{1}{c}A_\mu = \frac{1}{\sqrt{v}}\sum_{\mathbf{k}\lambda}e^{i\mathbf{k}\cdot\mathbf{r}}A_\mu(\mathbf{k}, \lambda, t) \qquad (1.86)$$

$$A_\mu(\mathbf{k}, \lambda, t) = (\frac{2\pi}{\omega_{\mathbf{k}}})^{\frac{1}{2}}\xi_\mu(\mathbf{k}, \lambda)(a_{\mathbf{k}\lambda}e^{-i\omega_{\mathbf{k}}t} + a^\dagger_{-\mathbf{k}\lambda}e^{i\omega_{\mathbf{k}}t}) \qquad (1.87)$$

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

potential represents the photon field. Two charges may interact via their common photon field or more directly through the instantaneous Coulomb interaction. **The division of the interaction between photons and Coulomb field is arbitrary— both interactions come from the same basic process.** The Hamiltonian (1.85) 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,

$$v_q = \frac{4\pi e^2}{q^2} \tag{1.88}$$

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

$$v_q(\omega) = \frac{v_q}{1 - v_q P(\mathbf{q}, \omega)} \tag{1.89}$$

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

$$\begin{aligned}
\nabla \cdot \mathbf{B} &= 0 \\
\nabla \times \mathbf{E} &= 0 \\
\nabla \cdot \mathbf{E} &= \frac{4\pi\rho}{\epsilon} \\
\nabla \times \mathbf{B} &= \frac{\epsilon}{c}\partial_t \mathbf{E} + \frac{4\pi}{c}\mathbf{j}
\end{aligned} \tag{1.90}$$

For the scalar and vector potentials

$$\begin{aligned}
\psi(\mathbf{r}) &= \frac{1}{\epsilon}\int \frac{d^3\mathbf{r}'\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \\
\nabla^2\mathbf{A} - \frac{\epsilon}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{A} &= -\frac{4\pi}{c}\mathbf{j}_t
\end{aligned} \tag{1.91}$$

Here the Coulomb Green's function is

$$\bar{v}_q = \frac{v_q}{\epsilon} \tag{1.92}$$

Regarding (1.89), it gives a formula for the dielectric function

$$\epsilon(\mathbf{q}, \omega) = 1 - v_q P(\mathbf{q}, \omega) \tag{1.93}$$

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

$$D_{\mu\nu}(\mathbf{k}, t - t') = -i\sum_\lambda \langle TA_\mu(\mathbf{k}, \lambda, t)A_\nu(-\mathbf{k}, \lambda, t')\rangle \tag{1.94}$$

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

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

where μ, ν are the x, y, z components, with vector potential in (1.87); the sum λ is the sum over the two transverse polarizations of the light, while ξ_μ are the polarization vectors for each component. At zero temperature,

$$D^0_{\mu\nu}(\mathbf{k}, t - t') = -\frac{2\pi i}{\omega_\mathbf{k}} e^{i\omega_\mathbf{k}|t-t'|} \sum_\lambda \xi_\mu \xi_\nu \qquad (1.95)$$

and with Fourier transform is

$$D^0(\mathbf{k}, \omega) = \frac{4\pi}{\omega^2 - \omega_\mathbf{k}^2 + i\delta} \sum_\lambda \xi_\mu \xi_\nu = \frac{4\pi[\delta_{\mu\nu} - (k_\mu k_\nu / k^2)]}{\omega^2 - \omega_\mathbf{k}^2 + i\delta} \qquad (1.96)$$

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.

$$D_{\mu\nu} = D^0_{\mu\nu} + \sum_{\lambda\delta} D^0_{\mu\lambda} \pi_{\lambda\delta} D_{\delta\nu} \qquad (1.97)$$

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

2

Nonzero Temperatures

2.1 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

$$\frac{\text{Tr}\left[e^{-\beta H}C_{\mathbf{p}\sigma}(t)C_{\mathbf{p}\sigma}^{\dagger}(t')\right]}{Tr(e^{-\beta H})} \tag{2.1}$$

$$C_{\mathbf{p}\sigma}(t) = e^{itH}C_{\mathbf{p}\sigma}e^{-itH} \tag{2.2}$$

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

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

The expansion of the series for bosons and fermions give

$$\eta_F(\xi_{\mathbf{p}}) = \frac{1}{e^{\beta\xi_{\mathbf{p}}} + 1} = \frac{1}{2} + \frac{1}{\beta}\sum_{n=-\infty}^{\infty}\frac{1}{(2n+1)i\pi/\beta - \xi_{\mathbf{p}}} \tag{2.3}$$

$$\eta_B(\omega_{\mathbf{q}}) = \frac{1}{e^{\beta\omega_{\mathbf{q}}} - 1} = -\frac{1}{2} + \frac{1}{\beta}\sum_{n=-\infty}^{\infty}\frac{1}{2ni\pi/\beta - \omega_{\mathbf{q}}} \tag{2.4}$$

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

$$p_n = (2n+1)\pi/\beta, \quad \omega_n = 2n\pi/\beta \tag{2.5}$$

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

Important knowledge, the expansion

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

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

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

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

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

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

with domain

$$-\beta \leq \tau \leq \beta \tag{2.6}$$

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

$$f(\tau) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty}\left[a_n \cos\left(\frac{n\pi\tau}{\beta}\right) + b_n \sin\left(\frac{n\pi\tau}{\beta}\right)\right] \tag{2.7}$$

where

$$a_n = \frac{1}{\beta}\int_{-\beta}^{\beta}d\tau f(\tau)\cos\left(\frac{n\pi\tau}{\beta}\right) \tag{2.8}$$

$$b_n = \frac{1}{\beta}\int_{-\beta}^{\beta}d\tau f(\tau)\sin\left(\frac{n\pi\tau}{\beta}\right) \tag{2.9}$$

or **equivently**. we have

$$f(i\omega_n) = \frac{1}{2}\beta(a_n + ib_n) \tag{2.10}$$

with

$$f(\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty}e^{-in\pi\tau/\beta}f(i\omega_n) \tag{2.11}$$

$$f(i\omega_n) = \frac{1}{2}\int_{-\beta}^{\beta}d\tau f(\tau)e^{in\pi\tau/\beta} \tag{2.12}$$

2.1.1   Boson

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

$$\text{boson}: f(\tau) = f(\tau+\beta), \quad -\beta < \tau < 0 \tag{2.13}$$

Further we have

$$f(i\omega_n) = \int_{0}^{\beta}d\tau e^{i\omega_n\tau}f(\tau)$$
$$f(\tau) = \frac{1}{\beta}\sum_{n}e^{-i\omega_n\tau}f(i\omega_n) \tag{2.14}$$
$$\omega_n = 2n\pi k_B T$$

2.1.2   Fermion

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

$$\text{fermions}: f(\tau) = -f(\tau+\beta), \quad -\beta < \tau < 0 \tag{2.15}$$

and the result give

$$f(i\omega_n) = \int_{0}^{\beta}d\tau e^{i\omega_n\tau}f(\tau)$$
$$f(\tau) = \frac{1}{\beta}\sum_{n}e^{-i\omega_n\tau}f(i\omega_n)3.23) \tag{2.16}$$
$$\omega_n = (2n+1)\pi k_B T$$

2.2 Matsubara Green's functions

The electron Green's function is defined as

$$
\begin{aligned}
\mathcal{G}(\mathbf{p}, \tau - \tau') &= -\langle T_\tau C_{\mathbf{p}\sigma}(\tau) C_{\mathbf{p}\sigma}^\dagger(\tau') \rangle && (2.17) \\
\mathcal{G}(\mathbf{p}, \tau - \tau') &= -\operatorname{Tr} \left[e^{-\beta(H - \mu N - \Omega)} T_\tau e^{\tau(H - \mu N)} C_{\mathbf{p}\sigma} e^{-(\tau - \tau')(H - \mu N)} \right. \\
&\quad \times \left. C_{\mathbf{p}\sigma}^\dagger e^{-\tau'(H - \mu N)} \right] && (2.18) \\
e^{-\beta\Omega} &= \operatorname{Tr}\left(e^{-\beta(H - \mu N)} \right) && (2.19)
\end{aligned}
$$

The definition is equivalent between (2.17) and (2.18), and it is the thermodynamic average, which is the trace over the complete set of states. The μ is the chemical potential and N is the particle number operator. A grand canonical ensemble is used, where the number of particles is variable. This many-particle system can be successfully used for one particle in an empty band. In this case, the analytical continuation si 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

$$
\begin{aligned}
\mathcal{G}(\mathbf{p}, \tau) &= -\langle T_\tau C_{\mathbf{p}\sigma}(\tau) C_{\mathbf{p}\sigma}^\dagger(0) \rangle && (2.20) \\
&= -\operatorname{Tr}\left[e^{-\beta(K - \Omega)} T_\tau (e^{\tau K} C_{\mathbf{p}\sigma} e^{-\tau K} C_{\mathbf{p}\sigma}^\dagger) \right] && (2.21) \\
\mathcal{G}(\mathbf{p}, i\omega_n) &= \int_0^\beta d\tau\, e^{i\omega_n \tau} \mathcal{G}(\mathbf{p}, \tau) && (2.22) \\
\mathcal{G}(\mathbf{p}, \tau) &= \frac{1}{\beta} \sum_n e^{-i\omega_n \tau} \mathcal{G}(\mathbf{p}, i\omega_n) && (2.23)
\end{aligned}
$$

For noninteracting Green's function, the τ evolution of the operators is[3]

$$
\begin{aligned}
C_{\mathbf{p}\sigma}(\tau) &= e^{\tau K_0} C_{\mathbf{p}\sigma} e^{-\tau K_0} = e^{-\xi_{\mathbf{p}}\tau} C_{\mathbf{p}\sigma} && (2.24) \\
C_{\mathbf{p}\sigma}^\dagger(\tau) &= e^{\tau K_0} C_{\mathbf{p}\sigma}^\dagger e^{-\tau K_0} = e^{\xi_{\mathbf{p}}\tau} C_{\mathbf{p}\sigma}^\dagger && (2.25)
\end{aligned}
$$

Then the Green's function is

$$
\mathcal{G}^0(\mathbf{p}, \tau) = -e^{-\xi_{\mathbf{p}}\tau}[\Theta(\tau) - \eta_F(\xi_{\mathbf{p}})] \tag{2.26}
$$

and

$$
\mathcal{G}^0(\mathbf{p}, i\omega_n) = \frac{1}{i\omega_n - \xi_{\mathbf{p}}} \tag{2.27}
$$

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

$$
\begin{aligned}
\mathcal{D}(\mathbf{q}, \tau - \tau') &= -\langle T_\tau \mathbf{A}(\mathbf{q}, \tau) \mathbf{A}(-\mathbf{q}, \tau') \rangle && (2.28) \\
\mathbf{A}(\mathbf{q}, \tau) &= e^{\tau H}(a_{\mathbf{q}} + a_{-\mathbf{q}}^\dagger) e^{-\tau H} && (2.29)
\end{aligned}
$$

and with the relation in (2.13), we have

$$\mathcal{D}(\mathbf{q}, \tau) = \mathcal{D}(\mathbf{q}, \tau + \beta) \quad -\beta < \tau < 0 \tag{2.30}$$

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

$$\mathcal{D}^0(\mathbf{q}, i\omega_n) = -\frac{2\omega_{\mathbf{q}}}{\omega_n^2 + \omega_{\mathbf{q}}} \tag{2.31}$$

Notice that it is almost identical to the zero-temperature case (1.45).

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

$$\mathcal{D}_{\mu\nu}(\mathbf{k}, \tau) = -\sum_{\lambda}\langle T_{\tau}\mathbf{A}_{\mu}(\mathbf{k}, \lambda, \tau)\mathbf{A}_{\nu}(-\mathbf{k}, \lambda, 0)\rangle \tag{2.32}$$

$$\mathbf{A}_{\mu}(\mathbf{k}, \lambda, 0) = \xi_{\mu}(\mathbf{k}, \lambda)(\frac{2\pi}{\omega_{\mathbf{k}}})(a_{\mathbf{k}\lambda} + a_{\mathbf{k}\lambda}^{\dagger}) \tag{2.33}$$

$$\mathcal{D}_{\mu\nu}^0(\mathbf{k}, i\omega_n) = -\frac{4\pi(\delta_{\mu\nu} - k_{\mu}k_{\nu}/k^2)}{\omega_n^2 + \omega_{\mathbf{k}}^2} \tag{2.34}$$

2.3   Retarded and advance Green's functions

The retarded and advanced Green's functions were introduced in 1.9. 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

$$\begin{aligned}
G_{ret}(\mathbf{p}, t - t') &= G_t(\mathbf{p}, t - t') - G^{<}(\mathbf{p}, t - t') \tag{2.35}\\
&= -i\Theta(t - t')\langle[C_{\mathbf{p}\sigma}(t)C_{\mathbf{p}\sigma}^{\dagger}(t') + C_{\mathbf{p}\sigma}^{\dagger}(t')C_{\mathbf{p}\sigma}(t)]\rangle\\
&= -i\Theta(t - t')\,\mathrm{Tr}\{e^{-\beta(K-\Omega)}[C_{\mathbf{p}\sigma}(t)C_{\mathbf{p}\sigma}^{\dagger}(t') + C_{\mathbf{p}\sigma}^{\dagger}(t')C_{\mathbf{p}\sigma}(t)]\}\\
K &= H - \mu N, \quad C_{\mathbf{p}\sigma}(t) = e^{iKt}C_{\mathbf{p}\sigma}e^{-iKt} \tag{2.36}
\end{aligned}$$

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

$$D_{ret}(\mathbf{q}, t - t') = -i\Theta(t - t')\langle A(\mathbf{q}, t)A(-\mathbf{q}, t') - A(-\mathbf{q}, t')A(\mathbf{q}, t)\rangle \tag{2.37}$$

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.

$$U = \sum_{ij} M_{ij} C_i^\dagger C_j \qquad (2.38)$$

$$V = \sum_{ijk} M_{ijk} C_i^\dagger C_j C_k \qquad (2.39)$$

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

$$\bar{U}_{ret}(t - t') = -i\Theta(t - t')\langle[U(t)U^\dagger(t') - U^\dagger(t')U(t)]\rangle \quad (2.40)$$
$$\bar{V}_{ret}(t - t') = -i\Theta(t - t')\langle[V(t)V^\dagger(t') + V^\dagger(t')V(t)]\rangle \quad (2.41)$$

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

$$G_{ret}(\mathbf{p}, E) = \int_{-\infty}^{\infty} dt\, e^{iE(t-t')} G_{ret}(\mathbf{p}, t - t') \qquad (2.42)$$

THe advanced Green's function for each is defined

$$G_{adv}(\mathbf{p}, t - t') = i\Theta(t - t')\langle[C_{\mathbf{p}\sigma}(t)C_{\mathbf{p}\sigma}^\dagger(t')$$
$$+ C_{\mathbf{p}\sigma}^\dagger(t')C_{\mathbf{p}\sigma}(t)]\rangle \qquad (2.43)$$
$$D_{adv}(\mathbf{q}, t - t') = i\Theta(t - t')\langle A(\mathbf{q}, t)A(-\mathbf{q}, t')$$
$$- A(-\mathbf{q}, t')A(\mathbf{q}, t)\rangle \qquad (2.44)$$

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.

$$U_{ret}(\omega) = U_{adv}^\dagger(\omega) \qquad (2.45)$$

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

$$i\omega_n \to \omega + i\delta \quad \mathcal{U}(i\omega_n) = U_{ret}(\omega) \qquad (2.46)$$

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:

$$A(\mathbf{p}, \omega) = -2\,\mathrm{Im}[G_{ret}(\mathbf{p}, \omega)] \qquad (2.47)$$

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

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

$$\mathcal{U}(i\omega_n) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\omega')}{i\omega_n - \omega'} \qquad (2.48)$$

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.

$$1 = \int \frac{d\omega}{2\pi} A(\mathbf{p}, \omega) \qquad (2.49)$$

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

$$G_{ret}^0(\mathbf{p}, E) = \frac{1}{E - \xi_{\mathbf{p}} + i\delta} \qquad (2.50)$$

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]

$$A^0(\mathbf{p}, E) = 2\pi\delta(E - \xi_{\mathbf{p}}) \qquad (2.51)$$

[4] $\dfrac{1}{E - \xi_{\mathbf{p}} + i\delta} = \dfrac{1}{E - \xi_{\mathbf{p}}} - 2\pi i\delta(E - \xi_{\mathbf{p}})$

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

$$n_{\mathbf{p}} = \int \frac{dE}{2\pi} \eta_F(E) A(\mathbf{p}, E) \qquad (2.52)$$

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

$$2N_{\mathbf{q}} + 1 = \langle A_{\mathbf{q}}^\dagger A_{\mathbf{q}} \rangle = \int \frac{d\omega}{2\pi} \eta_B(\omega) A(\mathbf{q}, \omega) \qquad (2.53)$$

The noninteracting phonon spectral function is

$$A^0(\mathbf{q}, \omega) = 2\pi[\delta(\omega - \omega_{\mathbf{q}}) - \delta(\omega + \omega_{\mathbf{q}})] \qquad (2.54)$$

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

$$\mathcal{G}(\mathbf{p}, ip_n) = \frac{1}{ip_n - \xi_{\mathbf{p}} - \Sigma(\mathbf{p}, ip_n)} \tag{2.55}$$

$$\mathcal{D}(\mathbf{q}, i\omega_n) = \frac{-2\omega_{\mathbf{q}}}{\omega_n^2 + \omega_{\mathbf{q}}^2 + 2\omega_{\mathbf{q}} P(\mathbf{q}, i\omega_n)} \tag{2.56}$$

Define the retarded self-energies according to (2.46)

$$ip_n \to E + i\delta \quad \Sigma(\mathbf{p}, ip_n) \to \Sigma_{ret}(\mathbf{p}, E) = \operatorname{Re}\Sigma_{ret} + i\operatorname{Im}\Sigma_{ret} \tag{2.57}$$

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

$$G_{ret}(\mathbf{p}, E) = \frac{1}{E + i\delta - \xi_{\mathbf{p}} - \Sigma_{ret}(\mathbf{p}, E)} \tag{2.58}$$

as derived from (2.46). The spectral function for the electron is rewritten in terms of the retarded self-energy,

$$A(\mathbf{p}, E) = \frac{-2\operatorname{Im}\Sigma_{ret}(\mathbf{p}, E)}{[E - \xi_{\mathbf{p}} - \operatorname{Re}\Sigma_{ret}(\mathbf{p}, E)]^2 + [\operatorname{Im}\Sigma_{ret}(\mathbf{p}, E)]^2} \tag{2.59}$$

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,

$$\Sigma(\mathbf{p}, Z) = C \ln[f(\mathbf{p}) - Z] \tag{2.60}$$

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

$$\Sigma(\mathbf{p}, ip_n) = C \ln[f(\mathbf{p}) - ip_n] \tag{2.61}$$

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

$$\Sigma_{ret}(\mathbf{p}, E) = C \ln|f(\mathbf{p}) - E| - i\pi C\Theta[E - f(\mathbf{p})] \tag{2.62}$$

and for advanced

$$\Sigma_{adv(\mathbf{p},E)} = C \ln|f(\mathbf{p}) - E| + i\pi C\Theta[E - f(\mathbf{p})] \tag{2.63}$$

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

$$G^*_{ret}(\mathbf{p}, E) = G_{adv}(\mathbf{p}, E) \tag{2.64}$$

[5] To get this relation

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

and also implies that

$$\Sigma_{ret}^*(\mathbf{p}, E) = \Sigma_{adv}(\mathbf{p}, E) \tag{2.65}$$

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

$$\Sigma(\mathbf{p}, Z) = C[f(\mathbf{p}) - Z]^{\frac{1}{2}} \tag{2.66}$$

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

$$\Sigma(\mathbf{p}, E + i\delta) \neq \Sigma(\mathbf{p}, E - i\delta) \tag{2.67}$$

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 $\operatorname{Im}\Sigma \neq 0$, then the spectral function is given by (2.59). In other regions where there is no branch cut, then take the limit of $\operatorname{Im} \to 0$ and obtain

$$\lim_{\operatorname{Im}\Sigma=0} A(\mathbf{p}, E) = 2\pi\delta(E - \xi_\mathbf{p} - \operatorname{Re}\Sigma_{ret}(\mathbf{p}, E)) \tag{2.68}$$

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

$$E(\mathbf{p}) - \mu = \xi_\mathbf{p} + \operatorname{Re}\Sigma(\mathbf{p}, E(\mathbf{p}) - \mu) \tag{2.69}$$

Assume that there is a problem in which (2.69) is satisfied when $\operatorname{Im}\Sigma = 0$. Then with the properties of delta function, the spectral function is written as

$$A(\mathbf{p}, E) = 2\pi Z(\mathbf{p})\delta(E - E(\mathbf{p}) + \mu) \tag{2.70}$$

$$Z(\mathbf{p}) = \frac{1}{\left|1 - \frac{\partial}{\partial E}\Sigma_{ret}(\mathbf{p}, E)\right|_{E=E(\mathbf{p})-\mu}} \tag{2.71}$$

The factor $Z(\mathbf{p})$ is called **renormalization factor**. Because of (2.49) 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 (2.69) may be used to define the effective mass. Assume that the noninteracting states are free particles

$$\xi_\mathbf{p} = \frac{p^2}{2m} - \mu = \varepsilon_\mathbf{p} - \mu \tag{2.72}$$

Furthermore, assume at low momentum that $E(\mathbf{p})$ in (2.69) varies quadratically wit momentum,

$$E(\mathbf{p}) = E_0 + \frac{p^2}{2m^*} + \mathcal{O}(p^4) \tag{2.73}$$

The proportionality constant is the inverse effective mass m^*

$$\frac{m}{m^*} = \frac{\partial E(\mathbf{p})}{\partial \varepsilon_{\mathbf{p}}} \tag{2.74}$$

from the definition of (2.69), we get

$$\frac{\partial E(\mathbf{p})}{\partial \varepsilon_{\mathbf{p}}} = \lim_{\varepsilon_{\mathbf{p}} \to 0} \left(1 + \frac{\partial}{\partial \varepsilon_{\mathbf{p}}} \operatorname{Re} \Sigma_{ret}(\mathbf{p}, E) + \left[\frac{\partial}{\partial E} \operatorname{Re} \Sigma_{ret}(\mathbf{p}, E) \right] \frac{\partial E(\mathbf{p})}{\partial \varepsilon_{\mathbf{p}}} \right) \tag{2.75}$$

With (2.74), the final term is arrived

$$\frac{m}{m^*} = \lim_{\varepsilon_{\mathbf{p}} \to 0} \left[\frac{1 + (\partial_{\varepsilon_{\mathbf{p}}}) \operatorname{Re} \Sigma_{ret}(\mathbf{p}, E_0 - \mu)}{1 - (\partial_{E_0}) \operatorname{Re} \Sigma_{ret}(\mathbf{p}, E_0 - \mu)} \right] \tag{2.76}$$

2.4   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.

$$-\frac{1}{\beta} \sum_m \mathcal{D}^0(\mathbf{q}, i\omega_m) \mathcal{G}^0(\mathbf{p}, ip_n + i\omega_m) = \frac{N_{\mathbf{q}} + \eta_F(\xi_{\mathbf{p}})}{ip_n - \xi_{\mathbf{p}} + \omega_{\mathbf{q}}}$$
$$+ \frac{N_{\mathbf{q}} + 1 - \eta_F(\xi_{\mathbf{p}})}{ip_n - \xi_{\mathbf{p}} - \omega_{\mathbf{q}}} \tag{2.77}$$

$$\frac{1}{\beta} \sum_n \mathcal{G}^0(\mathbf{p}, ip_n) \mathcal{G}^0(\mathbf{k}, ip_n + i\omega_m) = \frac{\eta_F(\xi_{\mathbf{p}}) - \eta_F(\xi_{\mathbf{k}})}{i\omega_m + \xi_{\mathbf{p}} - \xi_{\mathbf{k}}} \tag{2.78}$$

$$-\frac{1}{\beta} \sum_n \mathcal{G}^0(\mathbf{p}, ip_n) \mathcal{G}^0(\mathbf{k}, i\omega_m - ip_n) = \frac{1 - \eta_F(\xi_{\mathbf{p}}) - \eta_F(\xi_{\mathbf{k}})}{i\omega_m - \xi_{\mathbf{p}} - \xi_{\mathbf{k}}} \tag{2.79}$$

$$\frac{1}{\beta} \sum_n \mathcal{G}^0(\mathbf{p}, ip_n) = \eta_F(\xi_{\mathbf{p}}) \tag{2.80}$$

First consider the summation over a boson series, considering (2.77),

$$S = \frac{1}{\beta} \sum_m \frac{2\omega_{\mathbf{q}}}{\omega_m^2 + \omega_{\mathbf{q}}^2} \frac{1}{ip_n + i\omega_m - \xi_{\mathbf{p}}} \tag{2.81}$$

Denote this equation as

$$S = -\frac{1}{\beta} \sum_m f(i\omega_m) \tag{2.82}$$

where $f(i\omega_m)$ is the product of Green's function in (2.81). This summation si evaluated by a contour integration. The integral has the form,

$$I = \lim_{R\to\infty} \oint \frac{dz}{2\pi i} f(z)\eta_B(z) \qquad (2.83)$$

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

3
Appendix: Complex analysis

3.1 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.

3.1.1 Definition

The residue of a meromorphic function f at an isolated singularity a, denoted as $\text{Res}(f, a)$, is the unique value R such 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.

3.1.2 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 $dz \rightarrow d(e^{i\theta}) = ie^{i\theta} d\theta$. The result is

$$\oint_C z^k dz = \int_0^{2\pi} ie^{i(k+1)\theta} d\theta = \begin{cases} 2\pi i & (k = -1) \\ 0 & (\text{otherwise}) \end{cases}$$

Example.2 Consider the contour integral, where C is some simple

closed curve about 0.

$$\oint_C \frac{e^z}{z^5} dz$$
$$= \oint_C \frac{1}{z^5}(1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \dots)dz$$
$$= \oint_C \frac{1}{4!z} dz \frac{\pi i}{12}$$

The last formula is based on the previous result.

3.1.3   Calculating residues

For residue theorem,

$$\text{Res}(f, c) = \frac{1}{2\pi i} \oint_\gamma f(z)dz$$

where γ traces out a circle around c in a counterclockwise manner.

Removeable singularities

If function f can be continued to a holomorphic function on the whole disk, then $\text{Res}(f, c) = 0$. The converse is not generally true.

Simple poles

At a simple pole c, the residue of f is given by

$$\text{Res}(f, c) = \lim_{z \to c}(z - c)f(z)$$

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 $z = 1$,

$$\sin z = \sin 1 + \cos 1(z-1) + \frac{-\sin 1}{2!}(z-1)^2 + \dots$$

$$\frac{1}{z} = \frac{1}{(z-1)+1} = 1 - (z-1) + (z-1)^2 - (z-1)^3 + \dots$$

Multiplying those two series and introducing $1/(z-1)$ gives

$$\frac{\sin z}{z(z-1)} = \frac{\sin 1}{z-1} + (\cos 1 - \sin 1) + (z-1)\left(-\frac{\sin 1}{2!} - \cos 1 + \sin 1\right) + \dots$$

So the residue of $f(z)$ at $z = 1$ is $\sin 1$.

3.2 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,

$$\frac{1}{\omega + E_n - E_m + i\delta} = \mathcal{P}\frac{1}{\omega + E_n - E_m} - i\pi\delta(\omega + E_n - E_m)$$

3.3 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 ω, where χ_1 and χ_2 are real. Suppose this function is analytic in the upper half-plane of ω and vanishes like $1/|\omega|$ or faster as $|\omega| \to \infty$. 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

$$\chi_1(\omega) = \frac{2}{\pi}\mathcal{P}\int_{0}^{\infty}\frac{\omega'\chi_1(\omega')}{\omega'^2-\omega^2}d\omega'$$

$$\chi_2(\omega) = -=\frac{2\omega}{\pi}\mathcal{P}\int_{0}^{\infty}\frac{\chi_1(\omega')}{\omega'^2-\omega^2}d\omega'$$

4
Bibliography

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