Introduction to Green functions and many-body perturbation theory

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1 Motivation

The Green function methods for quantum many-body systems were mainly developed in the 1950's and early 60's. Before plunging into the formalism we briefly summarize some main motivations behind this development.

1.1 Connection to experiments

Here we will be very sketchy. Consider an experiment in which one exposes the system to some disturbance (whose strength is controlled by some external applied field $f(\boldsymbol{r}, t)$) and measures the response of the system. When the applied field is weak one expects the response to depend linearly on the applied field. This is called linear response. The "proportionality factor" is the associated response function. The basic equations can be shown to be (here we suppress all variables except the time variables)

$$\begin{aligned} H_{\text{tot}} &= H - f(t)O, && (1)\\ \langle O(t)\rangle &= \langle O\rangle + \int_{-\infty}^{\infty} \chi(t-t')f(t')dt', && (2)\\ \chi(t-t') &= -i\langle [O(t), O(t')]\rangle \theta(t-t'). && (3) \end{aligned}$$

Here H (H_{tot}) is the Hamiltonian of the system in the absence (presence) of the applied field $f(t)$, $\langle O(t)\rangle$ is the response (in terms of the operator O) of the system to the field, with $\langle O\rangle$ being the expectation value of O in the absence of the applied field (which often vanishes). The function $\chi(t)$ is a retarded response function (retarded means that it's only nonzero for $t > t'$, i.e. cause comes before effect). Other names sometimes used for such a quantity is susceptibility, correlation function or Green function. (As we will see there are many other, related quantities that are also called Green functions). Note that the expectation value in (3) is with respect to the undisturbed system, i.e. in the absence of the applied field.

For example the electrical conductivity $\sigma(\boldsymbol{q}, \omega)$ is related to a response function where the O's are given by the current operators, i.e. a retarded current-current correlation function. (Here the variables $\boldsymbol{q}$ and ω arise from taking Fourier transforms in space and time.) If time allows we will study the conductivity $\sigma(\boldsymbol{q}, \omega)$ in more detail later (see Secs. 4.9 and 4.10).

Retarded Green functions and functions related to these are thus central objects to calculate in many-body theory for comparing with experiments.

1.2 Divergences in the standard perturbation theory

One of the important early problems was to find the ground state energy of a gas of electrons interacting via the long-ranged Coulomb interaction in 3 dimensions. (To ensure charge neutrality this gas was embedded in a positive and uniform background charge.) Consider the kinetic energy and potential energy of this electron gas as a function of r_0, the average distance between two electrons (in 3D $r_0 \propto n^{-1/3}$ where n is the electron density). One can show that the kinetic energy per electron goes like $1/r_0^2$. and that the typical Coulomb interaction energy per electron goes like $1/r_0$. Thus for small r_0, i.e. a high-density gas, the kinetic energy dominates over the interaction energy, and one might hope that it is possible to treat the Coulomb interaction as a *perturbation* to the kinetic energy.[1] Thus in this limit one might hope that the ground state energy can be expressed in terms of a power series in the small dimensionless parameter $r_s = r_0/a_B$ (a_B is the Bohr radius) like

$$E_0 = \frac{K}{r_s^2}[1 + br_s + cr_s^2 + \ldots] \qquad \text{(anticipated, but turns out to be not quite right)} \qquad (4)$$

where K, a, b, c, etc. are constants. Indeed, 1st order perturbation theory gives a term of the form br_s in this series. But if one goes one step further and considers 2nd order perturbation theory, one finds a contribution which diverges like $\int_0 dq/q$, where q is the momentum transfer in the Fourier transform v_q of the Coulomb interaction ($v_q \propto 1/q^2$). That is, there is a logarithmic divergence from the lower limit 0 of the momentum transfers. This divergence is associated with the long range of the Coulomb interaction. Furthermore, if one examines higher order terms in the perturbation series one finds that they diverge even more strongly. Thus standard perturbation theory appears to be worthless.

On physical grounds, however, one does of course expect the energy of the interacting electron gas to be a finite and well-defined number, and no phase transitions occur as one "turns on" the repulsive interactions, so this failure of standard perturbation theory appears just to be a signal that the energy does not have a standard power series expansion in r_s. In 1957 Gell-Mann and Bruckner resolved this issue by using the recently developed many-body perturbation theory. Essentially what they did was to sum all the most divergent terms in the series (an infinite number of them) *before* doing the momentum integrals, and showed that one could then arrive at a result which was well-defined and finite (this is called a resummation of the perturbation series). They found that there was a term in the series for E_0 which is $\propto \ln r_s$, and thus indeed is not analytic at $r_s = 0$.

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[1] This assumes at the very least that the interaction doesn't cause any drastic changes to the system, such as a phase transition.

The solution of this problem thus requires one to include an infinite number of terms in the perturbation theory. Clearly one needs to develop a new method to be able to do this in an efficient way, and this is one of the main strengths of many-body perturbation theory. We will also see other examples where one needs to include an infinite number of terms in the perturbation theory.

2 The single-particle retarded Green function and its spectral function

Most response functions, e.g. the conductivity, involve retarded *two*-particle Green functions, in which the operator O in (3) involves the product of *two* creation/annihilation operators. However, we will start by discussing single-particle Green functions, as they are the simplest ones. Essentially, single-particle Green functions involve operators O which are a single creation or annihilation operator. In the fermionic case, the commutator in (3) is then replaced by an anticommutator in the definition of the retarded single-particle Green function.

2.1 Retarded, advanced, "greater", and "lesser" single-particle Green functions

The **retarded** single-particle Green function is defined as

$$G^R(x,t;x',t') \equiv -i\theta(t-t')\langle[\psi(x,t),\psi^\dagger(x',t')]_\pm\rangle. \tag{5}$$

The upper sign is for fermions, when $[A,B]_+ \equiv \{A,B\}$ is the anticommutator. The lower sign is for bosons, when $[A,B]_- \equiv [A,B]$ is the ordinary commutator. Furthermore, $x \equiv (\boldsymbol{r},\sigma)$, so that $\psi^\dagger(x) \equiv \psi^\dagger_\sigma(\boldsymbol{r})$ creates a particle at position $\boldsymbol{r}$ with spin projection σ (if the particle has a spin degree of freedom). We also define an **advanced** Green function as

$$G^A(x,t;x',t') \equiv +i\theta(t'-t)\langle[\psi(x,t),\psi^\dagger(x',t')]_\pm\rangle. \tag{6}$$

Note that the retarded function is nonzero only for $t > t'$ and the advanced function is nonzero only for $t < t'$. It is also convenient at this point to define two other types of Green functions, referred to as "G-greater" and "G-lesser":

$$\begin{aligned} G^>(x,t;x',t') &\equiv -i\langle\psi(x,t)\psi^\dagger(x',t')\rangle, && (7)\\ G^<(x,t;x',t') &\equiv -i(\mp)\langle\psi^\dagger(x',t')\psi(x,t)\rangle. && (8) \end{aligned}$$

In $G^<$ the upper sign is again for fermions and the lower for bosons. The retarded and advanced Green functions can then be expressed as

$$\begin{aligned} G^R(x,t;x',t') &= \theta(t-t')[G^>(x,t;x',t') - G^<(x,t;x',t')], && (9)\\ G^A(x,t;x',t') &= \theta(t'-t)[G^<(x,t;x',t') - G^>(x,t;x',t')]. && (10) \end{aligned}$$

2.2 The meaning of $\langle \cdots \rangle$ and the time dependence

We will consider a system with a macroscopic number of particles which is in thermodynamic equilibrium at some temperature T (which may be zero or nonzero). The average $\langle \cdots \rangle$ represents a thermal + quantum average in such a system. In general, there are two kinds of ensembles which may describe such systems: the canonical ensemble and the grand canonical ensemble. Let us summarize these in turn, starting with the simpler one, the canonical ensemble.

In the **canonical ensemble** the number of particles N in the system is fixed, and the system can exchange energy with a reservoir. The average energy of the system is determined by the temperature T. The quantum statistical-mechanical average of an arbitrary operator A is in this ensemble given by

$$\langle A\rangle = \frac{1}{Z}\sum_n \langle n|A|n\rangle e^{-\beta E_n} \tag{11}$$

Here $|n\rangle$ refer to the set of (normalized) eigenstates of the Hamiltonian H with eigenvalues E_n, $\beta = 1/k_B T$, and $Z = \sum_n e^{-\beta E_n}$ is the partition function. We can write the expectation value in a basis-independent way by defining the density matrix (calling it a matrix is misleading, but that is the standard name; it really is an operator)

$$\rho = \frac{1}{Z}e^{-\beta H} \tag{12}$$

and

$$Z = \text{Tr } e^{-\beta H}. \tag{13}$$

(Clearly $\text{Tr } \rho = 1$ as required for a density matrix.) With this definition we can write

$$\langle A\rangle = \text{Tr}(\rho A). \tag{14}$$

In the **grand canonical ensemble** the system does not have a fixed particle number. Instead, the system can exchange particles (in addition to energy) with a reservoir. Thus we need to introduce another parameter (in addition to the temperature T), namely the chemical potential μ, which determines the average number of particles in the system. The density matrix for this ensemble is given by

$$\rho = \frac{1}{Z}e^{-\beta(H-\mu N)} \tag{15}$$

where the partition function is

$$Z = \text{Tr } e^{-\beta(H-\mu N)}. \tag{16}$$

Here N is a number operator which counts the total number of particles. With these definitions of ρ and Z we again have

$$\langle A\rangle = \text{Tr}(\rho A). \tag{17}$$

To actually evaluate this trace it is convenient to use the basis consisting of eigenstates of the operator $H - \mu N$. Note that the total number of particles in such an eigenstate is definite (when H conserves the total number of particles), but can take an arbitrary nonnegative value.

In the following we will use the grand canonical ensemble. In regard to this there are some important things that should be pointed out:

- In this ensemble the time dependence of operators is defined to be determined by the operator $H - \mu N$, not H. This corresponds to measuring all single-particle energies with respect to the chemical potential μ. Thus we define

  $$A(t) \equiv e^{i(H-\mu N)t} A e^{-i(H-\mu N)t}. \tag{18}$$

- However, to save writing we will still write this as $A(t) = e^{iHt} A e^{-iHt}$. That is, H here will be implicitly understood to represent the operator $H - \mu N$.

- Similarly, instead of writing $e^{-\beta(H-\mu N)}$ we will write $e^{-\beta H}$.

- Finally, the eigenstates of the operator $H - \mu N$ (which we write as H!) will be written as $|n\rangle$ and the eigenvalues will be written as E_n. Thus we write

  $$H|n\rangle = E_n|n\rangle. \tag{19}$$

  As already mentioned above, the number of particles in such a many-body eigenstate is definite but can take any integer value from 0 to ∞.

In summary, whenever we refer to "the Hamiltonian" and "H" in the following, we really mean $H - \mu N$. (This is also what is done in the texts by Coleman and by Bruus and Flensberg when using the grand canonical ensemble.)

2.3 Some other forms of the Green functions

The Green functions defined so far are called **space-time** Green functions, because they involve the creation and annihilation of particles at definite locations in space and time. We can also define analogous Green functions in other bases than the spatial one (more precisely, space-spin basis when the particles have spin). For example, it will in many problems, especially those which are translationally invariant in space, be convenient to study Green functions which involve creation/annihilation of particles in a definite momentum state characterized by a momentum $\boldsymbol{k}$. Depending on the problem at hand, other Green functions, involving creation/annihilation of particles in other types of single-particle states, may also be useful. (For example, if the particles move in some external potential $U(x)$ it may be convenient to define Green functions which create/annihilate particles in eigenstates of $p^2/2m + U(x)$). Finally, it is also interesting to Fourier transform the Green functions in the time-frequency domain (Sec. 2.3.4).

2.3.1 Transformations to other bases

To relate these alternative Green functions to the space-time Green functions already defined, we need to know how to transform between bases. Thus we give a short repetition/summary of how to do this. Consider a basis $|\nu\rangle$ (e.g. $|\nu\rangle = |\boldsymbol{k}, \sigma\rangle$). We may write

$$|x\rangle = \sum_\nu |\nu\rangle\langle\nu|x\rangle = \sum_\nu \langle x|\nu\rangle^* |\nu\rangle = \sum_\nu \phi_\nu^*(x)|\nu\rangle, \tag{20}$$

where $\phi_\nu(x) \equiv \langle x|\nu\rangle$ is the single-particle *wavefunction* in the state $|\nu\rangle$. Writing $|x\rangle = \psi^\dagger(x)|0\rangle$ and $|\nu\rangle = c_\nu^\dagger|0\rangle$ (where $|0\rangle$ is the "vacuum" state containing no particles at all) we then have the following relation between the creation operators in the x-basis and the ν-basis:

$$\psi^\dagger(x) = \sum_\nu \phi_\nu^*(x) c_\nu^\dagger. \tag{21}$$

Taking the hermitian conjugate of this gives the relation between the corresponding annihilation operators:

$$\psi(x) = \sum_\nu \phi_\nu(x) c_\nu. \tag{22}$$

The most relevant example is when $|\nu\rangle = |\boldsymbol{k}, \sigma\rangle$. Then

$$\psi^\dagger(x) = \psi_\sigma^\dagger(\boldsymbol{r}) = \sum_{\boldsymbol{k},\sigma'} \underbrace{\phi_{\boldsymbol{k},\sigma'}^*(\boldsymbol{r},\sigma)}_{\phi_{\boldsymbol{k}}(\boldsymbol{r})\delta_{\sigma,\sigma'}} c_{\boldsymbol{k},\sigma'}^\dagger = \sum_{\boldsymbol{k}} \phi_{\boldsymbol{k}}^*(r) c_{\boldsymbol{k}\sigma}^\dagger = \frac{1}{\sqrt{\Omega}} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} c_{\boldsymbol{k},\sigma}^\dagger \tag{23}$$

and thus also

$$\psi_\sigma(\boldsymbol{r}) = \sum_{\boldsymbol{k}} \phi_{\boldsymbol{k}}(\boldsymbol{r}) c_{\boldsymbol{k}\sigma} = \frac{1}{\sqrt{\Omega}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} c_{\boldsymbol{k},\sigma}. \tag{24}$$

Here, to arrive at the last expressions in (23) and (24) we have taken the particles to live in a system which is a 3D cube of volume Ω with periodic boundary conditions, so

$$\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{\Omega}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}. \tag{25}$$

2.3.2 Green functions in other bases

We will illustrate how Green functions in different bases are related by looking at the retarded single-particle Green function. We have

$$\begin{aligned} G^R(x,t;x't') &= -i\theta(t-t')\langle[\psi(x,t), \psi^\dagger(x',t')]_\pm\rangle \\ &= -i\theta(t-t') \sum_{\nu\nu'} \phi_\nu(x)\phi_{\nu'}^*(x')\langle[c_\nu(t), c_{\nu'}^\dagger(t')]_\pm\rangle \\ &= \sum_{\nu\nu'} \phi_\nu(x)\phi_{\nu'}^*(x') G^R(\nu,t;\nu',t'), \end{aligned} \tag{26}$$

where we have defined the single-particle retarded Green function in the ν-basis as

$$G^R(\nu,t;\nu',t') = -i\theta(t-t')\langle[c_\nu(t), c_{\nu'}^\dagger(t')]_\pm\rangle. \tag{27}$$

2.3.3 $\boldsymbol{k}$-space Green function in translationally invariant systems

In a system which is translationally invariant in space, the space-time Green functions can not depend on $\boldsymbol{r}$ and $\boldsymbol{r}'$ separately, but only on their difference $\boldsymbol{r}-\boldsymbol{r}'$. In these systems it is natural to consider the $\boldsymbol{k}$-space Green function $G(\boldsymbol{k},\sigma,t;\boldsymbol{k}'\sigma',t')$, as it becomes diagonal in the $\boldsymbol{k}$ indices. This can be seen from (26), (23) and (24). We have

$$\begin{aligned} G^R(x,t;x',t') &= G(\boldsymbol{r},\sigma,t;\boldsymbol{r}',\sigma',t') = \frac{1}{\Omega}\sum_{\boldsymbol{k},\boldsymbol{k}'} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} G^R(\boldsymbol{k},\sigma,t;\boldsymbol{k}',\sigma',t') \\ &= \frac{1}{\Omega}\sum_{\boldsymbol{k},\boldsymbol{k}'} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}'} G^R(\boldsymbol{k},\sigma,t;\boldsymbol{k}',\sigma',t'). \qquad (28) \end{aligned}$$

As the lhs only depends on $\boldsymbol{r}-\boldsymbol{r}'$, the dependence on $\boldsymbol{r}'$ on the rhs must vanish, which means that the $\boldsymbol{k}$-space Green function is nonzero only when $\boldsymbol{k}=\boldsymbol{k}'$, i.e. $G^R(\boldsymbol{k},\sigma,t;\boldsymbol{k}',\sigma',t') = \delta_{\boldsymbol{k},\boldsymbol{k}'}G^R(\boldsymbol{k};\sigma,t;\sigma',t')$. Thus we get

$$G^R(\boldsymbol{r}-\boldsymbol{r}',\sigma,t;\sigma',t') = \frac{1}{\Omega}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} G^R(\boldsymbol{k};\sigma,t;\sigma',t') \qquad (29)$$

where

$$G^R(\boldsymbol{k};\sigma,t;\sigma',t') = -i\theta(t-t')\langle[c_{\boldsymbol{k},\sigma}(t), c^\dagger_{\boldsymbol{k},\sigma'}(t')]_\pm\rangle. \qquad (30)$$

2.3.4 Fourier transformed Green functions (in the time-frequency domain)

If the Hamiltonian does not depend explicitly on time, i.e. the Hamiltonian is translationally invariant in time, the Green functions will not depend on t and t' separately, but only on the difference $t-t'$. It is then convenient to Fourier transform the Green function in the time variable. This Fourier transform and its inverse are defined as

$$G(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega t} G(\omega), \qquad (31)$$

$$G(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} G(t). \qquad (32)$$

(Here we have suppressed all other variables than the time/frequency variables in the notation.)

2.4 Example: Green function for noninteracting electrons

We will now calculate the $\boldsymbol{k}$-space Green functions for noninteracting electrons. In this case, the Hamiltonian is given by

$$H = \sum_{\boldsymbol{k},\sigma} \xi_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} \qquad (33)$$

where $\xi_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} - \mu$ and μ is the chemical potential. Because H is diagonal in $\boldsymbol{k}$ and σ (the former property is due to the system being translationally invariant in space, as there is no external potential in the Hamiltonian), the Green functions will also be diagonal in $\boldsymbol{k}$ and σ. Taking this into account we consider the retarded Green function

$$G_0^R(\boldsymbol{k}, \sigma; t - t') = -i\theta(t - t')\langle\{c_{\boldsymbol{k}\sigma}(t), c^\dagger_{\boldsymbol{k}\sigma}(t')\}\rangle. \tag{34}$$

The subscript 0 on the Green function refers to the noninteracting nature of the Hamiltonian.

To calculate the Green function we need to work out the time dependence of the fermion operators. Since

$$c_{\boldsymbol{k}\sigma}(t) = e^{iHt} c_{\boldsymbol{k}\sigma} e^{-iHt}, \tag{35}$$

we have

$$\frac{dc_{\boldsymbol{k}\sigma}(t)}{dt} = i[H, c_{\boldsymbol{k}\sigma}(t)] = ie^{iHt} \underbrace{[H, c_{\boldsymbol{k}\sigma}]}_{-\xi_{\boldsymbol{k}} c_{\boldsymbol{k}\sigma}} e^{-iHt} = -i\xi_{\boldsymbol{k}} c_{\boldsymbol{k}\sigma}(t). \tag{36}$$

Integrating this differential equation gives

$$\begin{aligned} c_{\boldsymbol{k}\sigma}(t) &= e^{-i\xi_{\boldsymbol{k}} t} c_{\boldsymbol{k}\sigma}, & (37) \\ c^\dagger_{\boldsymbol{k}\sigma}(t) &= e^{i\xi_{\boldsymbol{k}} t} c^\dagger_{\boldsymbol{k}\sigma}. & (38) \end{aligned}$$

We see that the time dependence of the operators is very simple for noninteracting electrons. We now get for the greater Green functions:

$$\begin{aligned} G_0^>(\boldsymbol{k}, \sigma, t - t') &= -ie^{-i\xi_{\boldsymbol{k}} t} e^{i\xi_{\boldsymbol{k}} t'} \langle c_{\boldsymbol{k}\sigma} c^\dagger_{\boldsymbol{k}\sigma}\rangle = -ie^{-i\xi_{\boldsymbol{k}}(t-t')}(1 - \langle n_{\boldsymbol{k}\sigma}\rangle) \\ &= -ie^{-i\xi_{\boldsymbol{k}}(t-t')}(1 - n_F(\xi_{\boldsymbol{k}})), \end{aligned} \tag{39}$$

where

$$n_F(\omega) \equiv \frac{1}{e^{\beta\omega} + 1} \tag{40}$$

is the Fermi-Dirac distribution function. At zero temperature this becomes $n_F(\omega) = \theta(-\omega)$, hence a state $\boldsymbol{k}$ is occupied if $\epsilon_{\boldsymbol{k}} < \mu$ and empty if $\epsilon_{\boldsymbol{k}} > \mu$.

The calculation of the lesser Green function is very similar:

$$G_0^<(\boldsymbol{k}, \sigma, t - t') = +i\langle c^\dagger_{\boldsymbol{k}\sigma}(t') c_{\boldsymbol{k}\sigma}(t)\rangle = ie^{i\xi_{\boldsymbol{k}} t'} e^{-i\xi_{\boldsymbol{k}} t} \langle c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}\rangle = ie^{-i\xi_{\boldsymbol{k}}(t-t')} n_F(\xi_{\boldsymbol{k}}). \tag{41}$$

The retarded Green function can then be found from (9), which gives

$$G_0^R(\boldsymbol{k}, \sigma, t - t') = -i\theta(t - t') e^{-i\xi_{\boldsymbol{k}}(t-t')}. \tag{42}$$

Let us next consider the Fourier transform of this function, defined in (32):

$$G_0^R(\boldsymbol{k}\sigma, \omega) = -i\int_{-\infty}^{\infty} dt\ e^{i\omega t}\theta(t) e^{-i\xi_{\boldsymbol{k}} t} = -i\int_0^{\infty} dt\ e^{i(\omega - \xi_{\boldsymbol{k}})t}. \tag{43}$$

To make the integral converge at the upper limit we let $\omega \to \omega + i\eta$ where $\eta = 0^+$ is a positive infinitesimal. This gives

$$G_0^R(\boldsymbol{k}\sigma, \omega) = \frac{1}{\omega - \xi_{\boldsymbol{k}} + i\eta}. \tag{44}$$

We note that this Green function, considered as a function of ω for fixed $\boldsymbol{k}$, has a pole at $\omega = \xi_{\boldsymbol{k}} - i\eta$, i.e. at the excitation energy $\xi_{\boldsymbol{k}}$ of the system, except that the pole is just shifted infinitesimally off the real axis in the complex ω-plane and down into the lower half-plane. Thus the Fourier transform of the retarded Green function has the following properties: it is analytic in the upper half-plane, and the location of its poles (all in the lower half-plane) offer information about the excitation energies of the system. In the next section we will see that these are general features of the Fourier transform of the retarded Green function.

2.5 The Lehmann representation

We will now consider the "diagonal" (i.e. evaluated for $\nu' = \nu$) Green function $G^R(\nu, t; \nu, t') \equiv G^R(\nu; t, t') = G^R(\nu; t - t')$ for the fermionic case and derive what is called the Lehmann (or spectral) representation for its Fourier transform $G^R(\nu; \omega)$. We start with

$$G^>(\nu; t, t') = -i\langle c_\nu(t) c_\nu^\dagger(t')\rangle. \tag{45}$$

Next we write the explicit expressions for the average $\langle\cdots\rangle$ and for the time dependence of the operators. The trace involved in the average (see (17)) will be evaluated using the complete set of eigenstates $\{|n\rangle\}$ of H and the associated eigenvalues E_n. We also insert a resolution of the identity in terms of these eigenstates, i.e. $I = \sum_m |m\rangle\langle m|$ inbetween the operators $c_\nu(t)$ and $c_\nu^\dagger(t')$. (Note that although we don't know what these eigenstates *are*, we know that they *exist*, which is sufficient here.) This gives

$$\begin{aligned}
G^>(\nu; t, t') &= -i\frac{1}{Z}\sum_n e^{-\beta E_n}\langle n|c_\nu(t) c_\nu^\dagger(t')|n\rangle \\
&= -\frac{i}{Z}\sum_{n,m} e^{-\beta E_n}\langle n|e^{iHt} c_\nu e^{-iHt}|m\rangle\langle m|e^{iHt'} c_\nu^\dagger e^{-iHt'}|n\rangle \\
&= -\frac{i}{Z}\sum_{n,m} e^{-\beta E_n} e^{i(E_n - E_m)(t-t')}\underbrace{\langle n|c_\nu|m\rangle}_{\langle m|c_\nu^\dagger|n\rangle^*}\langle m|c_\nu^\dagger|n\rangle \\
&= -\frac{i}{Z}\sum_{n,m} e^{-\beta E_n} e^{i(E_n - E_m)(t-t')}|\langle m|c_\nu^\dagger|n\rangle|^2.
\end{aligned} \tag{46}$$

Following exactly the same steps to calculate $G^<(\nu; t, t') = i\langle c_\nu^\dagger(t') c_\nu(t)\rangle$, we get

$$\begin{aligned}
G^<(\nu; t, t') &= \frac{i}{Z}\sum_{n,m} e^{-\beta E_n} e^{i(E_m - E_n)(t-t')}|\langle n|c_\nu^\dagger|m\rangle|^2 \\
&= \frac{i}{Z}\sum_{n,m} e^{-\beta E_m} e^{i(E_n - E_m)(t-t')}|\langle m|c_\nu^\dagger|n\rangle|^2
\end{aligned} \tag{47}$$

where in the last expression we interchanged the names of the dummy summation variables n, m. This gives

$$\begin{aligned}
G^R(\nu; t - t') &= \theta(t - t')[G^>(\nu; t, t') - G^<(\nu; t, t')] \\
&= -i\theta(t - t')\frac{1}{Z}\sum_{n,m}\left(e^{-\beta E_n} + e^{-\beta E_m}\right) e^{i(E_n - E_m)(t-t')}|\langle m|c_\nu^\dagger|n\rangle|^2.
\end{aligned} \tag{48}$$

The Fourier transform of this is

$$\begin{aligned}
G^R(\nu,\omega) &= \int_{-\infty}^{\infty} dt\ e^{i\omega t} G^R(\nu,t) \\
&= -\frac{i}{Z}\sum_{n,m}\left(e^{-\beta E_n}+e^{-\beta E_m}\right)|\langle m|c_\nu^\dagger|n\rangle|^2 \int_{-\infty}^{\infty} dt\ \theta(t) e^{i(\omega+E_n-E_m)t} \\
&= -\frac{i}{Z}\sum_{n,m}\left(e^{-\beta E_n}+e^{-\beta E_m}\right)|\langle m|c_\nu^\dagger|n\rangle|^2 \int_{0}^{\infty} dt\ e^{i(\omega+E_n-E_m+i\eta)t}, \qquad (49)
\end{aligned}$$

i.e.,

$$G^R(\nu,\omega) = \frac{1}{Z}\sum_{n,m}\frac{|\langle m|c_\nu^\dagger|n\rangle|^2}{\omega+E_n-E_m+i\eta}\left(e^{-\beta E_n}+e^{-\beta E_m}\right). \qquad (50)$$

In this calculation we again let $\omega \to \omega + i\eta$ (where $\eta = 0^+$) to make the integral convergent. Eq. (50) is the Lehmann representation of $G^R(\nu,\omega)$. One can see that the singularities of $G^R(\nu,\omega)$ are poles located infinitesimally below the real axis at $\omega = E_m - E_n - i\eta$ (this pole exists provided the matrix element $\langle m|c_\nu^\dagger|n\rangle \neq 0$). Hence from the poles of $G^R(\nu,\omega)$ one can obtain information about the excitation energies $E_m - E_n$ associated with eigenstates $|m\rangle$ and $|n\rangle$ which are connected through the creation operator $c_\nu^\dagger$, i.e. eigenstates for which the state $|m\rangle$ has a finite overlap with the state $c_\nu^\dagger|n\rangle$. Here, clearly the eigenstate $|m\rangle$ has a single particle more than the eigenstate $|n\rangle$. Thus $G^R(\nu,\omega)$ gives information about the single-particle excitation spectrum.

2.6 The spectral function

In this section we will discuss a very important quantity called the (single-particle) spectral function $A(\nu,\omega)$, which is essentially the imaginary part of $G^R(\nu,\omega)$,[2]

$$A(\nu,\omega) \equiv -\frac{1}{\pi}\,\mathrm{Im}\,G^R(\nu,\omega). \qquad (51)$$

Using Eq. (50) and the fact that, for $\eta = 0^+$ and real x,

$$\mathrm{Im}\,\frac{1}{x+i\eta} = -\frac{\eta}{x^2+\eta^2} = -\pi\delta(x), \qquad (52)$$

we find that

$$A(\nu,\omega) = \frac{1}{Z}\sum_{n,m}|\langle m|c_\nu^\dagger|n\rangle|^2\left(e^{-\beta E_n}+e^{-\beta E_m}\right)\delta(\omega+E_n-E_m). \qquad (53)$$

It can be shown that $G^R(\nu,\omega)$ can be expressed in terms of the spectral function as follows:

$$G^R(\nu,\omega) = \int d\omega'\ \frac{A(\nu,\omega')}{\omega-\omega'+i\eta}. \qquad (54)$$

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[2] The prefactor $-1/\pi$ in (51) is a common, although not unique, convention. Some authors instead take the prefactor to be -2, which leads to factors of 2π differences in some of the following expressions.

A similar relation holds with $G^R(\nu,\omega)$ replaced by the *advanced* Green function $G^A(\nu,\omega)$ on the lhs and with $+i\eta$ replaced by $-i\eta$ on the rhs. From this one concludes that the Fourier transforms of the retarded and advanced Green functions are simply complex conjugates of each other (for real values of ω): $G^A(\nu,\omega) = [G^R(\nu,\omega)]^*$. One can also show that

$$\begin{aligned} iG^>(\nu,\omega) &= 2\pi\, A(\nu,\omega)[1-n_F(\omega)], &(55)\\ -iG^<(\nu,\omega) &= 2\pi\, A(\nu,\omega)n_F(\omega), &(56)\end{aligned}$$

which are known as the *fluctuation-dissipation theorem* for the fermionic single-particle Green functions. The proofs of Eqs. (54)-(56) will be left to a tutorial.

In the following we will for concreteness take $\nu = (\boldsymbol{k},\sigma)$.

2.6.1 Sum rule and physical interpretation

We will next show that the spectral function $A(\boldsymbol{k}\sigma,\omega)$ satisfies

$$\int_{-\infty}^{\infty} d\omega\, A(\boldsymbol{k}\sigma,\omega) = 1. \tag{57}$$

The proof goes as follows:

$$\begin{aligned}
\int_{-\infty}^{\infty} d\omega\; A(\boldsymbol{k}\sigma,\omega) &= \frac{1}{Z}\sum_{m,n} |\langle m|c^\dagger_{\boldsymbol{k}\sigma}|n\rangle|^2 \left(e^{-\beta E_n}+e^{-\beta E_m}\right) \underbrace{\int_{-\infty}^{\infty} d\omega\,\delta(\omega+E_n-E_m)}_{1}\\
&= \frac{1}{Z}\sum_{m,n} |\langle m|c^\dagger_{\boldsymbol{k}\sigma}|n\rangle|^2 \left(e^{-\beta E_n}+e^{-\beta E_m}\right)\\
&= \frac{1}{Z}\sum_{m,n} \langle m|c^\dagger_{\boldsymbol{k}\sigma}|n\rangle\langle n|c_{\boldsymbol{k}\sigma}|m\rangle \left(e^{-\beta E_n}+e^{-\beta E_m}\right)\\
&= \frac{1}{Z}\sum_{n,m} \left[e^{-\beta E_n}\langle n|c_{\boldsymbol{k}\sigma}|m\rangle\langle m|c^\dagger_{\boldsymbol{k}\sigma}|n\rangle + e^{-\beta E_m}\langle m|c^\dagger_{\boldsymbol{k}\sigma}|n\rangle\langle n|c_{\boldsymbol{k}\sigma}|m\rangle\right]\\
&= \frac{1}{Z}\left[\sum_n e^{-\beta E_n}\langle n|c_{\boldsymbol{k}\sigma}c^\dagger_{\boldsymbol{k}\sigma}|n\rangle + \sum_m e^{-\beta E_m}\langle m|c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma}|m\rangle\right]\\
&= \frac{1}{Z}\sum_n e^{-\beta E_n}\langle n|\underbrace{\left(c_{\boldsymbol{k}\sigma}c^\dagger_{\boldsymbol{k}\sigma}+c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma}\right)}_{=\{c_{\boldsymbol{k}\sigma},c^\dagger_{\boldsymbol{k}\sigma}\}=1}|n\rangle = \frac{1}{Z}\underbrace{\sum_n e^{-\beta E_n}}_{=Z} = 1. \qquad (58)
\end{aligned}$$

Eq. (57) is an example of a **sum rule**. A sum rule is an *exact* result for the frequency integral of a certain frequency-dependent quantity (typical examples being spectral functions of retarded Green functions, like $A(\boldsymbol{k}\sigma,\omega)$). In actual calculations for real systems, one is usually only able to get approximate results for such quantities, which may not satisfy the sum rule exactly. In such cases the extent to which the sum rule is approximately satisfied can be a useful measure of the quality of the approximations made.

The property (57) together with the fact that $A(\boldsymbol{k}\sigma,\omega) \geq 0$ (which can be seen from (53)) suggests that $A(\boldsymbol{k}\sigma,\omega)$ can be interpreted as a probability density. One can say (somewhat loosely speaking for the general interacting case) that $A(\boldsymbol{k}\sigma,\omega)d\omega$ is the probability that a fermion with momentum $\boldsymbol{k}$ has an energy in an infinitesimal energy window $d\omega$ about ω.

2.6.2 Spectral function for noninteracting fermions and Fermi liquids

Let us now investigate $A(\boldsymbol{k}\sigma,\omega)$ for a system of noninteracting fermions. We already calculated the retarded Green function for this case, $G_0^R(\boldsymbol{k}\sigma,\omega)$, in Eq. (44). It follows that the associated spectral function is a delta function,

$$A_0(\boldsymbol{k}\sigma,\omega) = \delta(\omega - \xi_{\boldsymbol{k}}). \tag{59}$$

Thus in this case the spectral function is nonzero only if the argument ω equals $\xi_{\boldsymbol{k}}$, which is the energy of a particle with quantum numbers $(\boldsymbol{k},\sigma)$ appearing in H_0. Therefore the energy of the particle is known *with certainty* when the momentum is given. This certainty is a reflection of the fact that in the noninteracting system, the many-body wavefunction is simply given by a **single** Slater determinant involving products of single-particle wavefunctions $\phi_{\boldsymbol{k}\sigma}(\boldsymbol{r})$ with associated energy $\xi_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} - \mu$. [It should be noted that for any quadratic Hamiltonian of the form $H_0 = \sum_\nu \xi_\nu c_\nu^\dagger c_\nu$ one finds the same result, i.e. $A_0(\nu,\omega) = \delta(\omega - \xi_\nu)$, so there's nothing special about choosing $\nu = (\boldsymbol{k},\sigma)$ here.]

In a large class of systems of interacting fermions, known as **Fermi liquids**, the spectral function can be written

$$A(\boldsymbol{k}\sigma,\omega) \approx \frac{Z_{\boldsymbol{k}}}{\pi}\frac{(1/2\tau_{\boldsymbol{k}})}{(\omega - \xi_{\boldsymbol{k}}^*)^2 + (1/2\tau_{\boldsymbol{k}})^2} + A_{\text{incoherent}}(\boldsymbol{k}\sigma,\omega). \tag{60}$$

Here $\tau_{\boldsymbol{k}}$ is a **lifetime**, $\xi_{\boldsymbol{k}}^*$ is a renormalized energy, and $Z_{\boldsymbol{k}}$ is a constant which is a positive number between 0 and 1. Compared to the noninteracting case, there is still a peak in the spectral function, represented by the first term in (60). However, the peak is now a Lorentzian instead of a delta function. Also, the width of the peak has broadened, the area under the peak has decreased (from 1 to Z_k), and the single-particle energies are renormalized. There is also an additional term $A_{\text{incoherent}}(\boldsymbol{k}\sigma,\omega)$ representing a continuum (i.e. not a peak) which must be there if $Z_{\boldsymbol{k}} \neq 1$ for the sum rule (57) to be satisfied.

A finite (i.e. not infinite) lifetime[3] $\tau_{\boldsymbol{k}}$ reflects the fact that in the presence of interactions the many-body wavefunction is a sum of many Slater determinants, which can be thought of as resulting from the fact that the interactions make the fermions scatter between different single-particle states $\phi_{\boldsymbol{k}\sigma}(\boldsymbol{r})$ (i.e. states with different $\boldsymbol{k}$'s); the lifetime $\tau_{\boldsymbol{k}}$ is thus a measure of the time between such scattering events. In a Fermi liquid, $1/\tau_{\boldsymbol{k}}$ approaches zero very fast as $|\boldsymbol{k}|$ approaches the Fermi momentum k_F. As a consequence, fermions close to the Fermi surface scatter very little, which can be shown to imply that treating them as essentially noninteracting is still qualitatively correct for many purposes. This is a very significant result since many experimentally measurable properties are at low temperatures essentially determined by the fermions at or near the Fermi surface. These properties are therefore not qualitatively changed by the electron-electron interactions.

The entities having energy $\xi_{\boldsymbol{k}}^*$ and lifetime $\tau_{\boldsymbol{k}}$ are called **quasi-particles**. As already noted, fermion systems in which this picture holds are called **Fermi liquids**, and the theory

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[3] Note that in the limit $\tau_{\boldsymbol{k}} \to \infty$ the first term in the spectral function again becomes a delta function.

describing them is known as Fermi liquid theory (which was first developed phenomenologically by Landau around 1957 and was subsequently given a microscopic foundation through the use of many-body perturbation theory in the following years).

We note that the identification and investigation of interacting fermionic systems which do *not* obey Fermi liquid theory is an important research question in current many-body physics. Such non-Fermi liquids by definition have a spectral function which can *not* be approximated by the form (60) and as a result they can therefore not be qualitatively understood in terms of a picture of noninteracting fermions. One prominent example of a non-Fermi liquid is the so-called **Luttinger liquid** which occurs in one spatial dimension.

2.6.3 Relation to momentum distribution (through weighted sum over ω) and to density of states (through sum over $\boldsymbol{k}$)

We will next find an exact expression for the quantity $\bar{n}_\nu \equiv \langle c_\nu^\dagger c_\nu \rangle$ in terms of a (weighted) frequency integral of the spectral function $A(\nu, \omega)$. We have

$$\begin{aligned} \bar{n}_\nu &\equiv \langle c_\nu^\dagger c_\nu \rangle = -iG^<(\nu, t=0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, \underbrace{e^{i\omega\cdot 0}}_{=1} \cdot \underbrace{(-i)G^<(\nu,\omega)}_{=2\pi A(\nu,\omega) n_F(\omega)} \\ &= \int_{-\infty}^{\infty} d\omega\, A(\nu,\omega) n_F(\omega), \end{aligned} \tag{61}$$

where we used (56). When $\nu = (\boldsymbol{k}\sigma)$ this gives a relation between the momentum distribution function $\bar{n}_{\boldsymbol{k}\sigma} \equiv \langle c_{\boldsymbol{k}\sigma}^\dagger c_{\boldsymbol{k}\sigma} \rangle$ and $A(\boldsymbol{k}\sigma, \omega)$:

$$\bar{n}_{\boldsymbol{k}\sigma} = \int_{-\infty}^{\infty} d\omega\, A(\boldsymbol{k}\sigma, \omega) n_F(\omega). \tag{62}$$

For a noninteracting system this gives $\bar{n}_{\boldsymbol{k}\sigma} = \int_{-\infty}^{\infty} d\omega\, \delta(\omega - \xi_{\boldsymbol{k}}) n_F(\omega) = n_F(\xi_{\boldsymbol{k}})$.

Another important quantity is the single-particle density of states $D(\omega)$ which is essentially the spectral function $A(\boldsymbol{k}, \omega)$ summed over all $\boldsymbol{k}$:

$$D(\omega) = \frac{1}{\Omega} \sum_{\boldsymbol{k},\sigma} A(\boldsymbol{k}\sigma, \omega). \tag{63}$$

The spectral function $A(\boldsymbol{k}, \omega)$ can be measured experimentally by tunneling spectroscopy (in this technique the differential conductance dI/dV at low temperatures gives information about the density of states $D(\omega)$) and Angle Resolved Photo-Emission Spectroscopy (ARPES). For details see Bruus and Flensberg, Ch. 8.4 and Coleman Ch. 10.7.2 and 10.7.3.

3 Imaginary-time (Matsubara) Green functions

3.1 Motivation

In most interacting systems, calculating physically interesting quantities like e.g. retarded Green functions and associated spectral functions is highly nontrivial and can usually only be accomplished approximately, e.g. in terms of many-body perturbation theory. For technical reasons it is useful to introduce what is known as **imaginary-time Green functions**, as it turns out that direct calculations of the retarded Green functions are impractical at finite temperatures. As we will see there is a rather simple mathematical relation between the imaginary-time Green functions and the retarded Green functions which allows one to obtain the latter from the former. In this section we develop these results for the case of single-particle Green functions, again focusing mainly on the fermionic case. The imaginary-time formalism is sometimes also referred to as the Matsubara formalism, and we will use these two names interchangeably.[4]

3.2 Imaginary-time single-particle Green function

The imaginary-time (or Matsubara) single-particle Green function is defined as

$$\mathcal{G}(\nu,\tau;\nu',\tau') \equiv -\langle T_\tau(c_\nu(\tau)c^\dagger_{\nu'}(\tau'))\rangle. \tag{64}$$

Here τ and τ' are real parameters satisfying $0 < \tau, \tau' < \beta$ where $\beta = 1/k_B T$ as usual. The time dependence of operators in the imaginary-time formalism is defined as

$$\begin{aligned} A(\tau) &\equiv e^{H\tau}Ae^{-H\tau}, & (65)\\ A^\dagger(\tau) &\equiv e^{H\tau}A^\dagger e^{-H\tau}. & (66)\end{aligned}$$

Compared to the usual real-time evolution defined in terms of the operators $e^{\pm iHt}$, it is as if we had set $it = \tau$. Since τ is real, this corresponds to t being imaginary; hence the name "imaginary-time." Note that τ being real means that $e^{\pm\tau H}$ are *not* unitary. This has the important implication that

$$A^\dagger(\tau) \neq (A(\tau))^\dagger. \tag{67}$$

Thus (65) and (66) are independent definitions and are not each other's adjoints, unlike the case for unitary real-time evolution.

The symbol T_τ in (64) is a time ordering operator which puts the operators in chronological order, with the earliest times furthest to the right, according to the following prescription:

$$T(c_\nu(\tau)c^\dagger_{\nu'}(\tau')) \equiv \begin{cases} c_\nu(\tau)c^\dagger_{\nu'}(\tau') & \text{if } \tau > \tau' \\ \epsilon c^\dagger_{\nu'}(\tau')c_\nu(\tau) & \text{if } \tau' > \tau. \end{cases} \tag{68}$$

Here $\epsilon = -1$ if the c's are fermion operators and $\epsilon = +1$ if they are boson operators. Thus in the fermionic case a minus sign is introduced upon interchanging the order of the operators while in the bosonic case there is no sign change.[5]

When the Hamiltonian is time-independent these Green functions will only depend on the time difference $\tau - \tau'$ and not on τ and τ' individually (as was also the case for the

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[4] There is also another formalism available which in contrast to the Matsubara formalism is only applicable at zero temperature and is therefore called the zero temperature formalism.

[5] This should not be confused with the standard commutation/anticommutation properties of bosonic/fermionic operators which in general only apply at *equal* times, while here the operators are evaluated at *different* times τ and τ'.

real-time Green functions considered in Sec. 2). This allows us to limit our consideration (without any loss of generality) to the function

$$\mathcal{G}(\nu,\nu';\tau) \equiv -\langle T_\tau(c_\nu(\tau)c^\dagger_{\nu'}(0))\rangle \tag{69}$$

where τ can now take values in the interval $-\beta < \tau < \beta$.

3.3 Periodicities in imaginary time. Fourier series and Matsubara frequencies

We will now show that the Matsubara Green functions obey the (anti-)periodicity conditions (here $\tau < 0$)

$$\mathcal{G}(\nu,\nu';\tau) = \mp\mathcal{G}(\nu,\nu';\tau+\beta) \tag{70}$$

where the upper (lower) sign is for fermions (bosons). To prove (70) we use the cyclic invariance of the trace operation,

$$\mathrm{Tr}(ABC\ldots XYZ) = \mathrm{Tr}(ZAB\ldots WXY) = \mathrm{Tr}(YZA\ldots VWX) \quad \text{etc.} \tag{71}$$

For the fermionic case this gives ($\tau < 0$)

$$\begin{aligned}
\mathcal{G}(\nu,\nu';\tau) &= -\langle T_\tau(c_\nu(\tau)c^\dagger_{\nu'}(0))\rangle = \langle c^\dagger_{\nu'}(0)c_\nu(\tau)\rangle \\
&= \frac{1}{Z}\mathrm{Tr}(e^{-\beta H}c^\dagger_{\nu'}e^{H\tau}c_\nu e^{-H\tau}) \\
&= \frac{1}{Z}\mathrm{Tr}(e^{H\tau}c_\nu e^{-H\tau}e^{-\beta H}c^\dagger_{\nu'}) \\
&= \frac{1}{Z}\mathrm{Tr}(\underbrace{e^{-\beta H}e^{\beta H}}_{=I}e^{H\tau}c_\nu e^{-H\tau}e^{-\beta H}c^\dagger_{\nu'}) \\
&= \frac{1}{Z}\mathrm{Tr}(e^{-\beta H}e^{H(\tau+\beta)}c_\nu e^{-H(\tau+\beta)}c^\dagger_{\nu'}) \\
&= \frac{1}{Z}\mathrm{Tr}(e^{-\beta H}c_\nu(\tau+\beta)c^\dagger_{\nu'}(0)) = \langle c_\nu(\underbrace{\tau+\beta}_{>0})c^\dagger_{\nu'}(0)\rangle \\
&= -\mathcal{G}(\nu,\nu';\tau+\beta) \quad \text{QED.}
\end{aligned} \tag{72}$$

The proof for the bosonic case is obviously very similar.

We can now use (70) twice to get $\mathcal{G}(\nu,\nu';-\beta) = \mp\mathcal{G}(\nu,\nu';0) = (\mp)^2\mathcal{G}(\nu,\nu';\beta) = \mathcal{G}(\nu,\nu';\beta)$. Hence the Matsubara Green function is periodic with period 2β on the interval $\tau \in (-\beta,\beta)$ and can therefore be expanded in a standard Fourier series on this interval, which can be written as

$$\mathcal{G}(\nu,\nu';\tau) = \frac{1}{\beta}\sum_{n\in\mathbb{Z}} e^{-i\tilde{\omega}_n\tau}\mathcal{G}(\nu,\nu';i\tilde{\omega}_n), \tag{73}$$

$$\mathcal{G}(\nu,\nu';i\tilde{\omega}_n) = \frac{1}{2}\int_{-\beta}^{\beta} d\tau e^{i\tilde{\omega}_n\tau}\mathcal{G}(\nu,\nu';\tau). \tag{74}$$

where the frequencies $\tilde{\omega}_n$[6] are given by $\tilde{\omega}_n = (2\pi n)/(2\beta) = \pi n/\beta$. Actually, because of the property (70) only a certain subset of the frequency components will be nonzero. This can be seen by splitting the integral in (74) into one over $(-\beta, 0)$ and one over $(0, \beta)$, using (70) in the first region to rewrite it too as an integral over the second region, and using the fact that $e^{-i\tilde{\omega}_n \beta} = e^{-i\pi n} = (-1)^n$:

$$\begin{aligned} \mathcal{G}(\nu,\nu';i\tilde{\omega}_n) &= \frac{1}{2}\left[\int_{-\beta}^{0} d\tau\; e^{i\tilde{\omega}_n\tau}\, \underbrace{\mathcal{G}(\nu,\nu';\tau)}_{\mp\mathcal{G}(\nu,\nu';\tau+\beta)} + \int_{0}^{\beta} d\tau\; e^{i\tilde{\omega}_n\tau}\mathcal{G}(\nu,\nu';\tau)\right] \\ &= \underbrace{\frac{1}{2}\left[\mp(-1)^n + 1\right]}\int_{0}^{\beta} d\tau\; e^{i\tilde{\omega}_n\tau}\mathcal{G}(\nu,\nu';\tau). \qquad (75) \end{aligned}$$

For fermions, the bracketed quantity is 1 if n is odd and 0 if n is even, while for bosons it's 1 if n is even and 0 if n is odd. Hence for fermions (bosons) only odd (even) values of n contribute in the Fourier series, which makes it natural to define

$$\omega_n \equiv \frac{(2n+1)\pi}{\beta} \quad \text{for fermions,} \tag{76}$$

$$\omega_n \equiv \frac{2n\pi}{\beta} \quad \text{for bosons} \tag{77}$$

where again n runs over *all* integers for both fermions and bosons. This gives our final result for the Fourier representation of the Matsubara Green functions:

$$\mathcal{G}(\nu,\nu';\tau) = \frac{1}{\beta}\sum_{\omega_n} e^{-i\omega_n\tau}\mathcal{G}(\nu,\nu';i\omega_n), \tag{78}$$

$$\mathcal{G}(\nu,\nu';i\omega_n) = \int_0^\beta d\tau\; e^{i\omega_n\tau}\mathcal{G}(\nu,\nu';\tau). \tag{79}$$

The frequencies ω_n are known as **Matsubara frequencies**. Note that they depend on temperature. They are discrete at finite temperature but become continuous in the limit of zero temperature ($\beta \to \infty$), when the spacing $2\pi/\beta$ between adjacent frequencies goes to zero. It has become customary to denote fermionic Matsubara frequencies by p_n or k_n and bosonic Matsubara frequencies by q_n or ω_n, which is a convention we will tend to follow from now on.

3.4 The connection between imaginary-time and retarded Green functions

We will next consider how one can obtain a retarded Green function from the corresponding imaginary-time Green function. The key is to calculate the Fourier transform $\mathcal{G}(i\omega_n)$ of the latter; then the retarded function $G^R(\omega)$ can be found from this by the substitution

$$i\omega_n \to \omega + i\eta \tag{80}$$

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[6] We have put a tilde on these frequencies because we are going to define a slightly different frequency variable ω_n below.

(where η is a positive infinitesimal), a procedure known as **analytic continuation**. This result follows from a comparison of the Lehmann representations for the imaginary-time and retarded Green functions. Since we considered the Lehmann representation for the fermionic diagonal retarded function $G^R(\nu,\omega) \equiv G^R(\nu,\nu;\omega)$ in Sec. 2.5 we will here consider the Lehmann representation for the corresponding Matsubara function $\mathcal{G}(\nu, ip_n) \equiv \mathcal{G}(\nu,\nu; ip_n)$. The result (80) is however valid also for the non-diagonal case, and for bosons, and also extends to more complicated Green functions than the single-particle one.

To calculate $\mathcal{G}(\nu, ip_n)$ we first need to find $\mathcal{G}(\nu,\tau)$. Following the same procedure as in Sec. 2.5 we have (we consider $\tau > 0$ only as that is sufficient to calculate $\mathcal{G}(\nu, ip_n)$)

$$\begin{aligned}\mathcal{G}(\nu,\tau) &= -\langle c_\nu(\tau) c_\nu^\dagger(0)\rangle \\ &= -\frac{1}{Z}\sum_{n,m} e^{-\beta E_n}\langle n|e^{H\tau}c_\nu e^{-H\tau}|m\rangle\langle m|c_\nu^\dagger|n\rangle \\ &= -\frac{1}{Z}\sum_{n,m} e^{-\beta E_n} e^{(E_n-E_m)\tau}|\langle m|c_\nu^\dagger|n\rangle|^2. \end{aligned} \tag{81}$$

Thus[7]

$$\begin{aligned}\mathcal{G}(\nu, ip_\ell) &= -\frac{1}{Z}\sum_{n,m} e^{-\beta E_n}|\langle m|c_\nu^\dagger|n\rangle|^2\int_0^\beta d\tau\; e^{(ip_\ell+E_n-E_m)\tau} \\ &= -\frac{1}{Z}\sum_{n,m} e^{-\beta E_n}|\langle m|c_\nu^\dagger|n\rangle|^2\,\frac{e^{(ip_\ell+E_n-E_m)\beta}-1}{ip_\ell+E_n-E_m} \\ &= \frac{1}{Z}\sum_{n,m}\frac{|\langle m|c_\nu^\dagger|n\rangle|^2}{ip_\ell+E_n-E_m}(e^{-\beta E_n}+e^{-\beta E_m}), \end{aligned} \tag{82}$$

where we used that

$$e^{ip_n\beta} = -1 \tag{83}$$

which follows from (76). Comparing (82) with (50) we see that indeed the Matsubara and retarded functions are simply related by (80).

3.5 Example: Noninteracting fermions

In this section we calculate the Matsubara Green function for noninteracting fermions. The Hamiltonian is given by

$$H_0 = \sum_\nu \xi_\nu c_\nu^\dagger c_\nu. \tag{84}$$

We denote the Matsubara function by $\mathcal{G}^{(0)}(\nu,\tau)$; the superscript 0 reflects the fact that the quadratic Hamiltonian is diagonal in the ν-basis; this makes the Matsubara function diagonal too. Using that

$$c_\nu(\tau) = e^{H_0\tau}c_\nu e^{-H_0\tau} = e^{-\xi_\nu\tau}c_\nu, \tag{85}$$

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[7] Since the index n is already "taken" we write ip_ℓ instead of ip_n for the Matsubara frequency here.

we find

$$\begin{aligned}
\mathcal{G}^{(0)}(\nu,\tau) &= -\langle T_\tau(c_\nu(\tau)c_\nu^\dagger(0))\rangle \\
&= -\theta(\tau)\langle c_\nu(\tau)c_\nu^\dagger(0)\rangle + \theta(-\tau)\langle c_\nu^\dagger(0)c_\nu(\tau)\rangle \\
&= -e^{-\xi_\nu\tau}[\theta(\tau)\langle c_\nu c_\nu^\dagger\rangle - \theta(-\tau)\langle c_\nu^\dagger c_\nu\rangle] \\
&= -e^{-\xi_\nu\tau}[\theta(\tau)(1-n_F(\xi_\nu)) - \theta(-\tau)n_F(\xi_\nu)]. \qquad (86)
\end{aligned}$$

Thus

$$\begin{aligned}
\mathcal{G}^{(0)}(\nu,ip_n) &= \int_0^\beta d\tau\; e^{ip_n\tau}\mathcal{G}^{(0)}(\nu,\tau) \\
&= -(1-n_F(\xi_\nu))\int_0^\beta d\tau\; e^{(ip_n-\xi_\nu)\tau} \\
&= \frac{1}{ip_n-\xi_\nu}\cdot\underbrace{(-1)(1-n_F(\xi_\nu))\left[e^{(ip_n-\xi_\nu)\beta}-1\right]}_{=1} \\
&= \frac{1}{ip_n-\xi_\nu} \qquad (87)
\end{aligned}$$

where we used (40) and (83). It is reassuring that if we now let $ip_n \to \omega + i\eta$ in this expression to obtain the retarded Green function, we get the same result (44) as we obtained earlier when calculating the retarded Green function directly for this case of noninteracting fermions.

3.6 Equation of motion approach for Matsubara Green functions

We will now develop an **equation of motion** approach to find the Matsubara single-particle Green function. This involves differentiating the Matsubara Green function with respect to τ, which will lead us to a differential equation obeyed by this function. We will see that for the case of quadratic Hamiltonians the differential equation is relatively simple in that it only involves single-particle Green functions. This differential equation can be transformed into an algebraic equation by Fourier transformation, for which a solution can be found in the form of an infinite series.

3.6.1 General Hamiltonians

Let us start by considering a fermionic system with a completely general Hamiltonian H and the Matsubara Green function $\mathcal{G}(\nu,\nu';\tau)$ where ν is some arbitrary basis:

$$\mathcal{G}(\nu,\nu';\tau) = -\langle T_\tau(c_\nu(\tau)c_{\nu'}^\dagger(0))\rangle. \qquad (88)$$

Differentiating this with respect to τ gives

$$\begin{aligned}
\frac{d}{d\tau}\mathcal{G}(\nu,\nu';\tau) &= -\frac{d}{d\tau}\left[\theta(\tau)\langle c_\nu(\tau)c_{\nu'}^\dagger(0)\rangle - \theta(-\tau)\langle c_{\nu'}^\dagger(0)c_\nu(\tau)\rangle\right] \\
&= -\delta(\tau)\underbrace{\langle(c_\nu(\tau)c_{\nu'}^\dagger(0) + c_{\nu'}^\dagger(0)c_\nu(\tau))\rangle}_{=\delta_{\nu\nu'}\quad(\tau=0)} - \left[\theta(\tau)\langle\frac{d}{d\tau}c_\nu(\tau)c_{\nu'}^\dagger(0)\rangle - \theta(-\tau)\langle c_{\nu'}^\dagger(0)\frac{d}{d\tau}c_\nu(\tau)\rangle\right] \\
&= -\delta(\tau)\delta_{\nu\nu'} - \left[\theta(\tau)\langle[H,c_\nu(\tau)]c_{\nu'}^\dagger(0)\rangle - \theta(-\tau)\langle c_{\nu'}^\dagger(0)[H,c_\nu(\tau)]\rangle\right], \qquad (89)
\end{aligned}$$

i.e.,

$$-\frac{d}{d\tau}\mathcal{G}(\nu,\nu';\tau) = \delta(\tau)\delta_{\nu\nu'} + \langle T_\tau([H,c_\nu(\tau)]c^\dagger_{\nu'}(0))\rangle. \tag{90}$$

To arrive at this result we used the equation of motion for $c_\nu(\tau)$,

$$\frac{dc_\nu(\tau)}{d\tau} = [H, c_\nu(\tau)] \tag{91}$$

which follows from (65). Note that the factor $\delta_{\nu\nu'}$ arose due to the delta function $\delta(\tau)$ which allowed us to set $\tau = 0$ in that term and then make use of the equal-time anticommutation relations.

If the Hamiltonian contains nontrivial interaction terms, such as terms that are quartic in the creation/annihilation operators (an example would be the Coulomb interaction between electrons), the second term on the rhs of (90) will involve higher-order Green functions than the single-particle one (e.g. two-particle Green functions). One can in turn find the equation of motion for these which will involve Green functions of even higher order, and so on. In order to make progress, this hierarchy of ever more complicated equations must then be "cut off" at some level by approximating the multi-particle Green function at that level as a product of lower-order Green functions.

In the following we will instead consider the simpler case of a quadratic Hamiltonian. Then, as we will see, the term on the rhs of (90) involving the expectation value of the time-ordered expression will just be another single-particle Green function. Thus in this case the equations of motion for the single-particle Green functions will constitute a "closed" system of equations.

3.6.2 Quadratic Hamiltonians

Assume that H is quadratic so that it can be written on the form

$$H = \sum_{\nu'\nu} h_{\nu'\nu} c^\dagger_{\nu'} c_\nu \tag{92}$$

which gives

$$[H, c_\nu(\tau)] = -\sum_{\nu'} h_{\nu\nu'} c_{\nu'}(\tau). \tag{93}$$

Inserting this into (90) one finds

$$-\frac{d}{d\tau}\mathcal{G}(\nu,\nu';\tau) = \delta(\tau)\delta_{\nu\nu'} + \sum_{\nu''} h_{\nu\nu''}\mathcal{G}(\nu'',\nu';\tau), \tag{94}$$

which is an equation of motion that only involves single-particle Green functions. Next we separate H into its diagonal part and non-diagonal parts,

$$h_{\nu\nu'} = \xi_\nu \delta_{\nu\nu'} + v_{\nu\nu'} \tag{95}$$

which gives

$$\left(-\frac{d}{d\tau} - \xi_\nu\right)\mathcal{G}(\nu,\nu';\tau) = \delta(\tau)\delta_{\nu\nu'} + \sum_{\nu''} v_{\nu\nu''}\mathcal{G}(\nu'',\nu';\tau). \tag{96}$$

This differential equation can now be turned into an algebraic equation by introducing the Fourier transform defined in (78)-(79). The lhs of (96) can then be written $(1/\beta)\sum_{p_n}(ip_n - \xi_\nu)e^{-ip_n\tau}\mathcal{G}(\nu,\nu';ip_n)$. Upon multiplying both sides of the equation by $e^{ip_m\tau}$ and integrating over τ from $\tau=0$ to $\tau=\beta$, one arrives at

$$(ip_m - \xi_\nu)\mathcal{G}(\nu,\nu';ip_m) = \delta_{\nu\nu'} + \sum_{\nu''} v_{\nu\nu''}\mathcal{G}(\nu'',\nu';ip_m) \tag{97}$$

where we used[8]

$$\begin{aligned} \frac{1}{\beta}\int_0^\beta d\tau\ e^{i(p_m-p_n)\tau} &= \delta_{mn}, & (98)\\ \int_0^\beta d\tau\ e^{ip_m\tau}\delta(\tau-0^+) &= 1. & (99) \end{aligned}$$

From (87) we have $ip_m - \xi_\nu = (\mathcal{G}^{(0)}(\nu;ip_m))^{-1}$, so that (97) can be rewritten as

$$\mathcal{G}(\nu,\nu';ip_m) = \mathcal{G}^{(0)}(\nu,ip_m)\delta_{\nu\nu'} + \mathcal{G}^{(0)}(\nu;ip_m)\sum_{\nu''} v_{\nu\nu''}\mathcal{G}(\nu'',\nu';ip_m). \tag{100}$$

Note that the Matsubara frequency ip_m is the same in all the Green functions in this equation, which makes it a little unnecessary to carry it along. To lighten the notation we will therefore drop it in the following.

3.6.3 Solution as perturbation series

Next we write an ansatz for the solution to Eq. (100) in the form of an infinite series,

$$\mathcal{G}(\nu,\nu') = \sum_{n=0}^{\infty}\mathcal{G}^{(n)}(\nu,\nu') \tag{101}$$

where $\mathcal{G}^{(n)}$ contains n powers of the non-diagonal matrix elements $v_{\nu_i\nu_j}$. When the non-diagonal part is zero, the solution of (100) is clearly just the unperturbed Green function, i.e.

$$\mathcal{G}^{(0)}(\nu,\nu') = \mathcal{G}^{(0)}(\nu)\delta_{\nu\nu'}. \tag{102}$$

---

[8] Eq. (99) requires some further explanation. One can regard the delta function $\delta(\tau)$ in Eq. (90) as the limit of a Lorentzian with a finite width and centered at $\tau=0$. It is then clear that only half of this function is inside the integration region, so $\int_0^\beta d\tau\ e^{ip_m\tau}\delta(\tau) = 1/2$. However, the result (90) is in fact not entirely correct as it stands. If $-(d/d\tau)\mathcal{G}$ has a delta function contribution at $\tau=0$, then because of the anti-periodicity (70) it should also have delta function contributions at $\tau=-\beta$ and $\tau=\beta$ with opposite signs from that at $\tau=0$. So if we integrate from 0 to β, the delta function at $\tau=\beta$ also gives contribution 1/2 (the minus sign in front of the delta function is cancelled by the factor $e^{ip_m\beta}=-1$ that is also in the integrand). Thus the total contribution from the two delta functions at $\tau=0$ and $\tau=\beta$ is $2\cdot 1/2 = 1$. We get the same result by keeping (90) as it is (i.e. not adding to it the delta function contributions at $\tau=\pm\beta$) and shifting $\mathcal{G}(\tau)$ by an infinitesimal amount to the right. Then the center of the delta function at $\tau=0$ is shifted to $\tau=0^+$ and thus it lies entirely inside the integration region, giving Eq. (99). In contrast, the delta function at $\tau=\beta$ is shifted to $\tau=\beta^+$ and thus gives no contribution to the integral anymore.

Inserting (101) into (100) and cancelling the zeroth order terms, one obtains the following recursion relation by equating equal powers of $v_{\nu_i\nu_j}$ on both sides:

$$\mathcal{G}^{(n)}(\nu,\nu') = \mathcal{G}^{(0)}(\nu) \sum_{\nu''} v_{\nu\nu''} \mathcal{G}^{(n-1)}(\nu'',\nu') \qquad (n \geq 1). \tag{103}$$

Iterating this, one finds

$$\mathcal{G}^{(1)}(\nu,\nu') = \mathcal{G}^{(0)}(\nu) v_{\nu\nu'} \mathcal{G}^{(0)}(\nu'), \tag{104}$$

$$\mathcal{G}^{(2)}(\nu,\nu') = \sum_{\nu_1} \mathcal{G}^{(0)}(\nu) v_{\nu\nu_1} \mathcal{G}^{(0)}(\nu_1) v_{\nu_1\nu'} \mathcal{G}^{(0)}(\nu'), \tag{105}$$

$$\mathcal{G}^{(3)}(\nu,\nu') = \sum_{\nu_1,\nu_2} \mathcal{G}^{(0)}(\nu) v_{\nu\nu_1} \mathcal{G}^{(0)}(\nu_1) v_{\nu_1\nu_2} \mathcal{G}^{(0)}(\nu_2) v_{\nu_2\nu'} \mathcal{G}^{(0)}(\nu'), \tag{106}$$

and, for general n,

$$\mathcal{G}^{(n)}(\nu,\nu') = \sum_{\nu_1,\dots,\nu_{n-1}} \mathcal{G}^{(0)}(\nu) v_{\nu\nu_1} \mathcal{G}^{(0)}(\nu_1) \dots \mathcal{G}^{(0)}(\nu_{n-1}) v_{\nu_{n-1}\nu'} \mathcal{G}^{(0)}(\nu'). \tag{107}$$

Thus in $\mathcal{G}^{(n)}$ there are $n+1$ factors of $\mathcal{G}^{(0)}$, n factors of $v_{\nu_i\nu_j}$, and $n-1$ summations over intermediate states ν_i.

4 Electrons in a disordered potential

4.1 Motivation

In this section we will consider the problem of electrons in a disordered potential. This is relevant to impurity scattering in a metal, which gives a contribution to the resistivity of the metal. However, calculating the resistivity is a problem involving two-particle Green function (the conductivity, which is the inverse of the resistivity, involves the current-current correlation function which is a two-particle retarded Green function). In this section we will focus on the simpler problem of studying the single-particle Green function. In fact, what we will eventually end up studying is an averaged version of this Green function, in which the positions of all the (randomly located) impurities have been averaged over. The analysis of this problem will give us our first exposure to important concepts like **Feynman diagrams** and the **self-energy**. We will see that the impurity scattering leads to a broadening of the spectral function (cf. the discussion in Sec. 2.6.2).

4.2 The impurity scattering Hamiltonian

We start by defining the Hamiltonian for this problem,

$$H = H_0 + V. \tag{108}$$

Here H_0 is the kinetic energy of the electrons, which is diagonal in the momentum basis,

$$H_0 = \sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}} \tag{109}$$

with $\xi_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} - \mu$. (We will drop the spin, since it doesn't play a crucial role in this problem and thus would just be another index to drag along.) The impurity potential is represented by V, which in first quantization is given by

$$V = \sum_{i=1}^{N_e} V(\boldsymbol{r}_i) \tag{110}$$

where the sum is over all electron coordinates $\boldsymbol{r}_i$ (N_e is the total number of electrons) and

$$V(\boldsymbol{r}) = \sum_{j=1}^{N} U(\boldsymbol{r} - \boldsymbol{R}_j). \tag{111}$$

Here $U(\boldsymbol{r})$ is the impurity potential from the individual impurities which are located at the positions $\boldsymbol{R}_j$ (N is the total number of impurities). Since V is a single-particle operator, its second quantized form is, like H_0, quadratic in the fermion operators, but unlike H_0 it is not diagonal in the $\boldsymbol{k}$-basis:

$$V = \sum_{\boldsymbol{k},\boldsymbol{k}'} \langle \boldsymbol{k}' | V(\boldsymbol{r}) | \boldsymbol{k} \rangle c^\dagger_{\boldsymbol{k}'} c_{\boldsymbol{k}} \tag{112}$$

where

$$\langle \boldsymbol{k}' | V(\boldsymbol{r}) | \boldsymbol{k} \rangle = \int d\boldsymbol{r} \phi^*_{\boldsymbol{k}'}(\boldsymbol{r}) V(\boldsymbol{r}) \phi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\Omega} \int d\boldsymbol{r}\; e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}} V(\boldsymbol{r}), \tag{113}$$

where we used (25). Inserting (111) gives

$$\begin{aligned}
\langle \boldsymbol{k}' | V(\boldsymbol{r}) | \boldsymbol{k} \rangle &= \frac{1}{\Omega} \sum_{j=1}^{N} \int d\boldsymbol{r}\; e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}} U(\underbrace{\boldsymbol{r} - \boldsymbol{R}_j}_{\equiv \boldsymbol{r}'}) \\
&= \frac{1}{\Omega} \sum_{j=1} \underbrace{\int d\boldsymbol{r}'\; e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}'} U(\boldsymbol{r}')}_{\text{independent of j}}\, e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{R}_j} \\
&= U(\boldsymbol{k}' - \boldsymbol{k}) \rho(\boldsymbol{k}' - \boldsymbol{k})
\end{aligned} \tag{114}$$

where we defined

$$\begin{aligned}
U(\boldsymbol{k}) &= \frac{1}{\Omega} \int d\boldsymbol{r} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} U(\boldsymbol{r}), && (115) \\
\rho(\boldsymbol{k}) &= \sum_{j=1}^{N} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_j}. && (116)
\end{aligned}$$

Note that all the information about the positions of the impurities lies in $\rho(\boldsymbol{k})$.

4.3 Perturbation series solution for the single-particle Matsubara Green function

To calculate the Green function for this problem we will make use of the equation-of-motion approach developed in Sec. 3.6. The Hamiltonian (108) is quadratic in the fermion operators, so the analysis in Secs. 3.6.2 and 3.6.3 is applicable, with

$$
\begin{aligned}
\nu &\rightarrow \boldsymbol{k}, &(117)\\
v_{\nu_i\nu_j} &\rightarrow U(\boldsymbol{k}_i-\boldsymbol{k}_j)\rho(\boldsymbol{k}_i-\boldsymbol{k}_j). &(118)
\end{aligned}
$$

Thus, using Eqs. (101) and (107) we get (again dropping the Matsubara frequencies in the Green functions)

$$\mathcal{G}(\boldsymbol{k},\boldsymbol{k}')=\sum_{n=0}^{\infty}\mathcal{G}^{(n)}(\boldsymbol{k},\boldsymbol{k}') \tag{119}$$

$$
\begin{aligned}
\mathcal{G}^{(n)}(\boldsymbol{k},\boldsymbol{k}') = \sum_{\boldsymbol{k}_1,\ldots,\boldsymbol{k}_{n-1}} & \mathcal{G}^{(0)}(\boldsymbol{k})U(\boldsymbol{k}-\boldsymbol{k}_1)\rho(\boldsymbol{k}-\boldsymbol{k}_1)\mathcal{G}^{(0)}(\boldsymbol{k}_1)\cdots\\
& \cdots\mathcal{G}^{(0)}(\boldsymbol{k}_{n-1})U(\boldsymbol{k}_{n-1}-\boldsymbol{k}')\rho(\boldsymbol{k}_{n-1}-\boldsymbol{k}')\mathcal{G}^{(0)}(\boldsymbol{k}'). \qquad (120)
\end{aligned}
$$

Note that $\mathcal{G}(\boldsymbol{k},\boldsymbol{k}')$ is not diagonal in $\boldsymbol{k}$. This is because the impurities make the system not translationally invariant.

4.4 Averaging over impurity locations

$\mathcal{G}(\boldsymbol{k},\boldsymbol{k}')$ is a function of the locations of all the impurities. Typically, however, we are not interested in the properties of the system for any particular impurity configuration. Instead we are more interested in **impurity-averaged properties**, which are obtained for a given quantity (e.g. the Green function) by averaging it over all possible impurity configurations. This impurity averaging also turns out to be a valid procedure for describing any real macroscopic system of interest for experimentally realizable temperatures, due to a property known as *self-averaging*.[9] Thus we will now consider how to carry out such an impurity average for the Matsubara Green function.

The locations of the various impurities will be assumed to be independent of each other, so that the probability distribution for the impurity configuration is simply a product of probability distributions for the location of individual impurities, which will be taken to be uniform in space. Hence the impurity average simply consists of averaging the positions of the N impurities over all space. Denoting the impurity-averaged Matsubara Green function by $\overline{\mathcal{G}}(\boldsymbol{k},\boldsymbol{k}')$ we thus have

$$\overline{\mathcal{G}}(\boldsymbol{k},\boldsymbol{k}')=\prod_{i=1}^{N}\left(\frac{1}{\Omega}\int d^3R_i\right)\mathcal{G}(\boldsymbol{k},\boldsymbol{k}'). \tag{121}$$

Being simply an integral over all impurity coordinates, the impurity average is clearly a linear operation, and can therefore be carried out for each term in the perturbation series (101) separately (i.e. the average of the sum is the sum of the averages), giving

$$\overline{\mathcal{G}}(\boldsymbol{k},\boldsymbol{k}')=\sum_{n=0}^{\infty}\overline{\mathcal{G}^{(n)}}(\boldsymbol{k},\boldsymbol{k}'). \tag{122}$$

---

[9] If you'd like more details, see the beginning of Sec. 12.4 in Bruus & Flensberg.

The only factors in Eq. (120) which depend on the impurity positions are the functions $\overline{\rho(\boldsymbol{q})}$. Thus to find $\overline{\mathcal{G}^{(n)}}(\boldsymbol{k},\boldsymbol{k}')$ we need to calculate the quantity $\overline{\rho(\boldsymbol{k}-\boldsymbol{k}_1)\rho(\boldsymbol{k}_1-\boldsymbol{k}_2)\dots\rho(\boldsymbol{k}_{n-1}-\boldsymbol{k}')}$. In the following we will consider how to do this for the lowest orders of n.

For $n=1$, we need to calculate

$$\begin{aligned}\overline{\rho(\boldsymbol{k}-\boldsymbol{k}')} &= \prod_{i=1}^{N}\left(\frac{1}{\Omega}\int d^3R_i\right)\rho(\boldsymbol{k}-\boldsymbol{k}') = \prod_{i=1}^{N}\left(\frac{1}{\Omega}\int d^3R_i\right)\sum_{j=1}^{N}e^{-i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}_j}\\ &= \sum_{j=1}^{N}\underbrace{\frac{1}{\Omega}\int d^3R_j\ e^{-i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}_j}}_{\delta_{\boldsymbol{k},\boldsymbol{k}'}}\cdot\prod_{i\neq j}\underbrace{\left(\frac{1}{\Omega}\int d^3R_i\right)}_{1} = N\delta_{\boldsymbol{k},\boldsymbol{k}'}. \end{aligned}\tag{123}$$

For $n=2$, we need to calculate

$$\begin{aligned}\overline{\rho(\boldsymbol{k}-\boldsymbol{k}_1)\rho(\boldsymbol{k}_1-\boldsymbol{k}')} &= \prod_{i=1}^{N}\left(\frac{1}{\Omega}\int d^3R_i\right)\sum_{j_1=1}^{N}e^{-i(\boldsymbol{k}-\boldsymbol{k}_1)\cdot\boldsymbol{R}_{j_1}}\sum_{j_2=1}^{N}e^{-i(\boldsymbol{k}_1-\boldsymbol{k}')\cdot\boldsymbol{R}_{j_2}}\\ &= \sum_{j_1=1}^{N}\sum_{j_2=1}^{N}\prod_{i=1}^{N}\left(\frac{1}{\Omega}\int d^3R_i\right)e^{-i(\boldsymbol{k}-\boldsymbol{k}_1)\cdot\boldsymbol{R}_{j_1}}e^{-i(\boldsymbol{k}_1-\boldsymbol{k}')\cdot\boldsymbol{R}_{j_2}}. \end{aligned}\tag{124}$$

For each term in the sum we must now distinguish between whether $j_1\neq j_2$ or $j_1=j_2$. If $j_1\neq j_2$, $N-2$ integrals give unity while the integrals over j_1 and j_2 give

$$\frac{1}{\Omega}\int d^3R_{j_1}e^{-i(\boldsymbol{k}-\boldsymbol{k}_1)\cdot\boldsymbol{R}_{j_1}}\ \frac{1}{\Omega}\int d^3R_{j_2}e^{-i(\boldsymbol{k}_1-\boldsymbol{k}')\cdot\boldsymbol{R}_{j_2}} = \delta_{\boldsymbol{k},\boldsymbol{k}_1}\delta_{\boldsymbol{k}_1,\boldsymbol{k}'}.\tag{125}$$

On the other hand, if $j_1=j_2$, $N-1$ integrals give unity while the integral over $j_1=j_2$ gives

$$\frac{1}{\Omega}\int d^3R_{j_1}\ e^{-i(\boldsymbol{k}-\boldsymbol{k}_1)\cdot\boldsymbol{R}_{j_1}}e^{-i(\boldsymbol{k}_1-\boldsymbol{k}')\cdot\boldsymbol{R}_{j_1}} = \frac{1}{\Omega}\int d^3R_{j_1}e^{-i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}_{j_1}} = \delta_{\boldsymbol{k},\boldsymbol{k}'}.\tag{126}$$

Therefore

$$\begin{aligned}\overline{\rho(\boldsymbol{k}-\boldsymbol{k}_1)\rho(\boldsymbol{k}_1-\boldsymbol{k}')} &= \sum_{j_1,j_2}\left[(1-\delta_{j_1,j_2})\delta_{\boldsymbol{k},\boldsymbol{k}_1}\delta_{\boldsymbol{k}_1,\boldsymbol{k}'}+\delta_{j_1,j_2}\delta_{\boldsymbol{k},\boldsymbol{k}'}\right]\\ &= (N^2-N)\delta_{\boldsymbol{k},\boldsymbol{k}_1}\delta_{\boldsymbol{k}_1,\boldsymbol{k}'}+N\delta_{\boldsymbol{k},\boldsymbol{k}'}. \end{aligned}\tag{127}$$

Here $N^2-N=N(N-1)$ can be approximated by N^2 as the error introduced is of order $1/N$ and thus very small in the limit of a large number of impurities, which is what we're considering here. Furthermore the product of Kronecker deltas can be rewritten as $\delta_{\boldsymbol{k},\boldsymbol{k}'}\delta_{\boldsymbol{k},\boldsymbol{k}_1}$. Hence we get

$$\overline{\rho(\boldsymbol{k}-\boldsymbol{k}_1)\rho(\boldsymbol{k}_1-\boldsymbol{k}')} = (N^2\delta_{\boldsymbol{k},\boldsymbol{k}_1}+N)\delta_{\boldsymbol{k},\boldsymbol{k}'}.\tag{128}$$

Let us also consider the $n=3$ case, for which we need to calculate

$$\begin{aligned}&\overline{\rho(\boldsymbol{k}-\boldsymbol{k}_1)\rho(\boldsymbol{k}_1-\boldsymbol{k}_2)\rho(\boldsymbol{k}_2-\boldsymbol{k}')} =\\ &= \sum_{j_1=1}^{N}\sum_{j_2=1}^{N}\sum_{j_3=1}^{N}\prod_{i=1}^{N}\left(\frac{1}{\Omega}\int d^3R_i\right)e^{-i(\boldsymbol{k}-\boldsymbol{k}_1)\cdot\boldsymbol{R}_{j_1}}e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{R}_{j_2}}e^{-i(\boldsymbol{k}_2-\boldsymbol{k}')\cdot\boldsymbol{R}_{j_3}}. \end{aligned}\tag{129}$$

The various cases we need to consider, and the delta functions obtained for each case, are: $j_1 \neq j_2 \neq j_3 \Rightarrow \delta_{\boldsymbol{k}\boldsymbol{k}_1}\delta_{\boldsymbol{k}_1\boldsymbol{k}_2}\delta_{\boldsymbol{k}_2\boldsymbol{k}'}$, $j_1 = j_2 \neq j_3 \Rightarrow \delta_{\boldsymbol{k}\boldsymbol{k}_2}\delta_{\boldsymbol{k}_2\boldsymbol{k}'}$, $j_1 \neq j_2 = j_3 \Rightarrow \delta_{\boldsymbol{k}\boldsymbol{k}_1}\delta_{\boldsymbol{k}_1\boldsymbol{k}'}$, $j_1 = j_3 \neq j_2 \Rightarrow \delta_{\boldsymbol{k}+\boldsymbol{k}_2,\boldsymbol{k}_1+\boldsymbol{k}'}\delta_{\boldsymbol{k}_1\boldsymbol{k}_2}$, $j_1 = j_2 = j_3 \Rightarrow \delta_{\boldsymbol{k}\boldsymbol{k}'}$. Doing the sums in (129) then gives

$$\overline{\rho(\boldsymbol{k}-\boldsymbol{k}_1)\rho(\boldsymbol{k}_1-\boldsymbol{k}_2)\rho(\boldsymbol{k}_2-\boldsymbol{k}')} = (N^3\delta_{\boldsymbol{k}\boldsymbol{k}_1}\delta_{\boldsymbol{k}_1\boldsymbol{k}_2} + N^2\delta_{\boldsymbol{k}\boldsymbol{k}_2} + N^2\delta_{\boldsymbol{k}\boldsymbol{k}_1} + N^2\delta_{\boldsymbol{k}_1\boldsymbol{k}_2} + N)\delta_{\boldsymbol{k}\boldsymbol{k}'} \quad (130)$$

where we have again made approximations like $N(N-1) \approx N^2$ etc and rewritten the delta function products in order to show that all terms contain a $\delta_{\boldsymbol{k}\boldsymbol{k}'}$.

4.5 Impurity-averaged Matsubara Green function: Perturbation series and Feynman diagrams

Each of the terms in the impurity averages will give rise to a term in the perturbation expansion for the Green function. Let us first note that all impurity averages we calculated contain a factor $\delta_{\boldsymbol{k}\boldsymbol{k}'}$, and this is true also for higher orders of n. Thus in contrast to the original Green function $\mathcal{G}(\boldsymbol{k},\boldsymbol{k}')$, the impurity-averaged Green function is diagonal in $\boldsymbol{k}$: $\overline{\mathcal{G}}(\boldsymbol{k},\boldsymbol{k}') = \overline{\mathcal{G}}(\boldsymbol{k})\delta_{\boldsymbol{k}\boldsymbol{k}'}$. This is a consequence of the fact that impurity averaging makes the system translationally invariant: The electrons see the same *average* environment everywhere in the system. The $\boldsymbol{k}$-diagonality is an important simplification resulting from the impurity average.

Apart from this, however, performing the impurity average may not appear at first sight to have made life much easier. It is clear from the averages we have just calculated that the number of terms at a given order, as well as the complexity and diversity of those terms, increase with the order n. How can we keep track of, and make sense of, this proliferation of ever more complicated terms? We will now introduce a graphical representation of the terms in the perturbation expansion for $\overline{\mathcal{G}}(\boldsymbol{k})$ which will be a crucial aid in this task. Thus, each term will be represented by a diagram (conventionally referred to as a **Feynman diagram**), and there will be specific rules (so-called **Feynman rules**) for translating the diagram version of the term into its corresponding mathematical expression (and vice versa). The diagrams will give us an intuitive physical interpretation of the terms in the perturbation expansion. In the beginning, as one familiarizes oneself with these concepts, one will need to start with the mathematical expressions and construct the diagrams from them. However, as one gains more experience one will be able to generate the diagrams first and then translate them into expressions, which will save a lot of time in the analysis.

4.5.1 Feynman rules for diagrams contributing to $\overline{\mathcal{G}^{(n)}}(\boldsymbol{k})$

By investigating the terms in the perturbation expansion for the impurity-averaged Green function, one can deduce the following Feynman rules.

Each diagram has

- $n+1$ directed full lines (representing electrons) laid end to end
- n directed dashed lines (representing interactions), which end at the junction between two electron lines, and begin at one of

- $m \leq n$ crosses (representing impurities).

Both the full (electron) lines and the dashed (interaction) lines are labelled by momenta. To generate all diagrams for a given m one connects the n interaction lines with the m crosses in all possible topologically different ways. One carries out this procedure for each m satisfying $1 \leq m \leq n$.

For a given diagram, the Feynman rules are:

- For each electron line of momentum $\boldsymbol{k}'$, associate a factor $\mathcal{G}^{(0)}(\boldsymbol{k}')$. The leftmost and rightmost electron lines both have momentum $\boldsymbol{k}$.
- For each interaction line of momentum $\boldsymbol{q}$, associate a factor $U(\boldsymbol{q})$.
- For each impurity cross, associate a factor N.
- At each electron vertex (junction between two electron lines and an interaction line), the momentum of the outgoing electron line must equal the sum of the momentum of the incoming electron line and the momentum of the incoming interaction line. I.e. there is momentum conservation at each electron vertex.
- At each impurity vertex (cross) the sum of the momenta of the connected outgoing interaction lines must equal zero. I.e. there is momentum conservation at each impurity vertex.
- Sum over all momenta that are left undetermined by momentum conservation.

4.5.2 Low-order Feynman diagrams

To illustrate these rules, we write down the expressions for all the terms in the series for orders $n = 1$, 2, and 3. At each order n, these are obtained simply by inserting the results for the impurity average at that order (calculated in the previous section) into Eq. (120). We list the terms in the same order as we listed the terms in the impurity averages in the previous section. The corresponding Feynman diagrams are shown in Fig. 1. You should make sure you understand how to translate between the series and the diagrams using the Feynman rules.[10]

For $n = 1$ we only have one term:

$$\mathcal{G}^{(0)}(\boldsymbol{k})NU(0)\mathcal{G}^{(0)}(\boldsymbol{k}) \qquad \text{(term 1)} \tag{131}$$

For $n = 2$ there are two terms:

$$\mathcal{G}^{(0)}(\boldsymbol{k})NU(0)\mathcal{G}^{(0)}(\boldsymbol{k})NU(0)\mathcal{G}^{(0)}(\boldsymbol{k}) \qquad \text{(term 2a)} \tag{132}$$

$$\sum_{\boldsymbol{k}_1}\mathcal{G}^{(0)}(\boldsymbol{k})NU(\boldsymbol{k}-\boldsymbol{k}_1)\mathcal{G}^{(0)}(\boldsymbol{k}_1)U(\boldsymbol{k}_1-\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k}) \qquad \text{(term 2b)} \tag{133}$$

---

[10] Note that there is also one diagram for order $n = 0$. This diagram, which has not been included in Fig. 1, is just an electron line and represents $\mathcal{G}^{(0)}(\boldsymbol{k})$.

For $n = 3$ there are five terms:

$$\mathcal{G}^{(0)}(\boldsymbol{k})NU(0)\mathcal{G}^{(0)}(\boldsymbol{k})NU(0)\mathcal{G}^{(0)}(\boldsymbol{k})NU(0)\mathcal{G}^{(0)}(\boldsymbol{k}) \qquad \text{(term 3a)} \tag{134}$$

$$\sum_{\boldsymbol{k}_1}\mathcal{G}^{(0)}(\boldsymbol{k})NU(\boldsymbol{k}-\boldsymbol{k}_1)\mathcal{G}^{(0)}(\boldsymbol{k}_1)U(\boldsymbol{k}_1-\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k})NU(0)\mathcal{G}^{(0)}(\boldsymbol{k}) \qquad \text{(term 3b)} \tag{135}$$

$$\sum_{\boldsymbol{k}_1}\mathcal{G}^{(0)}(\boldsymbol{k})NU(0)\mathcal{G}^{(0)}(\boldsymbol{k})NU(\boldsymbol{k}-\boldsymbol{k}_1)\mathcal{G}^{(0)}(\boldsymbol{k}_1)U(\boldsymbol{k}_1-\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k}) \qquad \text{(term 3c)} \tag{136}$$

$$\sum_{\boldsymbol{k}_1}\mathcal{G}^{(0)}(\boldsymbol{k})NU(\boldsymbol{k}-\boldsymbol{k}_1)\mathcal{G}^{(0)}(\boldsymbol{k}_1)NU(0)\mathcal{G}^{(0)}(\boldsymbol{k}_1)U(\boldsymbol{k}_1-\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k}) \qquad \text{(term 3d)} \tag{137}$$

$$\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2}\mathcal{G}^{(0)}(\boldsymbol{k})NU(\boldsymbol{k}-\boldsymbol{k}_1)\mathcal{G}^{(0)}(\boldsymbol{k}_1)U(\boldsymbol{k}_1-\boldsymbol{k}_2)\mathcal{G}^{(0)}(\boldsymbol{k}_2)U(\boldsymbol{k}_2-\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k}) \qquad \text{(term 3e)} \tag{138}$$

In each expression we have tried to keep the order of the factors as much as possible in accordance with the appearance of the corresponding diagram (this order is of course immaterial for the actual value of the expression).

Note that some of the diagrams in the perturbation series correspond to the same mathematical expression. Among the diagrams shown here, this is the case for diagrams 3b and 3c.

4.6 Irreducible diagrams, the self-energy, and the Dyson equation

By inspecting the terms in the perturbation series and the corresponding diagrams, one can see that some diagrams are composed by essentially concatenating, in various ways, diagrams appearing at lower order in the expansion. This implies that there exist diagrammatic "building blocks" which can be used to generate all the diagrams and thus the entire perturbation expansion. This will lead to some very essential further simplifications.

Let us first define the concept of an **irreducible diagram**. This is a diagram that *cannot* be cut in two pieces by only cutting a single *internal* electron line. (The leftmost and rightmost electron lines in a diagram are called external, all other electron lines are called internal.) If a diagram is not irreducible it is referred to as reducible. The irreducible diagrams in Fig. 1 are 1, 2b, 3d and 3e. All the others are reducible as they can be cut across an internal electron line (diagram 3a can in fact be cut in two different places). The cutting of a reducible diagram into two pieces along a single internal electron line is illustrated for diagram (3b) in Fig. 2.

Next we define the concept of a **self-energy diagram**. This is an irreducible diagram with the two *external* electron lines removed. Thus from Fig. 1 one finds one self-energy diagram at first order, one at second, and two at third order. We can find a mathematical expression for the self-energy diagram by using the Feynman rules. It is the same as that of the irreducible diagram it was constructed from except that the two factors of $\mathcal{G}^{(0)}(\boldsymbol{k})$ due to the external lines are removed.

Finally, we define the **self-energy** $\Sigma(\boldsymbol{k})$ as the sum of all self-energy diagrams (there is an infinite number of such diagrams). Denoting the self-energy diagrams as $\Sigma^{(i)}(\boldsymbol{k})$, $i = 1, 2, 3, \ldots$, the self-energy can be written

$$\Sigma(\boldsymbol{k}) = \sum_i \Sigma^{(i)}(\boldsymbol{k}). \tag{139}$$

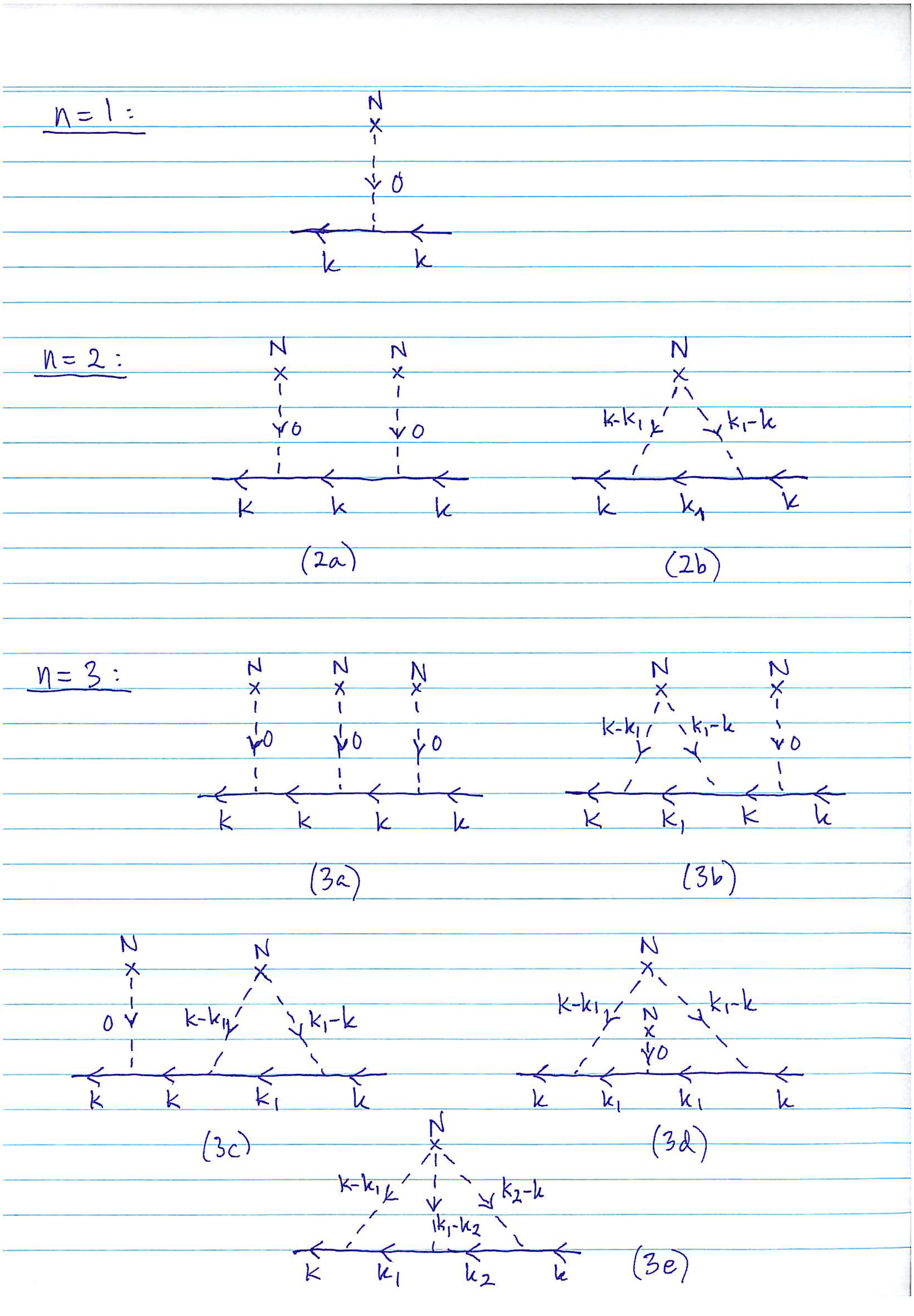

Figure 1: Feynman diagrams for $\overline{\mathcal{G}^{(n)}(\boldsymbol{k})}$ for orders $n = 1, 2, 3$. We have indicated the momenta of the unperturbed Green functions and of the interaction lines, and the factor N associated with each impurity.

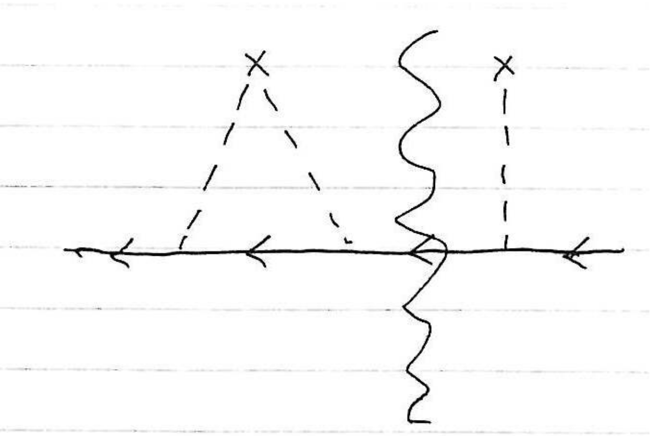

Figure 2: Cutting the reducible diagram (3b) into two pieces along the internal electron line (the cut is shown as a wiggly line).

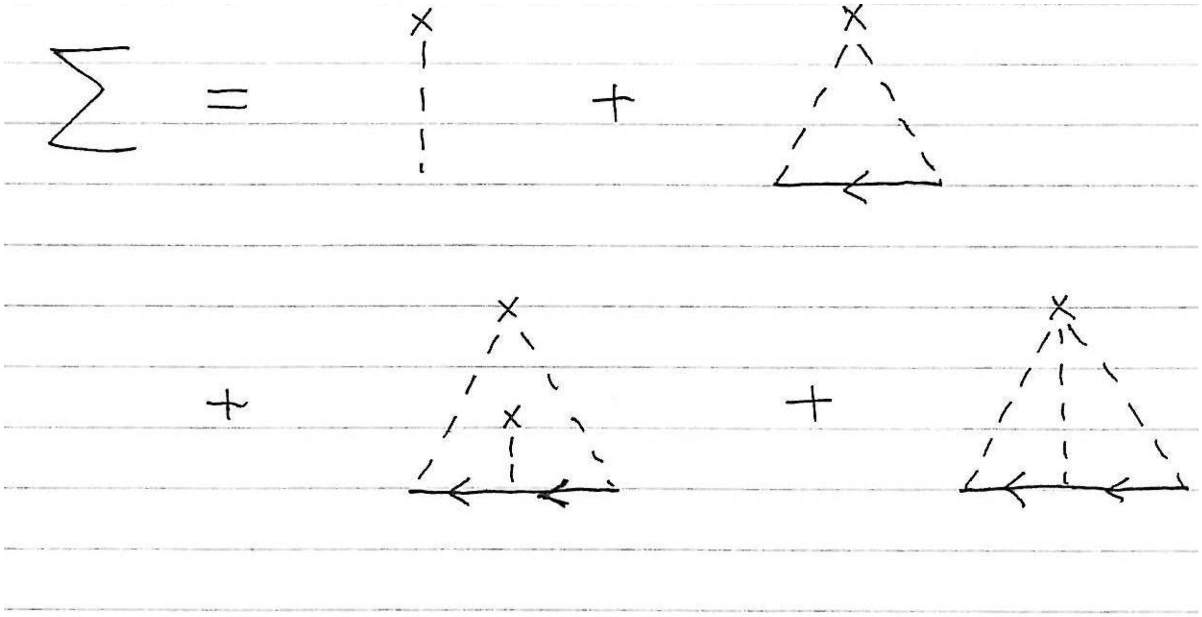

Figure 3: Self-energy up to and including terms of order $n = 3$.

The self-energy up to and including terms of order $n = 3$ is shown in Fig. 3.

An arbitrary term in $\overline{\mathcal{G}}(\boldsymbol{k})$ can now be written on the form (convince yourself that this is true, e.g. by looking at the diagrams in Fig. 1)

$$\mathcal{G}^{(0)}(\boldsymbol{k})\Sigma^{(i)}(\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k})\Sigma^{(j)}(\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k})\cdots\mathcal{G}^{(0)}(\boldsymbol{k})\Sigma^{(\ell)}(\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k}); \tag{140}$$

the number of self-energy factors here can be $0, 1, 2, \ldots$ depending on the term. Note that there is a factor of $\mathcal{G}^{(0)}$ on both sides of every self-energy factor, and that the momenta of all Green functions and self-energy factors are the same ($\boldsymbol{k}$). The entire perturbation expansion for $\overline{\mathcal{G}}(\boldsymbol{k})$ can then be obtained by summing over all such terms and over all the self-energy diagrams in each term:

$$\begin{aligned}
\overline{\mathcal{G}}(\boldsymbol{k}) &= \mathcal{G}^{(0)}(\boldsymbol{k}) + \sum_i \mathcal{G}^{(0)}(\boldsymbol{k})\Sigma^{(i)}(\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k}) + \sum_{i,j} \mathcal{G}^{(0)}(\boldsymbol{k})\Sigma^{(i)}(\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k})\Sigma^{(j)}(\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k}) \\
&+ \sum_{i,j,k} \mathcal{G}^{(0)}(\boldsymbol{k})\Sigma^{(i)}(\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k})\Sigma^{(j)}(\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k})\Sigma^{(k)}(\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k}) + \cdots \\
&= \mathcal{G}^{(0)}(\boldsymbol{k}) + \mathcal{G}^{(0)}(\boldsymbol{k})\Sigma(\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k}) + \mathcal{G}^{(0)}(\boldsymbol{k})\Sigma(\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k})\Sigma(\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k}) \\
&+ \mathcal{G}^{(0)}(\boldsymbol{k})\Sigma(\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k})\Sigma(\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k})\Sigma(\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k}) + \cdots \\
&= \mathcal{G}^{(0)}(\boldsymbol{k}) + \mathcal{G}^{(0)}(\boldsymbol{k})\Sigma(\boldsymbol{k})[\mathcal{G}^{(0)}(\boldsymbol{k}) + \mathcal{G}^{(0)}(\boldsymbol{k})\Sigma(\boldsymbol{k})\mathcal{G}^{(0)}(\boldsymbol{k}) + \cdots]. \qquad (141)
\end{aligned}$$

We recognize the expression inside square brackets as the expansion of $\overline{\mathcal{G}}(\boldsymbol{k})$ itself, so that we finally get

$$\overline{\mathcal{G}}(\boldsymbol{k}) = \mathcal{G}^{(0)}(\boldsymbol{k}) + \mathcal{G}^{(0)}(\boldsymbol{k})\Sigma(\boldsymbol{k})\overline{\mathcal{G}}(\boldsymbol{k}). \qquad (142)$$

This is the **Dyson equation**. It is easily solved to give

$$\overline{\mathcal{G}}(\boldsymbol{k}, ip_m) = \frac{1}{(\mathcal{G}^{(0)}(\boldsymbol{k}, ip_m))^{-1} - \Sigma(\boldsymbol{k}, ip_m)} = \frac{1}{ip_m - \xi_{\boldsymbol{k}} - \Sigma(\boldsymbol{k}, ip_m)}, \qquad (143)$$

where we have reinstated the ip_m variable which we dropped earlier.

In general the self-energy is complex. As we will see examples of later, the real part of the self-energy gives rise to a shift in the energy $\xi_{\boldsymbol{k}}$, while the imaginary part gives rise to a finite lifetime.

We have no hope of finding the exact Green function, as that would require calculating the exact self-energy as the sum of all self-energy diagrams. However, approximating the self-energy by the sum of just a subset (finite or infinite) of all the self-energy diagrams does give us an approximation for the Green function through the Dyson equation. Note that even when the number of self-energy diagrams included in this way is *finite* (e.g. we may include just one or two terms in the self-energy; see below), it still corresponds to summing an *infinite* number of terms in the expansion for the Green function, as seen by iterating the Dyson equation using the approximate self-energy.

4.7 Low-density weak-scattering approximation for the self-energy

We will now consider an approximation for the self-energy that is appropriate in the limit of low impurity density $n_{\text{imp}} \equiv N/\Omega$ and weak scattering potential $U(\boldsymbol{r})$. In this case it suffices to include the first two terms in the self-energy in Fig. 3. These are of first and second order in U (as they have one and two interaction lines, respectively) and are thus the leading terms at small U (as we'll see soon, the reason it's necessary to include the self-energy diagram of second order in U is because the first order term is rather trivial and does not give rise to a finite lifetime). They are also of first order in the impurity density n_{imp} because they only have one impurity cross; a self-energy diagram with m crosses will be of order n_{imp}^m. Self-energy diagrams with more than one cross can therefore be neglected in the low-density limit.

To understand why each impurity cross is associated with a factor $n_{\rm imp}$, first note that from the Feynman rules, a diagram of order n with m impurity crosses has n factors of $U(\boldsymbol{q}_i)$ and m factors of N. Let us separate out the inverse volume $1/\Omega$ from $U(\boldsymbol{q})$ (see Eq. (115)) by defining $U(\boldsymbol{q}) \equiv (1/\Omega)u(\boldsymbol{q})$. This shows that the diagram also comes with n factors of $1/\Omega$. Now consider the Feynman diagrams in Fig. 1. Note that a diagram of order n with m impurity crosses contains $n-m$ summations over internal momenta. This is valid in general, not just for the diagrams in this figure. We now associate one factor of $1/\Omega$ with each of these summations over an internal momentum; this uses up $n-m$ of these factors.[11] The remaining m factors of $1/\Omega$ are associated with the m impurity crosses. Thus each impurity cross comes with a factor $N/\Omega = n_{\rm imp}$.

Let us now evaluate the self-energy diagrams we will consider. We start with the first diagram in the self-energy in Fig. 3. Using the Feynman rules it is given by

$$\Sigma^{(1)}(\boldsymbol{k}, ip_n) = NU(0) = n_{\rm imp}u(0) \equiv n_{\rm imp}u \tag{144}$$

where we defined $u(0) \equiv u$. We see that in fact this diagram depends on neither $\boldsymbol{k}$ nor ip_n. When inserted into the Dyson equation, it is seen to just correspond to a constant energy shift $\xi_{\boldsymbol{k}} \to \xi_{\boldsymbol{k}} + \Sigma^{(1)}$.

The second diagram in Fig. 3 is a little more complicated. It is given by

$$\begin{aligned}\Sigma^{(2)}(\boldsymbol{k}, ip_n) &= N\sum_{\boldsymbol{k}_1} U(\boldsymbol{k}_1-\boldsymbol{k})U(\boldsymbol{k}-\boldsymbol{k}_1)\mathcal{G}^{(0)}(\boldsymbol{k}_1) = n_{\rm imp}\frac{1}{\Omega}\sum_{\boldsymbol{k}_1}|u(\boldsymbol{k}-\boldsymbol{k}_1)|^2\frac{1}{ip_n-\xi_{\boldsymbol{k}_1}}\\ &= -n_{\rm imp}\frac{1}{\Omega}\sum_{\boldsymbol{k}_1}|u(\boldsymbol{k}-\boldsymbol{k}_1)|^2\frac{\xi_{\boldsymbol{k}_1}+ip_n}{\xi_{\boldsymbol{k}_1}^2+p_n^2}.\end{aligned} \tag{145}$$

Let us for simplicity consider a very short-ranged potential $U(\boldsymbol{r})$, so that we may to a good approximation neglect the momentum dependence of $|u(\boldsymbol{k}-\boldsymbol{k}_1)|^2$ so that this factor can be taken outside the $\boldsymbol{k}_1$ summation. Next let us introduce the density of states

$$D(\xi) = \frac{1}{\Omega}\sum_{\boldsymbol{k}}\delta(\xi_{\boldsymbol{k}}-\xi). \tag{146}$$

This gives

$$\Sigma^{(2)}(\boldsymbol{k}, ip_n) = -n_{\rm imp}u^2\int_{-\infty}^{\infty}d\xi\; D(\xi)\frac{\xi+ip_n}{\xi^2+p_n^2}. \tag{147}$$

We will evaluate this integral approximately by replacing $D(\xi)$ by its value at the Fermi level $\xi = 0$ where $(\xi^2+p_n^2)^{-1}$ is largest. In this approximation the real part of $\Sigma^{(2)}$ will vanish, since the integrand becomes odd in ξ. We thus get

$$\Sigma^{(2)}(\boldsymbol{k}, ip_n) = -ip_n\; n_{\rm imp}u^2D(0)\underbrace{\int_{-\infty}^{\infty}\frac{d\xi}{\xi^2+p_n^2}}_{\pi/|p_n|} = -i\pi\frac{p_n}{|p_n|}n_{\rm imp}u^2D(0) = -\frac{i}{2\tau}\mathrm{sgn}(p_n), \tag{148}$$

where we have defined

$$\frac{1}{\tau} \equiv 2\pi\, n_{\rm imp}u^2D(0). \tag{149}$$

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[11] Therefore each summation over an internal momentum $\boldsymbol{k}_i$ can be written $(1/\Omega)\sum_{\boldsymbol{k}_i} = 1/(2\pi)^3\int d^3k_i$.

Inserting this into the Dyson equation gives

$$\overline{\mathcal{G}}(\boldsymbol{k}, ip_n) = \frac{1}{ip_n - \xi_{\boldsymbol{k}} - \Sigma(\boldsymbol{k}, ip_n)} = \frac{1}{ip_n - \xi_{\boldsymbol{k}} - n_{\mathrm{imp}}u + \frac{i}{2\tau}\mathrm{sgn}(p_n)}. \tag{150}$$

Below we will see that the parameter τ can be interpreted as a lifetime.

4.8 The impurity-averaged retarded Green function and its spectral function

We now want to find the impurity-averaged retarded Green function $\overline{G^R}(\boldsymbol{k}, \omega)$. From Sec. 3.4 we know that it is given by

$$\overline{G^R}(\boldsymbol{k}, \omega) = \overline{\mathcal{G}}(\boldsymbol{k}, ip_n)|_{ip_n \to \omega + i\eta}. \tag{151}$$

To do this analytic continuation we note that p_n appears in two places in (150): in the term ip_n and in the factor $\mathrm{sgn}(p_n)$. For the former the analytic continuation is just $ip_n \to \omega + i\eta$. For $\mathrm{sgn}(p_n)$ we first write this as a function of ip_n:

$$\mathrm{sgn}(p_n) = \mathrm{sgn}(\mathrm{Im}(ip_n)). \tag{152}$$

Thus the analytic continuation gives, for ω real,

$$\mathrm{sgn}(\mathrm{Im}(ip_n) \to \mathrm{sgn}(\mathrm{Im}(\omega + i\eta)) = \mathrm{sgn}(\eta) = +1, \tag{153}$$

where we used that $\eta = 0^+$. Thus for ω on the real axis,

$$\overline{G^R}(\boldsymbol{k}, \omega) = \frac{1}{\omega - \xi_{\boldsymbol{k}} - n_{\mathrm{imp}}u + \frac{i}{2\tau}}. \tag{154}$$

Here the infinitesimal imaginary term $i\eta$ in the denominator could be neglected in comparison to the finite imaginary term $i/(2\tau)$. Let us now calculate $\overline{G^R}(\boldsymbol{k}, t)$, given by

$$\overline{G^R}(\boldsymbol{k}, t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\; e^{-i\omega t}\overline{G^R}(\boldsymbol{k}, \omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\; \frac{e^{-i\omega t}}{\omega - \xi_{\boldsymbol{k}} - n_{\mathrm{imp}}u + \frac{i}{2\tau}}. \tag{155}$$

We can evaluate this integral using contour integration. We note that the integrand has a pole in the lower half plane at $\omega = \xi_{\boldsymbol{k}} + n_{\mathrm{imp}}u - \frac{i}{2\tau}$. From the factor $e^{-i\omega t} = \exp(-it\mathrm{Re}\,\omega)\exp(t\mathrm{Im}\,\omega)$ we see that for $t < 0$ we have to close the contour in the upper half plane. The contour then encloses no poles so that according to the residue theorem the integral is zero. On the other hand, when $t > 0$ we have to close the contour in the lower half plane. Using the residue theorem, we then pick up the residue of the pole in the lower half plane, giving

$$\overline{G^R}(\boldsymbol{k}, t) = \frac{1}{2\pi} \cdot 2\pi i(-1)e^{-i(\xi_{\boldsymbol{k}} + n_{\mathrm{imp}}u - \frac{i}{2\tau})t} \quad (t > 0), \tag{156}$$

here the (-1) comes from the contour being clockwise in this case. Thus we get

$$\overline{G^R}(\boldsymbol{k}, t) = -i\theta(t)e^{-i(\xi_{\boldsymbol{k}} + n_{\mathrm{imp}}u)t}e^{-t/(2\tau)}. \tag{157}$$

Thus the retarded Green function is decaying in time; the finite lifetime comes from a nonzero imaginary part of the self-energy. There is also a shift in the energy coming from the real part of the self-energy.

We can also find the spectral function of $\overline{G^R}(\boldsymbol{k},\omega)$:

$$\overline{A}(\boldsymbol{k},\omega) = -\frac{1}{\pi}\mathrm{Im}\,\overline{G^R}(\boldsymbol{k},\omega) = \frac{1}{\pi}\frac{1/2\tau}{(\omega-(\xi_{\boldsymbol{k}}+n_{\mathrm{imp}}u))^2+(1/2\tau)^2}. \tag{158}$$

This is a Lorentzian peaked at $\omega = \xi_{\boldsymbol{k}} + n_{\mathrm{imp}}u$ and with a width proportional to τ^{-1}. These results are interpreted as follows: The free electrons are turned into "*quasi-particles*" by the impurity scattering. The quasiparticles have an energy $\xi^*_{\boldsymbol{k}} = \xi_{\boldsymbol{k}} + n_{\mathrm{imp}}u$ and a finite lifetime τ.

4.9 An example of linear response theory and two-particle Green functions: The Kubo formula for the electrical conductivity

If an electric field of magnitude E is applied to a metal, the resulting current density J is given by

$$J = \sigma E \tag{159}$$

where σ is the conductivity. This is just a different way of writing Ohm's law $I = V/R$; the resistance R is proportional to the resistivity which is the inverse of the conductivity. Eq. (159) is an example of *linear response*; the response (J) to the applied field (E) is proportional to the applied field; the proportionality constant (σ) is thus an example of a response function (cf. Sec. 1.1).

We will show that the conductivity can be expressed in terms of a retarded current-current correlation function, which is a type of two-particle retarded Green function. The result we will arrive at is known as the Kubo formula for the conductivity. Let us start by considering a system with Hamiltonian H. For now this will be taken to be unspecified; the only thing we will assume is that it is not explicitly time-dependent. (Eventually we will take H to be given by the impurity scattering Hamiltonian (108)). Next we assume that this system is being acted on by some external applied field. We assume that the coupling of this applied field to the system occurs through a Hamiltonian H_{ext} which can have an explicit time dependence (which we don't indicate in the notation) because the applied field can vary with time. Furthermore we assume that H_{ext} is turned on "infinitely slowly", starting at time $t_0 = -\infty$, so that at that initial time the external field was not present and the system was then in the ground state of H. The total Hamiltonian is then

$$H_{\mathrm{tot}} = H + H_{\mathrm{ext}}. \tag{160}$$

The state $|\Psi(t)\rangle$ of the system evolves in time according to the time-dependent Schrödinger equation with H_{tot} as the Hamiltonian:

$$i\frac{\partial}{\partial t}|\Psi(t)\rangle = H_{\mathrm{tot}}|\Psi(t)\rangle, \tag{161}$$

where we have set $\hbar = 1$ as usual. Let us now define

$$|\Psi_H(t)\rangle = e^{iHt}|\Psi(t)\rangle. \tag{162}$$

One can show from (161) that the time evolution of $|\Psi_H(t)\rangle$ is given by

$$i\frac{\partial}{\partial t}|\Psi_H(t)\rangle = H_{\text{ext}}(t)|\Psi_H(t)\rangle \tag{163}$$

where we have defined

$$H_{\text{ext}}(t) \equiv e^{iHt}H_{\text{ext}}e^{-iHt}. \tag{164}$$

Note that the time dependence of $H_{\text{ext}}(t)$ comes from two sources: the factors $e^{\pm iHt}$ in its definition and the explicit time dependence of H_{ext} itself (which we haven't indicated in the notation). We see from (163) that if H_{ext} were zero, $|\Psi_H(t)\rangle$ would be time-independent. Eq. (163) can be integrated to give

$$|\Psi_H(t)\rangle = |\Psi_H(-\infty)\rangle - i\int_{-\infty}^{t} dt'\, H_{\text{ext}}(t')|\Psi_H(t')\rangle \tag{165}$$

where we have taken the initial time to be $-\infty$, when the external field was zero and we assume that the system was in the ground state of H. We will assume that H_{ext} is linear in the applied field. If it also were to contain terms of higher order in the applied field, those terms can be neglected since we only want to find the leading, i.e. linear, response to the applied field, which should be sufficient in the limit when the applied field is sufficiently weak. Thus it is sufficient to find $|\Psi_H(t)\rangle$ to linear order in H_{ext}. Since the 2nd term on the rhs in (165) already contains a factor H_{ext} we can therefore take $H_{\text{ext}} = 0$ when evaluating $|\Psi_H(t')\rangle$ in that integral, which gives [from (163)] $|\Psi_H(t')\rangle = |\Psi_H(-\infty)\rangle$. Defining $|\Psi_H(-\infty)\rangle = |\Psi_H\rangle$ (the ground state of H) we thus get to linear order in H_{ext},

$$|\Psi_H(t)\rangle = |\Psi_H\rangle - i\int_{-\infty}^{t} dt'\, H_{\text{ext}}(t')|\Psi_H\rangle. \tag{166}$$

Now let us find an expression for the expectation value of an operator $o(\boldsymbol{r})$ in the state $|\Psi(t)\rangle$,

$$O(\boldsymbol{r},t) \equiv \langle\Psi(t)|o(\boldsymbol{r})|\Psi(t)\rangle = \langle\Psi_H(t)|e^{iHt}o(\boldsymbol{r})e^{-iHt}|\Psi_H(t)\rangle = \langle\Psi_H(t)|o(\boldsymbol{r},t)|\Psi_H(t)\rangle. \tag{167}$$

Again, we just want the linear response, so inserting (166) and keeping only terms that are first order in H_{ext} gives

$$O(\boldsymbol{r},t) = \langle o(\boldsymbol{r},t)\rangle - i\int_{-\infty}^{t} dt'\,\langle[o(\boldsymbol{r},t), H_{\text{ext}}(t')]\rangle \tag{168}$$

where all the expectation values on the rhs are with respect to $|\Psi_H\rangle$, the ground state of H. This is an important point: The linear response is determined by an expectation value with respect to the *unperturbed* system (i.e. the system in the absence of the external applied field). This is as far as we can get on general grounds. To make further progress we must specify what $o(\boldsymbol{r})$ and H_{ext} are.

We will take $o(\boldsymbol{r})$ to be a component of the current operator[12] $\boldsymbol{j}(\boldsymbol{r})$ and H_{ext} to be the Hamiltonian describing how an electric field couples to the system to linear order. Let us

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[12] Strictly speaking we mean the current density operator, but for simplicity we will refer to it as the current operator.

first consider the current operator. For a system of "classical" electrons it would be given by

$$\boldsymbol{j}(\boldsymbol{r}) = \frac{e}{m}\sum_{i=1}^{N_e}(\boldsymbol{p}_i - e\boldsymbol{A}(\boldsymbol{r}_i))\delta(\boldsymbol{r}-\boldsymbol{r}_i). \tag{169}$$

Here e is the electron charge (i.e. $e = -|e| < 0$), m is the electron mass, $\boldsymbol{r}_i$ and $\boldsymbol{p}_i$ are the position and momentum of the i'th electron, and $\boldsymbol{A}$ is the vector potential. We are interested in the current response to an electric field $\boldsymbol{E}$ which can be expressed in terms of the vector potential as $\boldsymbol{E} = -\partial\boldsymbol{A}/\partial t$. The scalar electromagnetic potential ϕ is not needed and can be set to zero.

In "first quantization" the current operator can be written

$$\boldsymbol{j}(\boldsymbol{r}) = \boldsymbol{j}^P(\boldsymbol{r}) + \boldsymbol{j}^D(\boldsymbol{r}) \tag{170}$$

where

$$\begin{aligned}
\boldsymbol{j}^P(\boldsymbol{r}) &= \frac{e}{2m}\sum_i[\boldsymbol{p}_i\delta(\boldsymbol{r}-\boldsymbol{r}_i) + \delta(\boldsymbol{r}-\boldsymbol{r}_i)\boldsymbol{p}_i], &(171)\\
\boldsymbol{j}^D(\boldsymbol{r}) &= -\frac{e^2}{m}\sum_i\boldsymbol{A}(\boldsymbol{r}_i)\delta(\boldsymbol{r}-\boldsymbol{r}_i). &(172)
\end{aligned}$$

Here we have separated the current operator into a "paramagnetic" and "diamagnetic" part (this could have been done already in the classical expression above). In these expressions $\boldsymbol{r}_i$ and $\boldsymbol{p}_i$ are quantum-mechanical operators ($\boldsymbol{r}_i \to \boldsymbol{r}_i$, $\boldsymbol{p}_i \to -i\nabla_i$). Since they don't commute their order matters. This is why in $\boldsymbol{j}^P(\boldsymbol{r})$ they appear in a symmetrized way; this is necessary for $\boldsymbol{j}^P(\boldsymbol{r})$ to be a Hermitian operator.

In "second quantization" these current operators can be shown to be given by

$$\begin{aligned}
\boldsymbol{j}^P(\boldsymbol{r}) &= -\frac{ie}{2m}\sum_\sigma\left(\psi_\sigma^\dagger(\boldsymbol{r})\nabla\psi_\sigma(\boldsymbol{r}) - [\nabla\psi_\sigma^\dagger(\boldsymbol{r})]\psi_\sigma(\boldsymbol{r})\right), &(173)\\
\boldsymbol{j}^D(\boldsymbol{r}) &= -\frac{e^2}{m}\boldsymbol{A}(\boldsymbol{r})\sum_\sigma\psi_\sigma^\dagger(\boldsymbol{r})\psi_\sigma(\boldsymbol{r}), &(174)
\end{aligned}$$

where $\psi_\sigma^\dagger(\boldsymbol{r})$ and $\psi_\sigma(\boldsymbol{r})$ respectively create and annihilate an electron with spin projection σ at position $\boldsymbol{r}$.

Next let us consider how the vector potential enters the Hamiltonian. This happens through the term

$$\sum_i\frac{1}{2m}(\boldsymbol{p}_i - e\boldsymbol{A}(\boldsymbol{r}_i))^2. \tag{175}$$

This form is valid in both classical mechanics and quantum mechanics, if one interprets $\boldsymbol{r}_i$ and $\boldsymbol{p}_i$ appropriately (i.e. as operators in the latter case). In second quantization this term becomes

$$\frac{1}{2m}\sum_\sigma\int d\boldsymbol{r}\ \psi_\sigma^\dagger(\boldsymbol{r})(-i\nabla - e\boldsymbol{A}(\boldsymbol{r}))^2\psi_\sigma(\boldsymbol{r}). \tag{176}$$

From this H_{ext} can be extracted as the part that is linear in $\boldsymbol{A}$. This gives

$$H_{\text{ext}} = -\int d\boldsymbol{r} \boldsymbol{j}^P(\boldsymbol{r}) \cdot \boldsymbol{A}(\boldsymbol{r}) = -\int d\boldsymbol{r} \sum_{\beta=x,y,z} j^P_\beta(\boldsymbol{r}) A_\beta(\boldsymbol{r}). \tag{177}$$

Now we take $o(\boldsymbol{r}) = j_\alpha(\boldsymbol{r})$ in (168) where $\alpha = x$, y, or z. Inserting our expressions for the current operators and H_{ext} gives

$$J_\alpha(\boldsymbol{r}, t) = \langle j_\alpha(\boldsymbol{r}, t)\rangle - i \int_{-\infty}^{t} dt' \, \langle [j_\alpha(\boldsymbol{r}, t), -\int d\boldsymbol{r}' \sum_{\beta=x,y,z} j^P_\beta(\boldsymbol{r}', t') A_\beta(\boldsymbol{r}', t')]\rangle. \tag{178}$$

Here we have also introduced the explicit time dependence of $\boldsymbol{A}$ (which we haven't indicated earlier in order not to clutter the notation). However, this is not yet the linear response result. First of all, since the commutator already contains an explicit factor of $\boldsymbol{A}$, we can omit the diamagnetic part of $j_\alpha(\boldsymbol{r}, t)$ since it would lead to a contribution that is quadratic in $\boldsymbol{A}$. Thus we can replace $j_\alpha(\boldsymbol{r}, t) \to j^P_\alpha(\boldsymbol{r}, t)$ in the commutator. Second, $\langle j_\alpha(\boldsymbol{r}, t)\rangle = \langle j^D_\alpha(\boldsymbol{r}, t)\rangle$ since $\langle j^P_\alpha(\boldsymbol{r}, t)\rangle = 0$ (because there is no current in the absence of an electric field). We also use that

$$\langle \sum_\sigma \psi^\dagger(\boldsymbol{r}, t)\psi_\sigma(\boldsymbol{r}, t)\rangle = n(\boldsymbol{r}), \tag{179}$$

where $n(\boldsymbol{r})$ is the electron density at the point $\boldsymbol{r}$ (the expectation value is time-independent since H is time-independent). Furthermore, we can extend the upper limit in the t' integration to ∞ by introducing a factor $\theta(t - t')$ into the integrand. This gives

$$J_\alpha(\boldsymbol{r}, t) = -\sum_\beta \int_{-\infty}^{\infty} dt' \int d\boldsymbol{r}' \, \Pi^R_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}'; t - t') A_\beta(\boldsymbol{r}', t') - \frac{e^2}{m} n(\boldsymbol{r}) A_\alpha(\boldsymbol{r}, t), \tag{180}$$

where we have introduced the retarded current-current correlation function

$$\Pi^R_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}'; t - t') = -i\theta(t - t')\langle [j^P_\alpha(\boldsymbol{r}, t), j^P_\beta(\boldsymbol{r}', t']\rangle. \tag{181}$$

As indicated this correlation function depends only on the time *difference* $t - t'$ since H is time-independent. We now take the time Fourier transform of (180). The Fourier transform of the time convolution is the product of the Fourier transforms of each factor, giving

$$J_\alpha(\boldsymbol{r}, \omega) = -\sum_\beta \int d\boldsymbol{r}' \, \Pi^R_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}'; \omega) A_\beta(\boldsymbol{r}', \omega) - \frac{e^2}{m} n(\boldsymbol{r}) A_\alpha(\boldsymbol{r}, \omega). \tag{182}$$

Next, from $\boldsymbol{E}(\boldsymbol{r}, t) = -\partial \boldsymbol{A}(\boldsymbol{r}, t)/\partial t$ we get, for $\boldsymbol{A}(\boldsymbol{r}, t) = \boldsymbol{A}(\boldsymbol{r}, \omega)e^{-i\omega t} + \text{c.c.}$,

$$\begin{aligned} \boldsymbol{E}(\boldsymbol{r}, t) &= -\frac{\partial}{\partial t}(\boldsymbol{A}(\boldsymbol{r}, \omega)e^{-i\omega t} + \text{c.c.}) = -(-i\omega \boldsymbol{A}(\boldsymbol{r}, \omega)e^{-i\omega t} + c.c.) \equiv \boldsymbol{E}(\boldsymbol{r}, \omega)e^{-i\omega t} + \text{c.c.} \\ &\Rightarrow \boldsymbol{E}(\boldsymbol{r}, \omega) = i\omega \boldsymbol{A}(\boldsymbol{r}, \omega). \end{aligned} \tag{183}$$

Using this in (182) we can write

$$J_\alpha(\boldsymbol{r}, \omega) = \sum_\beta \frac{i}{\omega} \left[\int d\boldsymbol{r}' \, \Pi^R_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}'; \omega) E_\beta(\boldsymbol{r}', \omega) + \frac{e^2}{m} n(\boldsymbol{r}) \delta_{\alpha\beta} E_\beta(\boldsymbol{r}, \omega) \right]. \tag{184}$$

Finally, if we average over the impurity positions the system becomes translationally invariant, and therefore

$$
\begin{aligned}
\Pi^R(\boldsymbol{r},\boldsymbol{r}';\omega) &\rightarrow \bar{\Pi}^R(\boldsymbol{r},\boldsymbol{r}';\omega) = \bar{\Pi}^R(\boldsymbol{r}-\boldsymbol{r}',\omega), && (185)\\
n(\boldsymbol{r}) &\rightarrow \bar{n}(\boldsymbol{r}) = n, && (186)
\end{aligned}
$$

where $n = N_e/\Omega$ is the overall electron density. If we now do a space Fourier transform of (184), using that the Fourier transform of a convolution in space is the product of the Fourier transforms of each factor, we get

$$\bar{J}_\alpha(\boldsymbol{q},\omega) = \sum_\beta \sigma_{\alpha\beta}(\boldsymbol{q},\omega)E_\beta(\boldsymbol{q},\omega), \tag{187}$$

where the conductivity tensor is given by

$$\sigma_{\alpha\beta}(\boldsymbol{q},\omega) = \frac{i}{\omega}\left[\bar{\Pi}^R_{\alpha\beta}(\boldsymbol{q},\omega) + \frac{ne^2}{m}\delta_{\alpha\beta}\right]. \tag{188}$$

This is our final result for the conductivity, the Kubo formula.

4.10 Calculating the conductivity from the Kubo formula

Main steps involved in the calculation of the conductivity:

1. Define an imaginary-time (Matsubara) analogue to the retarded current-current correlation function:

   $$\pi_{\alpha\beta}(\boldsymbol{r}_1,\boldsymbol{r}_1';\tau_1-\tau_1') = -\langle T_\tau(j^P_\alpha(\boldsymbol{r}_1,\tau_1)j^P_\beta(\boldsymbol{r}_1',\tau_1'))\rangle. \tag{189}$$

   This is easier to calculate than the retarded function. Note that this Matsubara function is bosonic in the sense that it is periodic, not anti-periodic, when the time argument is translated by β. This is related to the fact that each current operator contains an even number (two) of fermionic operators. To get the retarded function from the imaginary-time function, one follows the conventional recipe of analytic continuation of the end result: $i\omega_n \rightarrow \omega + i\eta$.

2. The function (189) can be expressed as

   $$
   \begin{aligned}
   \pi_{\alpha\beta}(\boldsymbol{r}_1,\boldsymbol{r}_1';\tau_1-\tau_1') = \frac{e^2}{4m^2}\sum_{\sigma\sigma'}&(\nabla_{2'\beta}-\nabla_{1'\beta})(\nabla_{2\alpha}-\nabla_{1\alpha})\\
   &\langle T_\tau(\psi_\sigma(\boldsymbol{r}_2,\tau_2)\psi_{\sigma'}(\boldsymbol{r}_2',\tau_2')\psi^\dagger_{\sigma'}(\boldsymbol{r}_1',\tau_1')\psi^\dagger_\sigma(\boldsymbol{r}_1,\tau_1))\rangle_{\substack{\tau_2'=\tau_1^-,\ \boldsymbol{r}_2'=\boldsymbol{r}_1\\ \tau_2=\tau_1^-,\boldsymbol{r}_2=\boldsymbol{r}_1}},
   \end{aligned}
   \tag{190}
   $$

   where the time-ordered expression appearing here is a *two*-particle Matsubara Green function. To arrive at this result we have used that fermionic field operators that are all under a time-ordering symbol can be moved around freely if one introduces a minus sign every time two such field operators pass each other. (In this expression the derivatives act before the 2-coordinates are set equal to the 1-coordinates.)

3. Next, an important theorem called **Wick's theorem** can be used to express the time-ordered two-particle Green function in this expression as a sum of products of two time-ordered single-particle Green functions:

$$
\begin{aligned}
&\langle T_\tau(\psi_\sigma(\boldsymbol{r}_2,\tau_2)\psi_{\sigma'}(\boldsymbol{r}'_2,\tau'_2)\psi^\dagger_{\sigma'}(\boldsymbol{r}'_1,\tau'_1)\psi^\dagger_\sigma(\boldsymbol{r}_1,\tau_1))\rangle \\
&\quad= \langle T_\tau(\psi_\sigma(\boldsymbol{r}_2,\tau_2)\psi^\dagger_\sigma(\boldsymbol{r}_1,\tau_1))\rangle\langle T_\tau(\psi_{\sigma'}(\boldsymbol{r}'_2,\tau'_2)\psi^\dagger_{\sigma'}(\boldsymbol{r}'_1,\tau'_1))\rangle \\
&\quad- \langle T_\tau(\psi_\sigma(\boldsymbol{r}_2,\tau_2)\psi^\dagger_{\sigma'}(\boldsymbol{r}'_1,\tau'_1))\rangle\langle T_\tau(\psi_{\sigma'}(\boldsymbol{r}'_2,\tau'_2)\psi^\dagger_\sigma(\boldsymbol{r}_1,\tau_1))\rangle \\
&\quad= \mathcal{G}_{\sigma\sigma}(\boldsymbol{r}_2,\tau_2;\boldsymbol{r}_1,\tau_1)\mathcal{G}_{\sigma'\sigma'}(\boldsymbol{r}'_2,\tau'_2;\boldsymbol{r}'_1,\tau'_1) - \mathcal{G}_{\sigma\sigma'}(\boldsymbol{r}_2,\tau_2;\boldsymbol{r}'_1,\tau'_1)\mathcal{G}_{\sigma'\sigma}(\boldsymbol{r}'_2,\tau'_2;\boldsymbol{r}_1,\tau_1).
\end{aligned}
\tag{191}
$$

   This is a very significant simplification. Wick's theorem is valid when the expectation values are with respect to a Hamiltonian that is quadratic in fermion operators, as it is here. According to Wick's theorem, to arrive at this expression one pairs up creation operators with annihilation operators in all possible ways. The paired operators are then moved so they appear next to each other. In this process a minus sign is introduced every time two fermion operators are moved past each other. Thus the product of these signs gives the overall sign in front of the term. Next, the expectation value in each term factorizes into products of single-particle Green functions. Since we here have two creation and two annihilation operators, there are two different ways to pair them, which is why we get two terms in the sum on the rhs.

4. The first term in this expression gives, when substituted into (190), an expression involving $\langle j^P_\alpha(\boldsymbol{r}_1,\tau_1)\rangle\langle j^P_\beta(\boldsymbol{r}'_1,\tau'_1)\rangle$. This is zero because there is no current in the absence of an electric field. So only the second term in the pairing contributes to the conductivity.

5. We now Fourier transform to wavevector and Matsubara frequency space. Since we have reduced the problem to one involving a product of two single-particle Green functions, we can use the perturbation expansion we developed for this function in Sec. 4.3. Thus this product has a perturbation expansion given by the product of the perturbation expansions for each of the two single-particle Green functions.

6. We would like to find the conductivity $\sigma_{\alpha\alpha}(\boldsymbol{q}=0,\omega=0)\equiv\sigma$, i.e. the response to an electric field that is uniform in space and constant in time, for a system that is isotropic in space. We can set $\boldsymbol{q}=0$ directly. However, because ω appears in the denominator in (188) we cannot set $\omega=0$ directly. Instead we have to look at finite ω and take the limit $\omega\to 0$. This is however what we would have done anyway, since we first have to calculate the Matsubara function for an arbitrary $i\omega_n$ and then do the analytic continuation $i\omega_n\to\omega+i\eta$.

7. Next we do the impurity averaging. As for the single-particle Green function considered earlier, each term in the resulting expansion for $\bar{\pi}_{\alpha\alpha}(\boldsymbol{q}=0,i\omega_n)\equiv\bar{\pi}(i\omega_n)$ can be represented by a Feynman diagram. These will however look different from the ones for the single-particle Green function and will have different Feynman rules. The simplest diagram in this expansion is shown in Fig. 4(a) (it doesn't have any impurity scatterings). The upper and lower electron lines form a loop ("biting each other's tail"). There is conservation of momentum at each of the two vertices where the two

electron lines meet (shown as black dots). There is also conservation of the Matsubara frequency at each of these vertices. Note however that there is an external (bosonic) frequency $i\omega_n$ at each of these two vertices which makes the (fermionic) Matsubara frequencies of the two electron lines differ by ω_n. The internal fermionic Matsubara frequency ip_n goes in a loop and so is undetermined by frequency conservation. Hence there is a sum over ip_n.

8. The impurity averaging leads to two different classes of diagrams. Some examples of diagrams in the first class are shown in Fig. 4(b). In this class of diagrams, any given impurity in the diagram (represented by an impurity cross) scatters only with the upper line or only with the lower line. So any such diagram therefore contains a product of two Green function diagrams of the type we have seen before. All these diagrams can be summed exactly; the result is just given in terms of the product of the full Green functions for the upper and lower line. The mathematical expression for this sum is
$$\frac{2e^2}{3m^2\Omega}\sum_{\boldsymbol{k}}\boldsymbol{k}^2\frac{1}{\beta}\sum_{ip_n}\bar{\mathcal{G}}(\boldsymbol{k},ip_n+i\omega_n)\bar{\mathcal{G}}(\boldsymbol{k},ip_n). \tag{192}$$
Thus note that the Green functions in this expression are the full Green functions, not the unperturbed ($\mathcal{G}^{(0)}$) ones. The diagrammatic representation of this term is given in Fig. 4(c). The electron lines are drawn thick to indicate that they represent the full Green function. For obvious reasons this diagram is frequently referred to as "the bubble diagram".

9. In the second class of diagrams, there are impurities which scatter with both lines. These diagrams contain dashed interaction lines that straddle (via an impurity) both the upper and lower electron lines. Some examples of such diagrams are shown in Fig. 4(d). The set of these diagrams is referred to as **vertex corrections**. The types of vertex correction diagrams that can appear are dictated by our approximation for the self-energy. It turns out that for the approximation for the self-energy we used, which gave a momentum-independent self-energy, these vertex corrections cancel for the $\boldsymbol{q}=0$ conductivity we want to calculate. So it is sufficient to calculate only the bubble diagram. This is no longer true when using a more accurate, momentum-dependent, approximation for the self-energy, however.

10. The calculation of the bubble diagram is rather involved in itself, but won't be described in any detail here. The end result (after doing the analytic continuation) is that we find a conductivity given by
$$\sigma=\frac{ne^2\tau}{m} \tag{193}$$
where n is the electron density and τ is the lifetime defined in (149). This is of the same form that one gets from simple (classical) Drude theory.

5 Concluding remarks

Although in these introductory notes we have only had time to discuss one application of the Green function formalism, namely to electrons in a disordered potential, it is important to note that concepts and results like Feynman diagrams, the self-energy, and the Dyson equation, continue to be valid and central in applications of this formalism to other problems as well. For example, if one considers the problem of interacting electrons, and develops a perturbation expansion for the single-particle Green function of this problem, each term in the perturbation expansion can again be represented as a Feynman diagram. Although the appearance of these diagrams, and the Feynman rules, will be different from those of the impurity scattering problem, one can again define irreducible diagrams in exactly the same way (i.e. as Feynman diagrams that cannot be cut into two separate pieces by only cutting a single internal electron line) and from those one defines self-energy diagrams and then the self-energy as the sum of all self-energy diagrams. Furthermore, the Dyson equation relating the single-particle Green function and the self-energy continues to hold.

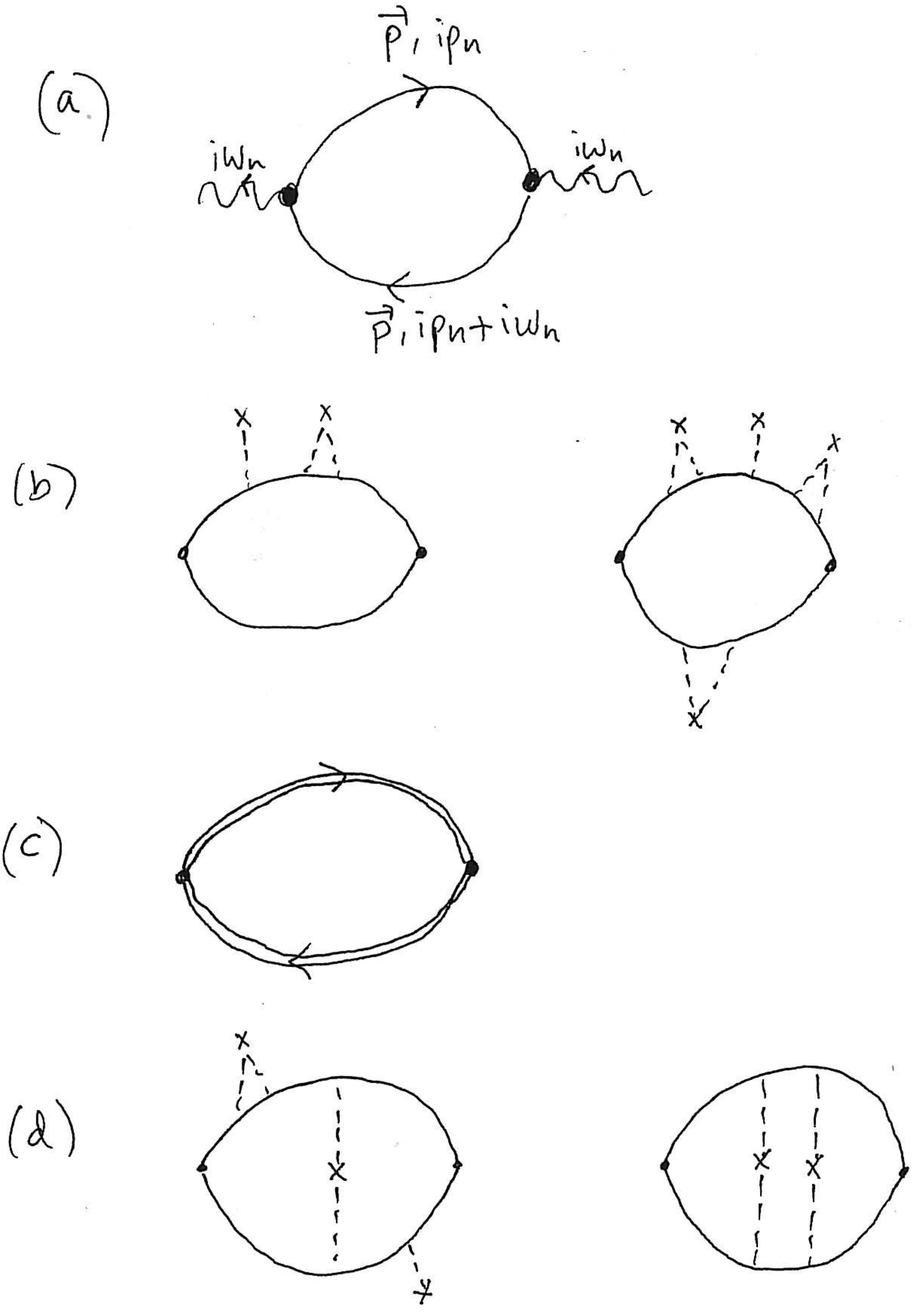

Figure 4: (a) The simplest diagram in the expansion for the Matsubara current-current correlation function $\bar{\pi}(i\omega_n)$. (b) Examples of diagrams in the first class. (c) Diagrammatic representation ("the bubble diagram") of the sum of all diagrams in the first class. (d) Examples of diagrams in the second class ("vertex corrections").