Lecture 5: The Non-Equilibrium Green Function Method

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Contents

1 Review of Equilibrium Green function formalism

In this section, we will review the Equilibrium Green function formalism and use it to introduce some of the nomenclature which we will require for the non-equilibrium formalism. We will introduce a time-ordered Green function on the special contour C^i. This will the basis for the following discussion of non-equilibrium Green functions.

1.1 Equilibrium Green functions

In a non-equilibrium theory the distribution function f will become an independent quantity. Therefore, in addition to the retarded and advanced Green functions, we need the correlation functions

$$G^{>}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = -i\langle \psi(\mathbf{x}_1, t_1)\psi^{\dagger}(\mathbf{x}_2, t_2)\rangle \tag{1}$$

$$G^{<}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = +i\langle \psi^{\dagger}(\mathbf{x}_2, t_2)\psi(\mathbf{x}_1, t_1)\rangle \tag{2}$$

They are related to the time-ordered Green function

$$\begin{aligned} G^{c}(\mathbf{x}_1, t_1;\mathbf{x}_2, t_2) &= -i\langle \mathcal{T}_t \psi(\mathbf{x}_1, t_1)\psi^{\dagger}(\mathbf{x}_2, t_2)\rangle \\ &= -i\Theta(t_1 - t_2)\langle \psi(\mathbf{x}_1, t_1)\psi^{\dagger}(\mathbf{x}_2, t_2)\rangle + i\Theta(t_2 - t_1)\langle \psi^{\dagger}(\mathbf{x}_2, t_2)\psi(\mathbf{x}_1, t_1)\rangle \\ &= \Theta(t_1 - t_2)(G^{>}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) + \Theta(t_2 - t_1)G^{<}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) \end{aligned}$$

Note that the retarded Green function can also be expressed by the two correlation functions

$$G^{r}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = \Theta(t_1 - t_2)(G^{>}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) - G^{<}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2)) \tag{3}$$

$$G^a(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = -\Theta(t_2 - t_1)(G^>(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) - G^<(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2)) \quad (4)$$

and $G^r - G^a = G^> - G^<$.

In thermal equilibrium these functions depend only on the time-difference $t = t_1 - t_2$. Introducing a Fourier transform (here we suppress the dependence on variables $\mathbf{x}_1, \mathbf{x}_2$ for the moment)

$$G(\omega) = \int_{-\infty}^{+\infty} e^{i\omega t} G(t) dt \quad (5)$$

one obtains the important relation between the two correlation functions

$$G^>(\omega) = -e^{\beta\omega} G^<(\omega) \quad (6)$$

and the spectral function

$$A(\omega) = i[G^r(\omega) - G^a(\omega)] = i[G^>(\omega) - G^<(\omega)] \quad (7)$$

we find

$$G^<(\omega) = if(\omega)A(\omega), \quad G^> = -i(1 - f(\omega))A(\omega) \quad (8)$$

where $f(\omega) = 1/\left(\exp(\beta\omega) + 1\right)$ is the Fermi function.

1.2 Perturbation theory for equilibrium Green functions

In order to calculate the Green function with help of a perturbation theory we split the Hamiltonian into $H = H_0 + V$ where H_0 describes a non-interacting electron system. Going over to the interaction representation the unitary operator for the time evolution between times t_0

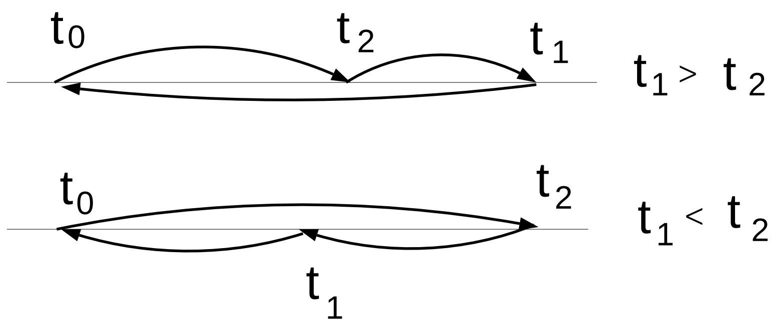

Figure 1: The contour C used for the perturbation theory in the time-evolution

and t becomes

$$e^{-iH(t-t_0)} = e^{-itH_0} S(t,t_0) e^{iH_0 t_0}, \quad S(t,t_0) = \mathcal{T} \exp\bigl(-i \int_{t_0}^{t} V_I(t') dt'\bigr) \tag{9}$$

where $O_I(t) = \exp(iH_0 t) O \exp(-iH_0 t)$. Here the time t_0 is some arbitrary reference time. We can set $t_0 = 0$. However, for later use in the case of a time dependent interaction it has to be chosen earlier than the switch-on time of the time-dependent interaction (i.e., $t_0 \to -\infty$).

For fixed time t_1, t_2 we then obtain

$$\langle \psi(t_1) \psi^\dagger(t_2) \rangle = \langle e^{iH_0 t_0} S(t_0,t_1) \psi_I(t_1) S(t_1,t_2) \psi_I^\dagger(t_2) S(t_2,t_0) e^{-iH_0 t_0} \rangle \tag{10}$$

which can also be written as

$$\langle \psi(t_1) \psi^\dagger(t_2) \rangle = \langle e^{iH_0 t_0} \mathcal{T}_C S_C \psi_I(t_1) \psi_I^\dagger(t_2) e^{-iH_0 t_0} \rangle, \;\; S_C = \mathcal{T} \exp\bigl(-i \int_C V_I(\tau) d\tau\bigr) \tag{11}$$

where C is the contour shown in Fig.1 and the time ordering operator $\mathcal{T}$ orders the interaction operators contained in S in the direction of the contour at the right places before, between, and behind the fermion operators at the fixed times t_1, t_2.

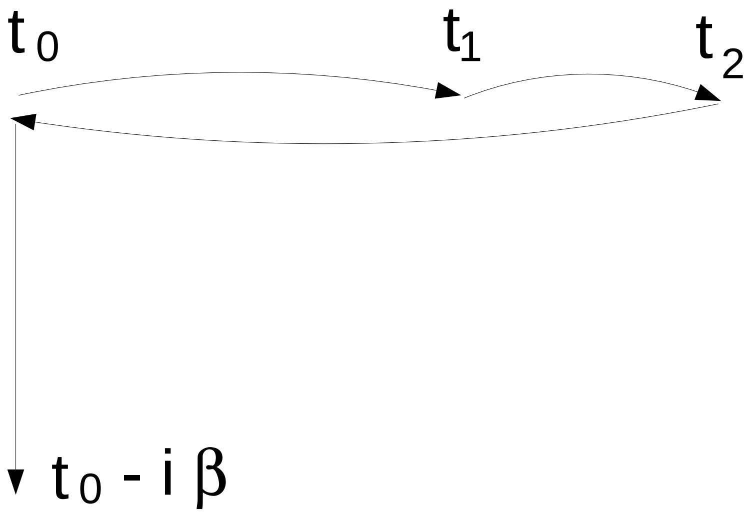

Figure 2: The contour C^i used for the perturbation theory including expansion of the statistical operator

Finally we have to expand also the statistical operator, which can be expressed by

$$e^{-\beta H} = e^{-i(t_0 - i\beta)H_0} S(t_0 - i\beta, t_0) e^{it_0 H_0} \tag{12}$$

Then

$$\langle \mathcal{T}_{C^i} \psi(t_1) \psi^\dagger(t_2) \rangle = \frac{\langle \mathcal{T}_{C^i} S_{C^i} \psi_I(t_1) \psi_I^\dagger(t_2) \rangle_0}{\langle \mathcal{T}_{C^i} S_{C^i} \rangle_0} \tag{13}$$

where now C^i is the contour shown in Fig. 2 and $\langle\rangle_0$ means a thermal average performed with the statistical operator $\rho_0 = e^{-\beta H_0}/Z_0$.

The time ordering contained in S means that a perturbation theory for the Green function can be formulated easily only for a Green function with time-ordered operators. Therefore we define a time ordered

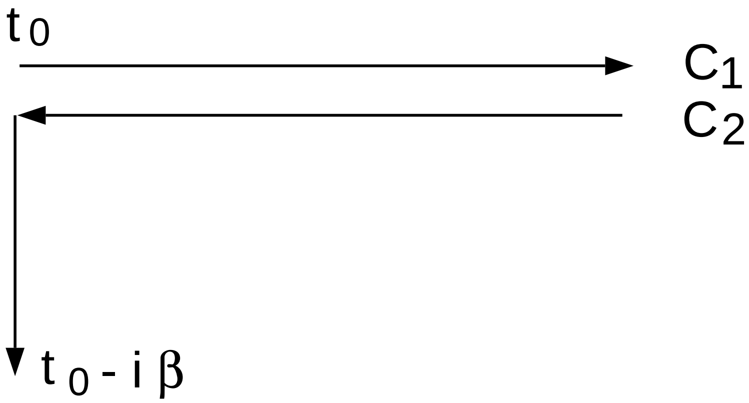

Figure 3: Contour C^i used for the perturbation expansion of the time-ordered Green function

Green function on the contour C^i:

$$G(\tau_1, \tau_2) = \begin{cases} -i\langle \psi(\tau_1)\psi^\dagger(\tau_2)\rangle & \text{for } \tau_1 >_c \tau_2 \\ +i\langle \psi^\dagger(\tau_2)\psi(\tau_1)\rangle & \text{for } \tau_1 <_c \tau_2 \end{cases} \tag{14}$$

where we distinguish between times τ_i on different parts of the contour (see Fig. 3).

Then for G the following perturbation expansion holds:

$$G(\tau_1, \tau_2) = -i \frac{\langle \mathcal{T}_{C^i} S_{C^i} \psi_I(\tau_1) \psi_I^\dagger(\tau_2)\rangle_0}{\langle \mathcal{T}_{C^i} S_{C^i}\rangle_0} \tag{15}$$

It is related to the real-time Green functions introduced above by

$$G(\tau_1, \tau_2) = \begin{cases} G^c(t_1, t_2) & \text{for } \tau_1, \tau_2 \in C_1 \\ G^>(t_1, t_2) & \text{for } \tau_1 \in C_2, \tau_2 \in C_1 \\ G^<(t_1, t_2) & \text{for } \tau_1 \in C_1, \tau_2 \in C_2 \\ G^{\bar{c}}(t_1, t_2) & \text{for } \tau_1, \tau_2 \in C_2 \end{cases} \tag{16}$$

The last being an antitime-ordered Green function. The retarded and advanced Green functions can be obtained from $G^>$ and $G^<$ in the usual way.

In thermal equilibrium it is possible to simplify this contour considerably: As in thermal equilibrium all Green functions depend only on the time difference we can replace C^i by a contour C^{th} which runs from t_0 to $t_0 - i\beta$, where we can set the real times two zero without loss of generality. One then defines a time-ordered Green function on the imaginary axis. The physical retarded and advanced Green functions are then obtained by an analytical continuation in frequency space. This is the Matsubara technique.

2 Introduction to Non-Equilibrium Green Function Formalism

2.1 Green functions with time dependent perturbation

A non-equilibrium situation is obtained if we add to the Hamiltonian H of the system a time-dependent perturbation H'_t describing for instance the interaction with an external time-dependent field:

$$\mathcal{H}_t = H + H'_t \tag{17}$$

with $H = H_0 + V$. We assume that the time dependent interaction H'_t vanishes for times $t < t_0$. The time dependent interaction can be treated by a perturbation expansion in a similar way as the internal

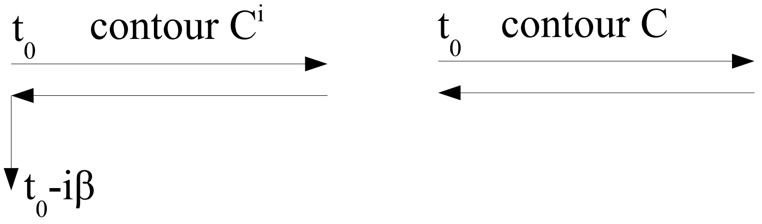

Figure 4: Contours C^i and C used for the double perturbation expansion of the non-equilibrium time-ordered Green function

interaction. The final result for the Green function can be written as a double expansion:

$$G(\tau_1, \tau_2) = -i \frac{\langle \mathcal{T}_{C^i} S_{C^i} S_C \psi_0(\tau_1) \psi_0^\dagger(\tau_2) \rangle_0}{\langle \mathcal{T}_{C^i} S_{C^i} S_C \rangle_0} \tag{18}$$

where

$$S_{C^i} = \exp\Big(-i \int_{C^i} d\tau V_I(\tau)\Big) \tag{19}$$

$$S_C = \exp\Big(-i \int_C d\tau H'_{\tau,I}(\tau)\Big) \tag{20}$$

and both interaction operators are Heisenberg operators constructed with H_0. Note that $H'_{\tau,0}$ contains an implicit time dependence through the external field. Here the contour C starts and ends at t_0, while the contour C^i starts at t_0 and ends at $t_0 - i\beta$.

The principal significance of this result is that for the time-ordered Green function on the contour C^i the usual perturbation expansion in form of Feynman graphs as in the case of equilibrium Green function can be applied. In particular if the Hamiltonian H_0 is bilinear in Fermionic operators Wick's theorem can be applied. It states that in each order of the perturbation theory the result for the Green function can be expressed by products of single particle Green functions of the non-interacting system. The same holds for the statistical operator. Therefore the denominator cancels against non-connected graphs in the numerator, leaving us with an expansion containing only connected graphs. For these, finally, a Dyson equation can be formulated, which will be the basis of the following discussion.

2.2 Dyson equation

In order to be specific let us assume a time-dependent interaction of the form

$$H'_t = \int dx \psi^\dagger(\mathbf{x}) U(\mathbf{x}, t) \psi(\mathbf{x}) \tag{21}$$

then the time-ordered Green function on the contour fulfills the following Dyson equation

$$\begin{aligned} G(1,2) &= G_0(1,2) + \int d3 G_0(1,2) U(3) G(3,2) \\ &+ \int d3 \int d4 G_0(1,3) \Sigma(3,4) G(4,2) \end{aligned} \tag{22}$$

where (i) is a short-hand notation for (x_i, τ_i) and $\int di = \int dx \int_{C^i} d\tau_i$. We did not specify the internal interaction further. It is contained in the (irreducible) self-energy Σ. The self-energy can be calculated and expressed by single-particle Green functions in any specific case. In principle the time-integrations have to be performed on the contour C^i. A simplification occurs if we put $t_0 \to -\infty$. Then the contribution from the path t_0 to $t_0 - i\beta$ can be neglected, if the internal interactions wash

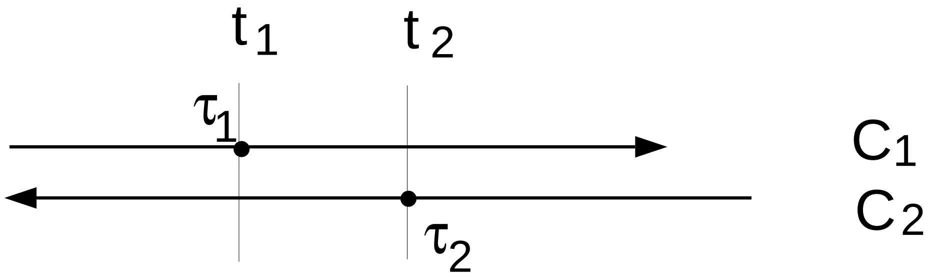

Figure 5: Relation between real times and times on the different branches of the Keldysh contour

out the memory of initial conditions. Then for the internal integrations we may use the contour C (Fig. 5) extending from $-\infty$ to $+\infty$ (part C_1) and back (part C_2). This will be called the Keldysh contour in the following.

There still remains the problem of expressing the integrations of products of different functions by integrations over the usual time axis $-\infty < t < +\infty$. This will be the task of the following section.

2.3 Langreth rules, Keldysh formalism

In the Dyson equations appear integrations over the contour of products of two and three functions. Let us start with the investigation of a folding of two functions of the form (here we suppress the dependence on the spatial variables)

$$C(\tau_1, \tau_2) = \int_C d\tau_3 A(\tau_1, \tau_3) B(\tau_3, \tau_2) \tag{23}$$

Our aim is to express this integral on C by integrals over the simple time-axis $-\infty < t < +\infty$. The result depends on the choice of variables on the contour. If we are interested, for instance, in $C^<(t_1, t_2)$ we place as in Fig. 5 τ_1 on C_1 and τ_2 on C_2 and evaluate the integrals on the contour. Then we obtain:

$$C^<(t_1, t_2) = \int_{-\infty}^{+\infty} dt \big[A^r(t_1, t) B^<(t, t_2) + A^<(t_1, t) B^a(t, t_2) \big] \tag{24}$$

For a derivation of this result we split the integrals:

$$C^<(t_1, t_2) = \int_{C_1} d\tau A(\tau_1, \tau) B(\tau, \tau_2) + \int_{C_2} d\tau A(\tau_1, \tau) B(\tau, \tau_2) \tag{25}$$

On C_1 the function B is a function $B^<$ while $A = A^c$. On C_2 the function A is a function $A^>$ while $B = B^{\bar{c}}$. Then for the first integral we obtain

$$\begin{aligned} \int_{C_1} d\tau A(\tau_1, \tau) B(\tau, \tau_2) &= \int_{-\infty}^{+\infty} dt A^c(t_1, t) B^<(t, t_2) \qquad (26) \\ &= \int_{-\infty}^{t_1} dt A^>(t_1, t) B^<(t.t_2) + \int_{t_1}^{+\infty} dt A^<(t_1, t) B^>(t, t_2) \end{aligned}$$

For the second integral we find

$$\begin{aligned} \int_{C_2} d\tau A(\tau_1, \tau) B(\tau, \tau_2) &= \int_{+\infty}^{-\infty} dt A^>(t_1, t) B^{\bar{c}}(t, t_2) \qquad (27) \\ &= -\int_{-\infty}^{t_2} dt A^>(t_1, t) B^>(t, t_2) - \int_{t_2}^{+\infty} dt A^>(t_1, t) B^<(t, t_2) \end{aligned}$$

Using the relations $A^r(t_1, t_2) = \Theta(t_1 - t_2)(G^>(t_1, t_2) - G^<(t_1, t_2))$ and $A^a(t_1, t_2) = -\Theta(t_2 - t_1)(G^>(t_1, t_2) - G^<(t_1, t_2))$ we can show the equivalence of the two results.

In a similar way we can show

$$C^>(t_1, t_2) = \int_{-\infty}^{+\infty} dt \big[A^r(t_1, t) B^>(t, t_2) + A^>(t_1, t) B^a(t, t_2) \big] \tag{28}$$

and

$$C^r(t_1,t_2) = \int_{-\infty}^{+\infty} dt A^r(t_1,t)B^r(t,t_2), \quad C^a(t_1,t_2) = \int_{-\infty}^{+\infty} dt A^a(t_1,t)B^a(t,t_2) \tag{29}$$

In the Dyson equation we also encounter a folding of the form

$$C(\tau_1,\tau_2) = \int_C d\tau A(\tau_1,\tau)U(\tau)B(\tau,\tau_2) \tag{30}$$

this is transformed into

$$C^<(t_1,t_2) = \int_{-\infty}^{+\infty} dt \big[A^r(t_1,t)U(t)B^<(t,t_2) + A^<(t_1,t)U(t)B^r(t,t_2)\big] \tag{31}$$

For a product of three functions we obtain similar rules, for instance, let

$$D(\tau_1,\tau_2) = \int_C d\tau_3 d\tau_4 A(\tau_1,\tau_3)B(\tau_3,\tau_4)C(\tau_4,\tau_2) \tag{32}$$

then

$$D^< = \int dt \big[A^r B^r C^< + A^r B^< C^a + A^< B^a C^a\big] \tag{33}$$

The rules for foldings of products can also be cast into matrix multiplication form (Keldysh matrices) by writing:

$$\hat{A} = \begin{pmatrix} A^r & A^K \\ 0 & A^a \end{pmatrix} \quad \text{and} \quad \hat{U} = U\tau_3 \tag{34}$$

where $A^K(1,1') = A^>(1,1') + A^<(1,1')$. Then in the above example

$$\hat{D} = \hat{A}\hat{B}\hat{C} \tag{35}$$

The rules needed to calculate the other self energy terms can be found in the review by Rammer and Smith.

As an example let us study the linear response of the density of free conduction electrons in a scalar potential. Here the self-energy is absent and we have the equation:

$$\delta G(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2) = \int_C d\tau_3 \int dx_3 G_0(\mathbf{x}_1,\tau_1;\mathbf{x}_3,\tau_3)U(\mathbf{x}_3,\tau_3)G_0(\mathbf{x}_3,\tau_3;\mathbf{x}_2,\tau_2) \tag{36}$$

The density is directly described by the function $n(\mathbf{x},t) = -iG^<(\mathbf{x},t;\mathbf{x},t)$. For this quantity we obtain

$$\begin{aligned} \delta n(\mathbf{x},t) \;&=\; \int dx_3 \int_{-\infty}^{+\infty} dt_3 \big[G_0^r(\mathbf{x}-\mathbf{x}_3,t-t_3)U(\mathbf{x}_3,t_3)G_0^<(\mathbf{x}_3-\mathbf{x},t_3-t) \\ &\qquad G_0^<(\mathbf{x}-\mathbf{x}_3,t-t_3)U(\mathbf{x}_3,t_3)G_0^a(\mathbf{x}_3-\mathbf{x},t_3-t)\big] \end{aligned} \tag{37}$$

where we already have used that the equilibrium Green functions depend only on the difference of arguments.

For a time-dependence of the scalar potential of the form

$$U(\mathbf{x},t) = \delta U \exp(i\mathbf{q}\cdot\mathbf{x} - i\Omega t) \tag{38}$$

and going over to a Fourier representation

$$G_0(x,t) = \frac{1}{N}\sum_k \int \frac{d\omega}{2\pi} G_0(\mathbf{k},\omega)\exp(i\mathbf{k}\cdot\mathbf{x} - i\omega t) \tag{39}$$

we find

$$\begin{aligned} \delta n(\mathbf{x},t) = -i\delta U \exp(i\mathbf{q}\cdot\mathbf{x} - i\Omega t)\frac{1}{N}\sum_{\mathbf{k}}\int\frac{d\omega}{2\pi}\big[G_0^r(\mathbf{k}+\mathbf{q},\omega+\Omega)G_0^<(\mathbf{k},\omega) \\ G_0^<(\mathbf{k}+\mathbf{q},\omega+\Omega)G_0^a(\mathbf{k},\omega)\big] \end{aligned}$$

Now we use the equilibrium relation:

$$G^<(\mathbf{k},\omega) = if(\omega)A(\mathbf{k},\omega) = 2\pi i f(\omega)\delta(\omega-\epsilon_{\mathbf{k}}+\mu), \quad G^{r,a}(\mathbf{k},\omega) = \frac{1}{\omega-\epsilon_{\mathbf{k}}+\mu\pm i\delta} \tag{40}$$

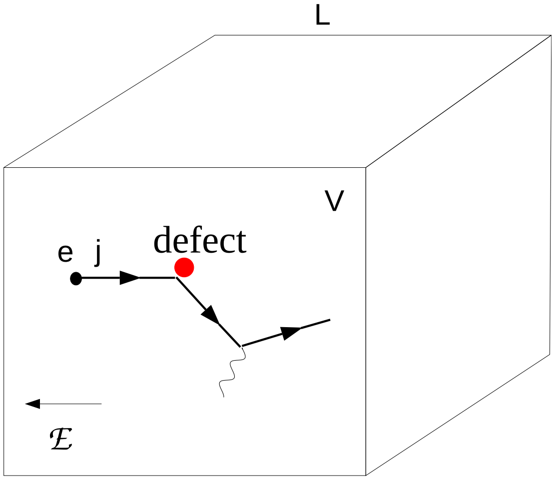

Figure 6: Electronic transport due to an applied field $\mathcal{E}$, is limited by inelastic collisions with lattice defects and phonons.

and obtain

$$\delta n(\mathbf{x},t) = \frac{1}{N}\sum_k \frac{f(\epsilon_{\mathbf{k}}-\mu) - f(\epsilon_{\mathbf{k+q}}-\mu)}{\Omega + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k+q}} + i\delta} U(\mathbf{x},t) \tag{41}$$

Here we recover the well-known Lindhard function.

3 Kinetic equations: The Boltzmann Equation

3.1 The Conventional Derivation

The nonequilibrium (but steady-state) situation of an electronic current in a metal driven by an external field is described by the Boltzmann equation. This differs from the situation of a system in equilibrium in that a constant deterministic current differs from random particle number fluctuations due to coupling to a heat and particle bath. Away from equilibrium ($\mathcal{E} \neq 0$) the distribution function may depend upon

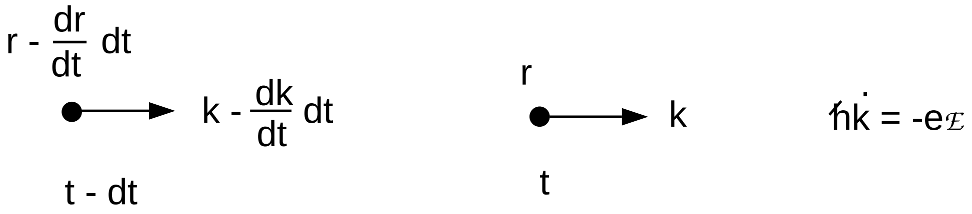

Figure 7: In lieu of scattering, particles flow without decay

$\mathbf{r}$ and t as well as $\mathbf{k}$ (or $E(\mathbf{k})$). Nevertheless, when $\mathcal{E} = 0$ we expect the distribution function of the particles in V to return to

$$f_0(\mathbf{k}) = f(\mathbf{r}, \mathbf{k}, t)|_{\mathcal{E}=0} = \frac{1}{e^{\beta(E(\mathbf{k})-E_F)} + 1} \tag{42}$$

To derive a form for $f(\mathbf{r}, \mathbf{k}, t)$, we will consider length scales larger than atomic distances, but smaller than distances in which the field changes significantly. In this way the system is considered essentially homogeneous with any inhomogeneity driven by the external field. Now imagine that there is no scattering (no defects, phonons), then since electrons are conserved

$$f(\mathbf{r}, \mathbf{k}, t) = f\left(\mathbf{r} - \mathbf{v}dt, \mathbf{k} \ + \frac{e\mathcal{E}}{\hbar}dt, t - dt\right) \tag{43}$$

Now consider defects and phonons (See Fig. 8) which can scatter a quasiparticle in one state at $\mathbf{r} \ - \mathbf{v} \ dt$ and time $t - dt$, to another at $\mathbf{r}$ and time t, so that $f(\mathbf{r}, \mathbf{k}, t) \neq f\left(\mathbf{r} - \mathbf{v}dt, \mathbf{k} + \frac{e\mathcal{E}}{\hbar}dt, tdt\right)$. We will express this scattering by adding a term.

$$f(\mathbf{r}, \mathbf{k}, t) = f\left(\mathbf{r} \ - \mathbf{v} \ dt, \mathbf{k} \ + e\mathcal{E}\frac{dt}{\hbar}, t - dt\right) \ + \left(\frac{\partial f}{\partial t}\right)_S dt \tag{44}$$

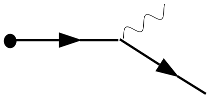

Figure 8: Scattering leads to quasiparticle decay.

For small dt we may expand

$$f(\mathbf{r},\mathbf{k},t) = f(\mathbf{r},\mathbf{k},t) - \mathbf{v}\;\cdot\;\nabla_r f + e\mathcal{E}\;\cdot\;\nabla_k \frac{f}{\hbar} - \frac{\partial f}{\partial t} + \left(\frac{\partial f}{\partial t}\right)_S \tag{45}$$

or

$$\frac{\partial f}{\partial t} + \mathbf{v}\;\cdot\;\nabla_r f - \frac{e}{\hbar}\mathcal{E}\;\cdot\;\nabla_k f = \left(\frac{\partial f}{\partial t}\right)_S \qquad \text{Boltzmann Equation} \tag{46}$$

3.2 Towards Transport in the Green Function Approach

We can give a more microscopic derivation of the Boltzmann equation employing the Green function approach. As above, we will assume that $U(\mathbf{x},t)$ is slowly dependent on $\mathbf{x}$ and t. Then it is expected that also e.g. the density $n(\mathbf{x},t) = -iG^<(\mathbf{x},t;\mathbf{x},t)$ slowly depends on these variables. We therefore introduce the so-called Wigner coordinates

$$T = (t_1 + t_2)/2, \quad t = t_1 - t_2, \quad \mathbf{X} = (\mathbf{x}_1 + \mathbf{x}_2)/2, \quad \mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2 \tag{47}$$

and express the Green functions $G(\mathbf{x}_1,t_1;\mathbf{x}_2,t_2)$ by these coordinates

$$G(\mathbf{x},t,\mathbf{X},T) := G(\mathbf{X}+\frac{\mathbf{x}}{2},T+\frac{t}{2};\mathbf{X}-\frac{\mathbf{x}}{2},T-\frac{t}{2}) \tag{48}$$

In equilibrium $G(\mathbf{x},t,\mathbf{X},T)$ depends only on the difference variables $\mathbf{x}$ and t and falls off or oscillates rapidly in these variables, while in non-equilibrium the dependence in $\mathbf{X}$ and T is induced by the perturbation $U(\mathbf{X},T)$.

In equilibrium we have introduced a Fourier transform with respect to the difference variables

$$G^<(\mathbf{k},\omega) = \int dt \int d^3x e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega t} G^<(\mathbf{x},t) \tag{49}$$

Previously in this lecture we found that the function $G^<(\mathbf{k},\omega)$ can be written as

$$G^<(\mathbf{k},\omega) = iA(\mathbf{k},\omega)f(\omega) \tag{50}$$

where $f(\omega)$ is the Fermi function and $A(\mathbf{k},\omega) = -2\mathrm{Im}G^r(\mathbf{k},\omega)$ is the spectral function, and

$$G^r(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} + \mu - \Sigma(\mathbf{k},\omega)} \tag{51}$$

In the absence of internal interactions ($\Sigma = 0$) we have $A(\mathbf{k},\omega) = 2\pi\delta(\omega - \epsilon_{\mathbf{k}} + \mu)$.

In the presence of a perturbation $U(\mathbf{X},T)$ a similar representation holds:

$$G^<(\mathbf{k},\omega,\mathbf{X},T) = iA(\mathbf{k},\omega,\mathbf{X},T)F(\mathbf{k},\omega,\mathbf{X},T) \tag{52}$$

with

$$A(\mathbf{k},\omega,\mathbf{X},T) = -2\mathrm{Im}G^r(\mathbf{k},\omega,\mathbf{X},T) \tag{53}$$

and a generalized distribution function $F(\mathbf{k},\omega,\mathbf{X},T)$.

In the quasiparticle approximation we assume that the electrons don't decay (or are very long lived) and that they have a well defined dispersion $\omega(\mathbf{k})$. In this case F does not depend on ω separately and can be replaced by a simpler distribution function $f(\mathbf{k},\mathbf{X},T)$. For this function we obtain the Boltzmann equation which is of the form

$$\Big(\frac{\partial f}{\partial T}+\frac{\partial \epsilon(\mathbf{k})}{\partial \mathbf{k}}\frac{\partial f}{\partial \mathbf{X}}-\frac{\partial U(\mathbf{X},T)}{\partial \mathbf{X}}\frac{\partial f}{\partial \mathbf{k}}\Big)=I\{f\} \tag{54}$$

with a scattering term $I\{f\}$, which in the case of impurity scattering is given by

$$I\{f\}=-2\pi c\sum_p |V(\mathbf{k}-\mathbf{p})|^2\delta(\epsilon_{\mathbf{k}}-\epsilon_p)(f(\mathbf{k},\mathbf{X},T)-f(\mathbf{p},\mathbf{X},T)) \tag{55}$$

In the remainder of this lecture we plan to show how this quasiclassical Boltzmann equation can be derived within the frame of a more general non-equilibrium theory.

3.3 Derivation of kinetic equations

We start from the Dyson equation in integral form on the Keldysh contour:

$$\begin{aligned} G(1,2) &= G_0(1,2)+\int d3 G_0(1,3)U(3)G(3,2) \\ &+ \int d3\int d4 G_0(1,3)\Sigma(3,4)G(4,2) \end{aligned} \tag{56}$$

or

$$\begin{aligned} G(1,2) &= G_0(1,2)+\int d3 G(1,3)U(3)G_0(3,2) \\ &+ \int d3\int d4 G(1,3)\Sigma(3,4)G_0(4,2) \end{aligned} \tag{57}$$

From this we obtain for the retarded Green function on the time-axis

$$
\begin{aligned}
&G^r(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = G_0^r(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) \\
&\quad + \int dt_3 \int dx_3 G_0^r(\mathbf{x}_1, t_1; \mathbf{x}_3, t_3) U(\mathbf{x}_3, t_3) G^r(\mathbf{x}_3, t_3; \mathbf{x}_2, t_2) \\
&\quad \int dt_3 \int dt_4 \int dx_3 \int dx_4 G_0^r(\mathbf{x}_1, t_1; \mathbf{x}_3, t_3) \Sigma^r(\mathbf{x}_3, t_3; x_4, t_4) G^r(x_4, t_4; \mathbf{x}_2, t_2)
\end{aligned}
$$

or using an abbreviated notation

$$
G^r = G_0^r + \{G_0^r U G^r\} + \{G_0^r \Sigma^r G^r\} \tag{58}
$$

where {} denotes a convolution in space and time with the same arguments as above.

For the lesser function $G^<$ we get a more complicated equation:

$$
G^< = G_0^< + \{G_0^r U G^< + G^< U G^a\} + \{G_0^r \Sigma^r G^< + G_0^r \Sigma^< G^a + G_0^< \Sigma^a G^a\} \tag{59}
$$

Similar equations are obtained if we start from the other form of the Dyson equation.

We now will transform the Dyson integral equation into a Dyson equation in differential form. Note that for non-interacting conduction electrons we have the following equation of motion for the Fermionic operator

$$
i \frac{\partial \psi(\mathbf{x}, t)}{\partial t} = H_0(\mathbf{x}) \psi(\mathbf{x}, t) \tag{60}
$$

Therefore we obtain for the Green functions the equations of motion

$$
\left[i \frac{\partial}{\partial t_1} - H_0(\mathbf{x}_1) \right] G_0^{r,a}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = \delta(t_1 - t_2) \tag{61}
$$

$$\Big[i\frac{\partial}{\partial t_1} - H_0(\mathbf{x}_1)\Big]G_0^<(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = 0 \tag{62}$$

where $H_0(\mathbf{x})$ is the Hamiltonian for non-interacting electrons. For free conduction electrons in a constant potential $H_0(\mathbf{x}) = -\nabla_x^2/2m - \mu$. The δ-function in the equation of motion for $G_0^{r,a}$ is due to the step-function in the definition. Similar equations hold if we differentiate with respect to the second time

$$\Big[-i\frac{\partial}{\partial t_2} - H_0(\mathbf{x}_2)\Big]G_0^{r,a}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = \delta(t_1 - t_2) \tag{63}$$

$$\Big[-i\frac{\partial}{\partial t_2} - H_0(\mathbf{x}_2)\Big]G_0^<(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = 0 \tag{64}$$

Then we obtain the equations of motion for G^r:

$$\begin{aligned}\Big[i\frac{\partial}{\partial t_1} - H_0(\mathbf{x}_1) - U(\mathbf{x}_1, t_1)\Big]G_0^r(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) &= \delta(t_1 - t_2) \\ &+ \int_{-\infty}^{+\infty} dt \int d^3x \Sigma^r(\mathbf{x}_1 t_1; x, t) G^r(x, t; \mathbf{x}_2, t_2)\end{aligned}$$

and a similar equation for G^a, while for $G^<$ (or $G^>$) we obtain the two equations

$$\begin{aligned}&\Big[i\frac{\partial}{\partial t_1} - H_0(\mathbf{x}_1) - U(\mathbf{x}_1, t_1)\Big]G_0^<(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = \\ &\int dt \int d^3x \Sigma^r(\mathbf{x}_1 t_1; \mathbf{x}, t) G^<(\mathbf{x}, t; \mathbf{x}_2, t_2) + \int dt \int d^3x \Sigma^<(\mathbf{x}_1 t_1; \mathbf{x}, t) G^a(\mathbf{x}, t; \mathbf{x}_2, t_2)\end{aligned} \tag{65}$$

$$\begin{aligned}&\Big[-i\frac{\partial}{\partial t_2} - H_0(\mathbf{x}_2) - U(\mathbf{x}_2, t_2)\Big]G_0^<(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = \\ &\int dt \int d^3x G^r(\mathbf{x}_1, t_1; \mathbf{x}, t) \Sigma^<(\mathbf{x}, t; \mathbf{x}_2, t_2) + \int dt \int d^3x G^<(\mathbf{x}_1, t_1; \mathbf{x}, t) \Sigma^a(\mathbf{x}, t; \mathbf{x}_2, t_2)\end{aligned} \tag{66}$$

In principle this is closed set of equations for the Green functions as soon as one has a well-defined expression for the self-energies. However, due to the many variables these equations of motion are very complicated.

3.4 Gradient expansion

Now we introduce the Wigner coordinates

$$T = (t_1 + t_2)/2, \quad t = t_1 - t_2, \quad \mathbf{X} = (\mathbf{x}_1 + \mathbf{x}_2)/2, \quad \mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2 \tag{67}$$

and express the Green functions by these coordinates

$$G(\mathbf{x}, t; \mathbf{X}, T) := G(\mathbf{X} + \frac{\mathbf{x}}{2}, T + \frac{t}{2}; X - \frac{\mathbf{x}}{2}, T - \frac{t}{2}) \tag{68}$$

Note that

$$\frac{\partial}{\partial T} G(\mathbf{x}, t; \mathbf{X}, T) = \Big(\frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2}\Big) G(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) \tag{69}$$

therefore a kinetic equation with respect to T is obtained if we subtract the two equations 65 and 66

$$\begin{aligned}\Big(i\frac{\partial}{\partial t_1} + i\frac{\partial}{\partial t_2} - H_0(\mathbf{x}_1) + H(\mathbf{x}_2) - U(\mathbf{x}_1, t_1) + U(\mathbf{x}_2, t_2)\Big) G^<(\mathbf{x}_1, t_1; \mathbf{x}_2, t_t) \\ = \{\Sigma^r G^< + \Sigma^< G^a - G^r \Sigma^< - G^< \Sigma^a\}\end{aligned} \tag{70}$$

where the products on r.h.s. of Eq. 70 are convolutions in space and time. If the variation of U is sufficiently slow we can make a gradient expansion

$$U(\mathbf{x}_1, t_1) - U(\mathbf{x}_2, t_2) \simeq \mathbf{x}\frac{\partial U(\mathbf{X}, T)}{\partial \mathbf{X}} + t\frac{\partial U(\mathbf{X}, T)}{\partial T} \tag{71}$$

This expansion (the factors t and $\mathbf{x}$) can be better handled if we go over to a Fourier representation with respect to the fast difference variables $\mathbf{x}, t$:

$$A(\mathbf{k}, \omega, \mathbf{X}, T) = \int dt \int d^3x e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega t} A(\mathbf{x}, t, \mathbf{X}, T) \tag{72}$$

then e.g.

$$\int dt \int d^3x e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega t} x A(\mathbf{x}, t, \mathbf{X}, T) = i\frac{\partial}{\partial k} A(\mathbf{k}, \omega, \mathbf{X}, T) \tag{73}$$

and the Fourier transform of the l.h.s. of Eq. 70 becomes

$$\Big(i\frac{\partial}{\partial t_1} + i\frac{\partial}{\partial t_2} - H_0(\mathbf{x}_1) + H(\mathbf{x}_2) - U(\mathbf{x}_1, t_1) + U(\mathbf{x}_2, t_2)\Big) G^<(\mathbf{x}_1, t_1; \mathbf{x}_2, t_t)$$
$$\rightarrow i\Big(\frac{\partial}{\partial T} + \frac{\partial \epsilon(\mathbf{k})}{\partial \mathbf{k}}\frac{\partial}{\partial \mathbf{X}} - \frac{\partial U(\mathbf{X}, T)}{\partial \mathbf{X}}\frac{\partial}{\partial \mathbf{k}} + \frac{\partial U(\mathbf{X}, T)}{\partial T}\frac{\partial}{\partial \omega}\Big) G^>(k, \omega, X, T)$$

where we have slightly generalized the Fourier transform of the Hamiltonian H_0 into a dispersion $\epsilon(k)$. Here we encounter already all the terms, except for the last term, which are contained in the driving term of the Boltzmann equation. Defining

$$\mathcal{L} := \Big(\frac{\partial}{\partial T} + \frac{\partial \epsilon(\mathbf{k})}{\partial \mathbf{k}}\frac{\partial}{\partial \mathbf{X}} - \frac{\partial U(\mathbf{X}, T)}{\partial \mathbf{X}}\frac{\partial}{\partial \mathbf{k}} + \frac{\partial U(\mathbf{X}, T)}{\partial T}\frac{\partial}{\partial \omega}\Big) \tag{74}$$

the equation of motion for the Green function $G^<$ now reads

$$i\mathcal{L}G^<(\mathbf{k}, \omega; \mathbf{X}, T) = \{\Sigma^r G^< + \Sigma^< G^a - G^r \Sigma^< - G^< \Sigma^a\} \tag{75}$$

Before we discuss the r.h.s. of Eq. 75, let us introduce an ansatz for the function $G^<$ which is similar in structure as in equilibrium:

$$G^<(\mathbf{k}, \omega, \mathbf{X}, T) = iA(\mathbf{k}, \omega, \mathbf{X}, T) F(\mathbf{k}, \omega, \mathbf{X}, T) \tag{76}$$

where $iA = G^r - G^a$ is the spectral function and F is a generalized distribution function. Within the gradient expansion the retarded and advanced Green function are easily calculated from Eq. 3 and the corresponding equations of motion

$$G^r(\mathbf{k}, \omega, \mathbf{X}, T) = \frac{1}{\omega - \epsilon_{\mathbf{k}} + \mu - U(\mathbf{X}, T) - \Sigma(\mathbf{k}, \omega, \mathbf{X}, T)} \tag{77}$$

$$A(\mathbf{k}, \omega, \mathbf{X}, T) = -2\mathrm{Im}G^r(\mathbf{k}, \omega, \mathbf{X}, T) \tag{78}$$

This result is remarkably simple. In order to obtain the Boltzmann equation we make a further approximation by neglecting the self-energy in the retarded Green function. Then we obtain the quasi-particle approximation:

$$A_0(\mathbf{k}, \omega, \mathbf{X}, T)) = 2\pi\delta(\omega - \epsilon_{\mathbf{k}} + \mu - U(\mathbf{X}, T)) \tag{79}$$

Of course, in this approximation the frequency ω of the distribution function $F(\mathbf{k}, \omega, \mathbf{X}, T)$ is no longer an independent variable. therefore in the quasiparticle approximation

$$G^<(\mathbf{k}, \omega, T, \mathbf{X}) = A_0(\mathbf{k}, \omega, \mathbf{X}, T) f(\mathbf{k}, \mathbf{X}, T) \tag{80}$$

Note that A_0 (as any function $y(\omega - \epsilon_{\mathbf{k}} + \mu - U(\mathbf{X}, T))$ is an eigenfunction of the differential operator of the Boltzmann equation:

$$\mathcal{L} A_0(\mathbf{k}, \omega, \mathbf{X}, T)) = 0 \tag{81}$$

Therefore

$$i\mathcal{L} G^<(\mathbf{k}, \omega, \mathbf{X}, T) = -A_0 \mathcal{L} f(\mathbf{k}, \mathbf{X}, T) \tag{82}$$

Now we turn to the scattering term, the r.h.s. of Eq. 75. The gradient expansion of convolutions can be performed systematically. For

$$C(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = \int dx' dt' A(\mathbf{x}_1, t_1; \mathbf{x}', t') B(\mathbf{x}', t'; \mathbf{x}_2, t_2) \tag{83}$$

one obtains

$$\begin{aligned} C(\mathbf{k}, \omega, \mathbf{X}, T) =& A(\mathbf{k}, \omega, \mathbf{X}, T) B(\mathbf{k}, \omega, \mathbf{X}, T) \\ & - \frac{i}{2}\Big(\frac{\partial A}{\partial T}\frac{\partial B}{\partial \omega} - \frac{\partial A}{\partial \omega}\frac{\partial B}{\partial T} - \frac{\partial A}{\partial \mathbf{X}}\frac{\partial B}{\partial \mathbf{k}} + \frac{\partial A}{\partial \mathbf{k}}\frac{\partial B}{\partial \mathbf{X}} \Big) \end{aligned}$$

Therefore, in the lowest approximation we write

$$\begin{aligned} &\{\Sigma^r G^< + \Sigma^< G^a - G^r \Sigma^< - G^< \Sigma^a\}(\mathbf{k}, \omega, \mathbf{X}, T) = \\ &= \Big(G^< (\Sigma^r - \Sigma^a) - (G^r - G^a)\Sigma^< \Big)(\mathbf{k}, \omega, \mathbf{X}, T) \end{aligned}$$

where we have replaced the convolutions by simple products. Then we obtain

$$A_0 \mathcal{L} f(\mathbf{k}, \mathbf{X}, T) = -\Big(G^< (\Sigma^r - \Sigma^a) - (G^r - G^a)\Sigma^< \Big)(\mathbf{k}, \omega, \mathbf{X}, T) \tag{84}$$

3.5 Self energy from impurity scattering

In the case of scattering from randomly distributed impurity scattering with an impurity scattering potential $V(\mathbf{q})$ the self energy is given in Born approximation

$$\Sigma^r(\mathbf{k}, \omega, \mathbf{X}, T) = c \sum_{\mathbf{p}} |V(\mathbf{k} - \mathbf{p})|^2 G^r(\mathbf{p}, \omega, \mathbf{X}, T) \tag{85}$$

This holds in a similar way also for the other Green functions. This form of the self-energy can be obtained from the corresponding Feynman graph expansion which holds on the Keldysh contour. Inserting now the ansatz for the $G^<$ function into the scattering term we find

$$A_0(\mathbf{k},\omega,\mathbf{X},T)\mathcal{L}f(\mathbf{k},\mathbf{X},T) = -c\sum_{\mathbf{p}} A_0(\mathbf{k},\omega,\mathbf{X},T)A_0(\mathbf{p},\omega,\mathbf{X},T)$$
$$|V(\mathbf{k}-\mathbf{p})|^2(f(\mathbf{k},\mathbf{X},T)-f(\mathbf{p},\mathbf{X},T))$$

Finally we integrate over ω to obtain

$$\mathcal{L}f(\mathbf{k},\mathbf{X},T) = -2\pi c\sum_{\mathbf{p}} |V(\mathbf{k}-\mathbf{p})|^2\delta(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{p}})(f(\mathbf{k},\mathbf{X},T)-f(\mathbf{p},\mathbf{X},T)) \tag{86}$$

This is the classical Boltzmann equation. The first term on the r.h.s. is the out-scattering term, the second term is the in-scattering term. The importance of this result is the validity of this equation for the distribution function also far from equilibrium. Their is no explicit reference to the temperature in the equation. It is contained only in the initial conditions, where $f(k,X,T) = f_0(\epsilon_{\mathbf{k}}-\mu)$ is the Fermi function. The δ-function which expresses energy conservation is due to the quasi-particle approximation of the spectrum function. Due to this approximation typical quantum effects which are contained in the frequency dependence of the distribution function get lost. There seems to be an inconsistency in the treatment of the self energy: we have neglected the self energy in the spectral function completely, while keeping it (in lowest order in the gradient expansion) in the scattering term. This defect can be cured partially by separating from the self energy those terms which lead to a renormalization of the single-particle excitation spectrum and those which lead to scattering.

Copies of these notes, supporting materials and links are available at http://www.physics.uc.edu/∼jarrell/Green . Much of the material came from standard texts and urls linked on the site.