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An Introduction to Nonequilibrium Many-Body Theory

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Nonequilibrium Perturbation Theory

The goal of this chapter is to construct the perturbation expansion for the 1-particle contour-ordered Green's function. First, we explain why the usual perturbation expansion on the Feynman contour (the real-time axis from $-\infty$ to ∞) or on the Matsubara contour (a segment on the imaginary-time axis from $-i\beta$ to $i\beta$) fails in general nonequilibrium situations.

1.1 Failure of Conventional Time-Ordered Perturbation Theory

The central goal of nonequilibrium many-body theory is to calculate real-time correlation functions. For example, we might want to calculate the 1-particle time-ordered Green's function,

$$iG(\mathbf{x},t;\mathbf{x}',t') = \langle T[\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')]\rangle = \operatorname{Tr}\rho T[\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')] \tag{1.1}$$

in the Heisenberg picture, where ρ is an arbitrary nonequilibrium density matrix and the Hamiltonian $\mathcal{H}(t)$ is in general time-dependent.

1.1.1 Equilibrium Many-Body Theory

In conventional equilibrium many-body theory, we know how to setup a perturbation theory to calculate this quantity. At zero temperature, the density matrix is

$$\rho = |\Psi_0\rangle\langle\Psi_0| \tag{1.2}$$

where $|\Psi_0\rangle$ is the exact ground state of a full interacting but time-independent Hamiltonian H. Then the time-ordered Green's function

$$iG(\mathbf{x},t;\mathbf{x}',t') = \langle\Psi_0|T[\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')]|\Psi_0\rangle \tag{1.3}$$

is given by conventional Feynman-Dyson perturbation theory,

$$iG(\mathbf{x},t;\mathbf{x}',t') = \frac{\langle \Phi_0|T[S(\infty,-\infty)\hat{\psi}(\mathbf{x},t)\hat{\psi}^\dagger(\mathbf{x}',t')]|\Phi_0\rangle}{\langle \Phi_0|S(\infty,-\infty)|\Phi_0\rangle} \tag{1.4}$$

where the caret denotes operators in the interaction picture with respect to a quadratic Hamiltonian H_0 where $H = H_0 + V$, $|\Phi_0\rangle$ is the ground state of H_0, and the S-matrix is

$$S(\infty,-\infty) = T\exp\left(-i\int_{-\infty}^{\infty} dt_1\, \hat{V}(t_1)\right) \tag{1.5}$$

The power series expansion of the S-matrix and the subsequent use of Wick's theorem generates the usual Feynman diagrams, of which the disconnected ones cancel against the phase factor in the denominator.

At finite temperatures, we use the coincidence in functional form of the thermal density matrix

$$\rho = \frac{e^{-\beta H}}{Z} \tag{1.6}$$

where $Z = \mathrm{Tr}\, e^{-\beta H}$ is the partition function, and the evolution operator $U(t) = e^{-iHt}$ to setup a perturbation theory in imaginary time. Here again, Wick's theorem can be used since each term in the perturbation expansion is an average over a noninteracting density matrix $\rho_0 = e^{-\beta H_0}/Z_0$ where $Z_0 = \mathrm{Tr}\, e^{-\beta H_0}$.

1.1.2 Failure of Conventional Techniques

These techniques seem quite powerful, so why can't we apply them to the more general problem of Eq. (1.1)?

Let us consider the Matsubara technique first. Out of equilibrium, there is no such thing as a temperature. As a result, in general the density matrix is not of exponential form, so there is no way we can use the Matsubara trick which consists in a simultaneous expansion of the density matrix and the time-evolution operator allowed by the coincidence in functional form of these two operators.

In the Feynman case, once again the density matrix is not a simple projector on the ground state as in Eq. (1.2).

These arguments are correct, but it is instructive to see in more detail where exactly does the mathematical construction of the above equilibrium perturbation expansions fail. We will try to construct an expansion of the nonequilibrium Green's function using the ordinary Feynman approach and see that it fails.

Consider a generic density matrix

$$\rho = \sum_{\Phi} p_\Phi |\Phi\rangle\langle\Phi| \tag{1.7}$$

where the $|\Phi\rangle$ can be arbitrary quantum states. First recall that in the Heisenberg picture, the density matrix does not evolve in time since its time evolution, given by the quantum Liouville equation, goes in a way opposite to that given by the Heisenberg equation of motion, so that the time evolution of ρ cancels out altogether. For convenience, we study one state at a time, namely we want to calculate the expectation value

$$iG_\Phi(\mathbf{x},t;\mathbf{x}',t') = \langle\Phi|T[\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')]|\Phi\rangle \tag{1.8}$$

and we can obtain the full Green's function by $G = \sum_\Phi p_\Phi G_\Phi$.

Now consider the following partition of the Hamiltonian $\mathcal{H}(t) = H + H'(t)$ where H is the unperturbed equilibrium Hamiltonian (but may still contain interactions) and all the time dependence is included in the nonequilibrium perturbation $H'(t)$. The field operator in the interaction picture is

$$\hat{\psi}(\mathbf{x},t) = e^{iHt}\psi(\mathbf{x})e^{-iHt} \tag{1.9}$$

and in the Heisenberg picture,

$$\psi(\mathbf{x},t) = \mathcal{U}^\dagger(t)\psi(\mathbf{x})\mathcal{U}(t) = \mathcal{S}(0,t)\hat{\psi}(\mathbf{x},t)\mathcal{S}(t,0) \tag{1.10}$$

where $\mathcal{S}(t,0) = e^{iHt}\mathcal{U}(t)$ and the evolution operator is

$$\mathcal{U}(t) = T\exp\left(-i\int_0^t dt_1\,\mathcal{H}(t_1)\right) \tag{1.11}$$

more generally, we have the S-matrix

$$\mathcal{S}(t,t') = e^{iHt}\mathcal{U}(t,t')e^{-iHt'} = T\exp\left(-i\int_{t'}^t dt_1\,\hat{H}'(t_1)\right) \tag{1.12}$$

where $\mathcal{U}(t,t') = T\exp\left(-i\int_{t'}^t dt_1\,\mathcal{H}(t_1)\right)$ and $\hat{H}'(t) = e^{iHt}H'(t)e^{-iHt}$ is the nonequilibrium perturbation in the interaction picture[1].

We substitute these relations into Eq. (1.8),

$$iG_\Phi(\mathbf{x},t;\mathbf{x}',t') = \langle\Phi|T[\mathcal{S}(0,t)\hat{\psi}(\mathbf{x},t)\mathcal{S}(t,0)\mathcal{S}(0,t')\hat{\psi}^\dagger(\mathbf{x}',t')\mathcal{S}(t',0)]|\Phi\rangle \tag{1.13}$$

Now the interaction picture state is given by

$$|\Phi(t)\rangle_I = \mathcal{S}(t,0)|\Phi(0)\rangle_I = \mathcal{S}(t,0)|\Phi\rangle \tag{1.14}$$

since all pictures coincide at $t = 0$. We can then say that

[1] We use curly letters for $\mathcal{U}$ and $\mathcal{S}$ to indicate that these operators take care of the full *nonequilibrium* Hamiltonian $\mathcal{H}$ with H' as the perturbation. Later upright letters U and S will be used for the corresponding operators taking care of the *equilibrium* Hamiltonian H with whatever interactions it may contain as the perturbation.

$$|\Phi\rangle = \mathcal{S}(0, \pm\infty)|\Phi(\pm\infty)\rangle_I \tag{1.15}$$

Putting everything together, we have

$$\begin{aligned} iG_\Phi(\mathbf{x}, t; \mathbf{x}', t') &= \langle\Phi(\infty)|_I \mathcal{S}(\infty, 0) \\ &\times T[\mathcal{S}(0, t)\hat{\psi}(\mathbf{x}, t)\mathcal{S}(t, t')\hat{\psi}^\dagger(\mathbf{x}', t')\mathcal{S}(t', 0)]\mathcal{S}(0, -\infty)|\Phi(-\infty)\rangle_I \end{aligned} \tag{1.16}$$

Now, the S-matrix $\mathcal{S}(\infty, -\infty)$ is itself a time-ordered product, so that we can write

$$iG_\Phi(\mathbf{x}, t; \mathbf{x}', t') = \langle\Phi(\infty)|_I T[\mathcal{S}(\infty, -\infty)\hat{\psi}(\mathbf{x}, t)\hat{\psi}^\dagger(\mathbf{x}', t')]|\Phi(-\infty)\rangle_I \tag{1.17}$$

making use of the group property of $\mathcal{S}(t, t')$.

So far everything is correct in a general nonequilibrium setting. At this point, the conventional Feynman expression Eq. (1.4) is obtained *only provided that the following crucial step holds*: $|\Phi(\infty)\rangle_I$ and $|\Phi(-\infty)\rangle_I$ differ only by a phase factor. This is true in equilibrium but breaks down out of equilibrium.

The reason is the following. In the conventional zero-temperature theory, we *adiabatically switch on and off* the interaction:

$$\mathcal{H}_\epsilon = H + e^{-\epsilon|t|}H' \tag{1.18}$$

where ϵ is a positive infinitesimal. We also choose $|\Phi\rangle$ to be $|\Psi_0\rangle$, the ground state of $\mathcal{H} = H + H'$. We assume this ground state to be nondegenerate. Since the time evolution is adiabatic, we can use the adiabatic theorem to say that $|\Phi(\pm\infty)\rangle_I = \lim_{\epsilon\to 0}\mathcal{S}_\epsilon(\pm\infty, 0)|\Psi_0\rangle$ are both eigenstates of H. Since $|\Psi_0\rangle$ is nondegenerate, these two states can differ by at most a phase factor,

$$|\Phi(\infty)\rangle_I = e^{iL}|\Phi(-\infty)\rangle_I \tag{1.19}$$

For definiteness, using the notation $|\Phi_0\rangle \equiv |\Phi(-\infty)\rangle_I$ it is easy to see that

$$e^{iL} = \langle\Phi_0|\mathcal{S}(\infty, -\infty)|\Phi_0\rangle \tag{1.20}$$

so that Eq. (1.17) gives Eq. (1.4) directly.

Out of equilibrium, the use of the adiabatic theorem is unjustified since under the assumption of a general time-dependent Hamiltonian $\mathcal{H}(t)$ the time evolution is *not* adiabatic. In the case that the Hamiltonian is time-independent but the density matrix is still arbitrary – the important case of a nonequilibrium steady state, we still cannot use the adiabatic theorem because the generic quantum states $|\Phi\rangle$ are not necessarily eigenstates of $\mathcal{H}$ and the adiabatic theorem applies only to eigenstates of the Hamiltonian. If we insist and expand the density matrix in the basis of eigenstates of $\mathcal{H}$, it is in general not diagonal in this basis,

$$\mathrm{Tr}\,\rho O = \sum_\Phi p_\Phi\langle\Phi|O|\Phi\rangle = \sum_{nn'}\rho_{nn'}\langle n|O|n'\rangle \tag{1.21}$$

so that even if $|n(\infty)\rangle_I = e^{iL_n}|n(-\infty)\rangle_I$, the appearance of crossed terms spoils the expansion. Finally, even if the ground state is assumed to be nondegenerate, excited states $|n\rangle$ appearing in the nonequilibrium density matrix ρ can be degenerate so they can be mixed by a non-Abelian Berry phase under adiabatic evolution, which once again invalidates the conventional procedure.

In brief, out of equilibrium $|\Phi(\infty)\rangle_I$ and $|\Phi(-\infty)\rangle_I$ are not simply related. This is obvious physically since when a system is driven out of equilibrium, its asymptotic future is quite different from its initial preparation in the remote past. The purpose of the various nonequilibrium contours such as the two-branch Schwinger-Keldysh contour is precisely to avoid any reference to the state in the asymptotic future $|\Phi(\infty)\rangle_I$ and base the expansion solely on $|\Phi(-\infty)\rangle_I$, the state in the asymptotic past.

1.2 The Schwinger-Keldysh Contour

This idea was pioneering by Schwinger [1], Craig [2], Mills [3], and popularized by Keldysh [4]. To get rid of the unwanted asymptotic future state $|\Phi(\infty)\rangle_I$ we simply use

$$|\Phi(\infty)\rangle_I = \mathcal{S}(\infty, -\infty)|\Phi(-\infty)\rangle_I \tag{1.22}$$

namely, we rewind the time evolution back to the asymptotic past. Equation (1.17) then becomes

$$iG_\Phi(\mathbf{x}, t; \mathbf{x}', t') = \langle\Phi(-\infty)|_I \mathcal{S}(-\infty, \infty) T[\mathcal{S}(\infty, -\infty)\hat{\psi}(\mathbf{x}, t)\hat{\psi}^\dagger(\mathbf{x}', t')]|\Phi(-\infty)\rangle_I \tag{1.23}$$

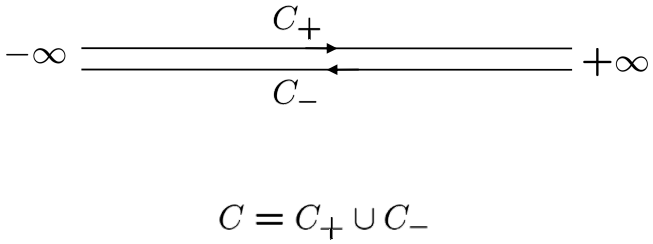

Fig. 1.1. Schwinger-Keldysh contour C.

Now we cannot simply push $\mathcal{S}(-\infty,\infty)$ past the time-ordering operator T and merge it with the forward evolution $\mathcal{S}(\infty,-\infty)$, since the whole backward evolution $\mathcal{S}(-\infty,\infty)$ lies to the left of the T-product. Left means later as far as time ordering is concerned. A clever way to kill these two birds with one stone is to introduce a *two-branch contour* C and ordering *along this contour* enforced by a *contour-ordering operator* T_c. This *Schwinger-Keldysh contour* (Fig. 1.1) consists of two oriented branches $C = C_+ \cup C_-$, the forward branch C_+ extending from $-\infty$ to ∞ and the backward branch C_- extending from ∞ to $-\infty$. We now extend the time variables t, t' to variables defined on this contour τ, τ', and define the fundamental object of nonequilibrium many-body theory, the contour-ordered Green's function,

$$iG(\mathbf{x},\tau;\mathbf{x}',\tau') = \langle T_c[\psi(\mathbf{x},\tau)\psi^\dagger(\mathbf{x}',\tau')]\rangle = \mathrm{Tr}\,\rho T_c[\psi(\mathbf{x},\tau)\psi^\dagger(\mathbf{x}',\tau')] \quad (1.24)$$

With variables and ordering along the contour C, the interaction picture expression corresponding to Eq. (1.23) is

$$iG_\Phi(\mathbf{x},\tau;\mathbf{x}',\tau') = \langle\Phi(-\infty)|_I T_c[\mathcal{S}_c(-\infty,-\infty)\hat{\psi}(\mathbf{x},\tau)\hat{\psi}^\dagger(\mathbf{x}',\tau')]|\Phi(-\infty)\rangle_I \quad (1.25)$$

where the contour S-matrix is

$$\mathcal{S}_c(-\infty,-\infty) \equiv T_c \exp\left(-i\oint_C d\tau_1\, \hat{H}'(\tau_1)\right) \quad (1.26)$$

where the integral is a line integral along the contour C. Note that there is no phase factor in the denominator as in the equilibrium theories since the contour S-matrix by itself (i.e. not in a T_c-ordered product) is actually unity.

According to our previous discussion, the full Green's function is now given by

$$iG(\mathbf{x},\tau;\mathbf{x}',\tau') = \mathrm{Tr}\,\rho(-\infty)T_c[\mathcal{S}_c(-\infty,-\infty)\hat{\psi}(\mathbf{x},\tau)\hat{\psi}^\dagger(\mathbf{x}',\tau')] \quad (1.27)$$

where we have a density matrix defined by

$$\rho(-\infty) = \sum_\Phi p_\Phi |\Phi(-\infty)\rangle_I \langle\Phi(-\infty)|_I \quad (1.28)$$

where now the states are not the Heisenberg states $|\Phi\rangle$ but the interaction picture states in the remote past $|\Phi(-\infty)\rangle_I$. From Eqs. (1.7) and (1.15), it is not hard to show that

$$\rho = \mathcal{S}(0,-\infty)\rho(-\infty)\mathcal{S}(-\infty,0) \quad (1.29)$$

So far this is rather general. Now, in the Keldysh theory we do adiabatically switch *on* the nonequilibrium perturbation V according to $e^{\epsilon t}$ from the remote past $t = -\infty$ to the present $t = 0$, but we do not switch it *off*. This enables us to study stationary nonequilibrium states, a long time after the system has

been driven out of equilibrium[2]. Because of the adiabatic switch-on procedure, $\rho(-\infty)$ can be identified as the density matrix of the system in the remote past when the nonequilibrium perturbation is turned off. It is then evolved in the usual way by the S-matrix $\mathcal{S}(0,-\infty)$ to a nonequilibrium density matrix ρ. One thus usually chooses $\rho(-\infty)$ to be an equilibrium distribution, $\rho(-\infty) = e^{-\beta H}/Z$.

1.3 The Closed Time Path Contour

In the previous section, we constructed the perturbation expansion such that the Green's function would be expressed as an average over the density matrix of the system in the *remote past* because this is what we know: because of the adiabatic switch-on procedure, we have $\rho(-\infty) = e^{-\beta H}/Z$ which is explicitly known. Indeed, the idea of the Keldysh technique is that we want to avoid reference to the general nonequilibrium density matrix ρ which is not usually explicitly known. However, this is not mandatory. If we actually know the density matrix ρ of the system at $t = 0$, then the early Eq. (1.13) is already enough:

$$iG(\mathbf{x},\tau;\mathbf{x}',\tau') = \mathrm{Tr}\,\rho T_c[\mathcal{S}_c(0,0)\hat{\psi}(\mathbf{x},\tau)\hat{\psi}^\dagger(\mathbf{x}',\tau')] \tag{1.30}$$

where ρ is now the full density matrix Eq. (1.7) at $t = 0$, and the contour over which the T_c operator and the S-matrix $\mathcal{S}_c$ are defined is the so-called *closed*

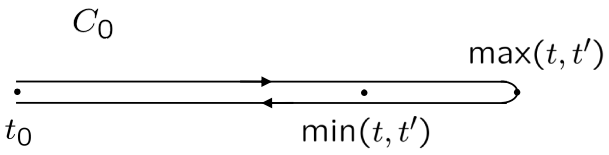

Fig. 1.2. Closed time path contour C_0.

[2] Actually, we may still study transient behavior in the Keldysh formalism, but provided we use an explicitly time-dependent Hamiltonian and there are no initial correlations, namely, the initial density matrix has to be noninteracting.

time path contour C_0 going from 0 to the latest of t or t', and then back to 0. Furthermore, there is nothing special about the time $t = 0$: we might have defined the Heisenberg and interaction pictures with respect to some other initial time t_0. Then the average would be over the density matrix at time t_0:

$$iG(\mathbf{x},\tau;\mathbf{x}',\tau') = \mathrm{Tr}\,\rho(t_0)T_c[\mathcal{S}_c(t_0,t_0)\hat{\psi}(\mathbf{x},\tau)\hat{\psi}^\dagger(\mathbf{x}',\tau')] \tag{1.31}$$

and the closed time path contour [5, 6] now goes from t_0 to the latest of t or t', and then back to t_0 (Fig. 1.2). To recover the Schwinger-Keldysh contour, we take the limit $t_0 \to -\infty$ and insert a factor of $\mathcal{S}(t,\infty)\mathcal{S}(\infty,t)$ or $\mathcal{S}(t',\infty)\mathcal{S}(\infty,t')$ in the perturbation expansion Eq. (1.13) to extend the contour to ∞, depending on whether t or t' is the latest. The density matrix is now $\rho(-\infty)$ and we invoke the adiabatic switch-on procedure to choose $\rho(-\infty) = e^{-\beta H}/Z$.

1.4 Interactions: the Kadanoff-Baym Contour

Equation (1.31) is in a form suitable for a perturbation expansion *provided* that $\rho(t_0)$ is a noninteracting (i.e., 1-particle) density matrix and that the field operators $\hat{\psi}, \hat{\psi}^\dagger$ in the interaction picture evolve with a noninteracting Hamiltonian H. Indeed, these are the conditions of applicability of Wick's theorem [7]. They are satisfied in the Keldysh theory if H is noninteracting since then $\rho(-\infty) = e^{-\beta H}/Z$ is a 1-particle density matrix. What if H contains interactions?

Let us first keep a general t_0 and assume that $\rho(t_0) = e^{-\beta H}/Z$ with H a general interacting Hamiltonian. We can always take $t_0 \to -\infty$ at the end to recover the Keldysh theory. We first break further the equilibrium Hamiltonian $H = H_0 + V$ into a noninteracting part H_0 and the interactions V. We want to express the interacting density matrix $e^{-\beta H}$ in terms of a noninteracting one $e^{-\beta H_0}$. We make use of Eqs. (1.11) and (1.12), but in imaginary time and with a general initial time t_0. Now the full (equilibrium) Hamiltonian is H. As mentioned earlier, we will therefore use upright letters U and S for the evolution and S-matrix respectively. The interaction and Heisenberg pictures are now defined with respect to the initial time t_0, meaning that $A(t) = e^{iH(t-t_0)}Ae^{-iH(t-t_0)}$ and $\hat{A}(t) = e^{iH_0(t-t_0)}Ae^{-iH_0(t-t_0)}$. Since H is time-independent, the evolution operator is simply $U(t,t_0) = e^{-iH(t-t_0)}$ and we have

$$S(t,t_0) = e^{iH_0(t-t_0)}U(t,t_0) \tag{1.32}$$

where the S-matrix is $S(t,t') = T\exp\left(-i\int_{t'}^{t} dt_1\,\hat{V}(t_1)\right)$. We then have

$$e^{-\beta H} = e^{-\beta H_0}S(t_0 - i\beta, t_0) \tag{1.33}$$

where here the S-matrix $S(t_0 - i\beta, t_0)$ evolves the density matrix along a contour $[t_0, t_0 - i\beta]$ on the imaginary axis. The Green's function Eq. (1.31) now assumes the form

$$iG(1,1') = \frac{1}{Z}\,\mathrm{Tr}\, e^{-\beta H_0} S(t_0 - i\beta, t_0) T_c[\mathcal{S}_c(t_0,t_0)\hat{\psi}_H(1)\hat{\psi}_H^\dagger(1')] \tag{1.34}$$

where for simplicity we denote space and time arguments by a collective index $1 \equiv (\mathbf{x}, \tau)$, $1' \equiv (\mathbf{x}', \tau')$. We have also explicitly indicated that the field operators still evolve according to the full H, see Eq. (1.9). They have to be brought to the current interaction picture defined with respect to H_0. This can be achieved as previously through the S-matrix,

$$\hat{\psi}_H(\mathbf{x}, t) = S(t_0, t)\hat{\psi}(\mathbf{x}, t)S(t, t_0) \tag{1.35}$$

where the caret without the subscript denotes the interaction picture with respect to H_0. Equation (1.34) thus becomes

$$\begin{aligned} iG(1,1') = \frac{1}{Z}\,\mathrm{Tr}\, e^{-\beta H_0} S(t_0 - i\beta, t_0) \\ \times T_c[\mathcal{S}_c(t_0,t_0)S(t_0,t)\hat{\psi}(1)S(t,t_0)S(t_0,t')\hat{\psi}^\dagger(1')S(t',t_0)] \end{aligned} \tag{1.36}$$

where we now see that the S-matrix for interactions S evolves along a *three-branch contour* $C^* = C_0 \cup [t_0, t_0 - i\beta]$ which is the *Kadanoff-Baym contour* [8] (Fig. 1.3). This contour goes from t_0 to the latest of t and t', back to t_0, and

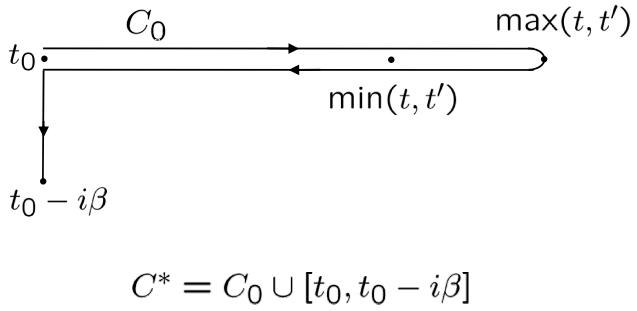

Fig. 1.3. Kadanoff-Baym contour C^*.

then down to $t_0 - i\beta$. We define an ordering operator T_{c^*} along this contour so that we can move the thermal S-matrix $S(t_0 - i\beta, t_0)$ into the contour-ordered product. We then obtain

$$iG(1,1') = \frac{\mathrm{Tr}\, e^{-\beta H_0} T_{c^*}[S_{c^*}(t_0 - i\beta, t_0)\mathcal{S}_c(t_0,t_0)\hat{\psi}(1)\hat{\psi}^\dagger(1')]}{\mathrm{Tr}\, e^{-\beta H_0} T_{c^*}[S_{c^*}(t_0 - i\beta, t_0)\mathcal{S}_c(t_0,t_0)]} \tag{1.37}$$

where in analogy with Eq. (1.26) we define a new contour-ordered S-matrix defined along the Kadanoff-Baym contour,

$$S_{c^*}(t_0 - i\beta, t_0) \equiv T_{c^*} \exp\left(-i \int_{C^*} d\tau_1 \, \hat{V}(\tau_1)\right) \tag{1.38}$$

We have written the partition function as

$$Z = \mathrm{Tr}\, e^{-\beta H} = \mathrm{Tr}\, e^{-\beta H_0} S(t_0 - i\beta, t_0) = \mathrm{Tr}\, e^{-\beta H_0} T_{c^*}[S_{c^*}(t_0 - i\beta, t_0)\mathcal{S}_c(t_0, t_0)] \tag{1.39}$$

since the S-matrices are already time-ordered on their respective contours, and since times on the $[t_0, t_0 - i\beta]$ strip are always later than times on C_0, we simply have $\mathcal{S}_c(t_0, t_0) = 1$ and $S_{c^*}(t_0 - i\beta, t_0) = S(t_0 - i\beta, t_0)$ even inside the T_{c^*}-ordered product. Note that the time arguments in Eq. (1.37) are defined on the three-branch Kadanoff-Baym contour C^*. Equation (1.37) is now fit for perturbation theory since by assumption the averages are with respect to a 1-particle density matrix $e^{-\beta H_0}$ and the field operators evolve according to the noninteracting H_0, so Wick's theorem can be applied.

The Kadanoff-Baym formalism is adequate for the study of initial correlations, namely the effect for times $t > t_0$ of having an interacting density matrix at time t_0, without the assumption $t \gg t_0$. The price to pay for this powerful formalism is that the Green's function is defined on a three-branch contour and has a complicated expression in terms of the simultaneous perturbation expansion of two S-matrices. However for many practical purposes this is overkill, and for steady-state problems we do not care about the effect of initial correlations. In many cases we can assume that correlations decay in time so that if we take the limit $t_0 \to -\infty$, at any finite time $t \gg t_0$ there is no signature left of the correlations in the initial density matrix $\rho(t_0)$. This is the Bogoliubov principle of weakening correlations, a general principle in nonequilibrium statistical mechanics. It is however advised to keep in mind that in some cases initial correlations can persist at long times due for example to the presence of metastable states.

1.4.1 Neglect of Initial Correlations and Schwinger-Keldysh Limit

For most practical purposes we can safely ignore the initial correlations when taking the limit $t_0 \to -\infty$. It has been shown [9, 10, 11] that neglecting initial correlations amounts to neglecting the imaginary strip $[t_0, t_0 - i\beta]$ in the Kadanoff-Baym contour, so we are back with the Schwinger-Keldysh contour (after having extended the closed time path contour as explained in section 1.3). In this limit, the S-matrices in the denominator of Eq. (1.37) are trivial and the denominator is just $\mathrm{Tr}\, e^{-\beta H_0}$. We thus have

$$iG(1, 1') = \mathrm{Tr}\, \rho_0 T_c[S_c(-\infty, -\infty)\mathcal{S}_c(-\infty, -\infty)\hat{\psi}(1)\hat{\psi}^\dagger(1')] \tag{1.40}$$

where the noninteracting density matrix is just

$$\rho_0 \equiv \frac{e^{-\beta H_0}}{\mathrm{Tr}\, e^{-\beta H_0}} \tag{1.41}$$

and $S_c(-\infty,-\infty)$ is just the Kadanoff-Baym contour-ordered S-matrix of Eq. (1.38) but neglecting the third branch of the contour and taking the limit $t_0 \to -\infty$,

$$S_c(-\infty,-\infty) \equiv T_c \exp\left(-i \oint_C d\tau_1\, \hat{V}(\tau_1)\right) \tag{1.42}$$

so that now all the ordering takes place along the Schwinger-Keldysh contour C. If the system is initially at zero temperature, we simply have

$$iG(1,1') = \langle \Phi_0 | T_c[S_c(-\infty,-\infty)\mathcal{S}_c(-\infty,-\infty)\hat{\psi}(1)\hat{\psi}^\dagger(1')] | \Phi_0 \rangle \tag{1.43}$$

with $|\Phi_0\rangle$ the noninteracting ground state of H_0. We see that we have now almost recovered Eq. (1.27), albeit with an additional S-matrix S_c containing the effect of the interactions V. We summarize both zero and finite-temperature results Eqs. (1.43) and (1.40) in the formula

$$iG(1,1') = \langle T_c[S_c(-\infty,-\infty)\mathcal{S}_c(-\infty,-\infty)\hat{\psi}(1)\hat{\psi}^\dagger(1')] \rangle \tag{1.44}$$

with the suitable expectation value. This is the essential starting point for calculations in Keldysh theory. The perturbation expansion can now be carried out, with both nonequilibrium terms $\hat{H}'$ from $\mathcal{S}_c$ (Eq. (1.26)) and interaction terms $\hat{V}$ from S_c (Eq. (1.38)) appearing in the expansion and in the ensuing Feynman diagrams. Let us remark here that the power of the Kadanoff-Baym and Keldysh approaches to nonequilibrium many-body theory – or more generally, to nonequilibrium field theory – lies in its structure being formally identical to that of usual equilibrium many-body theory, albeit with a time evolution and the corresponding perturbative expansion defined on a more general contour. Then most of the tools of quantum field theory can be applied: Feynman diagrams, integral equations for vertex functions such as the Dyson equation, etc.

1.5 Contour Dyson Equation

The whole perturbation expansion for the contour-ordered 1-particle Green's function on the nonequilibrium contour C can be resummed in the form of an integral equation, the Dyson equation:

$$\begin{aligned} G(1,1') &= G_0(1,1') + \int d2\, G_0(1,2)U(2)G(2,1') \\ &\quad + \int d2 \int d3\, G_0(1,2)\Sigma(2,3)G(3,1') \end{aligned} \tag{1.45}$$

$$\begin{aligned} G(1,1') &= G_0(1,1') + \int d2\, G(1,2)U(2)G_0(2,1') \\ &\quad + \int d2 \int d3\, G(1,2)\Sigma(2,3)G_0(3,1') \end{aligned} \tag{1.46}$$

where $G(1,1') \equiv -i\langle T_c[\psi(1)\psi^\dagger(1')]\rangle$ is the exact Green's function Eq. (1.24) and $G_0(1,1') \equiv -i\langle T_c[\hat{\psi}(1)\hat{\psi}^\dagger(1')]\rangle$ is the unperturbed Green's function with field operators in the interaction picture, $U(2)$ is a 1-particle potential and $\Sigma(2,3)$ is the 1-particle irreducible self-energy. The integral sign means a sum over all internal variables, $\int d2 \equiv \sum_{\sigma_2} \int d\mathbf{x}_2 \int_C d\tau_2$. For simplicity, we will use the following notation,

$$G = G_0 + G_0 U G + G_0 \Sigma G \tag{1.47}$$

$$G = G_0 + G U G_0 + G \Sigma G_0 \tag{1.48}$$

1.6 Initial Correlations with Arbitrary Initial Density Matrix

For the sake of completeness, let us just mention a few words about the most general problem (as far as I know) although we won't actually try to solve it in these lectures. Consider Eq. (1.31). In the Keldysh theory we let $t_0 \to -\infty$ and neglected initial correlations. In the Kadanoff-Baym theory we considered initial correlations by keeping a finite t_0, but we assumed that the initial density matrix $\rho(t_0)$ had the equilibrium form $\rho(t_0) = e^{-\beta H}/Z$ with H an interacting Hamiltonian. Now, what if $\rho(t_0)$ is a general, nonequilibrium, interacting density matrix? This corresponds to preparing the system in a correlated nonequilibrium state at a given time t_0 and observing the time evolution of the system for finite times $t > t_0$ without assuming $t \gg t_0$. People need that in the study of correlated plasmas for example. This problem has been studied by Fujita [9], Hall [10], Kukharenko and Tikhodeev [11], and Wagner [12] who gives a rather clear and comprehensive discussion. The idea is to use a modified Kadanoff-Baym contour. First, the general nonequilibrium density matrix can still be written in the form

$$\rho(t_0) = \frac{e^{-\lambda B}}{\mathrm{Tr}\, e^{-\lambda B}} \tag{1.49}$$

since it is positive definite and Hermitian, where λ is *not* the temperature and B is *not* the Hamiltonian but some general quantities. But because of the formal analogy to β and H, we can setup a perturbation expansion on a modified Kadanoff-Baym contour with the imaginary strip $[t_0 - i\lambda, t_0]$. This very general approach encompasses the Feynman, Matsubara, Schwinger-Keldysh, and Kadanoff-Baym approaches as special cases [12].

1.7 Relation to Real-Time Green's Functions

In all that follows, we will confine ourselves exclusively to the Keldysh approach [4, 14, 16, 13, 15] (but the equilibrium Hamiltonian H can still contain

interactions). Let us recap. Our initial goal is to calculate the real-time Green's function of Eq. (1.1),

$$iG(\mathbf{x},t;\mathbf{x}',t') = \langle T[\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')]\rangle = \mathrm{Tr}\,\rho T[\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')] \tag{1.50}$$

with operators in the Heisenberg picture with respect to the full nonequilibrium Hamiltonian $\mathcal{H}$ and a nonequilibrium density matrix ρ. We have defined a contour-ordered Green's function Eq. (1.24) with time arguments on a contour C,

$$iG(\mathbf{x},\tau;\mathbf{x}',\tau') = \langle T_c[\psi(\mathbf{x},\tau)\psi^\dagger(\mathbf{x}',\tau')]\rangle \tag{1.51}$$

and obtained a perturbation expansion for that Green's function in Eq. (1.44),

$$iG(\mathbf{x},\tau;\mathbf{x}',\tau') = \langle T_c[S_c(-\infty,-\infty)\mathcal{S}_c(-\infty,-\infty)\hat{\psi}(\mathbf{x},\tau)\hat{\psi}^\dagger(\mathbf{x}',\tau')]\rangle \tag{1.52}$$

with operators in the interaction picture with respect to the noninteracting part H_0 of the equilibrium Hamiltonian H. Now, how is the contour-ordered Green's function Eq. (1.51) related to the real-time Green's function Eq. (1.50)?

The answer is that depending on which branch the contour arguments τ, τ' belong to, different real-time Green's functions are obtained:

$$G(\mathbf{x},\tau;\mathbf{x}',\tau') = \begin{cases} G^T(\mathbf{x},t;\mathbf{x}',t') \equiv -i\langle T[\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')]\rangle & \text{if } \tau,\tau' \in C_+, \\ G^<(\mathbf{x},t;\mathbf{x}',t') \equiv i\langle \psi^\dagger(\mathbf{x}',t')\psi(\mathbf{x},t)\rangle & \text{if } \tau \in C_+, \tau' \in C_-, \\ G^>(\mathbf{x},t;\mathbf{x}',t') \equiv -i\langle \psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')\rangle & \text{if } \tau \in C_-, \tau' \in C_+, \\ G^{\tilde{T}}(\mathbf{x},t;\mathbf{x}',t') \equiv -i\langle \tilde{T}[\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')]\rangle & \text{if } \tau,\tau' \in C_-, \end{cases} \tag{1.53}$$

where G^T is the time-ordered Green's function of Eq. (1.50) and $\tilde{T}$ is an anti-time ordering operator which orders operators in the opposite way as T, so that $G^{\tilde{T}}$ is the anti-time-ordered Green's function. $G^{<,>}$ are the lesser and greater Green's functions, respectively. One then defines a 2×2 matrix Green's function in real time,

$$G = \begin{pmatrix} G^T & G^< \\ G^> & G^{\tilde{T}} \end{pmatrix} = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix} \tag{1.54}$$

It is not hard to show from the definitions that the following identities hold,

$$G^R = G^T - G^< = G^> - G^{\tilde{T}} \tag{1.55}$$

$$G^A = G^T - G^> = G^< - G^{\tilde{T}} \tag{1.56}$$

$$G^K = G^> + G^< = G^T + G^{\tilde{T}} \tag{1.57}$$

1.7.1 Larkin-Ovchinnikov Representation

In the so-called Larkin-Ovchinnikov representation [16], we perform a linear transformation on G to obtain another matrix $\hat{G}$,

$$\hat{G} = L\tau^3 G L^\dagger = \begin{pmatrix} G^R & G^K \\ 0 & G^A \end{pmatrix} \tag{1.58}$$

where $L = \frac{1}{\sqrt{2}}(\tau^0 - i\tau^2)$ where τ^i are the Pauli matrices (τ^0 is unity). $G^{R,A}$ are the retarded and advanced Green's functions,

$$G^R(\mathbf{x}, t; \mathbf{x}', t') = -i\theta(t - t')\langle\{\psi(\mathbf{x}, t), \psi^\dagger(\mathbf{x}', t')\}\rangle \tag{1.59}$$

$$G^A(\mathbf{x}, t; \mathbf{x}', t') = i\theta(t' - t)\langle\{\psi(\mathbf{x}, t), \psi^\dagger(\mathbf{x}', t')\}\rangle \tag{1.60}$$

and G^K is the Keldysh Green's function,

$$G^K(\mathbf{x}, t; \mathbf{x}', t') = -i\langle[\psi(\mathbf{x}, t), \psi^\dagger(\mathbf{x}', t')]\rangle \tag{1.61}$$

1.7.2 Langreth Theorem of Analytic Continuation

Consider the 'matrix products' occurring in Eqs. (1.45) and (1.46). These are convolution integrals on the two-branch contour. Consider first the following product of two contour-ordered quantities (such as Green's functions or self-energies),

$$C(1, 1') = \int d2A(1, 2)B(2, 1') \tag{1.62}$$

or in simple matrix notation,

$$C = AB \tag{1.63}$$

How do we convert this product to an integral over the real axis involving the real-time components of A and B? This is accomplished by the Langreth theorem [18, 19] which consists in a series of rules:

$$(AB)^{\lessgtr} = A^R B^{\lessgtr} + A^{\lessgtr} B^A \tag{1.64}$$

$$(AB)^{R,A} = A^{R,A} B^{R,A} \tag{1.65}$$

$$(ABC)^{\lessgtr} = A^R B^R C^{\lessgtr} + A^R B^{\lessgtr} C^A + A^{\lessgtr} B^A C^A \tag{1.66}$$

$$(ABC)^{R,A} = A^{R,A} B^{R,A} C^{R,A} \tag{1.67}$$

where the 'matrix products' on the right-hand side consist in summations over internal degrees of freedom (space and spin) and convolution integrals *on the real axis* from $-\infty$ to ∞. We are now completely rid of the contour; the 2×2 matrix structure takes care of the nonequilibrium physics and we can use ordinary real-time integrals. In particular, we can Fourier transform to frequency space in the case of a nonequilibrium steady state in which the Green's functions are time-translationally invariant, $G_{ij}(t, t') = G_{ij}(t - t')$.

We will not derive all these rules but only show how the first one can be obtained. Consider $C = AB$ on the Schwinger-Keldysh contour C. Then

$$
\begin{aligned}
C^<(t,t') &= \int_C d\tau_1\, A(t,\tau_1)B(\tau_1,t') \\
&= \int_{-\infty}^{\infty} dt_1\, A^T(t,t_1)B^<(t_1,t') + \int_{\infty}^{-\infty} dt_1\, A^<(t,t_1)B^{\tilde{T}}(t_1,t') \\
&= \int_{-\infty}^{\infty} dt_1 \left[A^T(t,t_1)B^<(t_1,t') - A^<(t,t_1)B^{\tilde{T}}(t_1,t')\right]
\end{aligned}
$$

From Eqs. (1.55) and (1.56), we know that $A^T = A^R + A^<$ and $B^{\tilde{T}} = B^< - B^A$, hence

$$
\begin{aligned}
C^<(t,t') &= \int_{-\infty}^{\infty} dt_1 \left[\left(A^R(t,t_1) + A^<(t,t_1)\right) B^<(t_1,t') - A^<(t,t_1)\left(B^<(t_1,t') - B^A(t_1,t')\right)\right] \\
&= \int_{-\infty}^{\infty} dt_1 \left[A^R(t,t_1)B^<(t_1,t') + A^<(t,t_1)B^A(t_1,t')\right]
\end{aligned}
$$

The other rules are obtained in a similar fashion. Usually, one writes down the diagrams as in conventional many-body theory and the corresponding analytic expressions involving contour-ordered Green's functions. Typically, these involve integrals over the contour. Then one translates these expressions in the real-time language using the Langreth rules. This is often referred to as 'analytic continuation' from the contour to the real-time axis in analogy with the Matsubara formalism. We feel this is somewhat pedantic since the Schwinger-Keldysh contour is not really a contour in the complex plane; it is only two counter-propagating copies of the real axis.

2

Quantum Kinetic Equations

We have now set up the necessary machinery to construct quantum kinetic equations which govern the evolution of correlation functions in a quantum many-body system driven out of equilibrium. We first say 'correlation functions' which are two-time objects instead of 'distribution functions' which are one-time objects because equations typically do not close for distribution functions. However equations for correlation functions are very complicated integral equations which can usually only be solved numerically. There however exists a variety of useful approximations which make the equations for distribution functions close.

We will thus first discuss the Keldysh and Kadanoff-Baym equations which are exact quantum kinetic equations for the nonequilibrium correlation functions of the system. Then we will introduce the Wigner transform, the gradient expansion and the gradient approximation which yield the quantum Boltzmann equation (QBE). As this equation is still rather complicated, further approximations can be made such as the quasiparticle and quasiclassical approximations. The QBE is still an equation for a four-parameter (two-point) correlation function $G^<(\mathbf{p}, \omega, \mathbf{R}, T)$. Expressed in terms of the Wigner distribution function $f^W(\mathbf{p}, \mathbf{R}, T) \equiv -iG^<(\mathbf{p}, t = 0, \mathbf{R}, T)$ which is a one-time function, the QBE does not close. One can however generate a closed equation for the Wigner distribution function by introducing the so-called generalized Kadanoff-Baym ansatz [17]. We will also recover the classical Boltzmann equation as a limiting case of the QBE.

We can actually understand from simple arguments why a kinetic equation for a quantum distribution function should have more terms than that for a classical distribution function. Recall how the classical Boltzmann equation is derived. Because of the incompressibility of phase space, the total rate of change of the classical distribution function $f(\mathbf{p}, \mathbf{R}, T)$ is equal to the rate of change of f due to collisions, say $\left(\frac{\partial f}{\partial T}\right)_{\text{coll}} \equiv I[f]$:

$$\frac{df}{dT} = I[f]$$

The Boltzmann equation is then obtained simply by using the chain rule for derivatives,

$$\left(\frac{\partial}{\partial T} + \mathbf{v}\cdot\nabla_{\mathbf{R}} + \mathbf{F}\cdot\nabla_{\mathbf{p}}\right) f = I[f] \tag{2.1}$$

since $d\mathbf{R}/dT = \mathbf{v}$ is the velocity and $d\mathbf{p}/dT = \mathbf{F}$ is the force from Newton's second law. In the quantum mechanical case, the distribution function also has an energy argument ω: $f = f(\mathbf{p}, \omega, \mathbf{R}, T)$. We thus generate an additional term in the corresponding Boltzmann equation:

$$\left(\frac{\partial}{\partial T} + \mathbf{v}\cdot\nabla_{\mathbf{R}} + \mathbf{F}\cdot\nabla_{\mathbf{p}} + \frac{d\omega}{dT}\frac{\partial}{\partial\omega}\right) f = I[f]$$

But the rate of change of energy is just the power, $d\omega/dT = P = \mathbf{F}\cdot\mathbf{v}$. Considering electric and magnetic fields, the force is just the Lorentz force $\mathbf{F} = e(\mathbf{E} + \mathbf{v}\times\mathbf{B})$, so $d\omega/dT = e\mathbf{E}\cdot\mathbf{v}$ since the magnetic force does no work. Hence we obtain [13]

$$\left[\frac{\partial}{\partial T} + \mathbf{v}\cdot\left(\nabla_{\mathbf{R}} + e\mathbf{E}\frac{\partial}{\partial\omega}\right) + e(\mathbf{E}+\mathbf{v}\times\mathbf{B})\cdot\nabla_{\mathbf{p}}\right] f = I[f] \tag{2.2}$$

We will see later in this chapter that this is essentially the structure of the QBE.

2.1 Keldysh Equation

We first apply the fourth Langreth rule Eq. (1.67) to the contour Dyson equations (1.47) and (1.48). We obtain

$$G^{R,A} = G_0^{R,A} + G_0^{R,A}UG^{R,A} + G_0^{R,A}\Sigma^{R,A}G^{R,A} \tag{2.3}$$
$$G^{R,A} = G_0^{R,A} + G^{R,A}UG_0^{R,A} + G^{R,A}\Sigma^{R,A}G_0^{R,A} \tag{2.4}$$

because a one-body potential U is proportional to a delta function in time (instantaneous) and is thus neither retarded nor advanced. Hence we see that the retarded and advanced nonequilibrium Green's functions obey Dyson equations which are formally identical to the equilibrium Dyson equations. If we now apply the third Langreth rule Eq. (1.66), we obtain

$$G^{<} = G_0^{<} + G_0^R U G^{<} + G_0^{<} U G^A + G_0^R \Sigma^R G^{<} + G_0^R \Sigma^{<} G^A + G_0^{<} \Sigma^A G^A$$
$$G^{<} = G_0^{<} + G^R U G_0^{<} + G^{<} U G_0^A + G^R \Sigma^R G_0^{<} + G^R \Sigma^{<} G_0^A + G^{<} \Sigma^A G_0^A$$

because the instantaneous one-body potential is diagonal in Keldysh space ($U^{<} = 0$). These two equations are the *Keldysh equations*. Integration over the real axis is understood, for example

$$(G_0^R U G^<)(\mathbf{x},t;\mathbf{x}',t') = \int_{-\infty}^{\infty} dt_1 \int d\mathbf{x}_1\, G_0^R(\mathbf{x},t;\mathbf{x}_1,t_1) U(\mathbf{x}_1,t_1) G^<(\mathbf{x}_1,t_1;\mathbf{x}',t')$$

and

$$\begin{aligned}(G_0^R \Sigma^R G^<)(\mathbf{x},t;\mathbf{x}',t') = \int_{-\infty}^{\infty} dt_1 \int d\mathbf{x}_1 \int_{-\infty}^{\infty} dt_2 \int d\mathbf{x}_2\, G_0^R(\mathbf{x},t;\mathbf{x}_1,t_1) \\ \times \Sigma^R(\mathbf{x}_1,t_1;\mathbf{x}_2,t_2) G^<(\mathbf{x}_2,t_2;\mathbf{x}',t')\end{aligned}$$

The Keldysh equations can be iterated. The infinite order iterate of either equation gives the same following explicit equation for $G^<$,

$$G^{\lessgtr} = [1 + G^R(U+\Sigma^R)] G_0^{\lessgtr} [1 + (U+\Sigma^A) G^A] + G^R \Sigma^{\lessgtr} G^A \tag{2.5}$$

which is the usual general form of the Keldysh equation.

We now digress a moment to study the free Green's functions $G_0^{<,>,R,A}$ more closely. They are propagators for a noninteracting Hamiltonian H_0. To be fully general, we consider a multiband one-particle Hamiltonian $H_0^{\mu\nu}(\mathbf{x}, -i\nabla)$ where μ, ν are band (and/or spin) indices. We however require that each $H_0^{\mu\nu}$ be a properly symmetrized function of the conjugate variables,

$$H_0^{\mu\nu}(\mathbf{x}, -i\nabla) = \sum_i \{f_i^{\mu\nu}(\mathbf{x}), g_i^{\mu\nu}(-i\nabla)\} + u^{\mu\nu}(\mathbf{x}) + v^{\mu\nu}(-i\nabla) \tag{2.6}$$

Then Hermiticity of the second quantized Hamiltonian,

$$H_0 = \sum_{\mu\nu} \int d\mathbf{x}\, \psi_\mu^\dagger(\mathbf{x}) H_0^{\mu\nu}(\mathbf{x}, -i\nabla) \psi_\nu(\mathbf{x}), \tag{2.7}$$

requires that[1]

$$H_0^{\mu\nu}(\mathbf{x}, -i\nabla) = H_0^{\nu\mu}(\mathbf{x}, i\nabla)^* \tag{2.8}$$

We use a matrix notation where $G_0^{\mu\nu}$ is represented by a matrix G_0 in band space. It is easy to show by application of the equation of motion technique that the contour-ordered propagator $G_0(\mathbf{x},\tau;\mathbf{x}',\tau')$ satisfies the following equations of motion[2] where matrix multiplication in band space is understood,

---

[1] Two remarks. First, in the case that the only imaginary quantities in $H_0^{\mu\nu}$ come from $-i\nabla$ (for example for a spin system without Zeeman term and in the absence of spin-orbit coupling), Eq. (2.8) requires the matrix $H_0^{\mu\nu}$ to be *symmetric*. Second, if $H_0^{\mu\nu}$ depends only on $\mathbf{x}$ and not on $-i\nabla$ (for example for a tight-binding model where $\mathbf{x}$ becomes a discrete variable and ∇ is replaced by finite differences), Eq. (2.8) requires the matrix $H_0^{\mu\nu}$ to be *Hermitian*.

[2] The delta function $\delta(\tau,\tau')$ is defined on the contour, such that $\delta^{R,A}(t,t') = \delta(t-t')$ and $\delta^{\lessgtr}(t,t') = 0$.

$$\Big(i\partial_\tau - H_0(\mathbf{x}, -i\nabla)\Big)G_0(\mathbf{x},\tau;\mathbf{x}',\tau') = \delta(\mathbf{x}-\mathbf{x}')\delta(\tau,\tau') \tag{2.9}$$

$$G_0(\mathbf{x},\tau;\mathbf{x}',\tau')\Big(-i\partial_{\tau'} - H_0(\mathbf{x}', i\nabla')\Big) = \delta(\mathbf{x}-\mathbf{x}')\delta(\tau,\tau') \tag{2.10}$$

where in Eq. (2.10) the derivatives $\partial_{\tau'}$ and ∇' act to the left. We do not write explicitly unit matrices in band space. If we take the real-time components of these contour equations, we obtain

$$\Big(i\partial_t - H_0(\mathbf{x}, -i\nabla)\Big)G_0^{R,A}(\mathbf{x},t;\mathbf{x}',t') = \delta(\mathbf{x}-\mathbf{x}')\delta(t-t') \tag{2.11}$$

$$\Big(i\partial_t - H_0(\mathbf{x}, -i\nabla)\Big)G_0^{<,>}(\mathbf{x},t;\mathbf{x}',t') = 0 \tag{2.12}$$

$$G_0^{R,A}(\mathbf{x},t;\mathbf{x}',t')\Big(-i\partial_{t'} - H_0(\mathbf{x}', i\nabla')\Big) = \delta(\mathbf{x}-\mathbf{x}')\delta(t-t') \tag{2.13}$$

$$G_0^{<,>}(\mathbf{x},t;\mathbf{x}',t')\Big(-i\partial_{t'} - H_0(\mathbf{x}', i\nabla')\Big) = 0 \tag{2.14}$$

We can write in simplified notation

$$\hat{G}_0^{-1}G_0^{R,A} = 1 \tag{2.15}$$

$$\hat{G}_0^{-1}G_0^{<} = 0 \tag{2.16}$$

$$G_0^{R,A}\hat{G}_0^{-1} = 1 \tag{2.17}$$

$$G_0^{<}\hat{G}_0^{-1} = 0 \tag{2.18}$$

where the action of the operator $\hat{G}_0^{-1}$ on the right and on the left is defined in Eqs. (2.11)-(2.14). These relations will be helpful in deriving the Kadanoff-Baym and quantum Boltzmann equations in the next section.

The Keldysh equations are used directly in mesoscopic transport for example, where one studies finite-sized nonequilibrium systems with important spatial and/or temporal inhomogeneities. Then the continuous spatial arguments $\mathbf{x}, \mathbf{x}'$ in the Green's functions are typically replaced by discrete site indices i, j (i.e. in a tight-binding representation) or by principal quantum numbers n, n' for discrete energy levels (i.e. in quantum dot physics). The Green's functions then become finite-sized matrices and the Keldysh equations become matrix equations. For a finite-sized system, it is possible to show that the Keldysh equation (2.5) becomes

$$G^{<} = G^R\hat{G}_0^{-1}G_0^{<}[1 + (U+\Sigma^A)G^A] + G^R\Sigma^{<}G^A \tag{2.19}$$

but the first term vanishes by Eq. (2.16), so that we have

$$G^{<} = G^R\Sigma^{<}G^A \tag{2.20}$$

which is the form of the Keldysh equation that is used in mesoscopic transport.

At the other side of the spectrum, if one wishes to study transport in macroscopic samples, i.e. transport in metals or bulk semiconductors, non-equilibrium (but not mesoscopic) superconductivity, etc., then it is usually more practical to use the Kadanoff-Baym equation and its ensuing Boltzmann-type approximations to be studied in the next sections [16]. Then one has to solve an (integro-)differential equation. It is easier to make approximations (such as near-homogeneous or slowly-varying perturbations, not too far from equilibrium) on the Kadanoff-Baym equation than on the Keldysh equation. Furthermore, a connection to conventional transport formalisms such as linear response theory (Kubo formula) can be made: transport coefficients calculated from the linearized quantum Boltzmann equation (which can be derived from the Kadanoff-Baym equation) in the steady-state limit are identical to those obtained in linear response theory.

2.2 Kadanoff-Baym Equation

With the help of these relations, we are now able to derive the Kadanoff-Baym equation from the Keldysh equations. If we act with $\hat{G}_0^{-1}$ on the left of the first Keldysh equation and on the right of the second Keldysh equation and use relations (2.15)-(2.18), we obtain

$$(\hat{G}_0^{-1} - U)G^< = \Sigma^R G^< + \Sigma^< G^A \tag{2.21}$$

$$G^<(\hat{G}_0^{-1} - U) = G^R \Sigma^< + G^< \Sigma^A \tag{2.22}$$

We now subtract these equations from one another:

$$[\hat{G}_0^{-1} - U, G^<] = \Sigma^R G^< + \Sigma^< G^A - G^R \Sigma^< - G^< \Sigma^A \tag{2.23}$$

We now introduce the nonequilibrium spectral function $A \equiv i(G^R - G^A)$ and the scattering rate, or linewidth, or imaginary part of the self-energy $\Gamma \equiv i(\Sigma^R - \Sigma^A)$. We also define symmetric combinations or real parts as $\mathrm{Re}\, G \equiv \frac{1}{2}(G^R + G^A)$ and $\mathrm{Re}\, \Sigma \equiv \frac{1}{2}(\Sigma^R + \Sigma^A)$. In terms of these quantities, Eq. (2.23) can be written as

$$[\hat{G}_0^{-1} - U, G^<] - [\mathrm{Re}\, \Sigma, G^<] - [\Sigma^<, \mathrm{Re}\, G] = -\tfrac{i}{2}\left(\{\Gamma, G^<\} - \{A, \Sigma^<\}\right)$$

However, as seen before, the Keldysh components $G^{R,A,<,>}$ and $\Sigma^{R,A,<,>}$ are not independent. With the relations $-iA = G^R - G^A = G^> - G^<$ and $-i\Gamma = \Sigma^R - \Sigma^A = \Sigma^> - \Sigma^<$ we can rewrite the equation as

$$[\hat{G}_0^{-1} - U - \mathrm{Re}\, \Sigma, G^<] - [\Sigma^<, \mathrm{Re}\, G] = \tfrac{1}{2}\left(\{\Sigma^>, G^<\} - \{G^>, \Sigma^<\}\right) \tag{2.24}$$

which is the *Kadanoff-Baym equation* [8, 13]. As we will see, the term on the left-hand side involving $[\hat{G}_0^{-1} - U, G^<]$ is a driving term, while the terms involving $\mathrm{Re}\, \Sigma$ and $\mathrm{Re}\, G$ describe renormalization effects. From a transport

point of view, they lead to renormalized transport coefficients and are neglected in the classical Boltzmann limit. The right-hand side is a collision term as will be seen. A similar Kadanoff-Baym equation can be derived for $G^>$. By subtracting the two equations, one obtains an equation for the spectral function,

$$[\hat{G}_0^{-1} - U - \mathrm{Re}\,\Sigma, A] - [\Gamma, \mathrm{Re}\,G] = 0 \tag{2.25}$$

which is used as a consistency check when one looks for approximate solutions to the Kadanoff-Baym equation.

The Kadanoff-Baym equation has to be supplemented by an equation for the retarded and advanced Green's functions. It is obtained in the same way, applying relations (2.15)-(2.18) to the nonequilibrium Dyson equations (2.3)-(2.4):

$$(\hat{G}_0^{-1} - U)G^R = 1 + \Sigma^R G^R \tag{2.26}$$

$$G^R(\hat{G}_0^{-1} - U) = 1 + G^R\Sigma^R \tag{2.27}$$

Add these two equations and dividing by 2 gives

$$\tfrac{1}{2}\{\hat{G}_0^{-1} - U, G^R\} = 1 + \tfrac{1}{2}\{\Sigma^R, G^R\} \tag{2.28}$$

In practice, because self-energies are typically functionals of the Green's function $\Sigma = \Sigma[G]$, the Kadanoff-Baym equation and the equations of motion (2.26)-(2.27) for G^R have to be solved self-consistently. Needless to say, this is a rather difficult task and one often has to resort to numerical techniques. Approximations have to be made for the self-energy functions. However, these approximations cannot be made blindly by choosing an arbitrary subset of diagrams since it is then possible to violate conservation laws as shown by Baym and Kadanoff. Self-energies should be derived from the Luttinger-Ward [20] functional Φ,

$$\Sigma[G] = \frac{\delta\Phi[G]}{\delta G} \tag{2.29}$$

The Luttinger-Ward functional $\Phi[G]$ is defined diagrammatically as the sum of all skeleton connected vacuum diagrams with free propagators G_0 replaced by exact propagators G. In practice, one keeps only a few diagrams in the diagrammatic expansion of Φ and then obtains the corresponding diagrammatic representation of the self-energy $\Sigma[G]$ by removing a fermion line G (which corresponds to functional differentiation in Eq. (2.29)). These so-called Φ-derivable approximations preserve conservation laws and are termed *conserving approximations* [21, 22, 8]. For interacting systems involving coupled degrees of freedom such as electrons and phonons, the electron self-energy Σ and phonon polarization Π should be derived from the same electron-phonon vertex Γ. This ensures that the same level of approximation is maintained for both the electron and phonon subsystems [23]. In general, gauge invariance implies the Ward identities which relate the self-energies and the vertex so that a given Φ-derivable approximation for the self-energy $\Sigma[G]$ defines a

fully consistent level of approximation for Green's functions, self-energies, and the vertex.

2.2.1 Wigner Representation and Gradient Expansion

We now move on to the gradient expansion of the Kadanoff-Baym equation [8, 16, 24]. The idea is to separate slow macroscopic variations from fast microscopic variations, and then perform a gradient expansion on the slow variables. In order to do that, we introduce mixed coordinates, the so-called Wigner representation:

$$\mathbf{r} \equiv \mathbf{x}_1 - \mathbf{x}_2, \quad \mathbf{R} \equiv \tfrac{1}{2}(\mathbf{x}_1 + \mathbf{x}_2) \tag{2.30}$$

$$t \equiv t_1 - t_2, \quad T \equiv \tfrac{1}{2}(t_1 + t_2) \tag{2.31}$$

so that a function $C(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2)$ becomes a function $\mathcal{C}(\mathbf{r}, t, \mathbf{R}, T)$. The fast 'relative' variables $(\mathbf{r}, t)$ will be Fourier transformed to $(\mathbf{k}, \Omega)$ while the slow 'center-of-mass' variables[3] $(\mathbf{R}, T)$ will serve for the gradient expansion. The Fourier transform is defined as

$$\begin{aligned} \mathcal{C}(\mathbf{k}, \Omega, \mathbf{R}, T) &\equiv \int dt \int d\mathbf{r}\, e^{i(\Omega t - \mathbf{k}\cdot\mathbf{r})} \mathcal{C}(\mathbf{r}, t, \mathbf{R}, T) \\ &= \int dt \int d\mathbf{r}\, e^{i(\Omega t - \mathbf{k}\cdot\mathbf{r})} C\left(\mathbf{R} + \tfrac{1}{2}\mathbf{r}, T + \tfrac{1}{2}t; \mathbf{R} - \tfrac{1}{2}\mathbf{r}, T - \tfrac{1}{2}t\right) \end{aligned} \tag{2.32}$$

We first work out the Wigner transform of the driving commutator term $[\hat{G}_0^{-1} - U, G^<]$. We have

$$\begin{aligned} [\hat{G}_0^{-1} - U, G^<]_{x_1,x_2} = &\left(i\frac{\partial}{\partial t_1} - H_0(\mathbf{x}_1, -i\nabla_1) - U(x_1)\right) G^<(x_1, x_2) \\ &- G^<(x_1, x_2)\left(-i\frac{\partial}{\partial t_2} - H_0(\mathbf{x}_2, i\nabla_2) - U(x_2)\right) \end{aligned}$$

and for convenience we use a four-vector notation $x^\mu_{1,2} = (t_{1,2}, \mathbf{x}_{1,2})$.

We want to study the dynamics of a system driven out of equilibrium by constant and uniform external electric $\mathbf{E}$ and magnetic $\mathbf{B}$ fields[4]. We first concentrate on the electric field and the magnetic field will be added later. The

[3] For example, consider a free propagator $g(t_1, t_2) = -ie^{-i\varpi(t_1 - t_2)}$ where ϖ is some characteristic frequency. Considered as a function of $t = \frac{1}{2}(t_1 - t_2)$ and $T = \frac{1}{2}(t_1 + t_2)$, this function has a fast variation with frequency 2ϖ in the t variable and is constant (infinitely slow variation) in the T variable. If we add a slow disturbance $\varpi \to \varpi + \Delta(t)$, there will start to be a weak dependence in T, but slower than the dependence in t.

[4] All the following derivations can be done for a general one-particle potential $U(x)$ but would lead to extremely cumbersome expressions. This doesn't have much interest anyway since the physically relevant perturbations are $\mathbf{E}$ and $\mathbf{B}$ fields.

one-particle potential $U(x)$ contains the electric field in the scalar potential gauge:

$$U(x) = -e\mathbf{E}\cdot\mathbf{x} \tag{2.33}$$

We have

$$\begin{aligned}[\hat{G}_0^{-1} - U, G^<]_{x_1,x_2} = &\left(i\frac{\partial}{\partial t_1} + i\frac{\partial}{\partial t_2}\right) G^<(x_1,x_2) - H_0(\mathbf{x}_1, -i\nabla_1)G^<(x_1,x_2) \\ &+G^<(x_1,x_2)H_0(\mathbf{x}_2, i\nabla_2) + e\mathbf{E}\cdot(\mathbf{x}_1-\mathbf{x}_2)G^<(x_1,x_2)\end{aligned}$$

The change of variables Eqs. (2.30) and (2.31) imply the following relations for the derivatives,

$$\frac{\partial}{\partial T} = \frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2}\,, \qquad \frac{\partial}{\partial t} = \frac{1}{2}\left(\frac{\partial}{\partial t_1} - \frac{\partial}{\partial t_2}\right),$$

and similar relations for the spatial derivatives. In Wigner coordinates we thus have

$$\begin{aligned}[\hat{G}_0^{-1} - U, G^<]_{\mathbf{r},t,\mathbf{R},T} = &i\frac{\partial}{\partial T}G^<(\mathbf{r},t,\mathbf{R},T) - H_0\left(\mathbf{R}+\tfrac{1}{2}\mathbf{r}, -i(\tfrac{1}{2}\nabla_{\mathbf{R}} + \nabla_{\mathbf{r}})\right)G^< \\ &+G^<H_0\left(\mathbf{R}-\tfrac{1}{2}\mathbf{r}, i(\tfrac{1}{2}\nabla_{\mathbf{R}} - \nabla_{\mathbf{r}})\right) + e\mathbf{E}\cdot\mathbf{r}G^<\end{aligned}$$

We now perform the Fourier transformation of the center-of-mass variables Eq. (2.32), which corresponds to the following substitutions,

$$i\frac{\partial}{\partial t} \to \Omega \tag{2.34}$$

$$-i\nabla_{\mathbf{r}} \to \mathbf{k} \tag{2.35}$$

$$t \to -i\frac{\partial}{\partial\Omega} \tag{2.36}$$

$$\mathbf{r} \to i\nabla_{\mathbf{k}} \tag{2.37}$$

We obtain

$$\begin{aligned}[\hat{G}_0^{-1} - U, G^<]_{\mathbf{k},\Omega,\mathbf{R},T} = &i\frac{\partial}{\partial T}G^<(\mathbf{k},\Omega,\mathbf{R},T) - H_0\left(\mathbf{R}+\tfrac{i}{2}\nabla_{\mathbf{k}}, \mathbf{k}-\tfrac{i}{2}\nabla_{\mathbf{R}}\right)G^< \\ &+G^<H_0\left(\mathbf{R}-\tfrac{i}{2}\nabla_{\mathbf{k}}, \mathbf{k}+\tfrac{i}{2}\nabla_{\mathbf{R}}\right) + ie\mathbf{E}\cdot\nabla_{\mathbf{k}}G^<\end{aligned}$$

We now perform a change of variables introduced by Mahan and Hänsch,

$$\omega = \Omega + e\mathbf{E}\cdot\mathbf{R} \tag{2.38}$$

which eliminates an unphysical $\propto \mathbf{E}\cdot\mathbf{R}$ term in the equation for G^R to be derived later. This change of variables implies the following substitutions,

$$\Omega \to \omega - e\mathbf{E}\cdot\mathbf{R} \tag{2.39}$$

$$\nabla_{\mathbf{R}} \to \nabla_{\mathbf{R}} + e\mathbf{E}\frac{\partial}{\partial\omega} \tag{2.40}$$

The derivative $\partial/\partial\omega$ is important and differentiates the QBE from the classical Boltzmann equation. We thus obtain the following final exact form for the driving commutator in the Wigner representation,

$$[\hat{G}_0^{-1} - U, G^<]_{\mathbf{k},\omega,\mathbf{R},T} = i\frac{\partial G^<}{\partial T} - H_0\left(\mathbf{R} + \tfrac{i}{2}\nabla_{\mathbf{k}}, \mathbf{k} - \tfrac{i}{2}\left(\nabla_{\mathbf{R}} + e\mathbf{E}\frac{\partial}{\partial\omega}\right)\right)G^< \\ + G^< H_0\left(\mathbf{R} - \tfrac{i}{2}\nabla_{\mathbf{k}}, \mathbf{k} + \tfrac{i}{2}\left(\nabla_{\mathbf{R}} + e\mathbf{E}\frac{\partial}{\partial\omega}\right)\right) + ie\mathbf{E}\cdot\nabla_{\mathbf{k}}G^< \tag{2.41}$$

where $G^< = G^<(\mathbf{k}, \omega, \mathbf{R}, T)$. We now see the importance of a proper ordering of the Hamiltonian since $[\mathbf{R}, \nabla_{\mathbf{R}}] \neq 0$ and $[\mathbf{k}, \nabla_{\mathbf{k}}] \neq 0$. The driving anti-commutator $\{\hat{G}_0^{-1} - U, G^R\}$ appearing in Eq. (2.28) for the retarded Green's function can be derived in a similar way. We simply quote the result:

$$\tfrac{1}{2}\{\hat{G}_0^{-1} - U, G^R\}_{\mathbf{k},\omega,\mathbf{R},T} = \omega G^R - \tfrac{1}{2}H_0\left(\mathbf{R} + \tfrac{i}{2}\nabla_{\mathbf{k}}, \mathbf{k} - \tfrac{i}{2}\left(\nabla_{\mathbf{R}} + e\mathbf{E}\frac{\partial}{\partial\omega}\right)\right)G^R \\ - \tfrac{1}{2}G^R H_0\left(\mathbf{R} - \tfrac{i}{2}\nabla_{\mathbf{k}}, \mathbf{k} + \tfrac{i}{2}\left(\nabla_{\mathbf{R}} + e\mathbf{E}\frac{\partial}{\partial\omega}\right)\right) \tag{2.42}$$

where as advertised the unphysical term $\mathbf{E}\cdot\mathbf{R}$ is removed by the Mahan-Hänsch transformation Eq. (2.38).

Having derived the driving terms in the Wigner representation, we must now see how to transform products of the form AB,

$$(AB)_{\mathbf{x}_1,t_1;\mathbf{x}_2,t_2} = \int dt' \int d\mathbf{x}'\, A(\mathbf{x}_1, t_1; \mathbf{x}', t')B(\mathbf{x}', t'; \mathbf{x}_2, t_2) \tag{2.43}$$

From the definition of the Wigner coordinates Eqs. (2.30-2.31), we have

$$A(\mathbf{x}_1, t_1; \mathbf{x}', t') = \mathcal{A}(\mathbf{x}_1 - \mathbf{x}', t_1 - t', \tfrac{1}{2}(\mathbf{x}_1 + \mathbf{x}'), \tfrac{1}{2}(t_1 + t')) \\ = \mathcal{A}\left(\mathbf{x}_1 - \mathbf{x}', t_1 - t', \mathbf{R} + \frac{\mathbf{x}' - \mathbf{x}_2}{2}, T + \frac{t' - t_2}{2}\right) \tag{2.44}$$

and similarly

$$B(\mathbf{x}', t'; \mathbf{x}_2, t_2) = \mathcal{B}(\mathbf{x}' - \mathbf{x}_2, t' - t_2, \tfrac{1}{2}(\mathbf{x}' + \mathbf{x}_2), \tfrac{1}{2}(t' + t_2)) \\ = \mathcal{B}\left(\mathbf{x}' - \mathbf{x}_2, t' - t_2, \mathbf{R} + \frac{\mathbf{x}' - \mathbf{x}_1}{2}, T + \frac{t' - t_1}{2}\right) \tag{2.45}$$

Since the derivative is the generator of translations, we have the following compact form for the usual Taylor expansion,

$$f(\mathbf{R} + \mathbf{a}, T + s) = e^{\mathbf{a}\cdot\nabla_{\mathbf{R}}}e^{s\partial_T}f(\mathbf{R}, T) \tag{2.46}$$

Using Eqs. (2.44,2.45,2.46), we can write Eq. (2.43) as

$$(AB)_{\mathbf{x}_1,t_1;\mathbf{x}_2,t_2} = \int dt' \int d\mathbf{x}'\, \mathcal{A}(\mathbf{x}_1-\mathbf{x}', t_1-t', \mathbf{R}, T) e^{-(\mathbf{x}_1-\mathbf{x}')\cdot\nabla^B_{\mathbf{R}}/2} e^{-(t_1-t')\partial^B_T/2} \times e^{(\mathbf{x}'-\mathbf{x}_2)\cdot\nabla^A_{\mathbf{R}}/2} e^{(t'-t_2)\partial^A_T/2} \mathcal{B}(\mathbf{x}'-\mathbf{x}_2, t'-t_2, \mathbf{R}, T) \tag{2.47}$$

where the superscripts A and B on the derivative operators $\nabla_{\mathbf{R}}, \partial_T$ indicate that they act on the function $\mathcal{A}$ and $\mathcal{B}$, respectively. The integral now has the form of a convolution product,

$$\int dt' \int d\mathbf{x}'\, \tilde{A}(\mathbf{x}_1-\mathbf{x}', t_1-t', \mathbf{R}, T)\tilde{B}(\mathbf{x}'-\mathbf{x}_2, t'-t_2, \mathbf{R}, T) = \tilde{A} * \tilde{B},$$

where

$$\tilde{A}(\mathbf{r}, t, \mathbf{R}, T) = \mathcal{A}(\mathbf{r}, t, \mathbf{R}, T) e^{-(\mathbf{r}\cdot\nabla^B_{\mathbf{R}} + t\partial^B_T)/2} \tag{2.48}$$

$$\tilde{B}(\mathbf{r}, t, \mathbf{R}, T) = e^{(\mathbf{r}\cdot\nabla^A_{\mathbf{R}} + t\partial^A_T)/2} \mathcal{B}(\mathbf{r}, t, \mathbf{R}, T) \tag{2.49}$$

We now take the Fourier transform, as defined in Eq. (2.32), of the convolution product, so that we have

$$(AB)_{\mathbf{k},\Omega,\mathbf{R},T} = \mathcal{F}\{\tilde{A} * \tilde{B}\} = \tilde{A}(\mathbf{k}, \Omega, \mathbf{R}, T)\tilde{B}(\mathbf{k}, \Omega, \mathbf{R}, T) \tag{2.50}$$

since the Fourier transform of a convolution product is the ordinary product of the Fourier transforms of the convoluted functions. We thus have

$$\tilde{A}(\mathbf{k}, \Omega, \mathbf{R}, T) = \int dt \int d\mathbf{r}\, e^{i(\Omega t - \mathbf{k}\cdot\mathbf{r})} \mathcal{A}(\mathbf{r}, t, \mathbf{R}, T) e^{-(\mathbf{r}\cdot\nabla^B_{\mathbf{R}} + t\partial^B_T)/2} \tag{2.51}$$

$$\tilde{B}(\mathbf{k}, \Omega, \mathbf{R}, T) = \int dt \int d\mathbf{r}\, e^{i(\Omega t - \mathbf{k}\cdot\mathbf{r})} e^{(\mathbf{r}\cdot\nabla^A_{\mathbf{R}} + t\partial^A_T)/2} \mathcal{B}(\mathbf{r}, t, \mathbf{R}, T) \tag{2.52}$$

Since a phase factor in a Fourier transform generates a translation,

$$\mathcal{F}\{e^{\mathbf{a}\cdot\mathbf{r}} e^{st} f(\mathbf{r}, t)\} = f(\mathbf{k} + i\mathbf{a}, \Omega - is) = e^{i\mathbf{a}\cdot\nabla_{\mathbf{k}}} e^{-is\partial_\Omega} f(\mathbf{k}, \Omega),$$

we obtain

$$\tilde{A}(\mathbf{k}, \Omega, \mathbf{R}, T) = \mathcal{A}(\mathbf{k}, \Omega, \mathbf{R}, T) e^{-i\nabla^B_{\mathbf{R}}\cdot\nabla^A_{\mathbf{k}}/2} e^{i\partial^B_T\partial^A_\Omega/2} \tag{2.53}$$

$$\tilde{B}(\mathbf{k}, \Omega, \mathbf{R}, T) = \mathcal{B}(\mathbf{k}, \Omega, \mathbf{R}, T) e^{i\nabla^A_{\mathbf{R}}\cdot\nabla^B_{\mathbf{k}}/2} e^{-i\partial^A_T\partial^B_\Omega/2} \tag{2.54}$$

Inserting these results in Eq. (2.50), we have

$$(AB)_{\mathbf{k},\Omega,\mathbf{R},T} = A(\mathbf{k}, \Omega, \mathbf{R}, T)\hat{\mathcal{G}}^{AB}(\mathbf{k}, \Omega, \mathbf{R}, T)B(\mathbf{k}, \Omega, \mathbf{R}, T) \tag{2.55}$$

where we have now dropped the curly letter notation $\mathcal{A}$ and $\mathcal{B}$ for simplicity, and we define the gradient operator $\hat{\mathcal{G}}^{AB}$ as

$$\hat{\mathcal{G}}^{AB}(\mathbf{k}, \Omega, \mathbf{R}, T) \equiv e^{-i(\partial^A_T\partial^B_\Omega - \partial^A_\Omega\partial^B_T - \nabla^A_{\mathbf{R}}\cdot\nabla^B_{\mathbf{k}} + \nabla^A_{\mathbf{k}}\cdot\nabla^B_{\mathbf{R}})/2}$$

As a mathematical aside, we note in passing that Eq. (2.55) corresponds to the Moyal or star product of two functions which is used in noncommutative

geometry and deformation quantization, and more generally in mathematics in the construction of deformed algebras.

So far, everything has been exact. In the so-called gradient approximation, we expand the exponential to first order in the gradients. We have

$$\hat{\mathcal{G}}^{AB}(\mathbf{k},\Omega,\mathbf{R},T) \simeq 1 - \frac{i}{2}\left(\frac{\partial^A}{\partial T}\frac{\partial^B}{\partial \Omega} - \frac{\partial^A}{\partial \Omega}\frac{\partial^B}{\partial T} - \nabla^A_{\mathbf{R}}\cdot\nabla^B_{\mathbf{k}} + \nabla^A_{\mathbf{k}}\cdot\nabla^B_{\mathbf{R}}\right)$$

so the basic expression of the gradient approximation is

$$\begin{aligned}(AB)_{\mathbf{k},\Omega,\mathbf{R},T} \simeq\ & A(\mathbf{k},\Omega,\mathbf{R},T)B(\mathbf{k},\Omega,\mathbf{R},T) \\ & -\frac{i}{2}\left(\frac{\partial A}{\partial T}\frac{\partial B}{\partial \Omega} - \frac{\partial A}{\partial \Omega}\frac{\partial B}{\partial T} - \nabla_{\mathbf{R}}A\cdot\nabla_{\mathbf{k}}B + \nabla_{\mathbf{k}}A\cdot\nabla_{\mathbf{R}}B\right)\end{aligned}$$

from Eq. (2.55). We can now write down the Kadanoff-Baym commutators and anticommutators in the Wigner representation under the gradient approximation as follows,

$$\begin{aligned}[A,B]_{\mathbf{k},\omega,\mathbf{R},T} = [A,B] &+ \frac{i}{2}\left(\left\{\frac{\partial A}{\partial \omega},\frac{\partial B}{\partial T}\right\} - \left\{\frac{\partial A}{\partial T},\frac{\partial B}{\partial \omega}\right\} - \{\nabla_{\mathbf{k}}A,\nabla_{\mathbf{R}}B\} + \{\nabla_{\mathbf{R}}A,\nabla_{\mathbf{k}}B\}\right) \\ &+\frac{i}{2}e\mathbf{E}\cdot\left(\left\{\frac{\partial A}{\partial \omega},\nabla_{\mathbf{k}}B\right\} - \left\{\nabla_{\mathbf{k}}A,\frac{\partial B}{\partial \omega}\right\}\right) \qquad (2.56)\end{aligned}$$

$$\begin{aligned}\{A,B\}_{\mathbf{k},\omega,\mathbf{R},T} = \{A,B\} &+ \frac{i}{2}\left(\left[\frac{\partial A}{\partial \omega},\frac{\partial B}{\partial T}\right] - \left[\frac{\partial A}{\partial T},\frac{\partial B}{\partial \omega}\right] - [\nabla_{\mathbf{k}}A,\nabla_{\mathbf{R}}B] + [\nabla_{\mathbf{R}}A,\nabla_{\mathbf{k}}B]\right) \\ &+\frac{i}{2}e\mathbf{E}\cdot\left(\left[\frac{\partial A}{\partial \omega},\nabla_{\mathbf{k}}B\right] - \left[\nabla_{\mathbf{k}}A,\frac{\partial B}{\partial \omega}\right]\right) \qquad (2.57)\end{aligned}$$

where on the right-hand side, these are ordinary matrix commutators and anticommutators, and we have performed the Mahan-Hänsch transformation Eq. (2.38).

2.3 Quantum Boltzmann Equation

We first discuss the QBE [24] in zero magnetic field, then add the magnetic field.

2.3.1 QBE with Electric Field

The QBE is now obtained merely as the Kadanoff-Baym equation (2.24) in the Wigner representation:

$$\begin{aligned}[\hat{G}_0^{-1} - U, G^<]_{\mathbf{k},\omega,\mathbf{R},T} = [\mathrm{Re}\,\Sigma, G^<]_{\mathbf{k},\omega,\mathbf{R},T} &+ [\Sigma^<, \mathrm{Re}\,G]_{\mathbf{k},\omega,\mathbf{R},T} \\ &+\tfrac{1}{2}\left(\{\Sigma^>, G^<\}_{\mathbf{k},\omega,\mathbf{R},T} - \{G^>,\Sigma^<\}_{\mathbf{k},\omega,\mathbf{R},T}\right) \qquad (2.58)\end{aligned}$$

where the left-hand side is given by Eq. (2.41) and the terms on the right-hand side are given by Eqs. (2.56) and (2.57). So far we have only rephrased the Kadanoff-Baym equation in Wigner coordinates and made the gradient approximation. Equation (2.58) is still valid to arbitrary order in the electric field and for both time and space-dependent (but slowly varying) perturbations. Note that this very general equation has in principle to be solved together with the equation for the retarded Green's function Eq. (2.28),

$$\tfrac{1}{2}\{\hat{G}_0^{-1} - U, G^R\}_{\mathbf{k},\omega,\mathbf{R},T} = 1 + \tfrac{1}{2}\{\Sigma^R, G^R\}_{\mathbf{k},\omega,\mathbf{R},T} \tag{2.59}$$

where the left-hand side is given in Eq. (2.42) and the anticommutator on the right-hand side is given by Eq. (2.57). Indeed, the nonequilibrium G^R enters the renormalization terms $\mathrm{Re}\, G$ and $\mathrm{Re}\, \Sigma$ (since $\Sigma^R = \Sigma^R[G^R]$) in Eq. (2.58).

It is obvious that this primary form of the QBE is extremely complicated and that not much progress can be made unless further approximations are introduced, otherwise one has to resort to numerical techniques. In addition, we have kept a fully general multiband Hamiltonian H_0 so far, but one can also restrict the analysis to a given class of Hamiltonians.

2.3.2 QBE with Electric and Magnetic Field

We now add the effect of a constant uniform magnetic field $\mathbf{B}$. Whereas the electric field $\mathbf{E}$ was introduced in Eq. (2.33) through the scalar potential, we now introduce the magnetic field through a vector potential,

$$\mathbf{A}(x) = -\tfrac{1}{2}\mathbf{x} \times \mathbf{B}$$

We also perform the Peierls substitution in the Hamiltonian,

$$H_0(-i\nabla) \to H_0(-i\nabla - e\mathbf{A}) = H_0\left(-i\nabla + \tfrac{1}{2}e\mathbf{x} \times \mathbf{B}\right) \tag{2.60}$$

We now proceed along similar steps as before. In Wigner coordinates, we have

$$\begin{aligned} H_0(x_1, -i\nabla_1 - e\mathbf{A}_1) &\to H_0\left(\mathbf{R} + \tfrac{1}{2}\mathbf{r}, -i(\tfrac{1}{2}\nabla_{\mathbf{R}} + \nabla_{\mathbf{r}}) + \tfrac{1}{2}e(\mathbf{R} + \tfrac{1}{2}\mathbf{r}) \times \mathbf{B}\right) \\ H_0(x_2, i\nabla_2 - e\mathbf{A}_2) &\to H_0\left(\mathbf{R} - \tfrac{1}{2}\mathbf{r}, i(\tfrac{1}{2}\nabla_{\mathbf{R}} - \nabla_{\mathbf{r}}) + \tfrac{1}{2}e(\mathbf{R} - \tfrac{1}{2}\mathbf{r}) \times \mathbf{B}\right) \end{aligned}$$

After Fourier transformation, we obtain terms like

$$H_0\left(\mathbf{R} \pm \tfrac{i}{2}\nabla_{\mathbf{k}}, \mathbf{k} + \tfrac{1}{2}e\mathbf{R} \times \mathbf{B} \mp \tfrac{i}{2}(\nabla_{\mathbf{R}} + \tfrac{1}{2}e\mathbf{B} \times \nabla_{\mathbf{k}})\right)$$

As before, we perform the Mahan-Hänsch transformation Eq. (2.38) which changes the derivative with respect to $\mathbf{R}$ according to Eq. (2.40), and obtain

$$H_0\left(\mathbf{R} \pm \tfrac{i}{2}\nabla_{\mathbf{k}}, \mathbf{k} + \tfrac{1}{2}e\mathbf{R} \times \mathbf{B} \mp \tfrac{i}{2}\left(\nabla_{\mathbf{R}} + e\mathbf{E}\frac{\partial}{\partial\omega} + \tfrac{1}{2}e\mathbf{B} \times \nabla_{\mathbf{k}}\right)\right)$$

The Mahan-Hänsch transformation got rid of the $\propto \mathbf{E} \cdot \mathbf{R}$ term. We now perform a similar extra transformation to get rid of the unphysical $\mathbf{R} \times \mathbf{B}$ term by introducing the kinematical momentum,

$$\mathbf{p} = \mathbf{k} + \tfrac{1}{2}e\mathbf{R}\times\mathbf{B} = \mathbf{k} - e\mathbf{A}(\mathbf{R}) \tag{2.61}$$

which implies $\nabla_{\mathbf{k}} \to \nabla_{\mathbf{p}}$ but modifies the $\mathbf{R}$ derivative once more,

$$\nabla_{\mathbf{R}} \to \nabla_{\mathbf{R}} + \tfrac{1}{2}e\mathbf{B}\times\nabla_{\mathbf{p}}$$

so that the final expression reads

$$H_0\left(\mathbf{R} \pm \tfrac{i}{2}\nabla_{\mathbf{p}}, \mathbf{p} \mp \tfrac{i}{2}\left(\nabla_{\mathbf{R}} + e\mathbf{E}\frac{\partial}{\partial\omega} + e\mathbf{B}\times\nabla_{\mathbf{p}}\right)\right)$$

Hence the generalization of Eq. (2.41) to include the magnetic field $\mathbf{B}$ is

$$\begin{aligned}[\hat{G}_0^{-1} - U, G^<]_{\mathbf{p},\omega,\mathbf{R},T} = i\frac{\partial G^<}{\partial T} &- H_0\left(\mathbf{R} + \tfrac{i}{2}\nabla_{\mathbf{p}}, \mathbf{p} - \tfrac{i}{2}\left(\nabla_{\mathbf{R}} + e\mathbf{E}\frac{\partial}{\partial\omega} + e\mathbf{B}\times\nabla_{\mathbf{p}}\right)\right)G^< \\ &+ G^< H_0\left(\mathbf{R} - \tfrac{i}{2}\nabla_{\mathbf{p}}, \mathbf{p} + \tfrac{i}{2}\left(\nabla_{\mathbf{R}} + e\mathbf{E}\frac{\partial}{\partial\omega} + e\mathbf{B}\times\nabla_{\mathbf{p}}\right)\right) \\ &+ ie\mathbf{E}\cdot\nabla_{\mathbf{p}}G^<\end{aligned} \tag{2.62}$$

and similarly the generalization of Eq. (2.42) is

$$\begin{aligned}\tfrac{1}{2}\{\hat{G}_0^{-1} - U, G^R\}_{\mathbf{p},\omega,\mathbf{R},T} = \omega G^R &- \tfrac{1}{2}H_0\left(\mathbf{R} + \tfrac{i}{2}\nabla_{\mathbf{p}}, \mathbf{p} - \tfrac{i}{2}\left(\nabla_{\mathbf{R}} + e\mathbf{E}\frac{\partial}{\partial\omega} + e\mathbf{B}\times\nabla_{\mathbf{p}}\right)\right)G^R \\ &- \tfrac{1}{2}G^R H_0\left(\mathbf{R} - \tfrac{i}{2}\nabla_{\mathbf{p}}, \mathbf{p} + \tfrac{i}{2}\left(\nabla_{\mathbf{R}} + e\mathbf{E}\frac{\partial}{\partial\omega} + e\mathbf{B}\times\nabla_{\mathbf{p}}\right)\right)\end{aligned} \tag{2.63}$$

All Green's functions and self-energies are now functions of $(\mathbf{p}, \omega, \mathbf{R}, T)$. The last thing to figure out is how Eqs. (2.56) and (2.57) are modified in the presence of the magnetic field. It is straightforward to show that the only changes are the substitution $\mathbf{k} \to \mathbf{p}$ and a new term linear in the magnetic field,

$$([A,B]_\pm)_{\mathbf{p},\omega,\mathbf{R},T} = ([A,B]_\pm)_{\mathbf{k},\omega,\mathbf{R},T}\Big|_{\mathbf{k}\to\mathbf{p}} + \tfrac{i}{2}e\mathbf{B}\cdot[\nabla_{\mathbf{p}}A \underset{,}{\times} \nabla_{\mathbf{p}}B]_\pm \tag{2.64}$$

where we use the notation

$$[\nabla_{\mathbf{p}}A \underset{,}{\times} \nabla_{\mathbf{p}}B]_\pm \equiv \nabla_{\mathbf{p}}A\times\nabla_{\mathbf{p}}B \pm \nabla_{\mathbf{p}}B\times\nabla_{\mathbf{p}}A \tag{2.65}$$

Then the QBE in the presence of both electric $\mathbf{E}$ and magnetic $\mathbf{B}$ fields is formally identical to Eq. (2.58),

$$\begin{aligned}[\hat{G}_0^{-1} - U, G^<]_{\mathbf{p},\omega,\mathbf{R},T} = [\mathrm{Re}\,\Sigma, G^<]_{\mathbf{p},\omega,\mathbf{R},T} &+ [\Sigma^<, \mathrm{Re}\,G]_{\mathbf{p},\omega,\mathbf{R},T} \\ &+ \tfrac{1}{2}\left(\{\Sigma^>, G^<\}_{\mathbf{p},\omega,\mathbf{R},T} - \{G^>, \Sigma^<\}_{\mathbf{p},\omega,\mathbf{R},T}\right)\end{aligned} \tag{2.66}$$

but with the definitions in Eqs. (2.62) and (2.64). Similarly, the equation for the retarded Green's function Eq. (2.59) becomes

$$\tfrac{1}{2}\{\hat{G}_0^{-1} - U, G^R\}_{\mathbf{p},\omega,\mathbf{R},T} = 1 + \tfrac{1}{2}\{\Sigma^R, G^R\}_{\mathbf{p},\omega,\mathbf{R},T} \tag{2.67}$$

together with Eqs. (2.63) and (2.64).

Equation (2.66) is the most general form of the quantum Boltzmann equation and makes no assumptions other than that of slowly varying disturbances. It is obvious that it is a rather complicated equation. Approximations should be introduced to bring it to a more tractable form. The first obvious approximation is to restrict the analysis to linear transport, that is, keep only terms to linear order in the electric field, while keeping terms to all orders in the magnetic field. Afterwards, approximations can branch off in different directions and depend on the problem at hand. In the next chapter, we discuss several useful approximate forms of the QBE.

2.3.3 One-Band Spinless Electrons

Most analytical work using the QBE is done for one-band spinless electrons. The single-particle Hamiltonian H_0 is of course

$$H_0(-i\nabla) = \frac{(-i\nabla)^2}{2m}$$

The driving terms Eqs. (2.62) and (2.63) become

$$[\hat{G}_0^{-1} - U, G^<]_{\mathbf{p},\omega,\mathbf{R},T} = i\left[\frac{\partial}{\partial T} + \mathbf{v}_\mathbf{p}\cdot\left(\nabla_\mathbf{R} + e\mathbf{E}\frac{\partial}{\partial\omega}\right) + e(\mathbf{E}+\mathbf{v}_\mathbf{p}\times\mathbf{B})\cdot\nabla_\mathbf{p}\right]G^<$$

$$\tfrac{1}{2}\{\hat{G}_0^{-1} - U, G^R\}_{\mathbf{p},\omega,\mathbf{R},T} = \left[\omega - \epsilon_\mathbf{p} + \frac{1}{8m}\left(\nabla_\mathbf{R} + e\mathbf{E}\frac{\partial}{\partial\omega} + e\mathbf{B}\times\nabla_\mathbf{p}\right)^2\right]G^R$$

where we have the usual definitions of the single-particle energies and velocities

$$\epsilon_\mathbf{p} = \frac{p^2}{2m}\,, \qquad \mathbf{v}_\mathbf{p} = \nabla_\mathbf{p}\epsilon_\mathbf{p} = \frac{\mathbf{p}}{m}.$$

We see that the driving term $[\hat{G}_0^{-1} - U, G^<]$ has indeed the form of Eq. (2.2) derived from simple considerations. We now consider the Kadanoff-Baym commutators Eq. (2.64). Consider first the anticommutator $\{A, B\}_{\mathbf{p},\omega,\mathbf{R},T}$. All the commutators in Eq. (2.57) vanish since the quantities are all scalars. Furthermore, the term proportional to $\mathbf{B}$ in Eq. (2.64) vanishes because of the antisymmetry of the cross product. Hence we have simply $\{A, B\}_{\mathbf{p},\omega,\mathbf{R},T} = 2AB$, and Eq. (2.67) becomes

$$\left[\omega - \epsilon_\mathbf{p} + \frac{1}{8m}\left(\nabla_\mathbf{R} + e\mathbf{E}\frac{\partial}{\partial\omega} + e\mathbf{B}\times\nabla_\mathbf{p}\right)^2 - \Sigma^R\right]G^R = 1 \tag{2.68}$$

The Kadanoff-Baym commutator in Eq. (2.64) becomes

$$[A,B]_{\mathbf{p},\omega,\mathbf{R},T} = i\left(\frac{\partial A}{\partial\omega}\frac{\partial B}{\partial T} - \frac{\partial A}{\partial T}\frac{\partial B}{\partial\omega} - \nabla_{\mathbf{p}}A\cdot\nabla_{\mathbf{R}}B + \nabla_{\mathbf{R}}A\cdot\nabla_{\mathbf{p}}B\right)$$
$$+ie\mathbf{E}\cdot\left(\frac{\partial A}{\partial\omega}\nabla_{\mathbf{p}}B - \nabla_{\mathbf{p}}A\frac{\partial B}{\partial\omega}\right) + ie\mathbf{B}\cdot(\nabla_{\mathbf{p}}A\times\nabla_{\mathbf{p}}B)$$

so that the QBE Eq. (2.66) becomes

$$i\left[\left(1-\frac{\partial\,\mathrm{Re}\,\Sigma}{\partial\omega}\right)\frac{\partial}{\partial T} + \frac{\partial\,\mathrm{Re}\,\Sigma}{\partial T}\frac{\partial}{\partial\omega} + (\mathbf{v}_{\mathbf{p}}+\nabla_{\mathbf{p}}\,\mathrm{Re}\,\Sigma)\cdot\left(\nabla_{\mathbf{R}} + e\mathbf{E}\frac{\partial}{\partial\omega}\right)\right.$$
$$\left.+e\left(\left(1-\frac{\partial\,\mathrm{Re}\,\Sigma}{\partial\omega}\right)\mathbf{E} + (\mathbf{v}_{\mathbf{p}}+\nabla_{\mathbf{p}}\,\mathrm{Re}\,\Sigma)\times\mathbf{B}\right)\cdot\nabla_{\mathbf{p}} - \nabla_{\mathbf{R}}\,\mathrm{Re}\,\Sigma\cdot\nabla_{\mathbf{p}}\right]G^{<}$$
$$-ie\mathbf{E}\cdot\left(\frac{\partial\Sigma^{<}}{\partial\omega}\nabla_{\mathbf{p}}\,\mathrm{Re}\,G - \frac{\partial\,\mathrm{Re}\,G}{\partial\omega}\nabla_{\mathbf{p}}\Sigma^{<}\right) - ie\mathbf{B}\cdot(\nabla_{\mathbf{p}}\Sigma^{<}\times\nabla_{\mathbf{p}}\,\mathrm{Re}\,G)$$
$$= \Sigma^{>}G^{<} - G^{>}\Sigma^{<} + i\left(\frac{\partial\Sigma^{<}}{\partial p^{\mu}}\frac{\partial\,\mathrm{Re}\,G}{\partial X_{\mu}} - \frac{\partial\Sigma^{<}}{\partial X^{\mu}}\frac{\partial\,\mathrm{Re}\,G}{\partial p_{\mu}}\right) \tag{2.69}$$

where we use the four-vector notation $p^{\mu} = (\omega,\mathbf{p})$ and $X^{\mu} = (T,\mathbf{R})$ with the Minkowski metric $\eta_{\mu\nu} = (+---)$.

Equation (2.69) is valid to arbitrary order in $\mathbf{E}$ and $\mathbf{B}$ fields. We see that the self-energy term $[\mathrm{Re}\,\Sigma, G^{<}]$ in the right-hand side of Eq. (2.66) has renormalized the velocity in the driving term,

$$\mathbf{v}_{\mathbf{p}} \to \mathbf{v}_{\mathbf{p}} + \nabla_{\mathbf{p}}\,\mathrm{Re}\,\Sigma = \nabla_{\mathbf{p}}(\epsilon_{\mathbf{p}} + \mathrm{Re}\,\Sigma),$$

and introduced the factor $\left(1-\frac{\partial\,\mathrm{Re}\,\Sigma}{\partial\omega}\right)$ reminiscent of the wavefunction renormalization factor Z^{-1} in Fermi liquid theory. The other term $[\Sigma^{<}, \mathrm{Re}\,G]$ gives some additional terms proportional to the $\mathbf{E}$ and $\mathbf{B}$ fields. The term $\Sigma^{>}G^{<} - G^{>}\Sigma^{<}$ on the left-hand side is a collision term.

3

Applications

We now consider a few applications of the nonequilibrium formalism.

3.1 Nonequilibrium Transport through a Quantum Dot

In this section we study nonequilibrium transport through a quantum dot connected to two external metallic leads (two-probe system). Let us first derive a general expression for the current through the dot in terms of Keldysh nonequilibrium Green's functions.

The Hamiltonian of the whole two-probe system is

$$\hat{H} = \sum_{\mathbf{k}\alpha\in L,R} \epsilon_{\mathbf{k}\alpha} c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + H_C[\{d^\dagger_n\},\{d_n\}] + \sum_{\mathbf{k}\alpha\in L,R,n} \left(t_{\mathbf{k}\alpha,n} c^\dagger_{\mathbf{k}\alpha} d_n + t^*_{\mathbf{k}\alpha,n} d^\dagger_n c_{\mathbf{k}\alpha} \right), \tag{3.1}$$

where $c^\dagger_{\mathbf{k}\alpha}$ ($c_{\mathbf{k}\alpha}$) is a fermionic creation (annihilation) operator for a single-particle momentum state $\mathbf{k}$ in channel α in the left or right metallic lead, and $d^\dagger_n, d_n$ are creation/annihilation operators for states in the quantum dot. H_C is the Hamiltonian of the quantum dot. For a noninteracting dot, H_C would be

$$H_C = \sum_{mn} h_{mn} d^\dagger_m d_n \tag{3.2}$$

For a dot with on-site repulsive interactions and a single site with spin-split levels ϵ_σ, we use the Anderson model,

$$H_C = \sum_\sigma \epsilon_\sigma d^\dagger_\sigma d_\sigma + U n_\uparrow n_\downarrow \tag{3.3}$$

with $n_\sigma = d^\dagger_\sigma d_\sigma$ is the number operator on the dot.

In any case, let us first derive a general expression for the current regardless of the presence of interactions in the dot. We however do require that the interactions, if any, be limited to the electrons inside the dot: the leads should

be noninteracting and there should be no interactions between electrons in the leads and electrons in the dot.

The full Hamiltonian is partitioned as explained in Chapter 1, i.e. $\mathcal{H} = H + H'$ where H is the equilibrium Hamiltonian and H' is the nonequilibrium perturbation. We also have to specify the initial noninteracting density matrix $\rho(-\infty)$. In the present problem, we have two possible ways of doing this partitioning:

- Choose H to be the Hamiltonian of the isolated leads and dot, and H' to be the coupling between the dots. The initial density matrix in the remote past $\rho(-\infty)$ is the product of the density matrices of the isolated systems in equilibrium:

$$\begin{aligned} H &= \sum_{\mathbf{k}\alpha\in L,R} \epsilon_{\mathbf{k}\alpha} c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + H_C[\{d^\dagger_n\},\{d_n\}] \\ H' &= \sum_{\mathbf{k}\alpha\in L,R,n} \Big(t_{\mathbf{k}\alpha,n} c^\dagger_{\mathbf{k}\alpha} d_n + t^*_{\mathbf{k}\alpha,n} d^\dagger_n c_{\mathbf{k}\alpha} \Big) \\ \rho(-\infty) &= \frac{1}{Z}\Big(e^{-\beta(H_L-\mu_L N_L)} \otimes \rho^{(0)}_C \otimes e^{-\beta(H_R-\mu_R N_R)} \Big) \end{aligned} \tag{3.4}$$

  where $H_{L,R}$ are the Hamiltonians of the isolated leads in equilibrium each with chemical potential $\mu_{L,R}$, and the initial density matrix of the dot[1] $\rho^{(0)}_C$ involves only the noninteracting part of the Hamiltonian of the dot H_C.
- Alternatively, we can choose H to be the Hamiltonian of the connected system in equilibrium at a single chemical potential μ. The nonequilibrium perturbation H' is then a one-body potential term which raises the single-particle energies by $\Delta_{L,R}$ in the leads. This represents the shift[2] in chemical potential $\mu \to \mu_{L,R} \equiv \mu + \Delta_{L,R}$. We then have

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[1] The obvious choice is $\rho^{(0)}_C = e^{-\beta(H^{(0)}_C - \mu_C N_C)}$ where $H^{(0)}_C$ is the noninteracting part of H_C but μ_C is unspecified. However this initial condition is included in $G^<_0$ which drops out of the Keldysh equation, see Section 2.1, so that the steady-state at any finite time $t > -\infty$ after the Keldysh adiabatic evolution is independent of μ_C. In particular, the steady-state current is independent of μ_C. This is a example of washing out of the initial conditions in the Keldysh formalism (even if here we are not even considering initial *correlations*). The steady-state nonequilibrium population of the dot will be given by the nonequilibrium Green's function of the dot $G^<$.

[2] To get the correct nonequilibrium self-consistent potential profile throughout the device including the dot, one would have to include Coulomb interactions in the Hamiltonian, at least at the Hartree (mean-field) level. Otherwise one can neglect interactions and add a term in the nonequilibrium perturbation to mimick the self-consistent potential profile, $\delta H' = \Delta d^\dagger d$ where $\Delta = \frac{\Delta_L + \Delta_R}{2}$, assuming a symmetric device.

$$H = \sum_{\mathbf{k}\alpha\in L,R} \epsilon_{\mathbf{k}\alpha} c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + H_C[\{d^\dagger_n\},\{d_n\}] + \sum_{\mathbf{k}\alpha\in L,R,n} \left(t_{\mathbf{k}\alpha,n} c^\dagger_{\mathbf{k}\alpha} d_n + t^*_{\mathbf{k}\alpha,n} d^\dagger_n c_{\mathbf{k}\alpha} \right)$$

$$H' = \sum_{\mathbf{k}\alpha\in L,R} \Delta_{L,R} c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha}$$

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

We will choose the first method which is well-suited to steady-state problems, while the second method is easier for time-dependent transport.

3.1.1 Expression for the Current

The current flowing through lead α is defined as

$$J_\alpha(t) \equiv -e\langle \dot{N}_\alpha \rangle, \tag{3.5}$$

where $N_\alpha = \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha}$ is the number operator for lead α and $e > 0$ is the electron charge. From the Heisenberg equation of motion $i\hbar\dot{N}_\alpha = [N_\alpha, H]$ and Eq. (3.1), we obtain

$$J_\alpha(t) = \frac{2e}{\hbar} \,\mathrm{Re} \sum_{\mathbf{k},n} t_{\mathbf{k}\alpha,n} G^<_{n,\mathbf{k}\alpha}(t,t), \tag{3.6}$$

where we have the mixed lesser Green's function $G^<_{n,\mathbf{k}\alpha}(t,t') = i\langle c^\dagger_{\mathbf{k}\alpha}(t') d_n(t)\rangle$. Using the Keldysh technique, we will obtain an expression for the mixed contour-ordered Green's function $G_{n,\mathbf{k}\alpha}(\tau,\tau') = -i\langle T_c\{d_n(\tau) c^\dagger_{\mathbf{k}\alpha}(\tau')\}\rangle$ and perform analytic continuation to real time to obtain the lesser function $G^<_{n,\mathbf{k}\alpha}(t,t')$.

For pedagogical reasons, let us first derive the expression from the usual perturbation expansion of the S-matrix and the subsequent application of Wick's theorem, and then obtain it from the path integral method which is more transparent.

3.1.2 Perturbation Expansion for the Mixed Green's Function

As explained, we define the unperturbed Hamiltonian as the first two terms of Eq. (3.1),

$$H = \sum_{\mathbf{k}\alpha} \epsilon_{\mathbf{k}\alpha} c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + H_C[\{d^\dagger_n\},\{d_n\}],$$

and the perturbation as the tunneling term,

$$H' = \sum_{\mathbf{k}\alpha,n} \left(t_{\mathbf{k}\alpha,n} c^\dagger_{\mathbf{k}\alpha} d_n + t^*_{\mathbf{k}\alpha,n} d^\dagger_n c_{\mathbf{k}\alpha} \right).$$

The perturbation expansion becomes

$$G_{n,\mathbf{k}\alpha}(\tau,\tau') = \sum_{l=0}^{\infty} \frac{(-i)^{l+1}}{l!} \oint_C d\tau_1 \cdots \oint_C d\tau_l \langle T_c\{\hat{d}_n(\tau)\hat{H}'(\tau_1)\cdots\hat{H}'(\tau_l)\hat{c}^\dagger_{\mathbf{k}\alpha}(\tau')\}\rangle, \tag{3.7}$$

where we have

$$\langle T_c\{\hat{d}_n(\tau)\hat{H}'(\tau_1)\cdots\hat{H}'(\tau_l)\hat{c}^\dagger_{\mathbf{k}\alpha}(\tau')\}\rangle = \prod_{i=1}^{l}\sum_{\mathbf{k}_i\alpha_i,n_i} \Big\langle T_c\Big\{\hat{d}_n(\tau)\Big(\hat{c}^\dagger_{\mathbf{k}_i\alpha_i}(\tau_i)t_{\mathbf{k}_i\alpha_i,n_i}\hat{d}_{n_i}(\tau_i) + \hat{d}^\dagger_{n_i}(\tau_i)t^*_{\mathbf{k}_i\alpha_i,n_i}\hat{c}_{\mathbf{k}_i\alpha_i}(\tau_i)\Big)\hat{c}^\dagger_{\mathbf{k}\alpha}(\tau')\Big\}\Big\rangle.$$

Wick's theorem can now be applied to correlators of $\hat{c},\hat{c}^\dagger$ fields since H is quadratic in these fields, whence the importance of the requirement that the leads be noninteracting. All the contractions involving the first term in $\hat{H}'(\tau_i)$ vanish, since $\hat{d}_n\hat{c}^\dagger_{\mathbf{k}_i\alpha_i} = 0$ and $\hat{d}_{n_i}\hat{c}^\dagger_{\mathbf{k}\alpha} = 0$ for the unconnected system, and the anomalous contractions $\hat{d}_n\hat{d}_{n_i}$ and $\hat{c}^\dagger_{\mathbf{k}_i\alpha_i}\hat{c}^\dagger_{\mathbf{k}\alpha}$ vanish because particle number is conserved. By Wick's theorem we thus have

$$\begin{aligned}
&\langle T_c\{\hat{d}_n(\tau)\hat{H}'(\tau_1)\cdots\hat{H}'(\tau_l)\hat{c}^\dagger_{\mathbf{k}\alpha}(\tau')\}\rangle \\
&= \prod_{i=1}^{l}\sum_{\mathbf{k}_i\alpha_i,n_i} t^*_{\mathbf{k}_i\alpha_i,n_i}\Big\langle T_c\Big\{\hat{d}_n(\tau)\hat{d}^\dagger_{n_i}(\tau_i)\hat{c}_{\mathbf{k}_i\alpha_i}(\tau_i)\hat{c}^\dagger_{\mathbf{k}\alpha}(\tau')\Big\}\Big\rangle \\
&= \sum_{\mathbf{k}_l\alpha_l,n_l} t^*_{\mathbf{k}_l\alpha_l,n_l}\langle T_c\{\hat{d}_n(\tau)\hat{H}'(\tau_1)\cdots\hat{H}'(\tau_{l-1})\hat{c}^\dagger_{\mathbf{k}_l\alpha_l,n_l}(\tau_l)\}\rangle\langle T_c\{\hat{c}_{\mathbf{k}_l\alpha_l}(\tau_l)\hat{c}^\dagger_{\mathbf{k}\alpha}(\tau')\}\rangle \\
&+ \sum_{\mathbf{k}_{l-1}\alpha_{l-1},n_{l-1}} t^*_{\mathbf{k}_{l-1}\alpha_{l-1},n_{l-1}}\langle T_c\{\hat{d}_n(\tau)\hat{H}'(\tau_1)\cdots\hat{H}'(\tau_{l-2})\hat{H}'(\tau_l)\hat{c}^\dagger_{\mathbf{k}_{l-1}}(\tau_{l-1})\}\rangle \\
&\times\langle T_c\{\hat{c}^\dagger_{\mathbf{k}_{l-1}\alpha_{l-1}}(\tau_{l-1})\hat{c}^\dagger_{\mathbf{k}\alpha}(\tau')\}\rangle + \ldots \\
&+ \sum_{\mathbf{k}_1\alpha_1,n_1} t^*_{\mathbf{k}_1\alpha_1,n_1}\langle T_c\{\hat{d}_n(\tau)\hat{H}'(\tau_2)\cdots\hat{H}'(\tau_l)\hat{c}^\dagger_{\mathbf{k}_1\alpha_1}(\tau_1)\}\rangle\langle T_c\{\hat{c}_{\mathbf{k}_1\alpha_1}(\tau_1)\hat{c}^\dagger_{\mathbf{k}\alpha}(\tau')\}\rangle,
\end{aligned}$$

where all the l terms are seen to yield the same contribution to the perturbation expansion Eq. (3.7) if the dummy integration variables $\tau_1,\ldots,\tau_l$ are relabeled. Choosing the labeling of the last term, we obtain

$$\begin{aligned}
G_{n,\mathbf{k}\alpha}(\tau,\tau') = \sum_{\mathbf{k}_1\alpha_1,n_1}\oint_C d\tau_1(-i)\sum_{l=1}^{\infty}\frac{(-i)^{l-1}}{(l-1)!}\oint_C d\tau_2\cdots\oint_C d\tau_l \\
\times\langle T_c\{\hat{d}_n(\tau)\hat{H}'(\tau_2)\cdots\hat{H}'(\tau_l)\hat{c}^\dagger_{\mathbf{k}_1\alpha_1}(\tau_1)\}\rangle t^*_{\mathbf{k}_1\alpha_1,n_1}(-i)\langle T_c\{\hat{c}_{\mathbf{k}_1\alpha_1}(\tau_1)\hat{c}^\dagger_{\mathbf{k}\alpha}(\tau')\}\rangle.
\end{aligned}$$

After relabeling the dummy integration variables once more, we see that the perturbation terms $\hat{H}'\cdots\hat{H}'$ give rise to the contour S-matrix Eq. (1.26), so that we finally have

$$G_{n,\mathbf{k}\alpha}(\tau,\tau') = \sum_m \oint_C d\tau_1\, G_{nm}(\tau,\tau_1)t^*_{\mathbf{k}\alpha,m}g_{\mathbf{k}\alpha}(\tau_1,\tau'), \tag{3.8}$$

where

$$G_{nm}(\tau,\tau') \equiv -i\langle T_c\{d_n(\tau)d_m^\dagger(\tau')\}\rangle = -i\langle T_c\{S_c(-\infty,-\infty)\hat{d}_n(\tau)\hat{d}_m^\dagger(\tau')\}\rangle, \tag{3.9}$$

is the contour-ordered Green's function of the scattering region, and we have

$$-i\langle T_c\{\hat{c}_{\mathbf{k}\alpha}(\tau)\hat{c}_{\mathbf{k}'\alpha'}^\dagger(\tau')\}\rangle = \delta_{\alpha\alpha'}\delta_{\mathbf{k}\mathbf{k}'}g_{\mathbf{k}\alpha}(\tau,\tau'),$$

because of translational invariance in the leads, where $g_{\mathbf{k}\alpha}(\tau,\tau') \equiv -i\langle T_c\{\hat{c}_{\mathbf{k}\alpha}(\tau)\hat{c}_{\mathbf{k}\alpha}^\dagger(\tau')\}\rangle$ is the contour-ordered Green's function of the (isolated) leads.

3.1.3 Path Integral Derivation of the Mixed Green's Function

The path integral can also be used in the Keldysh technique. The only difference is that the action is obtained by integrating the Lagrangian over the Schwinger-Keldysh contour C instead of over the real axis. The Lagrangian is

$$L(\bar{c},c,\bar{d},d) = \sum_{\mathbf{k}\alpha}\bar{c}_{\mathbf{k}\alpha}(i\partial_\tau - \epsilon_{\mathbf{k}\alpha})c_{\mathbf{k}\alpha} + \sum_n \bar{d}_n i\partial_\tau d_n - H_C[\{\bar{d}_n\},\{d_n\}] - \sum_{\mathbf{k}\alpha,n}\left(\bar{c}_{\mathbf{k}\alpha}t_{\mathbf{k}\alpha,n}d_n + \bar{d}_n t_{\mathbf{k}\alpha,n}^* c_{\mathbf{k}\alpha}\right) \tag{3.10}$$

To calculate the propagator $G_{n,\mathbf{k}\alpha}(\tau,\tau')$, it is appropriate to define the Keldysh generating functional $Z[\bar{\eta},J]$,

$$Z[\bar{\eta},J] = \mathrm{Tr}\,\rho T_c\left[e^{-i\oint_C d\tau\left(:\mathcal{H}: - \sum_n \bar{\eta}_n d_n - \sum_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha}^\dagger J_{\mathbf{k}\alpha}\right)}\right]$$

where $\bar{\eta}_n$ and $J_{\mathbf{k}\alpha}$ are Grassmann sources, and the normalization is such that $Z[0,0] = \mathrm{Tr}\,\rho \equiv Z$. The generating functional is useful because it can be used to generate the mixed correlation function,

$$iG_{n,\mathbf{k}\alpha}(\tau,\tau') = \frac{1}{Z}\frac{\delta^2 Z[\bar{\eta},J]}{\delta\bar{\eta}_n(\tau)\delta J_{\mathbf{k}\alpha}(\tau')}\bigg|_{\bar{\eta}=0,J=0} \tag{3.11}$$

The generating functional has a path integral representation,

$$Z[\bar{\eta},J] = \int \mathcal{D}[\bar{c},c,\bar{d},d]e^{i\left(S[\bar{c},c,\bar{d},d] + \oint_C d\tau(\bar{\eta}d + \bar{c}J)\right)}$$

where we use the shorthand notation $\bar{\eta}d \equiv \sum_n \bar{\eta}_n d_n$ and $\bar{c}J \equiv \sum_{\mathbf{k}\alpha}\bar{c}_{\mathbf{k}\alpha}J_{\mathbf{k}\alpha}$.

The d and the c fields are entangled in the Lagrangian Eq. (3.10). To disentangle them, we perform a shift of variables,

$$\bar{c}'_{\mathbf{k}\alpha}(\tau) \equiv \bar{c}_{\mathbf{k}\alpha}(\tau) - \sum_m \oint_C d\tau_1\, \bar{d}_m(\tau_1)t_{\mathbf{k}\alpha,m}^* g_{\mathbf{k}\alpha}(\tau_1,\tau)$$

$$c'_{\mathbf{k}\alpha}(\tau) \equiv c_{\mathbf{k}\alpha}(\tau) - \sum_m \oint_C d\tau_1\, g_{\mathbf{k}\alpha}(\tau,\tau_1)t_{\mathbf{k}\alpha,m}d_n(\tau_1)$$

where $g_{\mathbf{k}\alpha}(\tau,\tau_1)$ is the contour-ordered Green's function of the isolated leads defined earlier. It satisfies (see Eqs. (2.9) and (2.10) of the notes)

$$(i\partial_\tau - \epsilon_{\mathbf{k}\alpha})g_{\mathbf{k}\alpha}(\tau,\tau_1) = \delta(\tau,\tau_1)$$
$$g_{\mathbf{k}\alpha}(\tau,\tau_1)(-i\partial_{\tau_1} - \epsilon_{\mathbf{k}\alpha}) = \delta(\tau,\tau_1)$$

where in the second equation the derivative acts to the left. With this shift of variables, the Lagrangian becomes

$$L(\bar{c}',c',\bar{d},d) = \sum_{\mathbf{k}\alpha} \bar{c}'_{\mathbf{k}\alpha}(i\partial_\tau - \epsilon_{\mathbf{k}\alpha})c'_{\mathbf{k}\alpha} + L_0(\{\bar{d}_n\},\{d_n\}) - \sum_{\mathbf{k}\alpha,mn} \oint_C d\tau_1\, \bar{d}_m(\tau) t^*_{\mathbf{k}\alpha,m} g_{\mathbf{k}\alpha}(\tau,\tau_1) t_{\mathbf{k}\alpha,n} d_n(\tau_1)$$

where $L_0(\{\bar{d}_n\},\{d_n\}) = \sum_n \bar{d}_n i\partial_\tau d_n - H_C[\{\bar{d}_n\},\{d_n\}]$ is the Lagrangian of the isolated dot.

EXERCISE. Show this (hint: use integration by parts).

As a result, the action becomes

$$S[\bar{c}',c',\bar{d},d] = S_{\text{leads}}[\bar{c}',c'] + S_{\text{QD}}[\bar{d},d]$$

where

$$S_{\text{leads}}[\bar{c}',c'] \equiv \sum_{\mathbf{k}\alpha} \oint_C d\tau\, \bar{c}'_{\mathbf{k}\alpha}(i\partial_\tau - \epsilon_{\mathbf{k}\alpha})c'_{\mathbf{k}\alpha}$$

is the action of the isolated leads, and

$$S_{\text{QD}}[\bar{d},d] \equiv \oint_C d\tau\, L_0(\{\bar{d}_n\},\{d_n\}) - \sum_{\mathbf{k}\alpha,mn} \oint_C d\tau \oint_C d\tau_1\, \bar{d}_m(\tau) t^*_{\mathbf{k}\alpha,m} g_{\mathbf{k}\alpha}(\tau,\tau_1) t_{\mathbf{k}\alpha,n} d_n(\tau_1)$$

is an effective action for the quantum dot, which contains the effect of the external leads (bath). The source term $\bar{\eta}d$ is unaffected by the change of variables, but the source term $\bar{c}J$ becomes

$$\bar{c}J = \sum_{\mathbf{k}\alpha} \bar{c}_{\mathbf{k}\alpha}(\tau) J_{\mathbf{k}\alpha}(\tau) = \sum_{\mathbf{k}\alpha} \left(\bar{c}'_{\mathbf{k}\alpha}(\tau) + \sum_m \oint_C d\tau_1\, \bar{d}_m(\tau_1) t^*_{\mathbf{k}\alpha,m} g_{\mathbf{k}\alpha}(\tau_1,\tau) \right) J_{\mathbf{k}\alpha}(\tau)$$

The generating functional thus becomes

$$Z[\bar{\eta},J] = \int \mathcal{D}[\bar{c}',c',\bar{d},d] e^{iS_{\text{leads}}[\bar{c}',c']} e^{iS_{\text{QD}}[\bar{d},d]} e^{i\oint_C d\tau \left(\bar{\eta}d + (\bar{c}' + \bar{d}t^* g)J\right)}$$

where the integration measure $\mathcal{D}[\bar{c},c] = \mathcal{D}[\bar{c}',c']$ is invariant under the change of variables since it is only a shift.

We now perform the functional differentiation Eq. (3.11). This generates two terms. The first term is

$$\frac{1}{Z}\int \mathcal{D}[\bar{c}', c', \bar{d}, d] e^{iS_{\text{leads}}} e^{iS_{\text{QD}}} d_n(\tau)\bar{c}'_{\mathbf{k}\alpha}(\tau') = \langle T_c\{d_n(\tau)\hat{c}^\dagger_{\mathbf{k}\alpha}(\tau')\}\rangle$$

which is zero because it corresponds to the unconnected system (the action in the path integral is that of isolated leads). The second term is

$$\frac{1}{Z}\int \mathcal{D}[\bar{c}', c', \bar{d}, d] e^{iS_{\text{leads}}} e^{iS_{\text{QD}}} \sum_m \oint d\tau_1\, d_n(\tau)\bar{d}_m(\tau_1) t^*_{\mathbf{k}\alpha,m} g_{\mathbf{k}\alpha}(\tau_1, \tau')$$
$$= \sum_m \oint_C d\tau_1\, iG_{nm}(\tau, \tau_1) t^*_{\mathbf{k}\alpha,m} g_{\mathbf{k}\alpha}(\tau_1, \tau')$$

where

$$iG_{nm}(\tau, \tau_1) \equiv \langle T_c\{d_n(\tau)d^\dagger_m(\tau_1)\}\rangle = \frac{1}{Z}\int \mathcal{D}[\bar{c}', c', \bar{d}, d] e^{iS_{\text{leads}}} e^{iS_{\text{QD}}} d_n(\tau)\bar{d}_m(\tau_1)$$
$$= \frac{1}{Z}\int \mathcal{D}[\bar{c}, c, \bar{d}, d] e^{iS} d_n(\tau)\bar{d}_m(\tau_1)$$

is the exact Green's function of the connected dot. Hence we obtain

$$G_{n,\mathbf{k}\alpha}(\tau, \tau') = \sum_m \oint_C d\tau_1\, G_{nm}(\tau, \tau_1) t^*_{\mathbf{k}\alpha,m} g_{\mathbf{k}\alpha}(\tau_1, \tau')$$

which is just Eq. (3.8).

3.1.4 General Expression for the Current

In Eq. (3.6) for the current, we need the lesser mixed Green's function. We therefore apply the Langreth analytic continuation theorem Eq. (1.64) to Eq. (3.8) to get

$$G_{n,\mathbf{k}\alpha}(t, t') = \sum_m \int dt_1 \big(G^R_{nm}(t, t_1) t^*_{\mathbf{k}\alpha,m} g^<_{\mathbf{k}\alpha}(t_1, t') + G^<_{nm}(t, t_1) t^*_{\mathbf{k}\alpha,m} g^A_{\mathbf{k}\alpha}(t_1, t')\big)$$

We now assume steady state so that all the Green's functions depend only on the time difference, i.e. $G(t, t') = G(t - t')$. Then we get

$$G_{n,\mathbf{k}\alpha}(t, t) = \sum_m \int \frac{d\omega}{2\pi} \big(G^R_{nm}(\omega) t^*_{\mathbf{k}\alpha,m} g^<_{\mathbf{k}\alpha}(\omega) + G^<_{nm}(\omega) t^*_{\mathbf{k}\alpha,m} g^A_{\mathbf{k}\alpha}(\omega)\big) \quad (3.12)$$

The Green's functions of the isolated leads are

$$g^<_{\mathbf{k}\alpha}(\omega) = 2\pi i f_\alpha(\epsilon_{\mathbf{k}\alpha})\delta(\omega - \epsilon_{\mathbf{k}\alpha}) \quad (3.13)$$
$$g^A_{\mathbf{k}\alpha}(\omega) = \frac{1}{\omega - i\delta - \epsilon_{\mathbf{k}\alpha}} \quad (3.14)$$

where $f_\alpha(\epsilon) = (e^{\beta(\epsilon-\mu_\alpha)} + 1)^{-1}$ and the chemical potentials are those of the initial density matrix Eq. (3.4). We now substitute Eq. (3.12) in Eq. (3.6),

$$J_\alpha = \frac{2e}{\hbar}\,\mathrm{Re}\sum_{\mathbf{k},mn}\int\frac{d\omega}{2\pi}\,t^*_{\mathbf{k}\alpha,m}t_{\mathbf{k}\alpha,n}\big(g^<_{\mathbf{k}\alpha}(\omega)G^R_{nm}(\omega)+g^A_{\mathbf{k}\alpha}(\omega)G^<_{nm}(\omega)\big) \quad (3.15)$$

It is not hard to show from the definition of the Green's functions that the following relations hold,

$$G^<(\omega)^\dagger = -G^<(\omega)$$
$$G^R(\omega)^\dagger = G^A(\omega)$$

considering the Green's functions as matrices $G = G_{nm}$. Using these relations and Eqs. (3.13) and (3.14), we can show that Eq. (3.15) becomes [25]

$$J_\alpha = \frac{ie}{\hbar}\int\frac{d\omega}{2\pi}\,\mathrm{Tr}\,\Gamma_\alpha(\omega)\big\{f_\alpha(\omega)[G^R(\omega)-G^A(\omega)]+G^<(\omega)\big\} \quad (3.16)$$

where we define a linewidth function

$$\Gamma_{\alpha,mn}(\omega) \equiv 2\pi\rho_\alpha(\omega)t^*_{\alpha,m}(\omega)t_{\alpha,n}(\omega)$$

and we have introduced the density of states $\rho_\alpha(\omega) \equiv \sum_{\mathbf{k}}\delta(\omega-\epsilon_{\mathbf{k}\alpha})$ to convert the sum over $\mathbf{k}$ in Eq. (3.15) to an integral,

$$\sum_{\mathbf{k}} F(\epsilon_{\mathbf{k}\alpha}) = \int d\epsilon\,\rho_\alpha(\epsilon)F(\epsilon)$$

Equation (3.16) is an exact expression for the steady-state current through lead α of an arbitrary multiprobe system with interactions inside the dot (but not in the leads). However, the nonequilibrium Green's functions have to be calculated in the presence of interactions, and in the presence of the leads held at different chemical potentials.

For a two-probe system with proportionate couplings to the leads, $\Gamma_L(\omega) = \lambda\Gamma_R(\omega)$, one can arrive at a simpler expression. We first use the fact that in steady state, $J = J_L = -J_R$, so that we can write $J = xJ_L - (1-x)J_R$ for an arbitrary x. The current then reads

$$J = \frac{ie}{\hbar}\int\frac{d\omega}{2\pi}\,\mathrm{Tr}\,\Gamma_R\big[(\lambda x-(1-x))G^< + (\lambda x f_L-(1-x)f_R)(G^R-G^A)\big]$$

We then fix the arbitrary parameter $x = \frac{1}{1+\lambda}$ so that the first term vanishes and the current does not depend on $G^<$ anymore. We then obtain

$$J = \frac{ie}{\hbar}\int\frac{d\omega}{2\pi}[f_L(\omega)-f_R(\omega)]\,\mathrm{Tr}\left(\frac{\Gamma_L(\omega)\Gamma_R(\omega)}{\Gamma_L(\omega)+\Gamma_R(\omega)}\right)[G^R(\omega)-G^A(\omega)] \quad (3.17)$$

where the ratio is well-defined since the matrices Γ_L and Γ_R were assumed to be proportional.

3.1.5 Noninteracting Quantum Dot

We derive an alternate expression for the current in the case that there are no interactions in the dot. In this case, the retarded Green's function satisfies the Dyson equation

$$G^R = G_0^R + G_0^R \Sigma^R G^R, \tag{3.18}$$

where

$$\Sigma^R_{mn}(\omega) = \sum_{\mathbf{k}\alpha} t^*_{\mathbf{k}\alpha,m} g^R_{\mathbf{k}\alpha}(\omega) t_{\mathbf{k}\alpha,n} \tag{3.19}$$

is the noninteracting tunneling self-energy, with $\Gamma = \sum_\beta \Gamma_\beta = i(\Sigma^R - \Sigma^A)$. G_0^R is the equilibrium Green's function of the unconnected dot,

$$G_0^R(\omega) = (\omega + i\delta - h)^{-1}.$$

In other words, in the noninteracting case, the self-energy contains only the effect of the leads. From these equations it is easy to derive the identity,

$$G^R - G^A = -iG^R \Gamma G^A$$

The lesser Green's function follows from the Keldysh equation,

$$G^< = G^R \Sigma^< G^A$$

where the lesser self-energy is

$$\Sigma^< = i \sum_\beta f_\beta \Gamma_\beta \tag{3.20}$$

Consider a system with a single level, such that all quantities G, Γ, Σ are scalars. If we write $G^<$ in pseudoequilibrium form

$$G^< = i\bar{f} A$$

with $A = i(G^R - G^A) = G^R \Gamma G^A$ the spectral function, the pseudodistribution $\bar{f}$ is

$$\bar{f} = \frac{f_L \Gamma_L + f_R \Gamma_R}{\Gamma_L + \Gamma_R}$$

which is clearly not of equilibrium form if $f_L \neq f_R$.

Using the previous results, one can show that

$$J_\alpha = \frac{e}{h} \sum_\beta \int d\omega [f_\alpha(\omega) - f_\beta(\omega)] T_{\alpha\beta}(\omega)$$

where the transmission coefficient $T_{\alpha\beta}$ is

$$T_{\alpha\beta}(\omega) = \mathrm{Tr}\, \Gamma_\alpha(\omega) G^R(\omega) \Gamma_\beta(\omega) G^A(\omega)$$

which is the usual Landauer formula. Note that Landauer obtained this result heuristically while here it has been derived rigorously from the nonequilibrium formalism. Also, the Green's functions G^R and G^A have to be calculated out of equilibrium.

3.1.6 Interacting Quantum Dot: Anderson Model and Coulomb Blockade

In this section we consider on-site repulsive interactions in the dot [26, 27]. We assume that the couplings are proportionate $\Gamma_L \propto \Gamma_R$ so we use Eq. (3.17). The Hamiltonian of the quantum dot is the Anderson model Eq. (3.3),

$$H_C = \sum_\sigma \epsilon_\sigma d_\sigma^\dagger d_\sigma + U n_\uparrow n_\downarrow$$

Assuming that the couplings are diagonal in spin space, the current is

$$J = \frac{e}{\hbar} \sum_\sigma \int d\omega [f_L(\omega) - f_R(\omega)] \Gamma_{\sigma\sigma}(\omega) \left(-\frac{1}{\pi} \operatorname{Im} G^R_{\sigma\sigma}(\omega) \right)$$

where

$$G^R_{\sigma\sigma}(t) = -i\theta(t) \langle \{ d_\sigma(t), d_\sigma^\dagger(0) \} \rangle$$

is the nonequilibrium retarded Green's function of the dot (in the presence of the leads). This Green's function also satisfies a Dyson equation Eq. (3.18), but the self-energy now contains both contributions from the leads and from interactions in the dot. Both contributions are entangled in the exact self-energy which is not known. Obviously because of interactions the problem cannot be solved exactly. We will solve the problem approximately by using the equation of motion technique to obtain the exact Green's function $g^R_{\sigma\sigma}$ of the isolated interacting system, and calculate $G^R_{\sigma\sigma}$ from $g^R_{\sigma\sigma}$ by using the non-interacting tunneling self-energy Σ of the noninteracting Dyson equation Eq. (3.18). This is actually equivalent to performing a Hartree-Fock factorization of the higher correlation functions.

For simplicity, we denote the Green's function of the isolated dot (governed only by the Hamiltonian H_C) by

$$g^R_{\sigma\sigma}(t) = -i\theta(t) \langle \{ d_\sigma(t), d_\sigma^\dagger(0) \} \rangle_0$$

where the subscript $\langle \cdots \rangle_0$ indicates that the average is taken for the isolated dot. By taking a time derivative, we get

$$i \frac{\partial g^R_{\sigma\sigma}(t)}{\partial t} = \delta(t) + \theta(t) \langle \{ \dot{d}_\sigma(t), d_\sigma^\dagger(0) \} \rangle_0 \tag{3.21}$$

We use the Heisenberg equation of motion to obtain $\dot{d}_\sigma$,

$$i\dot{d}_\sigma = [d_\sigma, H_C] = \epsilon_\sigma d_\sigma + U[d_\sigma, n_\uparrow d_\downarrow] = \epsilon_\sigma d_\sigma + U d_\sigma n_{\bar{\sigma}} \tag{3.22}$$

where $\bar{\sigma} \equiv -\sigma$. Substituting this result in Eq. (3.21), we get

$$i \frac{\partial g^R_{\sigma\sigma}(t)}{\partial t} = \delta(t) + \epsilon_\sigma g^R_{\sigma\sigma}(t) + U g^{(2)}_{\sigma\sigma}(t) \tag{3.23}$$

where we define a 2-particle correlation function

$$g^{(2)}_{\sigma\sigma}(t) \equiv -i\theta(t)\langle\{d_\sigma(t)n_{\bar\sigma}(t), d^\dagger_\sigma(0)\}\rangle_0$$

We can also write down its own equation of motion,

$$i\frac{\partial g^{(2)}_{\sigma\sigma}}{\partial t} = \delta(t)\langle\{d_\sigma n_{\bar\sigma}, d^\dagger_\sigma\}\rangle_0 + \theta(t)\langle\{\dot d_\sigma(t)n_{\bar\sigma}(t), d^\dagger_\sigma(0)\}\rangle_0 + \theta(t)\langle\{d_\sigma(t)\dot n_{\bar\sigma}(t), d^\dagger_\sigma(0)\}\rangle_0$$

Since $[n_{\bar\sigma}, d_\sigma] = 0$, the first term is simply $\delta(t)\langle n_{\bar\sigma}\rangle$. The last term is zero since $n_{\bar\sigma}$ commutes with H_C. In the second term we substitute the result of Eq. (3.22), so that we finally get

$$i\frac{\partial g^{(2)}_{\sigma\sigma}}{\partial t} = \delta(t)\langle n_{\bar\sigma}\rangle + \epsilon_\sigma g^{(2)}_{\sigma\sigma}(t) + U g^{(2)}_{\sigma\sigma}(t) \tag{3.24}$$

In Fourier space, Eqs. (3.23) and (3.24) become

$$\begin{aligned}(\omega + i\delta - \epsilon_\sigma)g^R_{\sigma\sigma}(\omega) &= 1 + U g^{(2)}_{\sigma\sigma}(\omega)\\ (\omega + i\delta - \epsilon_\sigma - U)g^{(2)}_{\sigma\sigma}(\omega) &= \langle n_{\bar\sigma}\rangle\end{aligned}$$

Substituting the second equation in the first, we get

$$g^R_{\sigma\sigma}(\omega) = \frac{\langle n_{\bar\sigma}\rangle}{\omega + i\delta - \epsilon_\sigma - U} + \frac{1 - \langle n_{\bar\sigma}\rangle}{\omega + i\delta - \epsilon_\sigma}$$

which is the exact Green's function of the isolated dot. The corresponding spectral function has two peaks: one peak at $\omega = \epsilon_\sigma$ with spectral weight $1 - \langle n_{\bar\sigma}\rangle$ corresponding to the probability of the site being occupied by a single electron of spin σ, and a second peak at $\omega = \epsilon_\sigma + U$ with spectral weight $\langle n_{\bar\sigma}\rangle$ corresponding to double occupancy of the site with electrons of opposite spins.

To obtain the nonequilibrium Green's function $G^R_{\sigma\sigma}$ of the connected dot, we make the following ansatz: we take the interacting Green's function of the isolated dot $g^R_{\sigma\sigma}$ as the unperturbed Green's function G^R_0, and add the *noninteracting* tunneling self-energy Eq. (3.19):

$$G^R_{\sigma\sigma}(\omega) \simeq \frac{1}{[g^R_{\sigma\sigma}(\omega)]^{-1} - \Sigma^R(\omega)}$$

which gives the following result,

$$G^R_{\sigma\sigma}(\omega) = \frac{\omega + i\delta - \epsilon_\sigma - [1 - \langle n_{\bar\sigma}\rangle]U}{(\omega + i\delta - \epsilon_\sigma)(\omega + i\delta - \epsilon_\sigma - U) - (\omega + i\delta - \epsilon_\sigma - [1 - \langle n_{\bar\sigma}\rangle]U)\Sigma^R(\omega)} \tag{3.25}$$

In the simplest case, we neglect the energy dependence of the self-energy, and have $\Sigma^R = -i(\Gamma_L + \Gamma_R)/2$. Note that Eq. (3.25) is actually a self-consistent equation, if we take into account the change in spin population $\langle n_\sigma\rangle$ out of equilibrium. Indeed, $\langle n_\sigma\rangle$ is given out of equilibrium by

$$\langle n_\sigma \rangle = \langle d_\sigma^\dagger d_\sigma \rangle = \int \frac{d\omega}{2\pi i} G^<_{\sigma\sigma}(\omega)$$

where the lesser Green's function of the dot is given by the Keldysh equation which again involves $G^R_{\sigma\sigma}(\omega)$,

$$G^<_{\sigma\sigma}(\omega) = G^R_{\sigma\sigma}(\omega)\Sigma^<_{\sigma\sigma}(\omega)G^A_{\sigma\sigma}(\omega)$$

where $\Sigma^<$ is the lesser noninteracting tunneling self-energy Eq. (3.20).

Once $G^R_{\sigma\sigma}(\omega)$ is obtained by a numerical solution of the self-consistent equations, we can calculate the current J and the differential conductance dJ/dV as a function of bias voltage $V = (\mu_L - \mu_R)/e$. We can also add a gate potential V_g such that the single-particle energies are shifted, $\epsilon_\sigma \to \epsilon_\sigma + eV_g$.

In the following figures, we illustrate results for $\Gamma_L = \Gamma_R = 0.02$ eV, $\epsilon_\uparrow = -0.65$ eV, $\epsilon_\downarrow = -0.45$ eV and $U = 1$ eV at zero temperature. The chemical potentials are defined symmetrically $\mu_L = -\mu_R = eV_b/2$. The figures illustrate clearly the Coulomb blockade effect.

In Fig. 3.1, we display the Coulomb blockade diamond plot, the differential conductance dJ/dV as function of gate voltage and bias voltage. Note that linear response theory would give only the $V_b = 0$ line whereas with the nonequilibrium theory, we get the full bias-gate voltage diagram.

In Fig. 3.2, we plot two cuts of Fig. 3.1 along V_g, for two values of bias voltage: $V_b = 0$ (equilibrium case for which the differential conductance dJ/dV is just the equilibrium two-terminal conductance G), and $V_b = 1$ V (out of equilibrium: the equilibrium conductance peaks split due to the applied bias). Finally, in Fig. 3.3 we plot the current J itself as a function of V_g and V_b.

3.2 Linear Response for Steady-State and Homogeneous Systems

We now consider the limit of linear transport, that is, we keep only terms to first order in the electric field. We will study the QBE Eq. (2.69) in the absence[3] of magnetic field $\mathbf{B} = 0$, and for steady-state ($\partial/\partial T = 0$) and homogeneous ($\nabla_{\mathbf{R}} = 0$) systems. Consider first the equation for the retarded Green's function Eq. (2.68). Neglecting the possible dependence of the self-energy on the electric field which is a small effect, we have

$$G^R = \frac{1}{\omega - \epsilon_{\mathbf{p}} - \Sigma^R} + \mathcal{O}(E^2) \tag{3.26}$$

which to linear order in the electric field is just the equilibrium Green's function $G^R(\mathbf{p}, \omega)$. This simplifies drastically the solution of the QBE since all the retarded and advanced quantities can be taken in equilibrium. The QBE is

[3] The $\mathbf{B} \neq 0$ case can also be considered, but then the equilibrium Green's function has a dependence on the magnetic field which in general breaks translational invariance and makes things more complicated.

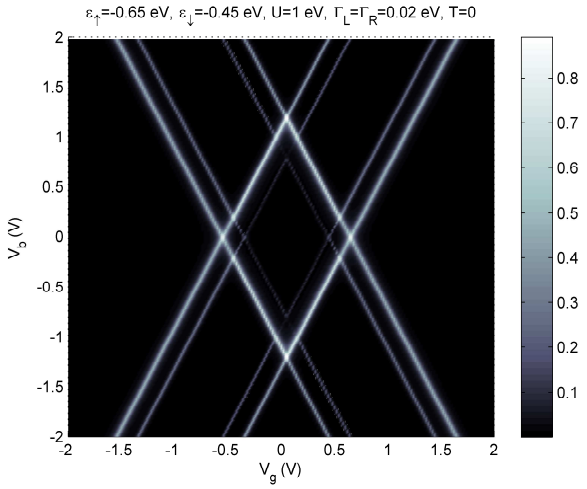

Fig. 3.1. Coulomb blockade diamond: differential conductance dJ/dV in units of e^2/h, as function of gate voltage V_g and bias voltage V_b. Note the doubling of the lines due to the level spacing $\Delta\epsilon = \epsilon_\downarrow - \epsilon_\uparrow = 0.2$ eV, and the large $U = 1$ eV spacing of the conductance peaks. The equilibrium conductance peaks at $V_b = 0$ split for nonzero applied bias $V_b \neq 0$ (see also Fig. 3.2).

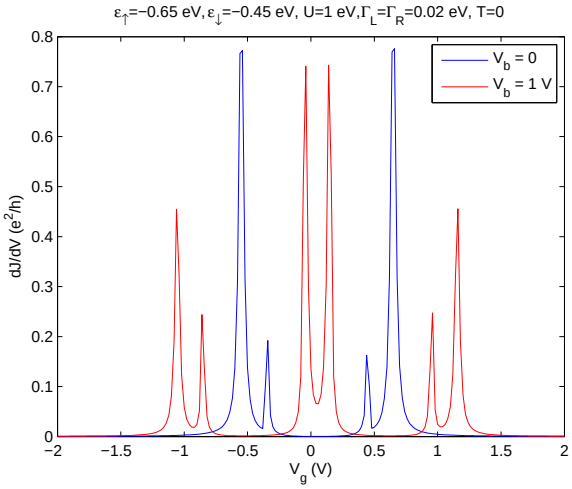

Fig. 3.2. Differential conductance dJ/dV as function of gate voltage V_g, both at equilibrium ($V_b = 0$) and out of equilibrium ($V_b \neq 0$).

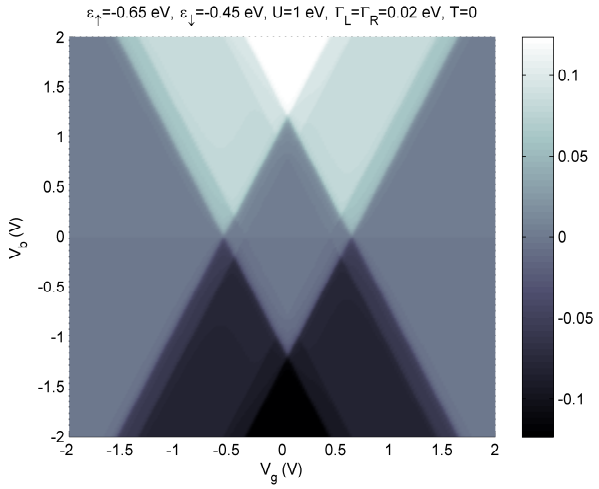

Fig. 3.3. Current J in units of e/h, as function of gate voltage V_g and bias voltage V_b.

$$e\mathbf{E}\cdot\left\{\left[\left(1-\frac{\partial\,\mathrm{Re}\,\Sigma}{\partial\omega}\right)\cdot\nabla_{\mathbf{p}}+(\mathbf{v}_{\mathbf{p}}+\nabla_{\mathbf{p}}\,\mathrm{Re}\,\Sigma)\frac{\partial}{\partial\omega}\right]G^{<}\right.$$
$$\left.-\frac{\partial\Sigma^{<}}{\partial\omega}\nabla_{\mathbf{p}}\,\mathrm{Re}\,G+\frac{\partial\,\mathrm{Re}\,G}{\partial\omega}\nabla_{\mathbf{p}}\Sigma^{<}\right\}=\Sigma^{<}A-\Gamma G^{<} \tag{3.27}$$

This equation can be drastically simplified in the linear response regime since the terms in the bracket on the left-hand side can be taken in equilibrium, since they are already multiplied by the electric field. This term can then be simplified by using the well-known equilibrium expressions,

$$G^{<}_{\mathrm{eq}}(\mathbf{p},\omega)=in_F(\omega)A(\mathbf{p},\omega)\,,\qquad \Sigma^{<}_{\mathrm{eq}}(\mathbf{p},\omega)=in_F(\omega)\Gamma(\mathbf{p},\omega)\,,$$
$$A(\mathbf{p},\omega)=\frac{\Gamma}{\sigma^2+(\Gamma/2)^2}\,,\qquad \mathrm{Re}\,G(\mathbf{p},\omega)=\frac{\sigma}{\sigma^2+(\Gamma/2)^2}\,, \tag{3.28}$$

where $\sigma(\mathbf{p},\omega)\equiv\omega-\epsilon_{\mathbf{p}}-\mathrm{Re}\,\Sigma$. In Eq. (3.27), all terms proportional to $n_F(\omega)$ vanish and we are left with

$$\tfrac{i}{2}A^2(\mathbf{p},\omega)\frac{\partial n_F}{\partial\omega}e\mathbf{E}\cdot\left[(\mathbf{v}_{\mathbf{p}}+\nabla_{\mathbf{p}}\,\mathrm{Re}\,\Sigma)\Gamma+\sigma\nabla_{\mathbf{p}}\Gamma\right]=\Sigma^{<}A-\Gamma G^{<} \tag{3.29}$$

Using equation (3.29) to derive transport coefficients is equivalent to using the Kubo formalism.

3.2.1 Example: Conductivity from Impurity Scattering

To illustrate how transport coefficients are calculated from the QBE, we study the simple example of the conductivity from impurity scattering in the dilute limit. The left-hand side of Eq. (3.29) contains equilibrium quantities as discussed before. The right-hand side (collision term) vanishes identically in equilibrium as is immediately seen from the relations (3.28). We keep only the terms $\mathcal{O}(E)$ in the collision term. As seen in Eq. (3.26), retarded quantities and the derived quantities $A=-2\,\mathrm{Im}\,G^R$ and $\Gamma=-2\,\mathrm{Im}\,\Sigma^R$ have no $\mathcal{O}(E)$ term, hence they are taken in equilibrium. Consequently, only the $\mathcal{O}(E)$ terms in the nonequilibrium functions $\Sigma^{<}$ and $G^{<}$ in the collision term are needed. Consider first the collision term. We consider the self-consistent Born approximation in which the usual equilibrium time-ordered self-energy is (Fig. 3.4)

$$\Sigma(\mathbf{p},\omega)=n_iV_{\mathbf{0}}+n_i\int\frac{d^3q}{(2\pi)^3}|V_{\mathbf{p}-\mathbf{q}}|^2G(\mathbf{q},\omega) \tag{3.30}$$

The nonequilibrium contour-ordered self-energy has the same structure, hence the nonequilibrium lesser self-energy is

$$\Sigma^{<}(\mathbf{p},\omega)=n_i\int\frac{d^3q}{(2\pi)^3}|V_{\mathbf{p}-\mathbf{q}}|^2G^{<}(\mathbf{q},\omega)$$

Consider expanding the nonequilibrium Green's function $G^{<}(\mathbf{p},\omega)$ as the equilibrium piece $G^{<}_{\mathrm{eq}}(\mathbf{p},\omega)$ plus a nonequilibrium piece $G^{<}_1(\mathbf{p},\omega)$:

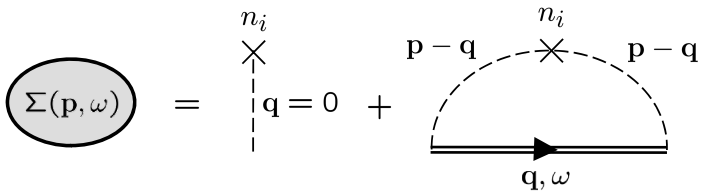

Fig. 3.4. Self-energy for impurity scattering in the self-consistent Born approximation.

$$G^<(\mathbf{p},\omega) = in_F(\omega)A(\mathbf{p},\omega) + G_1^<(\mathbf{p},\omega) \tag{3.31}$$

then the equilibrium part of the collision term vanishes as mentioned earlier, and the collision term is

$$\Sigma^< A - \Gamma G^< = \Sigma_1^< A - \Gamma G_1^< \equiv I[G_1^<]$$

where

$$\Sigma_1^<(\mathbf{p},\omega) = n_i \int \frac{d^3q}{(2\pi)^3} |V_{\mathbf{p}-\mathbf{q}}|^2 G_1^<(\mathbf{q},\omega)$$

We now make the following ansatz for the nonequilibrium part $G_1^<$,

$$G_1^<(\mathbf{p},\omega) = -iA(\mathbf{p},\omega)\frac{\partial n_F}{\partial \omega} e\mathbf{E}\cdot\mathbf{v}_{\mathbf{p}}\Lambda(\mathbf{p},\omega) \tag{3.32}$$

where $\Lambda(\mathbf{p},\omega)$ is a function to be determined. The collision term is then

$$\begin{aligned} I[G_1^<] = {} & iA(\mathbf{p},\omega)\Gamma(\mathbf{p},\omega)\frac{\partial n_F}{\partial \omega} \\ & \times e\mathbf{E}\cdot\left(\mathbf{v}_{\mathbf{p}}\Lambda(\mathbf{p},\omega) - \frac{n_i}{\Gamma(\mathbf{p},\omega)}\int \frac{d^3q}{(2\pi)^3}|V_{\mathbf{p}-\mathbf{q}}|^2 A(\mathbf{q},\omega)\mathbf{v}_{\mathbf{q}}\Lambda(\mathbf{q},\omega)\right) \end{aligned} \tag{3.33}$$

We now consider the left-hand side of Eq. (3.29). In the dilute limit, we neglect terms involving products of Γ and $\mathrm{Re}\,\Sigma$ since they are $\mathcal{O}(n_i^2)$. Hence we have

$$(\mathbf{v_p} + \nabla_\mathbf{p} \operatorname{Re} \Sigma)\Gamma + \sigma \nabla_\mathbf{p} \Gamma = \mathbf{v_p}\Gamma + (\omega - \epsilon_\mathbf{p})\nabla_\mathbf{p}\Gamma + \mathcal{O}(n_i^2) \to \mathbf{v_p}\Gamma$$

where in the last step we have neglected the term proportional to $\omega - \epsilon_\mathbf{p}$ since it is multiplied by $A^2(\mathbf{p},\omega)$ in Eq. (3.29) which is a strongly peaked function around $\omega = \epsilon_\mathbf{p}$ in the dilute limit ($\operatorname{Re}\Sigma \propto n_i$ is small). The QBE thus becomes

$$\begin{aligned}
&\tfrac{i}{2} A^2(\mathbf{p},\omega) \frac{\partial n_F}{\partial \omega} e\mathbf{E}\cdot\mathbf{v_p}\Gamma(\mathbf{p},\omega) = iA(\mathbf{p},\omega)\Gamma(\mathbf{p},\omega)\frac{\partial n_F}{\partial\omega} \\
&\times e\mathbf{E}\cdot\left(\mathbf{v_p}\Lambda(\mathbf{p},\omega) - \frac{n_i}{\Gamma(\mathbf{p},\omega)}\int \frac{d^3q}{(2\pi)^3}|V_{\mathbf{p}-\mathbf{q}}|^2 A(\mathbf{q},\omega)\mathbf{v_q}\Lambda(\mathbf{q},\omega)\right)
\end{aligned}$$

from which we extract an integral equation for the unknown function $\Lambda(\mathbf{p},\omega)$,

$$\mathbf{v_p}\Lambda(\mathbf{p},\omega) = \tfrac{1}{2}A(\mathbf{p},\omega)\mathbf{v_p} + \frac{n_i}{\Gamma(\mathbf{p},\omega)}\int\frac{d^3q}{(2\pi)^3}|V_{\mathbf{p}-\mathbf{q}}|^2 A(\mathbf{q},\omega)\mathbf{v_q}\Lambda(\mathbf{q},\omega)$$

which is reminiscent of the integral equation satisfied by the vector vertex function in the ladder approximation of the diagrammatic Kubo analysis. In fact, the approximations we have made on the QBE are equivalent to the ladder approximation in diagrammatic language.

The electric charge current $\mathbf{j}$ is given in general by

$$\mathbf{j}(\mathbf{R},T) = -ie\int\frac{d^3p}{(2\pi)^3}\,\mathbf{v_p}\int\frac{d\omega}{2\pi}\,G^<(\mathbf{p},\omega,\mathbf{R},T)$$

From the decomposition Eq. (3.31), the equilibrium piece will give a vanishing contribution and only $G_1^<$ in Eq. (3.32) will give a nonvanishing contribution to the current. We therefore obtain

$$\mathbf{j} = e^2\int\frac{d^3p}{(2\pi)^3}\int\frac{d\omega}{2\pi}\,\mathbf{v_p}(\mathbf{v_p}\cdot\mathbf{E})\left(-\frac{\partial n_F}{\partial\omega}\right)A(\mathbf{p},\omega)\Lambda(\mathbf{p},\omega)$$

from which the conductivity tensor is easily extracted,

$$\sigma_{\mu\nu} = \frac{e^2}{m^2}\int\frac{d^3p}{(2\pi)^3}\int\frac{d\omega}{2\pi}\,p_\mu p_\nu\left(-\frac{\partial n_F}{\partial\omega}\right)A(\mathbf{p},\omega)\Lambda(\mathbf{p},\omega)$$

which is equivalent to the Kubo formula result.

3.3 One-Band Electrons with Spin-Orbit Coupling

Consider a generic translationally invariant spin-$\frac{1}{2}$ Hamiltonian with spin-orbit coupling,

$$H_0(-i\nabla) = \frac{(-i\nabla)^2}{2m}\mathbb{1} + \boldsymbol{\lambda}(-i\nabla)\cdot\boldsymbol{\sigma} + \mu_B\mathbf{B}\cdot\boldsymbol{\sigma}$$

where $\boldsymbol{\lambda}(\mathbf{p})$ is odd in $\mathbf{p}$ in general due to time-reversal symmetry, but for simplicity we neglect higher-order terms and assume it is only linear in $\mathbf{p}$. Consider for example a two-dimensional electron gas with Rashba and Dresselhaus spin-orbit coupling,

$$H_{\rm SO} = \alpha(p_y\sigma_x - p_x\sigma_y) + \beta(p_x\sigma_x - p_y\sigma_y)$$

where α is the Rashba coupling and β is the linear Dresselhaus coupling. Then we simply have

$$\begin{aligned}\lambda_x(\mathbf{p}) &= \alpha p_y + \beta p_x\\ \lambda_y(\mathbf{p}) &= -(\alpha p_x + \beta p_y)\end{aligned}$$

Orbital magnetic effects are taken care of by the Peierls substitution Eq. (2.60). The Green's functions and self-energies in the Wigner representation are now 2×2 matrices. The Kadanoff-Baym driving term $[\hat{G}_0^{-1} - U, G^<]_{\mathbf{p},\omega,\mathbf{R},T}$ in the presence of electric and magnetic fields can be derived from the general expression Eq. (2.62). We obtain

$$\begin{aligned}[\hat{G}_0^{-1} - U, G^<]_{\mathbf{p},\omega,\mathbf{R},T} = i&\left[\frac{\partial}{\partial T} + \mathbf{v}_\mathbf{p}\cdot\left(\nabla_\mathbf{R} + e\mathbf{E}\frac{\partial}{\partial\omega}\right) + e(\mathbf{E}+\mathbf{v}_\mathbf{p}\times\mathbf{B})\cdot\nabla_\mathbf{p}\right]G^<\\ &-[(\boldsymbol{\lambda}+\mu_B\mathbf{B})\cdot\boldsymbol{\sigma}, G^<] + \tfrac{i}{2}\{\nabla_\mathbf{p}(\boldsymbol{\lambda}\cdot\boldsymbol{\sigma}), \nabla_\mathbf{R}G^<\}\\ &+\tfrac{i}{2}e\mathbf{E}\cdot\left\{\nabla_\mathbf{p}(\boldsymbol{\lambda}\cdot\boldsymbol{\sigma}), \frac{\partial G^<}{\partial\omega}\right\} - \tfrac{i}{2}e\mathbf{B}\cdot[\nabla_\mathbf{p}(\boldsymbol{\lambda}\cdot\boldsymbol{\sigma})\underset{,}{\times}\nabla_\mathbf{p}G^<]\end{aligned} \tag{3.34}$$

where $\mathbf{v}_\mathbf{p} = \mathbf{p}/m$ as before, we write simply $\boldsymbol{\lambda} \equiv \boldsymbol{\lambda}(\mathbf{p})$ and we use the notation of Eq. (2.65). The anticommutator is derived in a similar manner from Eq. (2.63),

$$\begin{aligned}\tfrac{1}{2}\{\hat{G}_0^{-1} - U, G^R\}_{\mathbf{p},\omega,\mathbf{R},T} = &\left[\omega - \epsilon_\mathbf{p} + \frac{1}{8m}\left(\nabla_\mathbf{R} + e\mathbf{E}\frac{\partial}{\partial\omega} + e\mathbf{B}\times\nabla_\mathbf{p}\right)^2\right]G^R\\ &-\tfrac{1}{2}\{(\boldsymbol{\lambda}+\mu_B\mathbf{B})\cdot\boldsymbol{\sigma}, G^R\} + \tfrac{i}{4}[\nabla_\mathbf{p}(\boldsymbol{\lambda}\cdot\boldsymbol{\sigma}), \nabla_\mathbf{R}G^R]\\ &+\tfrac{i}{4}e\mathbf{E}\cdot\left[\nabla_\mathbf{p}(\boldsymbol{\lambda}\cdot\boldsymbol{\sigma}), \frac{\partial G^R}{\partial\omega}\right] - \tfrac{i}{4}e\mathbf{B}\cdot\{\nabla_\mathbf{p}(\boldsymbol{\lambda}\cdot\boldsymbol{\sigma})\underset{,}{\times}\nabla_\mathbf{p}G^R\}\end{aligned} \tag{3.35}$$

The terms on the right-hand side of the QBE Eq. (2.66) and the equation for the retarded Green's function Eq. (2.67) are still given by the general Kadanoff-Baym commutators Eq. (2.64). Equations (3.34) and (3.35) are valid to arbitrary order in $\mathbf{E}$ and $\mathbf{B}$.

In the case of homogeneous ($\nabla_\mathbf{R} = 0$) transport in zero magnetic field $\mathbf{B} = 0$, the retarded Green's function picks up a contribution linear in the electric field, as opposed to the case of spinless electrons in section 3.2 where

the leading order was $\mathcal{O}(E^2)$, Eq. (3.26). This is because the commutator in Eq. (3.35)

$$\left[\nabla_{\mathbf{p}}(\boldsymbol{\lambda}\cdot\boldsymbol{\sigma}), \frac{\partial G^R}{\partial\omega}\right] \neq 0$$

does not vanish in general, hence the solution of Eq. (3.35) to linear order in $\mathbf{E}$ is not just the equilibrium Green's function.

3.4 Classical Boltzmann Limit

In this section, we derive the classical Boltzmann equation (2.1) from the QBE for 1-band spinless electrons, Eq. (2.69). First, we assume that the quantities $\mathrm{Re}\,\Sigma$ and $\mathrm{Re}\,G$ are essentially constant so that their derivatives vanish. In the QBE, these functions renormalize the transport coefficients that are found from the classical Boltzmann equation. We also perform the inverse of the change of variables Eq. (2.40), so that we are back with the untransformed frequency Ω. Hence we have

$$i\left[\frac{\partial}{\partial T} + \mathbf{v}_{\mathbf{p}}\cdot\nabla_{\mathbf{R}} + e(\mathbf{E}+\mathbf{v}_{\mathbf{p}}\times\mathbf{B})\cdot\nabla_{\mathbf{p}}\right] G^<(\mathbf{p},\Omega,\mathbf{R},T) = \Sigma^> G^< - G^>\Sigma^< \tag{3.36}$$

Consider Eq. (2.25) for the spectral function. It has been shown by Kadanoff and Baym that Eq. (2.25) for the nonequilibrium spectral function can be solved in the gradient approximation by the following ansatz,

$$A(\mathbf{p},\Omega,\mathbf{R},T) = \frac{\Gamma}{(\Omega-\epsilon_{\mathbf{p}}-\mathrm{Re}\,\Sigma-U(\mathbf{R}))^2+(\Gamma/2)^2}$$

where here $U(\mathbf{R}) = -e\mathbf{E}\cdot\mathbf{R}$. In the quasiparticle approximation, we assume that Γ is very small so that the spectral function approaches a delta function,

$$A(\mathbf{p},\Omega,\mathbf{R},T) = 2\pi\delta(\Omega-\epsilon_{\mathbf{p}}-\mathrm{Re}\,\Sigma-U(\mathbf{R})) \tag{3.37}$$

It is well-known that for equilibrium Green's functions, the fluctuation-dissipation theorem holds,

$$G^<(\mathbf{p},\Omega) = iA(\mathbf{p},\Omega)f(\Omega) \tag{3.38}$$

$$G^>(\mathbf{p},\Omega) = -iA(\mathbf{p},\Omega)[1-f(\Omega)] \tag{3.39}$$

where $f(\Omega)$ is the distribution function. Out of equilibrium we define a nonequilibrium quantity $F(\mathbf{p},\Omega,\mathbf{R},T)$ such that the nonequilibrium Green's functions $G^{<,>}(\mathbf{p},\Omega,\mathbf{R},T)$ satisfy analogous relations,

$$G^<(\mathbf{p},\Omega,\mathbf{R},T) = iA(\mathbf{p},\Omega,\mathbf{R},T)F(\mathbf{p},\Omega,\mathbf{R},T) \tag{3.40}$$

$$G^>(\mathbf{p},\Omega,\mathbf{R},T) = -iA(\mathbf{p},\Omega,\mathbf{R},T)[1-F(\mathbf{p},\Omega,\mathbf{R},T)] \tag{3.41}$$

Note that these relations are consistent with the exact relation $G^< - G^> = iA$ and merely constitute a definition of F. However, within the quasiparticle approximation Eq. (3.37), the Ω dependence of F is seen to be redundant because of the delta function and it is sufficient to consider a three-variable function $f(\mathbf{p}, \mathbf{R}, T) \equiv F(\mathbf{p}, \Omega, \mathbf{R}, T)$ which plays the role of a nonequilibrium distribution function. Equations (3.40,3.41) thus become

$$G^<(\mathbf{p}, \Omega, \mathbf{R}, T) = 2\pi i \delta(\Omega - \epsilon_{\mathbf{p}} - \mathrm{Re}\,\Sigma - U(\mathbf{R})) f(\mathbf{p}, \mathbf{R}, T) \tag{3.42}$$

$$G^>(\mathbf{p}, \Omega, \mathbf{R}, T) = -2\pi i \delta(\Omega - \epsilon_{\mathbf{p}} - \mathrm{Re}\,\Sigma - U(\mathbf{R}))[1 - f(\mathbf{p}, \mathbf{R}, T)] \tag{3.43}$$

where it is seen that the correlation functions $G^{<,>}$ contain information about the energy spectrum in addition to information about the nonequilibrium distribution. For a general spectral function $A(\mathbf{p}, \Omega, \mathbf{R}, T)$, the ansatz (3.40,3.41) with $F(\mathbf{p}, \Omega, \mathbf{R}, T) \equiv f(\mathbf{p}, \mathbf{R}, T)$ independent of Ω is called the *Kadanoff-Baym ansatz* [8]. We now substituting Eqs. (3.42) and (3.43) in Eq. (3.36) and integrate over all Ω, which is easy because of the delta functions. We obtain

$$\left(\frac{\partial}{\partial T} + \mathbf{v}_{\mathbf{p}} \cdot \nabla_{\mathbf{R}} + e(\mathbf{E} + \mathbf{v}_{\mathbf{p}} \times \mathbf{B}) \cdot \nabla_{\mathbf{p}} \right) f = I[f]$$

which is the classical Boltzmann equation (2.1), where the collision term $I[f]$ is

$$\begin{aligned} I[f] = &-i\Sigma^<(\mathbf{p}, \Omega, \mathbf{R}, T)\big|_{\Omega = \epsilon_{\mathbf{p}} + \mathrm{Re}\,\Sigma - e\mathbf{E}\cdot\mathbf{R}} [1 - f(\mathbf{p}, \mathbf{R}, T)] \\ &-i\Sigma^>(\mathbf{p}, \Omega, \mathbf{R}, T)\big|_{\Omega = \epsilon_{\mathbf{p}} + \mathrm{Re}\,\Sigma - e\mathbf{E}\cdot\mathbf{R}} f(\mathbf{p}, \mathbf{R}, T) \end{aligned}$$

We can also perform again the Mahan-Hänsch transformation Eq. (2.38),

$$\begin{aligned} I[f] = &-i\Sigma^<(\mathbf{p}, \omega, \mathbf{R}, T)\big|_{\omega = \epsilon_{\mathbf{p}} + \mathrm{Re}\,\Sigma} [1 - f(\mathbf{p}, \mathbf{R}, T)] \\ &-i\Sigma^>(\mathbf{p}, \omega, \mathbf{R}, T)\big|_{\omega = \epsilon_{\mathbf{p}} + \mathrm{Re}\,\Sigma} f(\mathbf{p}, \mathbf{R}, T) \end{aligned} \tag{3.44}$$

which can also be written simply as

$$I[f] = S^{\mathrm{in}}[1 - f] - S^{\mathrm{out}} f$$

where $S^{\mathrm{in}} = -i\Sigma^<$ is an in-scattering rate and $S^{\mathrm{out}} = i\Sigma^>$ is an out-scattering rate.

For the sake of definiteness, we investigate a simple example, where collisions are due to electrons scattering off static impurities in the dilute limit. We treat the interaction at the level of the self-consistent Born approximation. At this level the self-energy consists of one diagram with one resummed fermion line and two connected impurity lines. The equilibrium result for time-ordered quantities is well-known (Eq. (3.30)),

$$\Sigma(\mathbf{p}, \omega) = n_i V_{\mathbf{0}} + n_i \int \frac{d^3q}{(2\pi)^3} |V_{\mathbf{p}-\mathbf{q}}|^2 G(\mathbf{q}, \omega)$$

where $V_{\mathbf{k}}$ is the Fourier transform of the impurity scattering potential and n_i is the density of impurities. Since diagrammatic perturbation theory is formally the same in or out of equilibrium, the relation still holds for the Keldysh contour-ordered functions and the real-time components follow by the usual analytic continuation (which is trivial here since there are no products of contour-ordered quantities):

$$\Sigma^{<,>}(\mathbf{p},\omega,\mathbf{R},T) = n_i \int \frac{d^3q}{(2\pi)^3} |V_{\mathbf{p}-\mathbf{q}}|^2 G^{<,>}(\mathbf{q},\omega,\mathbf{R},T)$$

Substituting into the collision term Eq. (3.44) and using Eqs. (3.42,3.43), we obtain

$$I[f] = 2\pi n_i \int \frac{d^3q}{(2\pi)^3} |V_{\mathbf{p}-\mathbf{q}}|^2 \delta(\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{q}}) [f(\mathbf{q},\mathbf{R},T) - f(\mathbf{p},\mathbf{R},T)] \tag{3.45}$$

which is the standard result for impurity scattering. For weak electric fields, this collision term can be brought in the following form. Assume a homogeneous system. To linear order in $\mathbf{E}$, the distribution function is

$$f(\mathbf{p},T) = f_0(\mathbf{p}) + C(p,T)\mathbf{p}\cdot\mathbf{E} \tag{3.46}$$

where $f_0(\mathbf{p}) \equiv f_{\rm eq}(\epsilon_{\mathbf{p}})$ is the equilibrium distribution and $C(p,T)$ is a scalar function. Then

$$f(\mathbf{q},T) - f(\mathbf{p},T) = C(p,T)(\mathbf{q}-\mathbf{p})\cdot\mathbf{E}$$

since the delta function $\delta(\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{q}})$ in Eq. (3.45) enforces $\epsilon_{\mathbf{p}} = \epsilon_{\mathbf{q}}$ and $p = q$. Hence the collision term becomes

$$I[f] = -C(p,T)2\pi n_i \int \frac{d^3q}{(2\pi)^3} |V_{\mathbf{p}-\mathbf{q}}|^2 \delta(\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{q}})(\mathbf{p}-\mathbf{q})\cdot\mathbf{E} \tag{3.47}$$

Choose $\mathbf{p}$ along $\hat{\mathbf{z}}$, and parameterize $\mathbf{E}$ with (θ,ϕ) and $\mathbf{q}$ with (θ',ϕ'):

$$\begin{aligned}
\mathbf{p} &= p\hat{\mathbf{z}} \\
\mathbf{E} &= E(\sin\theta\cos\phi\,\hat{\mathbf{x}} + \sin\theta\sin\phi\,\hat{\mathbf{y}} + \cos\theta\,\hat{\mathbf{z}}) \\
\mathbf{q} &= p(\sin\theta'\cos\phi'\,\hat{\mathbf{x}} + \sin\theta'\sin\phi'\,\hat{\mathbf{y}} + \cos\theta'\,\hat{\mathbf{z}})
\end{aligned}$$

where we see that $\cos\theta' = \mathbf{p}\cdot\mathbf{q} \equiv \cos\theta_{\mathbf{p},\mathbf{q}}$. We get

$$(\mathbf{p}-\mathbf{q})\cdot\mathbf{E} = pE\big(\cos\theta(1-\cos\theta') - \sin\theta\sin\theta'\cos(\phi-\phi')\big)$$

In the integral over $\mathbf{q}$, the term $\cos(\phi-\phi')$ will vanish upon integration over ϕ', hence it can be omitted. Inserting the remaining first term in Eq. (3.47) and using Eq. (3.46), we get

$$I[f] = -\frac{f(\mathbf{p},T) - f_0(\mathbf{p})}{\tau_{\mathbf{p}}}$$

which is the usual form of the collision term in the relaxation time approximation, and the inverse relaxation time is

$$\frac{1}{\tau_{\mathbf{p}}} = 2\pi n_i \int \frac{d^3q}{(2\pi)^3} |V_{\mathbf{p}-\mathbf{q}}|^2 \delta(\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{q}}) \big(1 - \cos\theta_{\mathbf{p},\mathbf{q}}\big)$$

Notice the important factor $(1 - \cos\theta_{\mathbf{p},\mathbf{q}})$ which describes the effectiveness of large-angle scattering in destroying momentum.

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