

Nonequilibrium Green's Functions

Lecture notes: contour formalism, diagrams, Keldysh space, and quantum transport

E. Arrigoni

Institute of Theoretical and Computational Physics, TU Graz *

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Abstract

These notes cover the course on nonequilibrium Green's functions. Secs. 1–2 give suggested literature and motivate the subject. Part I (Secs. 3–7): the closed time (Keldysh) contour, the perturbation expansion and Feynman diagrams on the contour, the matrix (Keldysh-space) formulation with its retarded–advanced–Keldysh (RAK) representation, the noninteracting Green's functions, and the exactly solvable case of a single-particle potential. Part II (Secs. 8–12): a quench in a closed system and the role of dissipation, the resonant level coupled to one and two baths, the Landauer-type current formula, the interacting (Anderson) dot in the Hubbard-I approximation with Coulomb blockade, and the transient dynamics after a quantum quench. Sec. 13 then extends the diagrammatic toolbox to genuine electron–phonon and electron–electron vertices, in preparation for the derivation of the quantum Boltzmann equation in Sec. 14. They are typeset from the handwritten lecture notes (files 00–11 and the parallel `noneq-lecture` version); notational inconsistencies of the handwritten notes have been unified, and a few slips corrected – see the list in Appendix B. Standard references: the original papers by Keldysh [?] and Kadanoff–Baym [?] – with precursors by Martin–Schwinger [?] and Schwinger [?] – and the reviews and textbooks by Rammer and Smith [?], Haug and Jauho [?], Rammer [?], and Stefanucci and van Leeuwen [?], of which we mostly follow the first two. Throughout, $\hbar = 1$.

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1 Suggested literature

Before starting, a few pointers to the literature, with brief comments on what each source is useful for.

1.1 Equilibrium Green's functions

We take for granted the equilibrium (zero-temperature and finite-temperature) Green's-function formalism – contour ordering, Wick's theorem, Feynman diagrams, Dyson's equation – as developed in the companion course, whose notes are available online [?]:

<https://itp.tugraz.at/~arrigoni/vorlesungen/korrelations1/public/green.html>
(credentials: see teach center).

The present notes extend that formalism to systems out of equilibrium; see also the literature quoted there for the equilibrium case.

1.2 Nonequilibrium Green’s functions: textbooks and reviews

- **Haug and Jauho**, *Quantum Kinetics in Transport and Optics of Semiconductors* [?], (see teach center for the relevant chapters). This is our main reference: comprehensive and semiconductor-oriented in its applications, but the formalism developed in the early chapters is completely general and is the one we follow most closely.
- **Rammer and Smith**, short review article [?] (see teach center). A compact, historically important account of the same formalism from the transport-theory-of-metals perspective; a good complement to Haug–Jauho, in particular for the derivation of the Boltzmann equation from the Keldysh technique (Sec. 14).
- **Jauho’s lecture notes** [?], freely available online. A very pedagogical, self-contained introduction to the Keldysh nonequilibrium Green function technique; recommended as a first read alongside these notes.
- **Rammer**, *Quantum Field Theory of Non-equilibrium States* [?], and **Stefanucci and van Leeuwen**, *Nonequilibrium Many-Body Theory of Quantum Systems* [?]. Two more recent and more comprehensive textbooks, useful in particular for topics we only touch upon: initial correlations and the full Kadanoff–Baym contour (Sec. 3), and the connection to time-dependent density-functional theory.

1.3 Alternative approaches and applications

- **Kamenev**, Les Houches lecture notes [?]. A functional-integral (coherent-state path-integral) formulation of the Keldysh technique, complementary to the operator/diagrammatic approach used in these notes; it reaches the same retarded–advanced–Keldysh (RAK) structure of Sec. 5 from a different direction, and is recommended for a second, deeper pass on the formalism.
- **Jauho, Wingreen and Meir** [?]. Applies the formalism to time-dependent transport in resonant-tunneling semiconductor heterostructures; this is the paper behind the Landauer-type current formula of Sec. 10 and the transient dynamics of Sec. 12.
- **Ryndyk, Gutiérrez, Song and Cuniberti** [?]. Applies the same diagrammatic toolbox to transport at the molecular scale (molecular electronics), a natural extension of the nanostructure examples treated in Part II.
- **Brandbyge *et al.*** [?]. Combines nonequilibrium Green’s functions with density-functional theory (the “TranSIESTA” method) to obtain first-principles current–voltage characteristics of atomic-scale junctions – an example of how the formal machinery of this course becomes a quantitative, predictive tool.

2 Motivation: why nonequilibrium Green’s functions?

Equilibrium many-body theory answers a well-posed question: given a system described by a (possibly interacting) Hamiltonian h in thermal equilibrium, $\rho(h) = Z^{-1}e^{-\beta h}$, compute expectation values, correlation and response functions, spectral properties. Linear-response theory then extends this machinery to the leading effect of a *weak* external perturbation. This covers an enormous range of phenomena – conductivity, susceptibilities, optical spectra – but it structurally assumes that the system is at all times close to *some* equilibrium state.

Many situations of physical interest violate this assumption:

- A finite bias voltage or temperature difference drives a *steady* current through a nanostructure (quantum dot, molecule, nanowire); the bias is not infinitesimal, and the resulting steady state is not a thermal state of any simple reference Hamiltonian.
- A system is permanently coupled to two or more reservoirs held at different chemical potentials or temperatures (leads, phonon baths): by construction it never relaxes to global equilibrium.
- An ultrafast laser or THz pulse drives a system strongly and on time scales comparable to, or shorter than, its internal relaxation times (pump–probe spectroscopy, time-resolved ARPES); the transient, non-thermal state itself is the object of interest.
- A parameter of an otherwise isolated system is suddenly changed (a *quantum quench*): a lattice depth, an interaction strength, a magnetic field. One then asks how, or whether, and to what state the system subsequently relaxes – a question with no equilibrium analogue. Cold-atom experiments realize such quenches with remarkable control and isolation from the environment, and have become a standard testbed for this physics.

The common structural feature of all these examples is that we need $\langle O(t) \rangle = \text{Tr}[\rho O_H(t)]$ for an initial state ρ that is *not* the equilibrium density matrix of the Hamiltonian governing the time evolution – exactly the situation set up in Eq. (1) below, with $H'(t)$ an arbitrary, not necessarily weak or adiabatic, perturbation.

To handle this we need a perturbative and diagrammatic framework that does not rely on the system returning to, or remaining close to, a known equilibrium reference state. As we will see in Sec. 3, the fix – due to Schwinger, Keldysh, and Kadanoff and Baym – is to let time run forward *and back* along a closed contour. This has an important structural consequence, already visible in Sec. 5: whereas equilibrium theory needs only the retarded and advanced Green’s functions $G^{r,a}$ (spectral information), the nonequilibrium theory requires in addition the Keldysh component G^K , which encodes the actual, generally unknown, *occupation* of the states. In equilibrium the two pieces of information are related by the fluctuation–dissipation theorem, Eq. (66); out of equilibrium G^K becomes an independent quantity, to be determined self-consistently (e.g. via a kinetic equation, Sec. 14) together with the spectral functions. This is both the central technical difficulty and the central physical richness of the subject: the occupation of the states is no longer dictated by a temperature and a chemical potential, but becomes part of the answer.

The encouraging news, developed throughout Part I of these notes, is that essentially the entire machinery of equilibrium many-body theory – Wick’s theorem, Feynman diagrams, the linked-cluster theorem, self-energies, Dyson’s equation – carries over with only formal modifications once time is understood to run along the Keldysh contour. Part II then applies this machinery to concrete, solvable examples: a quantum quench, a level coupled to one or two particle reservoirs, the resulting steady-state current, and the effect of interactions.

3 The nonequilibrium problem and the Keldysh contour

3.1 Setup

We consider a many-body system described by the Hamiltonian

$$H(t) = h + H'(t), \quad h = H_0 + V, \quad (1)$$

where H_0 is a noninteracting (quadratic) Hamiltonian, V contains the interactions, and $H'(t)$ is an *arbitrary*, in general time-dependent, perturbation that is switched on at some time t_0 ,

$$H'(t) = 0 \quad \text{for } t < t_0. \quad (2)$$

For $t < t_0$ the system is in equilibrium with respect to h , described by the density matrix

$$\rho(h) = \frac{1}{Z} e^{-\beta h}, \quad Z = \text{Tr} e^{-\beta h}. \quad (3)$$

We are interested in expectation values at later times,

$$\langle O(t) \rangle = \text{Tr}[\rho(h) O_H(t)], \quad (4)$$

where $O_H(t)$ is the operator in the Heisenberg picture of the *full* Hamiltonian, $dO_H/dt = i[H_H(t), O_H(t)]$ (plus $\partial_t O$ for explicitly time-dependent operators). Note that, since H depends on time, $O_H(t) \neq e^{iHt} O e^{-iHt}$: the time evolution operator is the time-ordered exponential $U(t, t_0) = T \exp(-i \int_{t_0}^t H(t') dt')$ and $O_H(t) = U(t, t_0)^\dagger O U(t, t_0)$. We set $\hbar = 1$ throughout.

3.2 Interaction representation

When introducing an interaction representation one must specify with respect to which splitting of the Hamiltonian. Here we first take h as the unperturbed part and $H'(t)$ as the perturbation. Operators evolve with h ,

$$O_h(t) = e^{iht} O e^{-iht}, \quad (5)$$

which is nothing but the Heisenberg picture of the time-independent h ; we therefore denote it by the subscript h (the reason for this notation is that later we will use H_0 as the unperturbed Hamiltonian). States evolve with the remaining part; the corresponding time-evolution operator (“ S -matrix”) $S_h(t, t')$ is defined by

$$|\psi_h(t)\rangle = S_h(t, t') |\psi_h(t')\rangle, \quad i \frac{d}{dt} S_h(t, t') = H'_h(t) S_h(t, t'), \quad H'_h(t) = e^{iht} H'(t) e^{-iht}, \quad (6)$$

with solution

$$S_h(t, t_0) = T \exp\left(-i \int_{t_0}^t dt_1 H'_h(t_1)\right). \quad (7)$$

It obeys the group property $S_h(t_1, t_2) S_h(t_2, t_3) = S_h(t_1, t_3)$ and is unitary,

$$S_h(t_0, t) = S_h(t, t_0)^{-1} = S_h(t, t_0)^\dagger. \quad (8)$$

Since Heisenberg and interaction pictures coincide at t_0 ($O_H(t) = O_h(t)$ for $t \leq t_0$), one has

$$O_H(t) = S_h(t_0, t) O_h(t) S_h(t, t_0). \quad (9)$$

3.3 Failure of the equilibrium construction

We need expressions of the form (we take $T = 0$ for simplicity, so that the initial state is the ground state $|\Phi_0\rangle$ of h ; finite T is recovered below by other means)

$$\langle \Phi_0 | T A(t_1) B(t_2) \cdots | \Phi_0 \rangle, \quad (10)$$

with Heisenberg operators at times $t_i \geq t_0$. Proceeding as in the equilibrium case, i.e. inserting (9) and collecting the S -matrices inside the time ordering, one arrives at

$$\langle \Phi_0 | S_h(t_0, \infty) T [S_h(\infty, t_0) A_h(t_1) B_h(t_2) \cdots] | \Phi_0 \rangle. \quad (11)$$

In equilibrium one takes $t_0 = -\infty$ and switches the perturbation on and off adiabatically, $H'(t) = e^{-0^+|t|} V$. The Gell-Mann–Low theorem then guarantees $|\Phi_{+\infty}\rangle = S_h(+\infty, -\infty)|\Phi_0\rangle \propto |\Phi_0\rangle$ – the system returns to its (nondegenerate) ground state up to a phase – so the leftmost factor in (11) reduces to a trivial phase, which cancels against the denominator $\langle \Phi_0 | S | \Phi_0 \rangle$.

Out of equilibrium this fails: $H'(t)$ is arbitrary, it is neither switched on adiabatically nor switched off again, so the state at $t = +\infty$ bears no simple relation to $|\Phi_0\rangle$. Moreover, the leftmost operator $S_h(t_0, \infty)$ in (11) is *anti*-chronological and cannot be moved inside the time ordering. We are thus forced to keep the explicit evolution *back* from $+\infty$ to t_0 . (Instead of $+\infty$ we could as well turn back already at $\max(t_1, t_2, \dots)$.)

3.4 The Keldysh contour

The way out (Schwinger [?], Keldysh [?]) is to interpret the forward and backward evolutions in (11) as a single evolution along the closed time contour $C = C_1 \cup C_2$ of Fig. 1, which runs from t_0 to $+\infty$ (branch C_1) and back from $+\infty$ to t_0 (branch C_2).

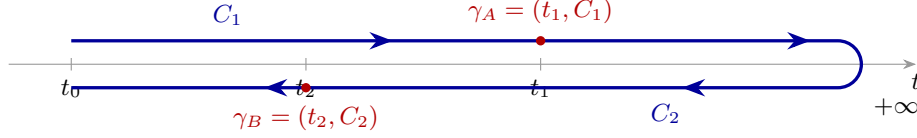


Figure 1: The Keldysh contour $C = C_1 \cup C_2$. A contour time $\gamma = (t, C)$ carries the physical time *and* the branch index. In the example shown, $\gamma_B >_c \gamma_A$ even though $t_2 < t_1$.

Each operator is assigned a *contour time*

$$\gamma = (t, C), \quad C \in \{C_1, C_2\}, \quad (12)$$

which specifies both the physical time and the branch on which it sits. The ordering along the contour, $\gamma_A >_c \gamma_B$ (“ γ_A later than γ_B on C ”), holds iff one of the three cases applies:

$$\begin{aligned} C_A = C_2, C_B = C_1 & \quad (\text{anything on } C_2 \text{ is later than anything on } C_1), \\ C_A = C_B = C_1, \quad t_A > t_B & \quad (\text{chronological on the forward branch}), \\ C_A = C_B = C_2, \quad t_A < t_B & \quad (\text{anti-chronological on the backward branch}). \end{aligned} \quad (13)$$

The *contour-ordering operator* T_C orders operators according to $>_c$; every transposition of two fermionic operators contributes a factor -1 . For two operators,

$$T_C A(\gamma_A) B(\gamma_B) = \begin{cases} A(\gamma_A) B(\gamma_B), & \gamma_A >_c \gamma_B, \\ \xi B(\gamma_B) A(\gamma_A), & \gamma_B >_c \gamma_A, \end{cases} \quad \boxed{\xi = +1 \text{ (bosons)}, \quad \xi = -1 \text{ (fermions)}} \quad (14)$$

(the sign ξ applies when both A and B are fermionic).¹

With these definitions, (11) becomes a contour-ordered expectation value,

$$\langle \Phi_0 | T A(t_1) B(t_2) \cdots | \Phi_0 \rangle = \langle \Phi_0 | T_C [S_C A_h(\gamma_1) B_h(\gamma_2) \cdots] | \Phi_0 \rangle, \quad \gamma_i = (t_i, C_1), \quad (15)$$

with the contour S -matrix

$$S_C \equiv S_h(t_0 C_2, t_0 C_1) = T_C \exp \left(-i \int_C d\gamma H'_h(\gamma) \right), \quad \int_C d\gamma = \int_{t_0}^{\infty} dt \Big|_{C_1} + \int_{\infty}^{t_0} dt \Big|_{C_2}. \quad (16)$$

The turning point $+\infty$ needs no branch label. Of course the operators need not be restricted to C_1 : (15) defines correlation functions for arbitrary contour arguments γ_i , which is the form needed for perturbation theory. Two comments:

- Exactly, and without invoking any adiabatic theorem,

$$\langle \Phi_0 | S_C | \Phi_0 \rangle = 1, \quad (17)$$

since $S_h(t_0 C_2, t_0 C_1) = S_h(t_0, \infty) S_h(\infty, t_0) = 1$: the backward evolution undoes the forward one.

- The same construction goes through for a mixed initial state $\rho(h)$; the average $\langle \cdots \rangle$ is then a trace with $\rho(h)$.

¹The handwritten notes use $\varepsilon \equiv -\xi$ (video version) and $\eta \equiv \xi$ (lecture version); here we use the single symbol ξ throughout, cf. Appendix B.

3.5 A quadratic reference Hamiltonian: adiabatic switching

To evaluate (15) perturbatively we will use Wick's theorem, which requires the unperturbed Hamiltonian to be *quadratic* — but $h = H_0 + V$ is not. At $T = 0$ we solve this by switching on the interaction V adiabatically starting from the infinite past:

$$H(t) = H_0 + V e^{\alpha t} + H'(t), \quad \alpha \rightarrow 0^+, \quad t_0 \rightarrow -\infty. \quad (18)$$

We now repeat the entire construction with the replacements

$$h \rightarrow H_0, \quad H'(t) \rightarrow W(t) \equiv V e^{\alpha t} + H'(t), \quad |\Phi_0\rangle \rightarrow |-\infty\rangle, \quad (19)$$

where $|-\infty\rangle$ is the ground state of H_0 , $H_0|-\infty\rangle = E_0|-\infty\rangle$, and interaction-picture operators evolve with H_0 : $A_0(t) \equiv A_{H_0}(t) = e^{iH_0 t} A e^{-iH_0 t}$. By the adiabatic switching, at the time when H' starts to act (nonadiabatically) the state has evolved from $|-\infty\rangle$ into the ground state of $h = H_0 + V$, so the physical situation of Sec. 1.1 is recovered (Fig. 2). The crucial gain is that the reference state and the free evolution now refer to the *quadratic* H_0 , so Wick's theorem applies.

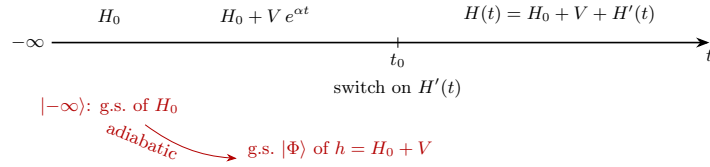


Figure 2: Preparation of the interacting ground state by adiabatically switching on V ; the arbitrary perturbation $H'(t)$ acts from t_0 on.

3.6 Further options and issues

For completeness we mention how the restrictions made above can be lifted; none of this will be needed in the following.

- *Initial correlations.* One may want to start at a *finite* t_0 from an arbitrary correlated density matrix ρ . Writing $\rho \propto e^{-\beta h}$, the Boltzmann factor is itself an evolution operator in imaginary time, and can be incorporated by appending a vertical (Matsubara) branch C_M running from t_0 down to $t_0 - i\beta$ (Fig. 3); this is the Kadanoff–Baym contour [?, ?].
- The vertical branch can be neglected when $t_0 \rightarrow -\infty$ and the interactions are switched on adiabatically (as in Sec. 1.5).
- A finite-temperature initial state can alternatively be produced by coupling the system to (noninteracting) heat baths; dissipation then erases the memory of the initial state. This is the route we will follow later in the course.

4 Perturbation expansion and Feynman diagrams

4.1 Expansion of the contour S -matrix

After the replacements of Sec. 1.5 the central object is

$$S \equiv S_{H_0}(-\infty C_2, -\infty C_1) = T_C \exp\left(-i \int_C W_0(\gamma) d\gamma\right), \quad W_0(t) = e^{iH_0 t} W(t) e^{-iH_0 t}, \quad (20)$$

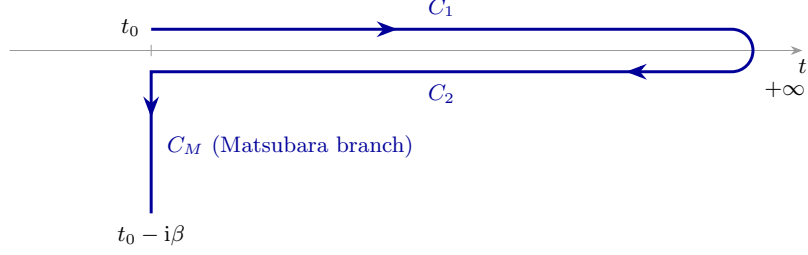


Figure 3: Contour with the additional imaginary-time branch C_M (Kadanoff–Baym contour), needed to treat initial correlations at finite t_0 .

which is expanded exactly as in ordinary perturbation theory,

$$S = T_C \left(1 - i \int_C W_0(\gamma) d\gamma - \frac{1}{2} \iint_C W_0(\gamma_1) W_0(\gamma_2) d\gamma_1 d\gamma_2 + \dots \right); \quad (21)$$

the only difference is that all time integrals run along the Keldysh contour.

4.2 The contour Green's function

We collect contour time and the remaining single-particle quantum numbers (position, spin, orbital, ...) into a single label

$$x = (\gamma, \vec{r}), \quad (22)$$

and define the *contour-ordered Green's function*

$$G(x_1, x_2) = -i \langle T_C c(x_1) c^\dagger(x_2) \rangle = \frac{-i \langle T_C S c_0(x_1) c_0^\dagger(x_2) \rangle_0}{\langle T_C S \rangle_0}, \quad (23)$$

where $\langle \dots \rangle_0 \equiv \langle -\infty | \dots | -\infty \rangle$ and $c_0, c_0^\dagger$ evolve with H_0 . The denominator actually equals 1, but it is convenient to keep it: it is the bookkeeping device behind the linked-cluster theorem below. Diagrammatically, (23) is represented by the two external points x_1, x_2 attached to the expansion of S (Fig. 4).



Figure 4: The Green's function: external points x_1, x_2 attached to the expanded S -matrix.

For a two-body, spin-independent, instantaneous interaction,

$$W(t) = \frac{1}{2} \int d\vec{r}_A d\vec{r}_B V(\vec{r}_A - \vec{r}_B) c^\dagger(\vec{r}_A) c^\dagger(\vec{r}_B) c(\vec{r}_B) c(\vec{r}_A), \quad (24)$$

each factor $\int_C W_0$ in (21) produces an interaction vertex $V(x_A, x_B) = V(\vec{r}_A - \vec{r}_B) \delta(\gamma_A, \gamma_B)$ whose two ends carry the *same* contour time ($\delta(\gamma, \gamma')$ is the contour delta function, discussed in Sec. 7).²

²The video notes write the interaction in the density–density form $c^\dagger c c^\dagger c$, which differs from the normal-ordered form (24) by a one-body term; we use (24) throughout.

4.3 Wick's theorem

Each term of the expansion contains T_C -ordered products of free (H_0 -evolved) creation and annihilation operators averaged in the noninteracting state $|\!-\infty\rangle$. For a quadratic H_0 , *Wick's theorem* [?] states that such averages decompose into the sum over all complete pairings (contractions) of the operators, each pairing giving the product of pair averages – i.e. of noninteracting Green's functions – with a sign ξ^P , where P is the number of transpositions of fermionic operators needed to bring the paired operators next to each other. In short: “*all lines have to be paired in all possible ways*”. For four operators,

$$\begin{aligned} \langle T_C c_0(x_1) c_0(x_2) c_0^\dagger(x_3) c_0^\dagger(x_4) \rangle_0 &= \langle T_C c_0(x_1) c_0^\dagger(x_4) \rangle_0 \langle T_C c_0(x_2) c_0^\dagger(x_3) \rangle_0 \\ &+ \xi \langle T_C c_0(x_1) c_0^\dagger(x_3) \rangle_0 \langle T_C c_0(x_2) c_0^\dagger(x_4) \rangle_0, \end{aligned} \quad (25)$$

represented graphically in Fig. 5. Anomalous contractions $\langle cc \rangle_0$ and $\langle c^\dagger c^\dagger \rangle_0$ vanish by particle-number conservation (they would be needed, e.g., for superconductors).



Figure 5: The two complete pairings of (25).

4.4 Low-order diagrams for G

At first order in V , inserting $S^{(1)} = -\frac{i}{2} \int dx_3 dx_4 V(x_3 - x_4) c_0^\dagger(x_3) c_0^\dagger(x_4) c_0(x_4) c_0(x_3)$ into the numerator of (23) and applying Wick's theorem produces the following classes of terms (note that x_3, x_4 are distinct points carrying the same contour time):

- the *exchange (Fock) diagram* of Fig. 6,

$$F(x_1, x_2) \equiv \int dx_3 dx_4 G_0(x_1, x_4) G_0(x_4, x_3) G_0(x_3, x_2) V(x_3 - x_4) \quad (26)$$

(we will use it again later);

- the *tadpole (Hartree) diagram* of Fig. 7,

$$\int dx_3 dx_4 G_0(x_1, x_3) G_0(x_3, x_2) G_0(x_4, x_4) V(x_3 - x_4); \quad (27)$$

- *disconnected* contributions such as Fig. 8,

$$G_0(x_1, x_2) \cdot P, \quad P = \int dx_3 dx_4 G_0(x_3, x_3) G_0(x_4, x_4) V(x_3 - x_4), \quad (28)$$

where the closed part P , without external legs, is called a *vacuum diagram* (another first-order vacuum diagram is $P' \propto \int G_0(x_3, x_4) G_0(x_4, x_3) V(x_3 - x_4)$).

Each of the connected diagrams occurs twice, with $x_3 \leftrightarrow x_4$ interchanged; the two contributions are topologically equivalent and equal, and cancel the factor $\frac{1}{2}$ of the vertex. The external variables x_1, x_2 are fixed; all internal variables are integrated (or summed) over, with times running along the contour.

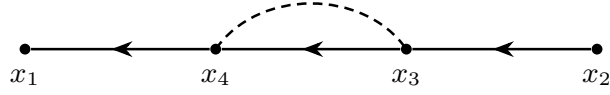


Figure 6: First-order exchange (Fock) diagram, Eq. (26).

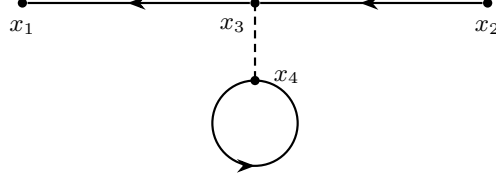


Figure 7: First-order tadpole (Hartree) diagram, Eq. (27).

At second order one finds, among others, the chain diagram of Fig. 9,

$$\int dx_3 \cdots dx_6 V(x_3 - x_4) V(x_5 - x_6) G_0(x_1, x_6) G_0(x_6, x_5) G_0(x_5, x_4) G_0(x_4, x_3) G_0(x_3, x_2), \quad (29)$$

as well as disconnected pieces such as $F(x_1, x_2) \cdot P$: disconnected contributions always factorize into products of lower-order connected diagrams and vacuum diagrams.

4.5 Linked-cluster theorem

The denominator $\langle T_C S \rangle_0$ of (23) contains no external points and thus consists of exactly the vacuum diagrams. When the ratio in (23) is evaluated order by order, the vacuum diagrams of the denominator cancel the disconnected contributions of the numerator. This is the *linked-cluster theorem*: in the end one only needs to evaluate *connected* diagrams,

$$G(x_1, x_2) = -i \langle T_C S c_0(x_1) c_0^\dagger(x_2) \rangle_0^{\text{connected}}. \quad (30)$$

4.6 Feynman rules

The diagrammatic elements are collected in Fig. 10; besides the electron propagator and the electron–electron interaction discussed so far, we list for later use the phonon propagator D_0 , the electron–phonon vertex g , and the single-particle potential u (Sec. 7).

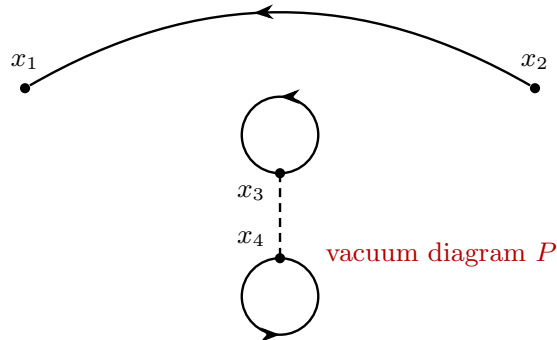


Figure 8: A disconnected first-order contribution: free propagation times the vacuum diagram P .

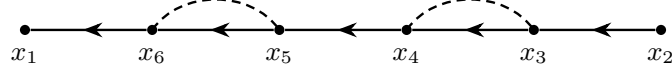


Figure 9: A second-order (chain) diagram.

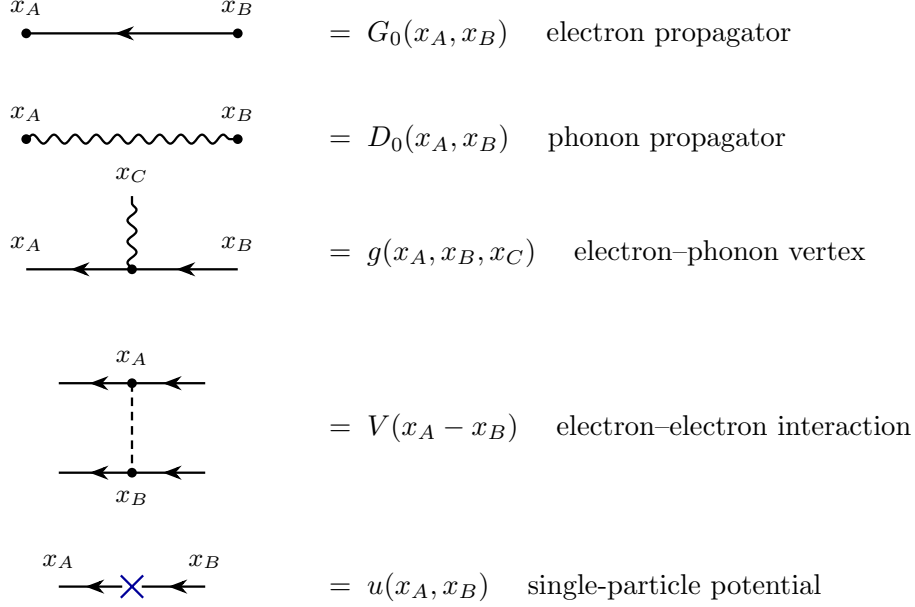


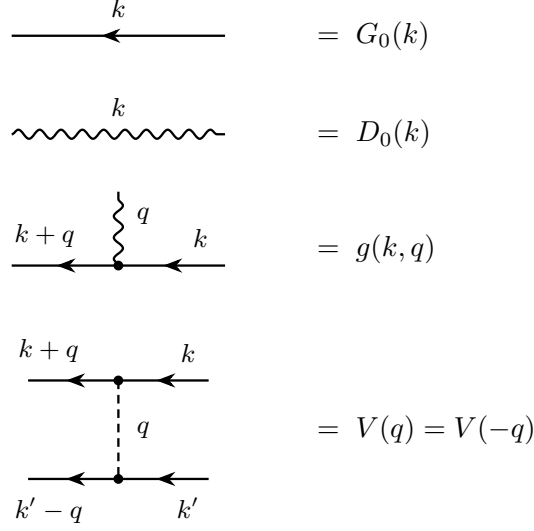
Figure 10: Diagrammatic elements in real space.

The rules to compute the contribution with m interaction vertices to $G(x_A, x_B)$ (see, e.g., Fetter–Walecka [?] or Mahan [1] for the equilibrium counterpart) are:

1. Draw all topologically inequivalent, *connected* diagrams starting at x_B and ending at x_A and containing m vertices.
2. Assign to the elements their values according to Fig. 10.
3. Multiply by $(-1)^F$, where F is the number of closed fermion loops, and by $i^{m/2}$, i.e. one factor i per interaction (V or phonon) line.³
4. Integrate (or sum) over all internal variables; time integrals run along the Keldysh contour.

In the presence of translation invariance it is convenient to Fourier transform to momentum space, and for time-independent situations (equilibrium, or a steady state) to frequency space; the elements then depend on $k = (\vec{k}, \omega)$ and momentum and/or frequency are conserved at every vertex (Fig. 11). The single-particle potential u breaks translation invariance in general and is then *not* momentum conserving. In general one may also use mixed representations: time + momentum, or frequency + position.

³ m counts the endpoints of interaction lines (for the electron–phonon interaction, the g -vertices), so $m/2$ is the number of interaction lines. A single-particle-potential cross carries *no* extra factor, as one easily checks by direct expansion; cf. Sec. 7.



momentum (and/or frequency) conservation at all vertices

Figure 11: Diagrammatic elements in momentum space.

4.7 Self-energy and Dyson's equation

Inspecting the expansion of G , the diagrams fall into two classes: *single-particle reducible* ones, which can be cut into two pieces by removing a single G_0 line, and *single-particle irreducible* (1PI) ones, which cannot. Define the *self-energy* $\Sigma(x_1, x_2)$ as the sum of all 1PI diagrams with the two external legs amputated (Fig. 12).



Figure 12: Lowest-order contributions to the self-energy (amputated): Hartree, Fock, single-particle potential, a second-order diagram, ...

Every diagram for G is either the bare line or a unique string of 1PI blocks connected by single G_0 lines; summing the resulting geometric series,

$$G = G_0 + G_0 * \Sigma * G_0 + G_0 * \Sigma * G_0 * \Sigma * G_0 + \dots, \quad (31)$$

one obtains *Dyson's equation* [?] (Fig. 13)

$$G(x_1, x_2) = G_0(x_1, x_2) + \int dx_3 dx_4 G_0(x_1, x_3) \Sigma(x_3, x_4) G(x_4, x_2) \quad (32)$$

or compactly $G = G_0 + G_0 * \Sigma * G$, where “ $*$ ” denotes the convolution over contour times together with the sum/integral over the internal quantum numbers. Collecting the 1PI blocks from the other side yields the equivalent “left” version $G = G_0 + G * \Sigma * G_0$.

For continuous variables the inverse of a two-point function is defined as the integral kernel A^{-1} with

$$\int A^{-1}(x_1, \bar{x}) A(\bar{x}, x_2) d\bar{x} = \delta(x_1, x_2); \quad (33)$$

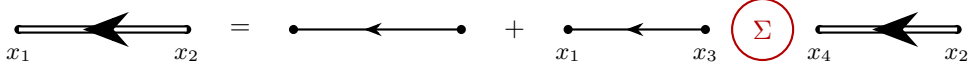


Figure 13: Dyson's equation. Double line: full G ; single line: G_0 .

for discrete indices it is the matrix inverse. With this notion, Dyson's equation can be solved formally:

$$G_0^{-1} = G^{-1} + \Sigma \quad \Longleftrightarrow \quad G = (G_0^{-1} - \Sigma)^{-1}. \quad (34)$$

In frequency space (steady state) and for a finite set of orbital indices this is a plain matrix relation and trivial to evaluate — the difficulty of the many-body problem is of course hidden in Σ .

5 Keldysh space

5.1 Branch-resolved Green's functions

For practical evaluations it is convenient to replace the contour arguments by ordinary times plus a discrete branch index, i.e. by a 2×2 matrix structure in *Keldysh space*. For the Green's function (and similarly for any two-point function) we write, with $\gamma_A = (t_A, C_A)$ and $\gamma_B = (t_B, C_B)$,

$$G(\gamma_A, \gamma_B) \longrightarrow \hat{G}(t_A, t_B) = \begin{pmatrix} G^T(t_A, t_B) & G^<(t_A, t_B) \\ G^>(t_A, t_B) & G^{\bar{T}}(t_A, t_B) \end{pmatrix}, \quad (35)$$

where the row (column) refers to the branch C_1 or C_2 of the first (second) argument, and

$$G^T(t_A, t_B) = -i \langle T c(t_A) c^\dagger(t_B) \rangle \quad (\text{time-ordered: both on } C_1), \quad (36)$$

$$G^{\bar{T}}(t_A, t_B) = -i \langle \bar{T} c(t_A) c^\dagger(t_B) \rangle \quad (\text{anti-time-ordered: both on } C_2), \quad (37)$$

$$G^<(t_A, t_B) = -i \xi \langle c^\dagger(t_B) c(t_A) \rangle \quad (\text{lesser: } t_A \text{ on } C_1, t_B \text{ on } C_2), \quad (38)$$

$$G^>(t_A, t_B) = -i \langle c(t_A) c^\dagger(t_B) \rangle \quad (\text{greater: } t_A \text{ on } C_2, t_B \text{ on } C_1), \quad (39)$$

with $\xi = +1$ for bosons and $\xi = -1$ for fermions as before. The assignment follows directly from the contour ordering: e.g. for t_A on C_1 and t_B on C_2 the operator $c^\dagger(t_B)$ is always later on the contour and T_C moves it to the left, at the price of a factor ξ ; this yields (38). (Remaining quantum numbers are suppressed; they simply come along as additional indices.)

5.2 Convolutions

In diagrams one constantly encounters contour convolutions,

$$C(\gamma_A, \gamma_B) = (A * B)(\gamma_A, \gamma_B) = \int_C d\gamma A(\gamma_A, \gamma) B(\gamma, \gamma_B). \quad (40)$$

Splitting the contour integral into its two branches and using that C_2 is run through backward,

$$C(\gamma_A, \gamma_B) = \int_{-\infty}^{+\infty} dt A(t_A C_A, t C_1) B(t C_1, t_B C_B) - \int_{-\infty}^{+\infty} dt A(t_A C_A, t C_2) B(t C_2, t_B C_B), \quad (41)$$

which in matrix notation reads

$$\hat{C}(t_A, t_B) = \int_{-\infty}^{+\infty} dt \hat{A}(t_A, t) \tau_3 \hat{B}(t, t_B), \quad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad (42)$$

the Pauli matrix τ_3 keeps track of the relative minus sign of the backward branch.

5.3 Keldysh rotation and the RAK representation

The four entries of (35) are not independent:

$$G^T + G^{\bar{T}} = G^> + G^<. \quad (43)$$

Exercise 5.1. Prove (43). (Hint: write the time orderings in terms of θ functions of $t_A - t_B$ and of $G^<, G^>.$)

One may therefore choose three independent linear combinations. There are several conventions; we use the transformation

$$\boxed{\underline{G} = L \tau_3 \hat{G} L^\dagger}, \quad L = \frac{1}{\sqrt{2}} (\tau_0 - i \tau_2) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad (44)$$

with $\tau_0 = \mathbb{1}$ and τ_i the Pauli matrices (L is unitary). The result is *upper triangular*,

$$\underline{G} = \begin{pmatrix} G^r & G^K \\ 0 & G^a \end{pmatrix}, \quad (45)$$

the *RAK (retarded-advanced-Keldysh) representation*, where

$$\begin{aligned} G^r &= G^T - G^< = G^> - G^{\bar{T}} \quad (\text{retarded}), \\ G^a &= G^T - G^> = G^< - G^{\bar{T}} \quad (\text{advanced}), \\ G^K &= G^< + G^> = G^T + G^{\bar{T}} \quad (\text{Keldysh}). \end{aligned} \quad (46)$$

Exercise 5.2. Verify (45) with (46), using (43).

Remark 5.1. Combining the definitions one finds the familiar forms

$$G^r(t_A, t_B) = -i \theta(t_A - t_B) \langle [c(t_A), c^\dagger(t_B)]_{-\xi} \rangle, \quad G^a(t_A, t_B) = +i \theta(t_B - t_A) \langle [c(t_A), c^\dagger(t_B)]_{-\xi} \rangle, \quad (47)$$

with $[A, B]_{-\xi} \equiv AB - \xi BA$ (anticommutator for fermions): G^r vanishes for $t_A < t_B$, G^a for $t_A > t_B$. G^r and G^a carry the spectral information; the Keldysh component G^K carries the information about the *occupation* of the states, which out of equilibrium is an independent quantity.

The rotation (44) is designed to also remove the τ_3 from convolutions: transforming (42),

$$\underline{C} = L \tau_3 \hat{C} L^\dagger = \int dt \underbrace{L \tau_3 \hat{A} L^\dagger}_A \underbrace{L \tau_3 \hat{B} L^\dagger}_B \implies \boxed{\underline{C}(t_A, t_B) = \int_{-\infty}^{+\infty} dt \underline{A}(t_A, t) \underline{B}(t, t_B)} \quad (48)$$

(insert $\mathbb{1} = L^\dagger L$ between $\tau_3 \hat{A}$ and $\tau_3 \hat{B}$): in the RAK representation convolutions are plain matrix products — no τ_3 any more.

Exercise 5.3. Fill in the steps leading to (48).

5.4 Some useful relations: triangular matrices

By (48), products of two-point functions in the RAK representation multiply like 2×2 upper-triangular matrices

$$\underline{B} = \begin{pmatrix} b_r & b_K \\ 0 & b_a \end{pmatrix}, \quad \underline{F} = \begin{pmatrix} f_r & f_K \\ 0 & f_a \end{pmatrix}, \quad (49)$$

where the entries $b_r, b_K, \dots$ may themselves be matrices (in orbital indices, time, $\dots$). The product preserves the triangular structure,

$$\underline{B} \underline{F} = \begin{pmatrix} b_r f_r & b_r f_K + b_K f_a \\ 0 & b_a f_a \end{pmatrix}, \quad (50)$$

i.e. retarded and advanced components simply multiply among themselves, while the Keldysh component mixes. Consequently the *inverse* $\underline{F} = \underline{B}^{-1}$, defined by $\underline{B} \underline{F} = \mathbb{1}$, is again triangular, with

$$\boxed{f_r = b_r^{-1}, \quad f_a = b_a^{-1}, \quad f_K = -b_r^{-1} b_K b_a^{-1}.} \quad (51)$$

(From the K component of $\underline{B} \underline{F} = \mathbb{1}$: $b_r f_K + b_K f_a = 0$.) These relations, closely related to the *Langreth rules* [?], will be used over and over, e.g. to solve Dyson's equation componentwise.

6 Noninteracting Green's functions

6.1 Setup

The noninteracting Green's functions are the building blocks of perturbation theory. Consider first a diagonal quadratic Hamiltonian,

$$H_0 = \sum_p \varepsilon_p c_p^\dagger c_p, \quad (52)$$

where p is a complete set of single-particle quantum numbers labelling the eigenstates of H_0 (for free particles: momentum and spin; for electrons in a crystal: crystal momentum, band and spin; etc.). The free (interaction-picture) evolution follows from

$$\frac{dc_p^\dagger}{dt} = i[H_0, c_p^\dagger] = i\varepsilon_p c_p^\dagger \quad \implies \quad c_p^\dagger(t) = e^{i\varepsilon_p t} c_p^\dagger(0), \quad c_p(t) = (c_p^\dagger(t))^\dagger = e^{-i\varepsilon_p t} c_p(0). \quad (53)$$

Exercise 6.1. Prove (53) (for fermions and for bosons).

All averages below are taken in the grand-canonical noninteracting equilibrium state at inverse temperature β and chemical potential μ (or, at $T = 0$, in the ground state $|\!-\infty\rangle$).

6.2 Retarded and advanced components

With the commutator notation $[A, B]_{-\xi} = AB - \xi BA$ (anticommutator for fermions),

$$G_0^r(p; t) = -i\theta(t) \langle [c_p(t), c_p^\dagger(0)]_{-\xi} \rangle = -i\theta(t) e^{-i\varepsilon_p t} \langle [c_p, c_p^\dagger]_{-\xi} \rangle = -i\theta(t) e^{-i\varepsilon_p t}. \quad (54)$$

Note that the (anti)commutator is a c -number, so G_0^r is *completely independent of the state*, i.e. of temperature, chemical potential, or any nonequilibrium distribution — it contains purely spectral information. Its Fourier transform, with a convergence factor $\delta \rightarrow 0^+$,

$$G_0^r(p, \omega) = -i \int dt e^{i(\omega - \varepsilon_p + i\delta)t} \theta(t) \quad \implies \quad \boxed{G_0^r(p, \omega) = \frac{1}{\omega - \varepsilon_p + i\delta}.} \quad (55)$$

Similarly,

$$G_0^a(p; t) = i\theta(-t) e^{-i\varepsilon_p t} = G_0^r(p; -t)^*, \quad \boxed{G_0^a(p, \omega) = \frac{1}{\omega - \varepsilon_p - i\delta} = G_0^r(p, \omega)^*}. \quad (56)$$

For a general (non-diagonal) quadratic Hamiltonian $H_0 = \sum_{pp'} h_{pp'} c_p^\dagger c_{p'}$ the Green's functions become matrices in (p, p') .

Exercise 6.2. Show that $G_0^a(\omega)_{pp'} = [G_0^r(\omega)_{p'p}]^*$, i.e. as a matrix $G_0^a(\omega) = G_0^r(\omega)^\dagger$.

Exercise 6.3. By introducing the unitary matrix U diagonalising h , derive the matrix expression

$$G_0^r(\omega) = [(\omega + i\delta) \mathbb{1} - h]^{-1}. \quad (57)$$

6.3 Greater and lesser components

These do depend on the state through the occupations. Using (53) and stationarity,

$$G_0^>(p t_A, p' t_B) = -i \langle c_p(t_A) c_{p'}^\dagger(t_B) \rangle = \delta_{pp'} G_0^>(p; t_A - t_B), \quad G_0^>(p; t) = -i e^{-i\varepsilon_p t} \bar{m}_p, \quad (58)$$

with

$$\bar{m}_p \equiv \langle c_p c_p^\dagger \rangle = 1 + \xi m_p, \quad m_p \equiv \langle c_p^\dagger c_p \rangle = \frac{1}{e^{\beta(\varepsilon_p - \mu)} - \xi} \quad (\text{Bose/Fermi function}). \quad (59)$$

Similarly (Exercise 6.4)

$$G_0^<(p; t) = -i \xi \langle c_p^\dagger(0) c_p(t) \rangle = -i \xi e^{-i\varepsilon_p t} m_p. \quad (60)$$

The Fourier transforms are sharp peaks at the level position, weighted by the occupation factors:

$$G_0^>(p, \omega) = -2\pi i \delta(\omega - \varepsilon_p) \bar{m}_p, \quad G_0^<(p, \omega) = -2\pi i \delta(\omega - \varepsilon_p) \xi m_p. \quad (61)$$

Exercise 6.4. Derive (60) and (61).

6.4 Keldysh component and the fluctuation–dissipation relation

From (46),

$$G_0^K(p; t) = G_0^>(p; t) + G_0^<(p; t) = -i e^{-i\varepsilon_p t} (\bar{m}_p + \xi m_p) = -i e^{-i\varepsilon_p t} (1 + 2\xi m_p), \quad (62)$$

so that

$$G_0^K(p, \omega) = -2\pi i \delta(\omega - \varepsilon_p) (1 + 2\xi m_p). \quad (63)$$

Since here m_p is a function of the level energy only, $m_p = m(\varepsilon_p)$, we can exploit the δ -function to replace $\varepsilon_p \rightarrow \omega$:

$$\boxed{G_0^K(p, \omega) = -2\pi i \delta(\omega - \varepsilon_p) s(\omega), \quad s(\omega) \equiv 1 + 2\xi m(\omega), \quad m(\omega) = \frac{1}{e^{\beta(\omega - \mu)} - \xi}.} \quad (64)$$

Using

$$\frac{1}{\omega - \varepsilon_p + i0^+} = \mathcal{P} \frac{1}{\omega - \varepsilon_p} - i\pi \delta(\omega - \varepsilon_p) \quad \implies \quad \text{Im } G_0^r(p, \omega) = -\pi \delta(\omega - \varepsilon_p), \quad (65)$$

Eq. (64) can be written as

$$\boxed{G_0^K(p, \omega) = 2i \text{Im } G_0^r(p, \omega) s(\omega) = [G_0^r(p, \omega) - G_0^a(p, \omega)] s(\omega).} \quad (66)$$

This is the (noninteracting) *fluctuation–dissipation relation*: in equilibrium the Keldysh component is completely fixed by the spectral functions $G^{r/a}$ and the equilibrium distribution encoded in $s(\omega)$. For fermions at $T = 0$,

$$s(\omega) = 1 - 2\theta(\mu - \omega) = \text{sign}(\omega - \mu). \quad (67)$$

Out of equilibrium, by contrast, G^K is an *independent* quantity: it carries the information on the actual (generally unknown) distribution function — this is precisely why the Keldysh formalism needs one more Green’s function than equilibrium theory.

Exercise 6.5. Extend (66) to a non-diagonal quadratic Hamiltonian (cf. Exercise 6.3): show that in equilibrium $G_0^K(\omega) = [G_0^r(\omega) - G_0^a(\omega)]s(\omega)$ holds as a matrix relation.

7 A single-particle potential: the exactly solvable case

7.1 The vertex

As the simplest application of the formalism — and an important building block for what follows — consider a noninteracting system perturbed by an arbitrary (possibly nonlocal and time-dependent) single-particle potential,

$$W_u(t) = \int d\vec{r}_A d\vec{r}_B u(\vec{r}_A, \vec{r}_B, t) c^\dagger(\vec{r}_A) c(\vec{r}_B). \quad (68)$$

In the expansion of the contour S -matrix, each factor $\int_C d\gamma W_{u,0}(\gamma)$ can be written with both operators carrying independent contour arguments,

$$\int_C d\gamma W_{u,0}(\gamma) = \int dx_A dx_B c_0^\dagger(x_A) u(x_A, x_B) c_0(x_B), \quad u(x_A, x_B) = \delta(\gamma_A, \gamma_B) u(\vec{r}_A, \vec{r}_B, t_A), \quad (69)$$

where $\int dx = \int_C d\gamma \int d\vec{r}$. Diagrammatically this is a vertex with one incoming and one outgoing fermion line — the *cross* of Fig. 10.

7.2 The contour delta function

The object $\delta(\gamma, \gamma_A)$ appearing in (69) is defined by

$$\int_C d\gamma \delta(\gamma, \gamma_A) f(\gamma) = f(\gamma_A). \quad (70)$$

Writing $\delta(\gamma, \gamma_A) = \delta_{CC_A} s_{C_A} \delta(t - t_A)$ with an unknown branch-dependent factor s_C and splitting $\int_C$ into the two branches (with the minus sign of the backward branch),

$$\int_{-\infty}^{\infty} dt \delta(t - t_A) \delta_{C_A C_1} s_{C_1} f(C_1, t) - \int_{-\infty}^{\infty} dt \delta(t - t_A) \delta_{C_A C_2} s_{C_2} f(C_2, t) \stackrel{!}{=} f(C_A, t_A), \quad (71)$$

one finds $s_{C_1} = +1$, $s_{C_2} = -1$, i.e.

$$\boxed{\delta(\gamma, \gamma_A) = \delta_{CC_A} (\tau_3)_{C_A C_A} \delta(t - t_A)} \quad (72)$$

the -1 on C_2 compensates the backward orientation of that branch.⁴

7.3 The cross in Keldysh space

By (72), in the branch (hat) representation the vertex (69) is the matrix

$$\hat{u}(t_A, t_B) = u(\vec{r}_A, \vec{r}_B, t_A) \delta(t_A - t_B) \tau_3, \quad (73)$$

and rotating to the RAK representation with (44),

$$\underline{u} = L \tau_3 \hat{u} L^\dagger = u(\vec{r}_A, \vec{r}_B, t_A) \delta(t_A - t_B) L \tau_3 \tau_3 L^\dagger \implies \boxed{\underline{u} = u(\vec{r}_A, \vec{r}_B, t_A) \delta(t_A - t_B) \mathbb{1}_{2 \times 2}}, \quad (74)$$

using $\tau_3 \tau_3 = \mathbb{1}$ and $LL^\dagger = \mathbb{1}$. Thus *the single-particle potential is proportional to the identity in RAK space* (“ r ” and “ a ” components equal to u , vanishing “ K ” component) — note that this holds in the RAK representation only, not in the hat representation.

⁴The handwritten notes write the branch sign as $(-1)^{C_A}$, which with the labels $C_A \in \{1, 2\}$ would give the wrong signs; $(\tau_3)_{CC}$ is what is meant, cf. Appendix B.

7.4 Exact Dyson equation

For a noninteracting system with the perturbation (68), the expansion of G contains only strings of crosses connected by G_0 lines (Fig. 14): the only single-particle *irreducible* diagram is the single cross itself, so

$$\boxed{\Sigma = u \text{ exactly,}} \quad (75)$$

and Dyson's equation resums the perturbative series exactly:

$$\underline{G} = \underline{G}_0 + \underline{G}_0 * \underline{u} * \underline{G}, \quad (76)$$

where “ $*$ ” now stands for the time convolution, the spatial integration (or orbital sum), *and* the 2×2 matrix product in Keldysh space.

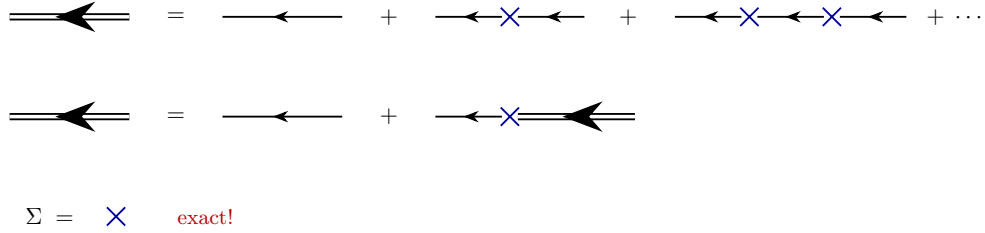


Figure 14: Diagrams with the single-particle potential: expansion, resummation, and the (exact) self-energy.

Since $\underline{u} \propto \mathbb{1}$ in RAK space, the triangular algebra of Sec. 5.4 immediately yields the component equations

$$G^r = G_0^r + G_0^r * u * G^r, \quad G^a = G_0^a + G_0^a * u * G^a, \quad G^K = G_0^K + G_0^r * u * G^K + G_0^K * u * G^a. \quad (77)$$

Exercise 7.1. Derive (77) from (76) using (50).

7.5 Outlook: steady state

A drastic simplification occurs in a *steady state*: if u is switched on at some time and thereafter remains time independent, one may expect the system to reach a stationary state (we will discuss later under which conditions this actually happens — coupling to baths plays a crucial role). Then all Green's functions depend on the time difference only, one can Fourier transform in time, and the convolutions in (77) become products: with the triangular-matrix inversion rules (51), Dyson's equation is solved algebraically, e.g. $G^r(\omega) = [G_0^r(\omega)^{-1} - u]^{-1}$. This is the starting point of the next part of the course, where we apply it to a simple model and to the coupling to baths.

8 A quench in a closed system: why dissipation matters

8.1 A sudden level shift

To appreciate the subtleties of the steady-state formalism we first apply it to the simplest imaginable “nonequilibrium” problem: a closed system whose levels are suddenly shifted,

$$H_0 = \sum_p \varepsilon_p c_p^\dagger c_p, \quad \hat{V} = \theta(t - t_0) \sum_p v_p c_p^\dagger c_p. \quad (78)$$

(We consider fermions; before t_0 the system is in equilibrium at μ, T .) Assuming that some time after t_0 a *steady state* is reached, all Green's functions depend on time differences only

and we can work in frequency space. The perturbation is a single-particle potential, diagonal in p , so by Sec. 7 the self-energy is exact, $\underline{\Sigma}_{pp'} = \delta_{pp'} v_p \mathbb{1}$, and Dyson's equation $\underline{G}^{-1} = \underline{g}^{-1} - \underline{\Sigma}$ can be solved with the triangular-matrix rules (51). For each p (we drop the index), using $(\underline{g}^{-1})^K = -g^{r-1} g^K g^{a-1} = (g^{r-1} - g^{a-1}) s(\omega)$:

$$G^r = (g^{r-1} - v)^{-1} = \frac{1}{\omega - \varepsilon - v + i\delta}, \quad G^a = (G^r)^*, \quad (79)$$

and, since v drops out of the difference $g^{r-1} - g^{a-1} = G^{r-1} - G^{a-1}$,

$$G^K = -G^r (G^{r-1} - G^{a-1}) s(\omega) G^a = (G^r - G^a) s(\omega), \quad s(\omega) = 1 - 2f(\omega - \mu) : \quad (80)$$

the fluctuation-dissipation form survives, *with the original equilibrium distribution centred at the old μ .*

8.2 Occupations: comparison with the exact solution

The equal-time Keldysh component gives the occupations: from $G_{pp'}^K(t=0) = -i\delta_{pp'} + 2i\langle c_p^\dagger c_p \rangle$,

$$\langle c_p^\dagger c_p \rangle = \frac{\delta_{pp'}}{2} - \frac{i}{2} G_{pp'}^K(t=0) = \frac{\delta_{pp'}}{2} - \frac{i}{2} \int \frac{d\omega}{2\pi} G_{pp'}^K(\omega). \quad (81)$$

With (80) and $G^r - G^a = -2\pi i \delta(\omega - \varepsilon_p - v_p)$,

$$\langle c_p^\dagger c_p \rangle = \frac{1}{2} \left(1 - s(\varepsilon_p + v_p) \right) = f(\varepsilon_p + v_p - \mu). \quad (82)$$

This is *wrong*: since $[\hat{V}, c_p^\dagger c_p] = 0$, the sudden shift cannot change any occupation. The exact result is a rigidly shifted band with unchanged filling, i.e. a new chemical potential $\mu' = \mu + v$ (for a uniform shift $v_p = v$); the NEGF steady state (82) instead describes a band *refilled down to the old μ* (Fig. 15).

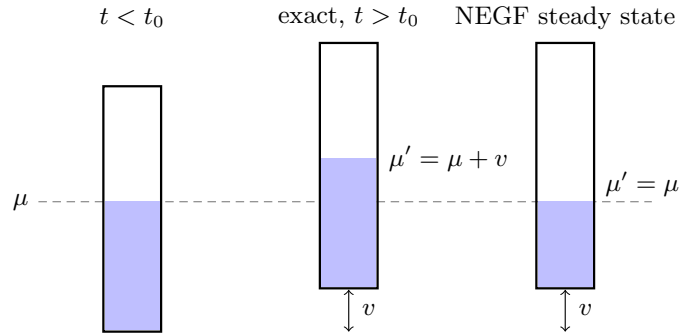


Figure 15: Sudden shift of a filled band: exact result (occupations unchanged, $\mu' = \mu + v$) versus the naive NEGF steady state (refilled to the original μ).

8.3 Resolution: order of limits

Where did we cheat? In assuming a steady state: *a closed system without dissipation never reaches one.* Tracing through the calculation, the culprit is the innocuous-looking Keldysh component of the inverse,

$$(\underline{g}^{-1})^K = (g^{r-1} - g^{a-1}) s(\omega) = 2i \delta s(\omega), \quad (83)$$

which is “in principle zero” as $\delta \rightarrow 0^+$ — but the problem is ill posed: sandwiched between $G^r \cdots G^a$, whose product develops a pole $\sim 1/\delta$ on resonance, it produces the finite result (80). The steady-state formalism thus implicitly performs the limits in the order

$$t \rightarrow \infty \quad \text{first,} \quad \delta \rightarrow 0^+ \quad \text{second :} \quad (84)$$

the convergence factor δ acts as an *artificial infinitesimal dissipation* — an infinitesimally coupled bath at the original μ, T — which re-equilibrates the system on the (arbitrarily long) time scale $1/\delta$. For the closed system this “re-equilibration” is spurious. The lesson: *physically meaningful steady states require genuine dissipation*, i.e. coupling to infinite baths, which is where we turn now. When such a finite coupling Γ is present, the δ of the Green’s functions is superseded by Γ and the artefact disappears.

9 Coupling to a bath: the resonant level model

9.1 The model

We now attach the small system to a genuinely dissipative environment: an infinite bath (“lead”). The *noninteracting resonant level model* consists of a single level (“dot”) d with energy Δ coupled to a continuum of lead levels (Fig. 16; for the moment ignore the right lead):

$$H_0 = \sum_p \varepsilon_p c_p^\dagger c_p + \Delta d^\dagger d, \quad V = \sum_p V_p (c_p^\dagger d + d^\dagger c_p). \quad (85)$$

For $t < t_0$ the coupling is off and each region is separately in equilibrium, in general with different temperatures and chemical potentials (μ_L, T_L for the lead, μ_c, T_c for the level). At t_0 the coupling V is switched on; for $t - t_0$ large a steady state is reached — this time a legitimate one, since the infinite bath provides dissipation. It is convenient to use a uniform notation $d \equiv c_{p=0}$.

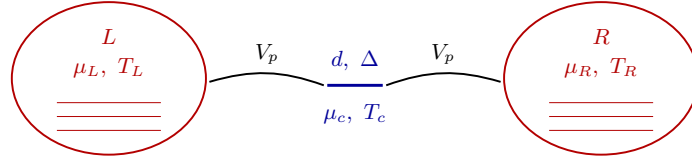


Figure 16: Resonant level coupled to two leads. In this section only the left lead is present; the right lead is added in Sec. 10.

9.2 Projection of Dyson’s equation: embedding self-energy

The coupling V is a single-particle “potential”, so Dyson’s equation is exact (Sec. 7); all objects are 2×2 RAK matrices and, in the steady state, functions of ω :

$$\underline{G} = \underline{g} + \underline{g} \underline{V} \underline{G}, \quad \text{i.e.} \quad \underline{G}_{pp_1} = \underline{g}_{pp_1} + \sum_{p_2 p_3} \underline{g}_{pp_2} \underline{V}_{p_2 p_3} \underline{G}_{p_3 p_1}, \quad (86)$$

where $\underline{g}$ is the $V = 0$ Green’s function, diagonal in the indices, $\underline{g}_{pp'} \propto \delta_{pp'}$, and $\underline{V}_{pp'} = V_{pp'} \mathbb{1}$ with $V_{0p} = V_{p0} = V_p$ the only nonzero elements. Projecting onto the level ($p = p' = 0$) and eliminating $\underline{G}_{p0} = \underline{g}_{pp} V_{p0} \underline{G}_{00}$ ($p \neq 0$):

$$\underline{G}_{00} = \underline{g}_{00} + \underline{g}_{00} \tilde{\Sigma} \underline{G}_{00}, \quad \boxed{\tilde{\Sigma}(\omega) = \sum_p V_{0p} \underline{g}_{pp}(\omega) V_{p0}}, \quad (87)$$

with the solution

$$\underline{G}_{00} = (\underline{g}_{00}^{-1} - \tilde{\Sigma})^{-1}. \quad (88)$$

$\tilde{\Sigma}$ is called the *embedding* (or hybridization) self-energy: the only single-particle-irreducible d - d process is one hop into the lead, free propagation there, and one hop back. Equation (88) is exact.

9.3 Retarded component: level shift and broadening

Taking the retarded component of (88) (the triangular algebra of Sec. 5.4 at work), with $g_{00}^r(\omega)^{-1} = \omega - \Delta + i0^+$ and, for simplicity, $V_p = V$:

$$\tilde{\Sigma}^r(\omega) = V^2 \sum_p g_{pp}^r(\omega) = V^2 \sum_p \mathcal{P} \frac{1}{\omega - \varepsilon_p} - i\pi V^2 \sum_p \delta(\omega - \varepsilon_p) \equiv R_L(\omega) - i\Gamma_L(\omega), \quad (89)$$

where $\rho_L(\omega) = \sum_p \delta(\omega - \varepsilon_p)$ is the lead density of states and

$$\Gamma_L(\omega) = \pi V^2 \rho_L(\omega) \geq 0. \quad (90)$$

Hence

$$\boxed{G_{00}^r(\omega) = \frac{1}{\omega - E(\omega) + i\Gamma_L(\omega)}, \quad E(\omega) = \Delta + R_L(\omega).} \quad (91)$$

The real part R_L describes a *shift* of the level, the imaginary part Γ_L a *broadening*: the finite escape rate into the bath gives the level a finite lifetime. The spectral function $A_{00}(\omega) = -\frac{1}{\pi} \text{Im } G_{00}^r(\omega) = \frac{1}{\pi} \Gamma_L / [(\omega - E)^2 + \Gamma_L^2]$ is a (generalized) Lorentzian of width Γ_L centred at E , normalized to $\int d\omega A_{00} = 1$.

9.4 Keldysh component: the bath dictates the distribution

For the Keldysh component, (88) and (51) give

$$G_{00}^K = -G_{00}^r (\underline{g}_{00}^{-1} - \tilde{\Sigma})^K G_{00}^a = G_{00}^r \left(\tilde{\Sigma}^K - (\underline{g}_{00}^{-1})^K \right) G_{00}^a. \quad (92)$$

As in Sec. 8, $(\underline{g}_{00}^{-1})^K = (g_{00}^{r-1} - g_{00}^{a-1}) s_c(\omega) = 2i0^+ s_c(\omega)$ is infinitesimal, where $s_c(\omega) = 1 - 2f(\omega, \mu_c, T_c)$ carries the *initial* distribution of the level. Now, however, it may safely be dropped: it competes with $\tilde{\Sigma}^K$, which has a *finite* imaginary part $\propto \Gamma_L$ (and G_{00}^r has no poles on the real axis for $\Gamma_L > 0$). Physically, dropping $(\underline{g}_{00}^{-1})^K$ means that μ_c and T_c — the initial preparation of the small central region — do not affect the steady state, as expected for a finite system coupled to an infinite bath. Contrast this with the pathology of Sec. 8, where the corresponding term was the *only* source of the Keldysh component. With

$$\tilde{\Sigma}^K(\omega) = V^2 \sum_p g_{pp}^K = V^2 \sum_p (g_{pp}^r - g_{pp}^a) s_L(\omega) = -2i\Gamma_L(\omega) s_L(\omega), \quad s_L(\omega) = 1 - 2f(\omega, \mu_L, T_L), \quad (93)$$

one finds

$$\boxed{G_{00}^K(\omega) = -2i\Gamma_L(\omega) |G_{00}^r(\omega)|^2 s_L(\omega) = (G_{00}^r(\omega) - G_{00}^a(\omega)) s_L(\omega) = -2\pi i A_{00}(\omega) s_L(\omega),} \quad (94)$$

where we used $G^r - G^a = 2i \text{Im } G^r = -2i\Gamma_L |G^r|^2$.

Exercise 9.1. Prove the second equality in (94).

Equation (94) is a fluctuation–dissipation relation with the distribution *of the bath*: in the steady state the level has simply thermalized with the lead. With a single bath, nonequilibrium was only a transient — the steady state is an equilibrium one.

9.5 Occupation of the level

Using (81) and (94),

$$\langle d^\dagger d \rangle = \frac{1}{2} - \frac{i}{2} \int \frac{d\omega}{2\pi} G_{00}^K(\omega) = \frac{1}{2} - \frac{1}{2} \int d\omega A_{00}(\omega) s_L(\omega) = \int d\omega A_{00}(\omega) f_L(\omega), \quad (95)$$

using $\int d\omega A_{00} = 1$: the occupation is the overlap of the spectral function with the Fermi function of the bath (Fig. 17). In the *wide-band limit* (WBL), $\Gamma_L(\omega) = \Gamma$ and $R_L = 0$ constants, at $T = 0$:⁵

$$\langle d^\dagger d \rangle = \frac{1}{\pi} \int_{-\infty}^{\mu_L} \frac{\Gamma d\omega}{(\omega - \Delta)^2 + \Gamma^2} = \frac{1}{2} + \frac{1}{\pi} \arctan \frac{\mu_L - \Delta}{\Gamma}. \quad (96)$$

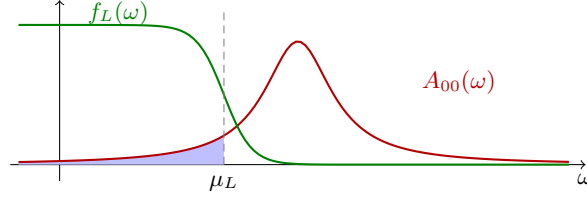


Figure 17: Occupation of the level as the overlap $\int A_{00}(\omega) f_L(\omega) d\omega$.

Exercise 9.2. Using the left version of Dyson's equation, $\underline{G} = \underline{g} + \underline{G} \underline{V} \underline{g}$, derive closed expressions for $\underline{G}_{0p}$, $\underline{G}_{p0}$ and $\underline{G}_{pp'}$ in terms of $\underline{G}_{00}$ and lead quantities.

Exercise 9.3. Add a second level f to the dot, $H_c = \Delta (c_0^\dagger c_0 + f^\dagger f) + T (c_0^\dagger f + f^\dagger c_0)$, with bath and coupling as before (only c_0 couples to the bath). Derive a closed expression for $\underline{G}_{ff}$.

Exercise 9.4. Semi-infinite chain. For $H = v \sum_{n=0}^{\infty} (c_n^\dagger c_{n+1} + \text{h.c.})$, treat the bond v_0 between sites 0 and 1 as the perturbation and express $\underline{G}_{00}$ in terms of the Green's function $\underline{g}_{11}$ of the chain with the bond removed. Realizing that $\underline{g}_{11} = \underline{G}_{00}$, obtain a self-consistent (recursive) equation for $\underline{G}_{00}$ and compute the spectral function.

10 Two baths: steady-state transport

10.1 Two reservoirs

With a single bath the steady state turned out to be an equilibrium state: the central region thermalizes with the reservoir. Do we ever obtain *true* nonequilibrium in the steady state? Yes — with *two (or more) infinite reservoirs* kept at different chemical potentials and/or temperatures, so that a current flows through the central region forever.

Formally the extension is trivial. We use the Hamiltonian (85) with the convention that $p < 0$ labels the left lead (μ_L, T_L) and $p > 0$ the right lead (μ_R, T_R) (Fig. 16). The embedding self-energy simply splits into the two contributions,

$$\underline{G}_{00} = (\underline{g}_{00}^{-1} - \underline{\tilde{\Sigma}})^{-1}, \quad \underline{\tilde{\Sigma}} = \underline{\tilde{\Sigma}}_L + \underline{\tilde{\Sigma}}_R, \quad \underline{\tilde{\Sigma}}_\alpha = \sum_{p \in \alpha} V_{0p} \underline{g}_{pp} V_{p0}. \quad (97)$$

The retarded components are as in (89), $\tilde{\Sigma}_\alpha^r = R_\alpha(\omega) - i\Gamma_\alpha(\omega)$ with $\Gamma_\alpha = \pi V^2 \rho_\alpha(\omega)$, so

$$G_{00}^r(\omega) = \left(\omega - E(\omega) + i\Gamma(\omega) \right)^{-1}, \quad E = \Delta + \sum_\alpha R_\alpha, \quad \Gamma = \sum_\alpha \Gamma_\alpha : \quad (98)$$

in the spectral properties only the *total* bath density of states $\rho_L + \rho_R$ enters.

⁵The handwritten notes (file 06a) miss the prefactor $1/\pi$ in this integral; cf. Appendix B.

10.2 Keldysh component: an average that is no equilibrium

The Keldysh component instead keeps track of which bath supplies which electrons:

$$G_{00}^K = |G_{00}^r|^2 \sum_{\alpha=L,R} (-2i \Gamma_{\alpha}(\omega) s_{\alpha}(\omega)), \quad s_{\alpha}(\omega) = 1 - 2f(\omega, \mu_{\alpha}, T_{\alpha}). \quad (99)$$

Using $G_{00}^r - G_{00}^a = -2i \Gamma |G_{00}^r|^2$, this can be written in pseudo-equilibrium form,

$$\boxed{G_{00}^K(\omega) = (G_{00}^r - G_{00}^a) s_{\text{av}}(\omega), \quad s_{\text{av}}(\omega) = \frac{\Gamma_L(\omega) s_L(\omega) + \Gamma_R(\omega) s_R(\omega)}{\Gamma_L(\omega) + \Gamma_R(\omega)},} \quad (100)$$

but the coupling-weighted distribution s_{av} does *not* correspond to any equilibrium $\mu_{\text{av}}, T_{\text{av}}$: at $T_L = T_R = 0$, for instance, it describes a double-step distribution. This is genuine steady-state nonequilibrium.

10.3 Current

The most interesting observable is the current [?, ?]. The current flowing out of lead L is $\hat{I}_L = -e d\hat{N}_L/dt$ with $\hat{N}_L = \sum_{p<0} c_p^\dagger c_p$ (we take the electron charge as $-e$ conventions aside; overall signs cancel in the final result):

$$\hat{I}_L = -e i [H, \hat{N}_L] = -ie \sum_{p<0} V_p (c_0^\dagger c_p - c_p^\dagger c_0). \quad (101)$$

The expectation value follows from the equal-time off-diagonal Keldysh component, $\langle c_p^\dagger c_0 \rangle = -\frac{i}{2} G_{0p}^K(t=0)$ (cf. (81)), giving

$$I_L = e \sum_{p<0} V_p \text{Re } G_{0p}^K(t=0) = e \int \frac{d\omega}{2\pi} \sum_{p<0} V_p \text{Re } G_{0p}^K(\omega). \quad (102)$$

The mixed function follows from the (left) Dyson equation, $\underline{G}_{0p} = \underline{G}_{00} \underline{V}_{0p} \underline{g}_{pp}$; with the product rule $(\underline{A} \underline{B})^K = A^r B^K + A^K B^a$ and (100),

$$\sum_{p<0} V_p G_{0p}^K = G_{00}^r (-2i \Gamma_L) s_L + (G_{00}^r - G_{00}^a) (R_L + i \Gamma_L) s_{\text{av}}, \quad (103)$$

where we used $\sum_{p<0} V_p^2 g_{pp}^r = R_L - i \Gamma_L$ (and its conjugate for g^a). Taking the real part, the terms with R_L drop and

$$I_L = \frac{e}{\pi} \int d\omega \Gamma_L \text{Im } G_{00}^r (s_L - s_{\text{av}}). \quad (104)$$

Finally, from (100), $s_L - s_{\text{av}} = \frac{\Gamma_R}{\Gamma} (s_L - s_R)$, and with $s_{\alpha} = 1 - 2f_{\alpha}$, $\text{Im } G_{00}^r = -\Gamma |G_{00}^r|^2$:

$$\boxed{I_L = \frac{2e}{\pi} \int d\omega \Gamma_L(\omega) \Gamma_R(\omega) |G_{00}^r(\omega)|^2 (f_L(\omega) - f_R(\omega)) = \frac{e}{2\pi} \int d\omega T(\omega) (f_L(\omega) - f_R(\omega)),} \quad (105)$$

a Landauer-type formula with the transmission function

$$T(\omega) = 4 \Gamma_L \Gamma_R |G_{00}^r(\omega)|^2 \leq 1 \quad (106)$$

(the maximum $T = 1$ is reached on resonance for symmetric coupling $\Gamma_L = \Gamma_R$; note $e/2\pi = e/h$ in ordinary units). Remarks:

- I_R is obtained by exchanging $L \leftrightarrow R$, whence $I_L = -I_R$: the current is conserved.
- The integrand is the product of the occupation difference $f_L - f_R$, the joint density of states $\propto \Gamma_L \Gamma_R \propto \rho_L \rho_R$, and the transmission probability $\propto |G_{00}^r|^2$. At low temperature only the *transport window* $\mu_R < \omega < \mu_L$ contributes (Fig. 18).

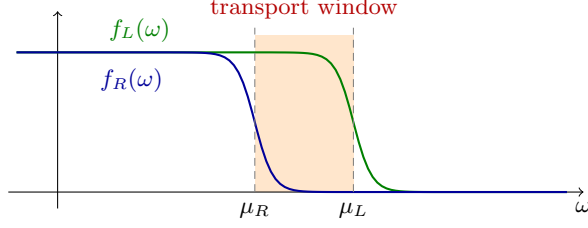


Figure 18: Only frequencies in the transport window between μ_R and μ_L (where $f_L \neq f_R$) contribute to the current.

11 Electron–electron interaction: Anderson model and Hubbard-I

11.1 Single-impurity Anderson model

We now include the electron–electron interaction in the central region (quantum dot). The prototypical model is the *single-impurity Anderson model* [?] (for its nonequilibrium transport see Meir–Wingreen–Lee [?]): a spinful level with on-site repulsion U , coupled to noninteracting leads,

$$H_0 = \sum_{p,\sigma} \varepsilon_p c_{p\sigma}^\dagger c_{p\sigma} + \varepsilon_d \sum_{\sigma} d_{\sigma}^\dagger d_{\sigma}, \quad V = \sum_{p,\sigma} V_p (c_{p\sigma}^\dagger d_{\sigma} + d_{\sigma}^\dagger c_{p\sigma}), \quad H_U = U n_{d\uparrow} n_{d\downarrow}, \quad (107)$$

with $\varepsilon_d = \Delta - U/2$ (so that Δ is the particle–hole–symmetric reference). This model produces, among other things, *Coulomb blockade* and the *Kondo effect*; here we treat it in the simplest nontrivial approximation, following the “Hubbard-I” [?] or “cluster perturbation theory” logic (see also Haug–Jauho [?]).

11.2 Diagram structure and the Hubbard-I approximation

Two structural facts organize the diagrams: (i) the interaction U attaches to d -lines only; (ii) the hybridization V_p only connects c - with d -lines. It is therefore convenient to distinguish d - and c -type propagators, and to define the d – d self-energy $\tilde{\Sigma}$ as the sum of all diagrams that cannot be cut in two by breaking a d -line; then

$$\underline{G}_{dd} = \underline{g}_{dd} + \underline{g}_{dd} \tilde{\Sigma} \underline{G}_{dd}. \quad (108)$$

Two exactly summable subsets of $\tilde{\Sigma}$ are (Fig. 19):

- the diagrams with no U : exactly the embedding self-energy of Sec. 9, $\tilde{\Sigma}(U=0) = \sum_p V_{0p} \underline{g}_{pp} V_{p0}$;
- the diagrams with no V : the self-energy of the isolated (“atomic”) interacting level — exactly solvable, since the atomic problem is.

The *Hubbard-I approximation* consists in keeping just these two classes,

$$\boxed{\tilde{\Sigma} \approx \tilde{\Sigma}(V=0) + \tilde{\Sigma}(U=0)}; \quad (109)$$

the first neglected diagram contains both U and V . Taking a larger central cluster instead of a single site turns this into *cluster perturbation theory* (cf. Balzer–Potthoff [?]).

$$\tilde{\Sigma} \approx \text{Diagram: } \text{X} \text{---} \text{wavy line} \text{---} \text{X} + \text{Diagram: } \text{red circle with } U \text{ inside}$$

$$\tilde{\Sigma}(U=0) = V_{0p} g_{pp} V_{p0}$$

$$\tilde{\Sigma}(V=0): \text{ all pure-}U \text{ diagrams (atomic limit, exact)}$$

Figure 19: Hubbard-I approximation for the d - d self-energy.

11.3 The atomic problem: equations of motion

We need the Green's function of the isolated level, $H_{\text{at}} = \varepsilon_d \sum_{\sigma} n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}$. One could use exact diagonalization and the Lehmann representation; here we use the *equations of motion*. For $g^r(t) = -i\theta(t)\langle\{d_{\uparrow}(t), d_{\uparrow}^{\dagger}(0)\}\rangle$:

$$i\partial_t g^r(t) = \delta(t) + \varepsilon_d g^r(t) + U g^{(2)}(t), \quad g^{(2)}(t) = -i\theta(t)\langle\{n_{d\downarrow} d_{\uparrow}(t), d_{\uparrow}^{\dagger}\}\rangle, \quad (110)$$

using $\partial_t d_{\uparrow} = i[H_{\text{at}}, d_{\uparrow}] = -i(\varepsilon_d + U n_{d\downarrow}) d_{\uparrow}$.

Exercise 11.1. Verify this commutator.

In general (110) starts an infinite hierarchy; here it *closes*, because $[H_{\text{at}}, n_{d\downarrow}] = 0$ (so $n_{d\downarrow}$ is time independent) and $n_{d\downarrow}^2 = n_{d\downarrow}$:

$$i\partial_t g^{(2)}(t) = \delta(t)\langle n_{d\downarrow} \rangle + (\varepsilon_d + U) g^{(2)}(t) \implies g^{(2)}(\omega) = \frac{\langle n_{d\downarrow} \rangle}{\omega - \varepsilon_d - U}, \quad (111)$$

(all $\omega \rightarrow \omega + i0^+$), and hence

$$\boxed{g_{\text{at}}^r(\omega) = \frac{\langle n_{d\downarrow} \rangle}{\omega - \Delta - \frac{U}{2}} + \frac{1 - \langle n_{d\downarrow} \rangle}{\omega - \Delta + \frac{U}{2}} :} \quad (112)$$

two poles (the *Hubbard levels*) at $\omega = \Delta \pm U/2$, with weights $\langle n_{d\downarrow} \rangle$ and $1 - \langle n_{d\downarrow} \rangle$. The advanced function has $\omega \rightarrow \omega - i0^+$, and $g_{\text{at}}^K = (g_{\text{at}}^r - g_{\text{at}}^a) s(\omega)$. As in the noninteracting case, $(g_{\text{at}}^{-1})^K = (g_{\text{at}}^{r-1} - g_{\text{at}}^{a-1}) s(\omega)$ is nonzero only at the poles of g_{at}^r and hence infinitesimal: it can be neglected once the level is coupled to the leads.

11.4 Coupling to the leads

The atomic self-energy is extracted from $\underline{g}_{dd}^{-1} - \tilde{\Sigma}(V=0) = \underline{g}_{\text{at}}^{-1}$, so that within Hubbard-I

$$\underline{G}_{dd} = \left(\underline{g}_{dd}^{-1} - \tilde{\Sigma}(V=0) - \tilde{\Sigma}(U=0) \right)^{-1} = \left(\underline{g}_{\text{at}}^{-1} - \sum_p V_{0p} g_{pp} V_{p0} \right)^{-1}. \quad (113)$$

The retarded part reads, with R, Γ as before,

$$G_{dd}^r(\omega) = \left(g_{\text{at}}^r(\omega)^{-1} - R(\omega) + i\Gamma(\omega) \right)^{-1}. \quad (114)$$

For $R, \Gamma \ll U$ the structure is dominated by the two atomic poles. Expanding near $\omega \approx \Delta + U/2$,

$$G_{dd}^r(\omega) \approx \frac{\langle n_{\downarrow} \rangle}{\omega - \Delta - \frac{U}{2} - R\langle n_{\downarrow} \rangle + i\Gamma\langle n_{\downarrow} \rangle}, \quad (115)$$

and similarly near $\Delta - U/2$ with weight $1 - \langle n_{\downarrow} \rangle$: each Hubbard level is *shifted* by R times its weight and *broadened* by Γ times its weight. The spectral function $A_{dd} = -\frac{1}{\pi} \text{Im } G_{dd}^r$ shows two peaks of widths $\Gamma_1 = \Gamma(1 - \langle n_{\downarrow} \rangle)$ and $\Gamma_2 = \Gamma\langle n_{\downarrow} \rangle$ (Fig. 20).

11.5 Current and Coulomb blockade

The calculation of the Keldysh component and of the current proceeds exactly as in Sec. 10: since the dot contribution to Σ^K is infinitesimal, only the leads contribute,

$$G_{dd}^K = |G_{dd}^r|^2 \sum_{\alpha} (-2i \Gamma_{\alpha} s_{\alpha}) = (G_{dd}^r - G_{dd}^a) s_{av}(\omega), \quad (116)$$

with the same s_{av} as in (100) (this also determines $\langle n_{\downarrow} \rangle$ self-consistently), and the current is again of Landauer form: at $T = 0$ and $\mu_R < \mu_L$,

$$I = 2\pi e V^2 \int_{\mu_R}^{\mu_L} d\omega A_{dd}(\omega) \frac{\rho_L^0(\omega) \rho_R^0(\omega)}{\rho_L^0(\omega) + \rho_R^0(\omega)}. \quad (117)$$

All effects of the interaction enter through G_{dd}^r , i.e. through the spectral function A_{dd} . In the tunneling regime (V , hence Γ , small) the peaks of A_{dd} are narrow: the current is strongly suppressed *except* when one of the resonances $\Delta \mp U/2$ lies inside the transport window $[\mu_R, \mu_L]$. This is the *Coulomb blockade* effect: sweeping the level position ε_d (the gate voltage), the conductance shows a pair of peaks separated by U (Fig. 20).

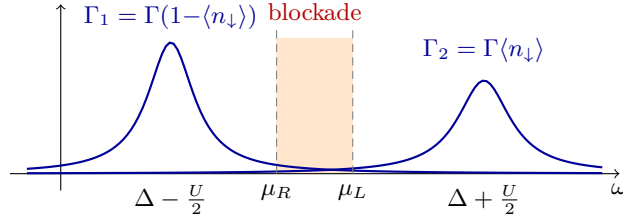


Figure 20: Hubbard-I spectral function of the Anderson model: two peaks of weight $1 - \langle n_{\downarrow} \rangle$ and $\langle n_{\downarrow} \rangle$, widths Γ_1, Γ_2 . If no peak lies in the transport window, the current is blocked (Coulomb blockade).

Exercise 11.2. Fill in the steps leading to G_{dd}^K above.

12 Time dependence: relaxation after a quantum quench

So far we have computed steady-state properties. The same machinery gives access to the full *transient* dynamics after a quantum quench (the general time-dependent transport formalism is due to Jauho–Wingreen–Meir [?]). We reproduce here in detail the accompanying note “Time-dependence for a quantum quench” (file 09); see also Stefanucci–Almbladh [?] and Cini [?] for alternative derivations.

12.1 Dyson equation and time-domain calculus

We consider a central region of N levels described by a quadratic Hamiltonian

$$H = c^\dagger \varepsilon c, \quad c = (c_1, \dots, c_N)^T, \quad (118)$$

with ε an $N \times N$ matrix, suddenly coupled at $t = 0$ to noninteracting baths (“quantum quench”), $V(t) = V \theta(t)$. The (exact) Dyson equation, in both its left and right forms, reads

$$G = g + g \circ \tilde{\Sigma} \circ G = g + G \circ \tilde{\Sigma} \circ g, \quad g^{-1} \circ G = I + \tilde{\Sigma} \circ G, \quad G \circ g^{-1} = I + G \circ \tilde{\Sigma}, \quad (119)$$

where $\tilde{\Sigma}$ is the embedding (hybridization) self-energy generated by the baths. (There are no two-body interactions here; the only self-energy is the embedding one, exact by Sec. 9.) Its retarded component is

$$G_r = g_r + g_r \circ \tilde{\Sigma}_r \circ G_r, \quad \text{equivalently} \quad g_r^{-1} \circ G_r = I + \tilde{\Sigma}_r \circ G_r. \quad (120)$$

Since the quench breaks time-translation invariance, we work directly in the time domain, where two-time functions compose by convolution and the identity/inverse are defined accordingly:

$$A = B \circ C \Leftrightarrow A(t_1, t_2) = \int dt B(t_1, t) C(t, t_2), \quad I(t_1, t_2) = \delta(t_1 - t_2), \quad A = B^{-1} \Leftrightarrow A \circ B = I. \quad (121)$$

12.2 Unperturbed retarded Green's function

We start from the unperturbed ($\tilde{\Sigma} = 0$) retarded Green's function

$$g_r(t_1, t_2) = -i \theta(t_1 - t_2) \langle \{c(t_1), c^\dagger(t_2)\} \rangle. \quad (122)$$

Keeping for the moment a possibly time-dependent $\varepsilon(t)$, and using $\dot{c}(t_1) = i[H(t_1), c(t_1)]$ with $[H, c] = -\varepsilon c$, its equation of motion is

$$\begin{aligned} \partial_{t_1} g_r(t_1, t_2) &= -i \delta(t_1 - t_2) \underbrace{\langle \{c(t_1), c^\dagger(t_1)\} \rangle}_{=1} + \theta(t_1 - t_2) \langle \{[H(t_1), c(t_1)], c^\dagger(t_2)\} \rangle \\ &= -i \delta(t_1 - t_2) - \varepsilon(t_1) \theta(t_1 - t_2) \langle \{c(t_1), c^\dagger(t_2)\} \rangle = -i \delta(t_1 - t_2) - i \varepsilon(t_1) g_r(t_1, t_2), \end{aligned} \quad (123)$$

i.e.

$$\boxed{(i\partial_{t_1} - \varepsilon(t_1)) g_r(t_1, t_2) = \delta(t_1 - t_2)} \quad \Longleftrightarrow \quad g_r^{-1}(t_1, t_2) = (i\partial_{t_1} - \varepsilon(t_1)) \delta(t_1 - t_2). \quad (124)$$

The last equality identifies the inverse of g_r in the sense of (121). With the initial condition $g_r(t_1^+, t_1) = -i$ (from the equal-time anticommutator), the solution of (124) is

$$g_r(t_1, t_2) = -i \theta(t_1 - t_2) T \exp\left(-i \int_{t_2}^{t_1} \varepsilon(t) dt\right), \quad (125)$$

where T is the time-ordering, needed because the matrix $\varepsilon(t)$ need not commute with itself at different times. *From here on we take ε time-independent*, so that $g_r(t_1, t_2) = -i \theta(t_1 - t_2) e^{-i\varepsilon(t_1 - t_2)}$.

12.3 Retarded Green's function after the quench

The bath self-energy is switched on together with $V(t) = V\theta(t)$:

$$\tilde{\Sigma}(t_1, t_2) = V(t_1) g_{\text{bath}}(t_1 - t_2) V^\dagger(t_2) = \theta(t_1) \theta(t_2) V g_{\text{bath}}(t_1 - t_2) V^\dagger \equiv \theta(t_1) \theta(t_2) \tilde{\tilde{\Sigma}}(t_1 - t_2), \quad (126)$$

which is time-translation invariant *once both times are positive*. Writing (120) explicitly,

$$G_r(t_1, t_2) = g_r(t_1 - t_2) + \int dt_3 dt_4 g_r(t_1 - t_3) \theta(t_3) \theta(t_4) \tilde{\tilde{\Sigma}}_r(t_3 - t_4) G_r(t_4, t_2), \quad (127)$$

we distinguish three cases.

Both times positive ($t_2 \geq 0$). Since every factor is retarded, the times are ordered $t_1 > t_3 > t_4 > t_2 \geq 0$, so the θ 's in (127) are redundant and all quantities are time-translation invariant. A Fourier (Laplace) transform turns the convolution into a product; with $z = \omega + i0^+$,

$$\boxed{\bar{G}_r(z) = (g_r(z)^{-1} - \bar{\tilde{\Sigma}}_r(z))^{-1} = (z - \varepsilon - \bar{\tilde{\Sigma}}_r(z))^{-1}}. \quad (128)$$

We denote by $\bar{\tilde{\Sigma}}_r, \bar{G}_r$ the time-translation-invariant functions valid for both times positive,

$$\bar{G}_r(t_1, t_2) = \bar{G}_r(t_1 - t_2) = G_r(t_1, t_2) \quad (t_1, t_2 \geq 0), \quad (129)$$

and reserve the argument z for their Fourier (Laplace) transform.

Both times negative ($0 \geq t_1 \geq t_2$). The bath is not yet coupled, so $G_r = g_r$.

Mixed times ($t_1 > 0 \geq t_2$). We use (120) with (124); since $\delta(t_1 - t_2) = 0$ here,

$$(i\partial_{t_1} - \varepsilon) G_r(t_1, t_2) = \int dt_3 \bar{\tilde{\Sigma}}_r(t_1 - t_3) \theta(t_3) G_r(t_3, t_2). \quad (130)$$

For fixed t_2 this has the form (191) of Appendix A with $f(t_1) \equiv G_r(t_1, t_2)$ and $h = 0$; its solution (196) translates to

$$\boxed{G_r(t_1, t_2) = i G_r(t_1, 0) G_r(0, t_2) = i G_r(t_1, 0) g_r(0, t_2) \quad (t_1 \geq 0, t_2 \leq 0)}, \quad (131)$$

using $G_r(0, t_2) = g_r(0, t_2)$ for $t_2 \leq 0$. The same argument generalizes to any ordered triple, giving the *composition (semigroup) rule*

$$\boxed{G_r(t_1, t_3) = i G_r(t_1, t_2) G_r(t_2, t_3), \quad t_1 \geq t_2 \geq t_3}. \quad (132)$$

(The prefactor i compensates the two $-i$ normalizations of the retarded functions; one checks it on the bare g_r .) The advanced function follows from

$$G_a(t_1, t_2) = G_r(t_2, t_1)^\dagger. \quad (133)$$

Exercise 12.1 (9.1). Calculate the time-dependent G_r for a bath with a Lorentzian density of states.

12.4 Keldysh Green's function

Neglecting as usual g_k^{-1} , the Keldysh components of the left and right Dyson equations (119) are

$$g_r^{-1} \circ G_k = \tilde{\Sigma}_r \circ G_k + \tilde{\Sigma}_k \circ G_a \Rightarrow G_r^{-1} \circ G_k = \tilde{\Sigma}_k \circ G_a, \quad G_k \circ g_a^{-1} = G_k \circ \tilde{\Sigma}_a + G_r \circ \tilde{\Sigma}_k \Rightarrow G_k \circ G_a^{-1} = G_r \circ \tilde{\Sigma}_k. \quad (134)$$

Propagating the first time. The first equation of (134) at $t_1 > 0, t_2 = 0$ reads

$$\left((g_r^{-1} - \tilde{\Sigma}_r) \circ G_k \right) (t_1, 0) = \int dt_3 \tilde{\Sigma}_k(t_1, t_3) G_a(t_3, 0). \quad (135)$$

The right-hand side vanishes: the advanced $G_a(t_3, 0)$ forces $t_3 < 0$, but there $\tilde{\Sigma}_k = 0$ by (126). Hence $G_k(t_1, 0)$ obeys the homogeneous equation

$$(i\partial_{t_1} - \varepsilon) G_k(t_1, 0) - \int_0^\infty dt_3 \bar{\tilde{\Sigma}}_r(t_1 - t_3) G_k(t_3, 0) = 0, \quad (136)$$

of the form (191) with $f(t_1) = G_k(t_1, 0)$ and $h = 0$. Its solution (196) is

$$G_k(t, 0) = i G_r(t, 0) g_k(0, 0) = G_r(t, 0) (1 - 2n_0), \quad (137)$$

where we used $G_k(0, 0) = g_k(0, 0)$ (since $V = 0$ for negative times) and the equilibrium equal-time value $g_k(0, 0) = -i(1 - 2n_0)$, with n_0 the initial occupation (matrix) of the central region.

Propagating the second time. For arbitrary $t_1, t_2 > 0$ we propagate the second argument using the second equation of (134). It is convenient to take its Hermitian conjugate (which also exchanges the time arguments) and use $G_a^\dagger = G_r$, giving $G_r^{-1} \circ G_k^\dagger = \tilde{\Sigma}_k^\dagger \circ G_a$, i.e.

$$(i\partial_{t_1} - \varepsilon) G_k^\dagger(t_1, t_2) - \int_0^\infty dt_3 \tilde{\Sigma}_r(t_1 - t_3) G_k^\dagger(t_3, t_2) = \underbrace{\int_0^{t_2} dt_3 \tilde{\Sigma}_k^\dagger(t_1, t_3) G_a(t_3, t_2)}_{h(t_1, t_2)}. \quad (138)$$

For $t_1 > t_2 > 0$ the right-hand side no longer vanishes; since $\tilde{\Sigma}_k$ and G_a are already known, $h(t_1, t_2)$ is an explicit inhomogeneity. Equation (138) again has the form (191), with solution (196)

$$G_k^\dagger(t_1, t_2) = i G_r(t_1, 0) G_k^\dagger(0, t_2) + \int_0^\infty dt_3 G_r(t_1 - t_3) h(t_3, t_2) \quad (t_1, t_2 > 0). \quad (139)$$

Taking the Hermitian conjugate, exchanging $t_1 \leftrightarrow t_2$, inserting the explicit h from (138), and using $G_a(t_1, t_2) = G_r(t_2, t_1)^\dagger$ together with (137) yields the symmetric result

$$G_k(t_1, t_2) = -i G_r(t_1, 0) (1 - 2n_0) G_r(t_2, 0)^\dagger + \int_0^{t_2} dt_3 \int_0^{t_1} dt_4 G_r(t_1 - t_4) \tilde{\Sigma}_k(t_4 - t_3) G_r(t_2 - t_3)^\dagger, \quad (140)$$

valid for $t_1, t_2 > 0$: a first term propagating the memory of the initial state, and a double integral fed by the baths.

12.5 Wide-band limit

For several baths α in the wide-band limit the retarded contribution is frequency independent, $\tilde{\Sigma}_{r\alpha}(\omega) = -i\Gamma_\alpha$, so that

$$\tilde{\Sigma}_r(z) = -i\Gamma, \quad \Gamma = \sum_\alpha \Gamma_\alpha. \quad (141)$$

The Fourier transform of (128) then gives a simple exponential decay,

$$\bar{G}_r(t) = -i\theta(t) e^{-i\varepsilon t - \Gamma t}, \quad (142)$$

and, e.g. for $t_1 > 0, t_2 < 0$, (131) gives $G_r(t_1, t_2) = -i e^{-i\varepsilon(t_1 - t_2) - \Gamma t_1}$.⁶

Exercise 12.2 (9.2). Verify (142) by Fourier-transforming $\bar{G}_r(z) = (z - \varepsilon + i\Gamma)^{-1}$.

The Keldysh components are less trivial: $\tilde{\Sigma}_{k\alpha}(\omega) = -2i\Gamma_\alpha s_\alpha(\omega)$. Taking baths at $T = 0$ with chemical potentials μ_α , so that $s_\alpha(\omega) = \text{sign}(\omega - \mu_\alpha)$, the Fourier transform gives

$$\tilde{\Sigma}_{k\alpha}(t_1 - t_2) = -\frac{2\Gamma_\alpha}{\pi} \frac{e^{-i\mu_\alpha(t_1 - t_2)}}{t_1 - t_2}, \quad (143)$$

and the total $\tilde{\Sigma}_k$ is the sum over baths.

⁶The source note writes $\bar{G}_r(t) = e^{-i\varepsilon t - \Gamma t}$, dropping the $-i\theta(t)$; we keep it, as it is required for consistency with the composition rule (132), cf. Appendix B.

Exercise 12.3 (9.3). Verify (143) (use the Fourier transform of the sign function, $\int d\omega e^{-i\omega t} \text{sign } \omega = -2i\mathcal{P}(1/t)$).

Of particular interest is the time-dependent occupation $n(t)$ of the central region, given by the equal-time Keldysh function, $-i(1 - 2n(t)) = G_k(t, t)$. Setting $t_1 = t_2 = t$ in (140) and inserting (142),

$$G_k(t, t) = -ie^{-2\Gamma t} (1 - 2n_0) + e^{-2\Gamma t} \int_0^t dt_3 \int_0^t dt_4 e^{\Gamma(t_3+t_4)} e^{i\varepsilon(t_4-t_3)} \sum_{\alpha} \tilde{\tilde{\Sigma}}_{k\alpha}(t_4 - t_3). \quad (144)$$

The first term is the contribution of the initial occupation, which decays with rate 2Γ ; the second drives the central region toward the steady-state occupation set by the baths. This closes the circle with Secs. 8–9: it is precisely the finite dissipation Γ that erases the memory of the initial state and renders the steady state — and with it the whole steady-state formalism — meaningful.⁷

13 Interaction vertices: electron–phonon and the contact electron–electron vertex

So far the only vertex we have studied in detail is the single-particle potential u of Sec. 7, with one incoming and one outgoing fermion line. We now turn to genuine *interaction* vertices with more legs: the electron–phonon vertex, and an effective, instantaneous electron–electron vertex built from it. This material follows Rammer and Smith [?]; the general classification of vertices in the classical/quantum (Larkin–Ovchinnikov) basis is discussed systematically by Kamenev [?] (Sec. 1). These vertices are the building blocks for diagrammatic corrections beyond the mean-field (Hartree–Fock/Hubbard-I) treatment of Sec. 11, and in particular for the collision integral of the quantum Boltzmann equation derived in Sec. 14.

13.1 The electron–phonon vertex on the contour

Consider the electron–phonon coupling

$$W_{ep} = \int d\vec{x}_1 d\vec{x}_2 d\vec{x}_3 c^\dagger(\vec{x}_1) c(\vec{x}_2) \rho(\vec{x}_3) g(\vec{x}_1, \vec{x}_2, \vec{x}_3), \quad (145)$$

where $\rho(\vec{x}_3)$ stands for either the phonon annihilation or the phonon creation operator, $\rho \in \{b, b^\dagger\}$ – i.e. (145) really represents two vertices (*absorption* and *emission*), treated separately below. Inserted into the contour S -matrix, $S_{ep} = \int_C d\gamma \hat{W}_{ep}(\gamma)$ with $\hat{W}_{ep}(\gamma)$ the interaction-picture form of (145) evaluated at the single contour time γ . Exactly as for the single-particle potential (Sec. 7), we give each of the three operators its own independent contour argument and enforce their equality by inserting $\prod_{i=1}^3 \delta(\gamma - \gamma_i) d\gamma_i$:

$$S_{ep} = \int dx_1 dx_2 dx_3 c^\dagger(x_1) c(x_2) \rho(x_3) g(x_1, x_2, x_3), \quad g(x_1, x_2, x_3) \equiv \delta(\gamma_1 - \gamma_3) \delta(\gamma_2 - \gamma_3) g(\vec{x}_1, \vec{x}_2, \vec{x}_3), \quad (146)$$

where $x_i = (\gamma_i, \vec{x}_i)$ as usual. Diagrammatically this is a 3-point *contact* vertex, Fig. 21 (left): nonzero only when all three contour times coincide, exactly as the cross was nonzero only for $\gamma_A = \gamma_B$.

⁷Reinstating the $-i\theta$ normalization (142), a careful evaluation of the double integral gives the phase $e^{+i\varepsilon(t_4-t_3)}$ shown here; the source note carries $e^{-i\varepsilon(t_4-t_3)}$, cf. Appendix B.

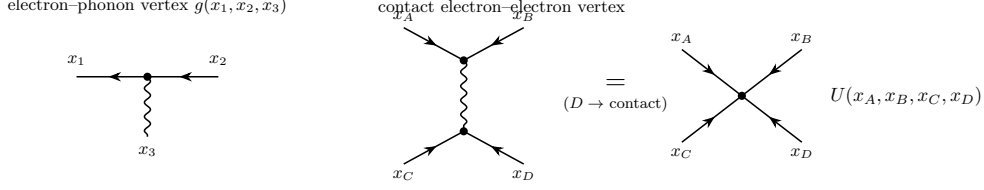


Figure 21: Left: the electron–phonon vertex, Eq. (146). Right: the contact electron–electron vertex obtained by gluing two electron–phonon vertices with a contact phonon propagator, Eq. (155).

13.2 Branch (hat) representation

Consider a diagram built with one g vertex, e.g.

$$\int G(x_A, x_1) G(x_2, x_B) D(x_3, x_C) g(x_1, x_2, x_3) dx_1 dx_2 dx_3. \quad (147)$$

Writing everything in the branch (hat) representation of Sec. 5, with $\tilde{x}_i = (t_i, \vec{x}_i)$ the contour-time argument stripped of its branch label and $\eta_i \in \{1, 2\}$ the branch label itself, the contour integrals split as $\int_C d\gamma = \sum_\eta \eta \int dt$ (Eq. (42), with the shorthand $\eta \equiv (\tau_3)_{\eta\eta} = \pm 1$ used both for the branch label and for its sign). Equation (147) becomes

$$\int \hat{G}(\tilde{x}_A, t\tilde{x}_1)_{\eta_A \eta_1} \hat{G}(t\tilde{x}_2, \tilde{x}_B)_{\eta_2 \eta_B} \hat{D}(t\tilde{x}_3, \tilde{x}_C)_{\eta_3 \eta_C} dt \hat{v}_{\eta_1 \eta_2}^{\eta_3}(\tilde{x}_1, \tilde{x}_2, \tilde{x}_3), \quad (148)$$

where the branch-index structure of the vertex, read off from (146), is

$$\boxed{\hat{v}_{\eta_1 \eta_2}^{\eta_3} = \eta_1 \delta_{\eta_1 \eta_2} \delta_{\eta_2 \eta_3}.} \quad (149)$$

All three branch indices are forced equal, $\eta_1 = \eta_2 = \eta_3 \equiv \eta$, and the vertex carries an extra sign $\eta = (\tau_3)_{\eta\eta}$ – the same mechanism that produced the τ_3 in the contour delta function (72): a vertex, like a delta function, is local on the contour, so all of its legs necessarily sit on the same branch, and the branch sum $\int_C = \sum_\eta \eta \int dt$ contributes precisely one such sign per vertex.

13.3 RAK representation: a selection rule

We now transform (149) to the RAK representation, i.e. we ask which combinations of RAK legs ($A, B, C \in \{1, 2\}$, with 1 the retarded/advanced-type index and 2 the Keldysh-type index of Sec. 5) give a nonzero vertex. From $\underline{G} = L\tau_3\hat{G}L^\dagger$ one has $\hat{G} = \tau_3 L^\dagger \underline{G} L$ (Sec. 5), i.e. the row index of $\hat{G}$ is dressed by $\tau_3 L^\dagger$ and the column index by L . Attaching this to each of the three legs of (149) (leg 1 is a column index, legs 2,3 are row indices) and summing over the single shared branch label η gives the RAK-space vertex

$$\tilde{v}_{ABC} = \sum_{\eta=1,2} \eta L_{A\eta} (L^\dagger)_{\eta B} (L^\dagger)_{\eta C} g, \quad (150)$$

where A is the RAK index paired with leg 1 and B, C those paired with legs 2,3. This is a finite sum, computable explicitly from

$$L = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad L^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}. \quad (151)$$

Exercise 13.1. Evaluate the sum (150) explicitly for all eight combinations $A, B, C \in \{1, 2\}$ and show that

$$\tilde{v}_{ABC} = \frac{g}{\sqrt{2}} \times \begin{cases} 1, & \text{an odd number of } A, B, C \text{ equal } 1, \\ 0, & \text{an even number of } A, B, C \text{ equal } 1. \end{cases} \quad (152)$$

(Hint: write $L_{A\eta} = s \sigma_L(A, \eta)$ and $(L^\dagger)_{\eta B} = s \sigma_R(\eta, B)$ with $s = 1/\sqrt{2}$ and $\sigma = \pm 1$ signs read off from $L, L^\dagger$; check that for $\eta = 1$ all six signs are $+1$, while for $\eta = 2$ each sign is -1 exactly when the corresponding index equals 1; the $\eta = 2$ term is then $-s^3(-1)^{n_1}$ with n_1 the number of indices among A, B, C equal to 1, and the $\eta = 1$ term is always $+s^3$.)

Equation (152) is a *selection rule*: not every combination of retarded/advanced-type (1) and Keldysh-type (2) legs is allowed at the vertex. This is the same structural phenomenon as the well-known theorem that, in the classical/quantum basis, an interaction vertex must carry an odd number of “quantum” legs (see Kamenev [?] for the general statement and proof via the normalization $\langle T_C S \rangle_0 = 1$); the precise index that plays the role of “quantum” differs between our (uniform, upper-triangular) RAK convention and the mixed convention commonly used for bosonic fields, but the underlying causality structure – and the vanishing of the all-retarded/advanced vertex combinations forbidden by (152) – is the same.

13.4 Contact electron–electron vertex from phonon exchange

As an application, and to make contact with the electron–electron interaction used in Sec. 11, we construct an effective electron–electron vertex by gluing two electron–phonon vertices with a phonon propagator, then taking the phonon propagator to be *instantaneous* (frequency independent), $\underline{D} = D_0 \mathbb{1}$ – i.e. $D^r = D^a = D_0$, $D^K = 0$, exactly the same RAK structure as the single-particle potential, Eq. (74). (Such a D is of course not a physical equilibrium phonon propagator – it violates the fluctuation–dissipation relation, Eq. (66) – but it is a legitimate and standard model for a contact, Hubbard-type, instantaneous electron–electron repulsion, obtained by integrating out an auxiliary bosonic field with $D_0 = U$ or $D_0 = -U$, cf. Sec. 11.)

Gluing two vertices (152) through the (diagonal) phonon line, the contact electron–electron vertex is

$$U_{B_1 A_2; B'_1 A'_2} = D_0 \sum_{C=1,2} \tilde{v}_{B_1 A_2 C} \tilde{v}_{B'_1 A'_2 C}, \quad (153)$$

with B_1, A_2 (resp. B'_1, A'_2) the RAK indices of the two fermion legs at the first (resp. second) vertex. Using (152),

$$\tilde{v}_{B_1 A_2, 1} = \frac{g}{\sqrt{2}} \delta_{B_1 A_2}, \quad \tilde{v}_{B_1 A_2, 2} = \frac{g}{\sqrt{2}} (1 - \delta_{B_1 A_2}), \quad (154)$$

(for $C = 1$: $B_1, A_2, 1$ has an odd number of 1’s iff $B_1 = A_2$; for $C = 2$: iff $B_1 \neq A_2$), so the two terms of (153) are mutually exclusive and

$$U_{B_1 A_2; B'_1 A'_2} = \frac{D_0 g^2}{2} \left[\delta_{B_1 A_2} \delta_{B'_1 A'_2} + (1 - \delta_{B_1 A_2})(1 - \delta_{B'_1 A'_2}) \right]. \quad (155)$$

The vertex is nonzero only when the two fermion pairs are of the *same type*: either both “diagonal” ($B_1 = A_2$ and $B'_1 = A'_2$, both retarded/advanced-type) or both “off-diagonal” ($B_1 \neq A_2$ and $B'_1 \neq A'_2$, both mixed retarded–Keldysh type) – itself a special case of the general selection rule (152) applied to the four-point object, consistent with what one would find starting directly from the electron–electron interaction (24) of Sec. 2 and repeating the present construction with u -type crosses on each leg instead of g -vertices.

Exercise 13.2. Check directly, by summing over the phonon leg C in (153) using (154), that the cross terms $\tilde{v}_{B_1 A_2, 1} \tilde{v}_{B'_1 A'_2, 2}$ never contribute, and that (155) follows.

13.5 Outlook

The vertex (155) (and, more generally, the genuine momentum- and frequency-dependent electron–electron and electron–phonon vertices of (24) and (145)) is what is needed to go beyond the mean-field (Hartree–Fock, Hubbard-I) approximation of Sec. 11: dressing the self-energy with one or more of these vertices at second order and beyond generates the leading corrections to the mean-field self-energy, and – after a gradient expansion of the resulting Dyson equation – the *collision integral* of the quantum Boltzmann equation, to which we turn next (Sec. 14).

14 Derivation of the quantum Boltzmann equation

The Boltzmann equation is the standard semiclassical tool to describe transport in weakly nonequilibrium systems. We now derive it, together with an explicit microscopic expression for its collision term, from the nonequilibrium Green’s-function formalism developed so far – following Haug and Jauho [?] (with minor differences of notation), see also Rammer and Smith [?] and, for the impurity-averaging technique, Bruus and Flensberg [?].

14.1 The classical Boltzmann equation

Let $f(\vec{R}, \vec{p}, t)$ be the single-particle distribution function, so that $f d^3 R d^3 p$ is the number of particles in the corresponding phase-space volume element at time t (band indices and crystal momentum can be added straightforwardly). In equilibrium, for a homogeneous system, $f = f_F(\varepsilon_{\vec{p}})$, the Fermi function. For a quantum system $\Delta R, \Delta P$ cannot be taken infinitesimal but must be coarse-grained, $\Delta R \Delta P \gg \hbar$ – this restriction will reappear, made precise, in Sec. 14.7 below.

Consider the action of an external potential $U(\vec{R}, t)$.⁸ The semiclassical equations of motion are

$$\dot{\vec{p}} = \vec{F} = -\vec{\nabla}_R U(\vec{R}, t), \quad \dot{\vec{R}} = \vec{v} = \vec{\nabla}_p \varepsilon(\vec{p}). \quad (156)$$

In the absence of scattering between particles, f is simply transported along classical trajectories,

$$f(\vec{R}, \vec{p}, t) = f(\vec{R} - \vec{v} \Delta t, \vec{p} - \vec{F} \Delta t, t - \Delta t), \quad (157)$$

which, to linear order in Δt , gives $\Delta t (\vec{v} \cdot \vec{\nabla}_R f + \vec{F} \cdot \vec{\nabla}_p f + \partial_t f) = 0$. If, in addition, scattering modifies f by $(\Delta f)_S = (\partial f / \partial t)_S \Delta t$, one obtains the *Boltzmann equation*

$$\boxed{\vec{v} \cdot \vec{\nabla}_R f + \vec{F} \cdot \vec{\nabla}_p f + \frac{\partial f}{\partial t} = \left(\frac{\partial f}{\partial t} \right)_S}. \quad (158)$$

The left-hand side (the *streaming* or *transport* term) is purely kinematic; the right-hand side (the *collision* or *scattering* term) encodes the microscopic dynamics. We now derive (158) – including a first-principles expression for the collision term – from the Dyson equation of Sec. 13 and earlier.

⁸This plays exactly the role of the single-particle potential $u(\vec{r}_A, \vec{r}_B, t)$ of Sec. 7, here restricted to a local (diagonal, multiplicative) potential, $U(\vec{R}, t) \equiv u(\vec{R}, \vec{R}, t)$; it is unrelated to the four-point contact vertex $U_{B_1 A_2; B'_1 A'_2}$ of Sec. 13, which carries a different tensor structure.

14.2 From Dyson's equation to the generalized Kadanoff–Baym equation

Since the system is, in general, neither time- nor space-translation invariant, all objects below are matrices (integral kernels) in real time and space; products denote convolutions, $C(x_1, x_2) = \int dx_3 A(x_1, x_3) B(x_3, x_2)$, with $x_i = (t_i, \vec{r}_i)$. Write Dyson's equation (34), splitting the self-energy into the contribution of the external potential U (a one-body term, as in Sec. 7) and the remainder Σ ,

$$G = G_0 + G_0 (\Sigma + U) G \quad \implies \quad (G_0^{-1} - U) G = \mathbb{1} + \Sigma G, \quad (159)$$

all as 2×2 matrices in Keldysh (RAK) space, Sec. 5. The retarded $(1, 1)$ component of (159) gives (using triangularity, cf. (50))

$$(G_0^{r-1} - U - \Sigma^r) G^r = \mathbb{1}, \quad (160)$$

and the Keldysh component, using $G_0^{K-1} = 0$ (the noninteracting Keldysh component has no inverse, cf. Sec. 6),

$$(G_0^{r-1} - U) G^K + (G_0^{-1} - U)^K G^a = \Sigma^r G^K + \Sigma^K G^a. \quad (161)$$

Similarly, the “right” Dyson equation $G = G_0 + G (\Sigma + U) G_0$ gives the Keldysh component

$$G^K (G_0^{a-1} - U) = G^r \Sigma^K + G^K \Sigma^a. \quad (162)$$

Subtracting (162) from (161) eliminates the (singular, and mutually equal once coupled to a dissipative continuum – cf. the discussion after Eq. (34) and in Sec. 9) bare inverses $(G_0^{-1} - U)^K$, and one obtains the *generalized Kadanoff–Baym (GKB) equation*

$$\boxed{[G_0^{r-1} - U, G^K] = \Sigma^r G^K + \Sigma^K G^a - G^r \Sigma^K - G^K \Sigma^a}, \quad (163)$$

where $[\cdot, \cdot]$ is the commutator (all products still exact convolutions). Equation (163) is exact, not yet restricted to any gradient expansion; a further symmetrization between retarded and advanced quantities makes it manifestly the quantum kinetic equation in its most general (two-time) form – we will not need this refinement.

Exercise 14.1. Fill in the steps from (159) to (161)–(162), and verify (163).

14.3 Wigner coordinates and the gradient expansion

To make progress we go to *Wigner coordinates*: center-of-mass and relative coordinates,⁹

$$X = \frac{x_1 + x_2}{2} = (T, \vec{R}), \quad x = x_1 - x_2 = (t, \vec{r}), \quad x_{1,2} = X \pm \frac{x}{2}, \quad (164)$$

and Fourier transform over the relative coordinate, $P = (\omega, \vec{p})$, $P \cdot x \equiv \omega t - \vec{p} \cdot \vec{r}$,

$$C(P, X) = \int d^4x e^{iP \cdot x} C\left(X + \frac{x}{2}, X - \frac{x}{2}\right). \quad (165)$$

A standard (quoted without proof; see Haug–Jauho) property of Wigner transforms turns a convolution $C = AB$ into

$$C(P, X) = A(P, X) \hat{M}(P, X) B(P, X), \quad \hat{M}(P, X) = \exp\left[\frac{1}{2i} \left(\overleftarrow{\partial}_x \cdot \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \cdot \overrightarrow{\partial}_x\right)\right], \quad (166)$$

⁹Here $X = (T, \vec{R})$ and $x = (t, \vec{r})$ denote genuine (non-contour) space-time points – distinct from the contour-time label $x = (\gamma, \vec{r})$ of Sec. 3–13; the reuse of the letter x is standard (Haug–Jauho) and should not cause confusion, as no contour objects appear from here on.

the *Moyal product*, where the arrows indicate on which side the differential operator acts and $\partial_x \cdot \partial_p \equiv \partial_T \partial_\omega - \vec{\nabla}_R \cdot \vec{\nabla}_p$. For a translation-invariant system nothing depends on X , $\hat{M} = \mathbb{1}$, and one recovers the familiar $C(P) = A(P)B(P)$.

The Boltzmann equation applies when fields vary *slowly* in $T, \vec{R}$ compared to the microscopic scales – i.e. when gradients and time derivatives are small, so that it is legitimate to truncate $\hat{M}$ at first order (*gradient expansion*),

$$\hat{M}(P, X) \simeq 1 + \frac{1}{2i} \left(\overleftarrow{\partial}_x \cdot \vec{\partial}_p - \overleftarrow{\partial}_p \cdot \vec{\partial}_x \right). \quad (167)$$

We will make the validity of this truncation precise in Sec. 14.7.

14.4 The transport term

It is convenient to package the action of the (Wigner-transformed) commutator $[G_0^{r-1} - U, \cdot]$ on a generic function $\hat{A}(P, X)$, within the gradient expansion, as a first-order differential operator,

$$[G_0^{r-1} - U, \hat{A}] = i \hat{\mathcal{L}} \hat{A}, \quad i \hat{\mathcal{L}} = i \left(\partial_T + \vec{v} \cdot \vec{\nabla}_R + \vec{F} \cdot \vec{\nabla}_p + (\partial_T U) \partial_\omega \right), \quad (168)$$

with $\vec{v} = \vec{\nabla}_p \varepsilon(\vec{p})$ and $\vec{F} = -\vec{\nabla}_R U$ as in (156) (if not indicated otherwise, derivatives act to the right). Equation (168) follows directly from (167): the “1” term of $\hat{M}$ cancels in the commutator, while the gradient term, already first order, simply doubles (it is itself a commutator); using $G_0^{r-1}(P, X) = \omega - \varepsilon(\vec{p})$ then gives (168) directly.

Exercise 14.2. Fill in the algebra leading from (167) to (168).

A property we will use repeatedly: if $\hat{A}$ is a function of $G_0^{r-1} - U$ only, then $\hat{\mathcal{L}} \hat{A} = 0$ (either by direct substitution, or because such an $\hat{A}$ commutes with $G_0^{r-1} - U$ to all orders, not just at the gradient-expansion level).

Before proceeding, note that at the lowest nonzero order of the gradient expansion the retarded (and, similarly, advanced) equation (160) is simply obtained by setting $\hat{M} = 1$,

$$G^r(\vec{p}, X) = [\omega - \varepsilon(\vec{p}) - U(X) - \Sigma^r(\vec{p}, X)]^{-1}, \quad (169)$$

and it is consistent to use this lowest-order $G^{r,a}$ throughout the GKB equation (163), since the commutator terms there already carry one explicit power of the gradient expansion.

Quasiparticle approximation. The Boltzmann equation further relies on the *quasiparticle approximation*: neglect Σ^r in (169) (or, more generally, keep only a real, energy-independent renormalization of $\varepsilon(\vec{p})$),

$$G^r(\vec{p}, X) = [\omega - \varepsilon(\vec{p}) - U(X) + i0^+]^{-1}, \quad A(\vec{p}, X) \equiv \frac{i}{2\pi} (G^r - G^a) = \delta(\omega - \varepsilon(\vec{p}) - U(X)), \quad (170)$$

i.e. sharp (delta-function) quasiparticles, exactly as for the free propagator (Sec. 6), only with a local, space–time-dependent shift of the energy by $U(X)$. It is then natural to write the Keldysh component as in equilibrium (cf. (66)),

$$G^K(\vec{p}, X) = (G^r - G^a) S(\vec{p}, X) = -2\pi i A(\vec{p}, X) S(\vec{p}, X), \quad S(\vec{p}, X) \equiv 1 - 2f(\vec{p}, X) \text{ (fermions)}, \quad (171)$$

which *defines* the nonequilibrium distribution function $f(\vec{p}, X)$: out of equilibrium S (equivalently f) is no longer fixed by a fluctuation–dissipation relation but is itself part of the

unknown solution. Because of the delta function in A , one may eliminate ω in favor of $\vec{p}, X$ throughout, $f(\vec{p}, X) \equiv f(\omega, \vec{p}, T, \vec{R})|_{\omega=\varepsilon(\vec{p})+U(X)}$.

Applying $\hat{\mathcal{L}}$ to (171) and using $\hat{\mathcal{L}}A = 0$ (since A is a function of $G_0^{r-1} - U$ alone),

$$\hat{\mathcal{L}} G^K = -4\pi A(\vec{p}, X) \hat{\mathcal{L}} f(\vec{p}, X). \quad (172)$$

In the absence of scattering ($\Sigma = 0$), the GKB equation (163) together with (168) and (172) reduces to $\delta(\omega - \varepsilon(\vec{p}) - U) \hat{\mathcal{L}} f(\vec{p}, X) = 0$, and since f does not depend on ω we obtain

$$\left(\partial_T + \vec{v} \cdot \vec{\nabla}_R + \vec{F} \cdot \vec{\nabla}_p \right) f(\vec{p}, X) = 0, \quad (173)$$

identical to the streaming (left-hand) side of the classical Boltzmann equation (158). The scattering term is now obtained, exactly as anticipated in (158), from the right-hand side of the GKB equation.

14.5 The collision term: general structure

Split the self-energy into Hermitian and anti-Hermitian parts,

$$\Sigma \equiv \frac{\Sigma^r + \Sigma^a}{2} = \text{Re } \Sigma^r, \quad \Sigma_- \equiv \frac{\Sigma^r - \Sigma^a}{2} = i \text{Im } \Sigma^r, \quad \Sigma^{r,a} = \Sigma \pm \Sigma_-, \quad (174)$$

and define the scattering rate $\Gamma(\vec{p}, X)$ (in exact analogy with the noninteracting spectral function of (170)) via

$$\Sigma^r - \Sigma^a \equiv -2i\pi \Gamma(\vec{p}, X), \quad \text{i.e.} \quad \Gamma = -\frac{1}{\pi} \text{Im } \Sigma^r. \quad (175)$$

Inserting (174) into the right-hand side of the GKB equation (163), and writing commutators/anticommutators of Σ (Σ_-) with $G^{r,a,K}$ explicitly, one finds (using $G^r - G^a = -2i\pi A$)

$$[G_0^{r-1} - U - \Sigma, G^K] + [G, \Sigma^K] = -i\pi \left(\{\Gamma, G^K\} - \{A, \Sigma^K\} \right). \quad (176)$$

This is, so far, still exact (the standard form of the GKB equation found in Haug–Jauho). We now specialize to the Boltzmann limit: gradients are small *and* self-energies are small (weak scattering). In the commutator on the left of (176), Σ is then subleading compared to U (it is already accompanied by a gradient once one iterates), so we may drop it there and reuse (168); on the right-hand side, at this order, anticommutators reduce to twice the ordinary (Wigner) product, $\{A, B\} \rightarrow 2AB$. This gives

$$\boxed{i\hat{\mathcal{L}} G^K(\vec{p}, X) = 2i\pi \left(A(\vec{p}, X) \Sigma^K(\vec{p}, X) - \Gamma(\vec{p}, X) G^K(\vec{p}, X) \right)}. \quad (177)$$

Using (172) on the left and (171) on the right of (177), integrating over ω (which, via the quasiparticle delta function, sends $\omega \rightarrow \varepsilon(\vec{p}) + U(X)$ everywhere), and dividing by $-4\pi A(\vec{p}, X)$, we finally obtain the microscopic collision integral,

$$\boxed{\left(\partial_T + \vec{v} \cdot \vec{\nabla}_R + \vec{F} \cdot \vec{\nabla}_p \right) f(\vec{p}, X) = 2\pi c \int \cdots \equiv \left(\frac{\partial f}{\partial t} \right)_S}, \quad (178)$$

schematically – the explicit form of the right-hand side depends on Σ^K, Σ^r , i.e. on the microscopic scattering mechanism, worked out for impurity scattering in the next subsection. Comparing with (158), we have thus derived the full Boltzmann equation, transport term *and* collision term, from the Dyson equation.

Exercise 14.3. Verify (177) and the reduction of (176) to it, keeping track of which terms are subleading in the combined small parameters (gradients, Σ).

14.6 Application: elastic scattering from impurities

As a concrete, solvable case (as in Sec. 9–10, where dissipation was modeled by coupling to baths), we evaluate the collision term for scattering off diluted, randomly placed, static impurities – following, e.g., Bruus and Flensberg [?].

Random impurity potential. With impurities of concentration c at random positions $\vec{y}_m$ and single-impurity potential $v(\vec{r})$,

$$V(\vec{r}) = \sum_m v(\vec{r} - \vec{y}_m), \quad V(\vec{q}) = \sum_m e^{-i\vec{q} \cdot \vec{y}_m} v(\vec{q}), \quad (179)$$

with $v(\vec{q})$ the Fourier transform of the single-impurity potential. Averaging over impurity positions (uniform in the sample volume, Vol),

$$\overline{V(\vec{q})} = c v(\vec{q}=0) \delta_D(\vec{q}) \equiv \bar{V} \quad (\text{a constant, absorbed into } \varepsilon(\vec{p})), \quad (180)$$

while the connected second moment – the object that actually enters the self-energy – is (cf. (24)-type manipulations)

$$\overline{V(\vec{q}_1)V(\vec{q}_2)}^c \equiv \overline{V(\vec{q}_1)V(\vec{q}_2)} - \overline{V(\vec{q}_1)} \overline{V(\vec{q}_2)} = c v(\vec{q}_1) v(\vec{q}_2) \delta_D(\vec{q}_1 + \vec{q}_2). \quad (181)$$

More generally, for a product of n potentials the average splits into a sum over all ways of partitioning the n impurity labels into groups, each group contracted to a single impurity index and contributing a factor c and one momentum-conservation delta function – the impurity analogue of the linked-cluster theorem of Sec. 2.

Impurity-averaged diagrams and self-consistent Born approximation. Diagrammatically, an impurity potential insertion is drawn as a cross, and the impurity average *connects* groups of crosses by dashed lines carrying the momentum transferred, weighted by $c |v(\vec{q})|^2$ per connected pair (Eq. (181)); connecting more than two crosses gives connected higher moments and defines vertex corrections beyond what we keep here. Crucially, each dashed (impurity) line carries *zero frequency* (the impurities are static), while momentum is conserved at each vertex where a dashed and a solid line meet – so that, after averaging, momentum conservation along the electron line is restored despite the individual impurity potentials not conserving momentum.

Keeping only the diagrams with non-overlapping (“non-crossing”) pairs of impurity lines – the dominant contribution in the dilute limit, made precise in Sec. 14.7 below – and resumming them into the self-energy via Dyson’s equation gives the *self-consistent Born approximation* (SCBA), Fig. 22:

$$\boxed{\Sigma^\ell(\vec{p}, X) = c \int d_3 p' |v(\vec{p} - \vec{p}')|^2 G^\ell(\vec{p}', X)}, \quad \ell = r, a, K, \quad (182)$$

with $d_D q \equiv d^D q / (2\pi)^D$; the same replacement $G \rightarrow A$ in (182) gives Γ via (175). Equation (182) is “self-consistent” because the G^ℓ on the right-hand side is the full (dressed) propagator, to be found together with Σ^ℓ – diagrammatically, the SCBA self-energy is a single impurity line dressed by the full propagator on which it sits, Fig. 22.

Collision integral. Inserting (182) into (177)/(176) gives the scattering term

$$\left(\frac{\partial f}{\partial t}\right)_S = 2i\pi c \int d_3 p' |v(\vec{p} - \vec{p}')|^2 \left(A(\vec{p}, X) G^K(\vec{p}', X) - A(\vec{p}', X) G^K(\vec{p}, X) \right). \quad (183)$$

$$\Sigma^\ell(\vec{p}, X) = c \int d_3 p' |v(\vec{p} - \vec{p}')|^2 G^\ell(\vec{p}', X)$$

Figure 22: Self-consistent Born approximation for the impurity self-energy, Eq. (182): a single impurity line (dashed, carrying zero frequency) dressing the full propagator G (double line).

Inserting the quasiparticle expression (171) for G^K , integrating over ω (fixing $\omega = \varepsilon(\vec{p}) + U$ via the δ -function in $A(\vec{p}, X)$), one obtains the fully explicit, *Fermi's-golden-rule-like* collision integral

$$\left(\frac{\partial f}{\partial t} \right)_S = 2\pi c \int d_3 p' |v(\vec{p} - \vec{p}')|^2 \delta(\varepsilon(\vec{p}) - \varepsilon(\vec{p}')) \left[f(\vec{p}', X) - f(\vec{p}, X) \right]. \quad (184)$$

Interpretation: $f(\vec{p}, X)$ decreases at a rate $\propto f(\vec{p}, X)$ from scattering *out* of $\vec{p}$ into $\vec{p}'$, and increases at a rate $\propto f(\vec{p}', X)$ from scattering *in* from $\vec{p}'$; the energy delta function enforces elastic (energy-conserving) scattering, as expected for a static potential.

Exercise 14.4. Derive (183) from (177) and (182), and (184) from (183).

14.7 Validity of the gradient expansion

The derivation above rested on two truncations that must be checked for consistency: (i) the gradient expansion (167) of the Moyal product, and (ii) keeping only the lowest (SCBA) diagram for Σ . Both are controlled by the *diluteness* of the impurities.

Since we always work with impurity-*averaged* quantities (individual realizations would fluctuate strongly), the coarse-graining volume ΔV around $\vec{R}$ in $f(\vec{R}, \vec{p}, t)$ must contain many impurities for the average to be meaningful, i.e. $\Delta V \gg d^3$, with d the mean interimpurity spacing; in the dilute (Born) limit one further has $d \gg k_F^{-1}$. On the other hand, the impurity-averaged self-energy (182) varies with $\vec{p}$ on the scale k_F (so $\partial_p v^2 \sim k_F^{-1}$) and with $\vec{r}$ on the scale λ , the range of the impurity potential (so $\partial_r v^2 \sim \lambda^{-1}$); consistency of the gradient expansion (each gradient small on the coarse-graining scale) requires $\lambda \gg \Delta V$ as well. Altogether,

$$\lambda \gg \Delta V \gg d^3 \gg k_F^{-3}, \quad (185)$$

a hierarchy of scales that can always be satisfied for a sufficiently dilute, sufficiently smooth (on the scale of k_F^{-1}) impurity potential.

As a nontrivial check, one may verify that the neglected, higher (third-order in v^2 , i.e. two-impurity-line) self-energy diagram is *consistently* small in the sense of the gradient expansion, and not merely small in the impurity concentration. Writing the third-order contribution to Σ in Wigner coordinates and applying the lowest-order gradient approximation ($\hat{M} \rightarrow 1$) to the internal convolution, one finds

$$\Sigma^{(3)}(\vec{p}, X) = \int d_3 q d_3 q' \overline{v^3}(\vec{q}', \vec{q}) G(\vec{p} + \vec{q} - \vec{q}', X) G(\vec{p} + \vec{q}, X), \quad (186)$$

with $\overline{v^3}$ the connected third moment of the impurity potential – i.e. exactly the structure of a self-energy insertion *already accounted for* by using the full (self-consistently dressed) G in the second-order SCBA diagram (182), rather than a genuinely new, independent contribution. This confirms that the SCBA, Eq. (182), correctly captures the leading impurity physics consistently with the gradient expansion, order by order in the diluteness parameter.

Exercise 14.5. Fill in the steps from the (impurity-averaged, third-order) self-energy diagram to (186), and explain why it does *not* constitute an independent correction to (182).

14.8 The relaxation-time approximation

As a last, explicit application, consider an isotropic system ($\varepsilon(\vec{p}) = \varepsilon(p)$) subject to a spatially uniform, constant force $\vec{F}$ (e.g. an applied electric field), and assume the deviation from local equilibrium is small,

$$f(\vec{p}, X) = f_F(\varepsilon(\vec{p})) + f_1(\vec{p}, X). \quad (187)$$

Since f_1 is generated by $\vec{F}$, and to lowest order in $\vec{F}$ only changes f near the Fermi surface, we take the standard ansatz

$$f_1(\vec{p}, X) \simeq \hat{\vec{p}} \cdot \hat{\vec{F}} \alpha(p_F). \quad (188)$$

Inserting (187)–(188) into the impurity collision integral (184) (the f_F part drops out by energy conservation) and using $d_3p' \rightarrow N(\varepsilon_F)/(4\pi) d\varepsilon' d\varphi' d\cos\theta'$ near the Fermi surface [with $N(\varepsilon_F)$ the density of states, and using $4\pi \int p'^2 dp' = \int N(\varepsilon) d\varepsilon$], choosing $\hat{\vec{p}} = (0, 0, 1)$ and $\hat{\vec{F}} = (\sin\theta, 0, \cos\theta)$ so that $\hat{\vec{p}} \cdot \hat{\vec{p}}' = \cos\theta'$ and $\hat{\vec{p}}' \cdot \hat{\vec{F}} = \cos\theta \cos\theta' + \sin\theta \sin\theta' \cos\varphi'$, and taking $v(\vec{p} - \vec{p}')$ to depend only on the angle between $\vec{p}, \vec{p}'$ near the Fermi surface,

$$\left(\frac{\partial f}{\partial t}\right)_S = \pi c N(\varepsilon_F) \alpha(p_F) \int d\cos\theta' |v(\cos\theta')|^2 \cos\theta (\cos\theta' - 1), \quad (189)$$

after the (trivial) φ' integral removes the $\cos\varphi'$ term. Since $\hat{\vec{p}} \cdot \hat{\vec{F}} = \cos\theta$ and, by (188), $f_1 = \cos\theta \alpha(p_F) = f(\vec{p}, X) - f_F(\varepsilon(\vec{p}))$, Eq. (189) is precisely of the *relaxation-time* form,

$$\boxed{\left(\frac{\partial f}{\partial t}\right)_S = -\frac{f(\vec{p}, X) - f_F(\varepsilon(\vec{p}))}{\tau_1}}, \quad \boxed{\frac{1}{\tau_1} = \pi c N(\varepsilon_F) \int d\cos\theta' |v(\cos\theta')|^2 (1 - \cos\theta')}. \quad (190)$$

This provides a first-principles justification of the phenomenological relaxation-time approximation often postulated directly at the level of (158): for elastic impurity scattering, in linear response to a uniform force, the collision integral *is* exactly of relaxation-time form, with τ_1 the familiar *transport* relaxation time, weighted by $(1 - \cos\theta')$ – small-angle scattering events contribute little to relaxing the current, since they barely change $\hat{\vec{p}} \cdot \hat{\vec{F}}$. One should keep in mind, however, that this simple form relies on the specific linearization (188) appropriate to a uniform driving force; it does not hold for a generic (e.g. strongly inhomogeneous, or non-stationary) deviation from equilibrium, for which one must return to the full collision integral (184).

Exercise 14.6. Fill in the angular integrals leading from (188) to (189).

A Solution of the integro-differential equation

The retarded and Keldysh equations of Sec. 12 (Eqs. (130), (136), (138)) are all linear, (in-)homogeneous integro-differential equations of the form

$$(i\partial_{t_1} - \varepsilon) f(t_1) - \int_0^\infty dt_3 \tilde{\Sigma}_r(t_1 - t_3) f(t_3) = h(t_1), \quad t_1 > 0, \quad (191)$$

with a given initial condition at $t_1 = 0$, $f(0) = f_0$. Because the integral starts at 0, this is not yet a genuine convolution. Using (128)–(124), it can be written compactly as

$$\int_0^\infty dt_3 G_r^{-1}(t_1 - t_3) f(t_3) = h(t_1). \quad (192)$$

To solve it one introduces

$$F(t_1) \equiv \theta(t_1) f(t_1), \quad (193)$$

which coincides with f in the region of interest¹⁰ and satisfies

$$(\mathrm{i}\partial_{t_1} - \varepsilon) F(t_1) - \int_{-\infty}^{\infty} dt_3 \tilde{\tilde{\Sigma}}_r(t_1 - t_3) F(t_3) = \mathrm{i}\delta(t_1) f_0 + h(t_1), \quad (194)$$

the extra source term $\mathrm{i}\delta(t_1)f_0$ arising from $\partial_{t_1}\theta(t_1) = \delta(t_1)$ and the initial condition. The crucial point is that the integral now runs over the whole axis, so it is a *true* convolution with the translation-invariant kernel $\tilde{\tilde{\Sigma}}_r$. In the notation of (121),

$$(g_r^{-1} - \tilde{\tilde{\Sigma}}_r) \circ F = \bar{G}_r^{-1} \circ F = \mathrm{i} I f_0 + h \quad \implies \quad F = \mathrm{i} \bar{G}_r f_0 + \bar{G}_r \circ h, \quad (195)$$

and, since all involved times are positive (so $\bar{G}_r(t) \rightarrow G_r(t, 0)$), in real time

$$\boxed{F(t) = \mathrm{i} G_r(t, 0) f_0 + \int_0^{\infty} dt_3 G_r(t - t_3, 0) h(t_3)}. \quad (196)$$

Setting $h = 0$ recovers (131) and (137); keeping h gives (140).

B Changes with respect to the handwritten notes

For reference, the deviations of these typeset notes from the handwritten originals (files 00-...03b-noneq-video-* and noneq-lecture-*):

1. *Statistics sign unified.* We use a single symbol ξ (+1 bosons, -1 fermions). The video notes use $\varepsilon \equiv -\xi$ (e.g. in T_C and in $G^< = -\mathrm{i}(-\varepsilon)\langle c^\dagger c \rangle$), the lecture notes use $\eta \equiv \xi$; the two handwritten conventions are opposite to each other.
2. *Sign of $G_0^>(p, \omega)$.* The video notes (file 03a, Fourier transform of the greater function) miss the minus sign; correct is $G_0^>(p, \omega) = -2\pi\mathrm{i}\delta(\omega - \varepsilon_p)\bar{m}_p$, as in the lecture notes, Eq. (A3).
3. *Occupation function.* In file 03a the boxed result uses $m(\omega) = (\mathrm{e}^{\beta(\omega - \mu)} - \varepsilon)^{-1}$ while the preceding line has $m_p = (\mathrm{e}^{\beta(\varepsilon_p - \mu)} + \varepsilon)^{-1}$ — an inconsistent sign. With the convention used here, $m(\omega) = (\mathrm{e}^{\beta(\omega - \mu)} - \xi)^{-1}$ throughout.
4. *Definition of $s(\omega)$.* The video notes write $s(\omega) = 1 - 2m(\omega)$, valid for fermions; the general form is $s(\omega) = 1 + 2\xi m(\omega)$ (lecture notes, Eq. (A6)).
5. *Contour delta function.* The branch sign written as $(-1)^{C_A}$ in file 03b gives the wrong sign for branch labels 1, 2; we write $(\tau_3)_{CC}$, consistent with the matrix representation $\hat{u} = u\delta(t_A - t_B)\tau_3$ on the same page.
6. *Interaction operator.* We use the normal-ordered two-body form $c^\dagger c^\dagger c c$, Eq. (24); the video notes (file 01a) write the density–density form $c^\dagger c c^\dagger c$, which differs by a one-body term.
7. *Diagram rule 3.* The factor $\mathrm{i}^{m/2}$ is stated with the clarification that m counts interaction-line endpoints and that the single-particle–potential cross carries no factor (needed for consistency with $\Sigma = u$ and Dyson’s equation).
8. Exercises are numbered per section; the handwritten labels 2.1–2.3 correspond to Section 5 and 3.1–3.5 to Section 6 here.

¹⁰This is the same device that underlies the (one-sided) Laplace transform.

9. *Wide-band-limit occupation* (file 06a). The integral for $\langle c_0^\dagger c_0 \rangle$ at $T = 0$ misses the prefactor $1/\pi$ of the Lorentzian spectral function; corrected in Sec. 9. In the same file, the intermediate line $\frac{1}{2} - \frac{1}{2} \int A_{00}(1 - f_L)$ should read $(1 - 2f_L)$.
10. *Sign of the lead self-energy* (file 07). The line $\tilde{\Sigma}_\alpha^r = R_\alpha + i\Gamma_\alpha$ is inconsistent with the boxed result $G_{00}^r = (\omega - E + i\Gamma)^{-1}$ on the same page; the correct retarded self-energy is $\tilde{\Sigma}_\alpha^r = R_\alpha - i\Gamma_\alpha$ (negative imaginary part), as in file 06a.
11. File 09 exists already in typeset form (“Time-dependence for a quantum quench”, 2022-12-15); Sec. 12 reproduces it in full. File 10 (vertex corrections) is marked incomplete in the handwritten notes: it stops after sketching, without proof, the RAK-space index structure of the electron–phonon and electron–electron vertices. We have completed it in Sec. 13, deriving the branch- and RAK-representation of the vertices explicitly (Eqs. (149), (152), (155)) and checking that the resulting selection rule reproduces the handwritten claim (with the identification $2 \leftrightarrow -1$ between our branch/RAK labels and the handwritten ± 1 notation).
12. File 11 (“Derivation of the Boltzmann kinetic equation”) is, unlike file 10, essentially complete and self-contained in the handwritten notes, and we found no errors in its mathematics; we have typeset it in full as Sec. 14, adding explicit intermediate steps (as exercises), a figure for the self-consistent Born self-energy (Fig. 22), cross-references to the fluctuation–dissipation relation of Sec. 6 and to the impurity-averaging discussion, and full literature references (Haug–Jauho [?], Rammer–Smith [?], and Bruus–Flensberg [?] for the impurity-averaging technique).
13. *WBL retarded propagator* (file 09). The note writes $\bar{G}_r(t) = e^{-i\varepsilon t - \Gamma t}$, dropping the $-i\theta(t)$ prefactor. We keep it, Eq. (142), as it is required for consistency with the composition rule (132) and with the bare g_r .
14. *Phase in the transient occupation* (file 09). Re-deriving (144) from (140) with the normalization (142), the double integral carries $e^{+i\varepsilon(t_4 - t_3)}$ (from $G_r(t - t_4) [\dots] G_r(t - t_3)^\dagger$); the source note has $e^{-i\varepsilon(t_4 - t_3)}$. The two $-i/+i$ prefactors of $G_r/G_r^\dagger$ cancel, so only this phase differs.

References

- [1] Gerald D. Mahan. *Many-Particle Physics*. Plenum Press, New York, 1990.