Introduction to the Keldysh nonequilibrium Green function technique

A. P. Jauho

I. BACKGROUND

The Keldysh nonequilibrium Green function technique is used very widely to describe transport phenomena in mesoscopic systems. The technique is somewhat subtle, and a rigorous treatment would require much more time than we have at our disposal, see, for example, the text-book by Haug and Jauho [1]. The goal of these lectures is to give a rough idea of how the technique works, and illustrate it with a few simple examples. Our main application is to calculate the current through a resonant-tunneling diode; this calculation can be done in a number of different ways, such as the Landauer-Büttiker formalism, or by a Master Equation approach, and our hope is that studying this exactly solvable problem by different methods will give insight to the different formalisms.

II. REVIEW OF PERTURBATION EXPANSION OF THE GREEN FUNCTION

I will assume that the audience is familiar with equilibrium Green functions on the level as discussed in Many-Particle Physics I (Transport in Nanostructures) [2]. Nevertheless, I summarize some of the central features here.

We start by defining a time-ordered (also called causal) zero-temperature single-particle Green function

$$G(x, t; x', t') = \frac{-i}{\hbar} \frac{\langle \Psi_0 | T\{\psi_H(x, t)\psi_H^\dagger(x', t')\} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \ . \tag{1}$$

Next, recall the various representation pictures of quantum mechanics:

- **Schrödinger picture:** the wavefunctions are time-dependent: $i\frac{\partial}{\partial t}\psi(t) = H\psi(t)$; the operators are constant.

- **Heisenberg picture:** The wavefunctions are constant; the operators are time-dependent: $\mathcal{O}(t) = e^{iHt}\mathcal{O}(0)e^{-iHt}$.

- **Interaction picture:** The wavefunctions develop under the influence of the "difficult" interaction part of the Hamiltonian $H = H_0 + V$: $\hat{\psi}(t) = e^{iH_0 t}e^{-iHt}\psi(0)$. The operators develop under the influence of the "easy" non-interacting Hamiltonian H_0 only: $\hat{\mathcal{O}}(t) = e^{iH_0 t}\hat{\mathcal{O}}(0)e^{-iH_0 t}$. [9]

The time-development of the interaction picture is often expressed in terms of a U operator (or matrix):

$$\hat{\psi}(t) = U(t)\psi(0), \qquad U(t) = e^{iH_0 t}e^{-iHt} \ . \tag{2}$$

We next introduce the S-matrix, which changes the wavefunction from $\hat{\psi}(t')$ to $\hat{\psi}(t)$:

$$\hat{\psi}(t) = S(t, t')\hat{\psi}(t') \ . \tag{3}$$

Thus,

$$S(t, t') = U(t)U^\dagger(t') \ . \tag{4}$$

The S-matrix obeys the group property $S(t, t') = S(t, t'')S(t'', t')$. Furthermore, the S-matrix can be expressed as a time-ordered product [for a derivation based on the equation of motion for S, see [2],[3],[4]:

$$S(t, t') = Te^{-i\int_{t'}^{t} dt_1 \hat{V}(t_1)} \ . \tag{5}$$

The definition for the Green function contains a difficulty: It involves the exact ground state of the system. But this is one of the things we want to compute with the Green function! To make any progress, we must express the exact ground state $|\Psi_0\rangle$ in terms of quantities we know, for example the non-interacting ground state $|\Phi_0\rangle$. This connection is formed by the Gell-Mann and Low theorem:

$$|\Psi_0\rangle = S(0, -\infty)|\Phi_0\rangle \ , \tag{6}$$

The proof for this relation is rather subtle (see Ref.[5], pp. 61–64) and we do not reproduce it here. In analogy with (6), we have

$$\langle \Psi_0 | = \langle \Phi_0 | S(\infty, 0) \ . \tag{7}$$

The object $\langle \Phi_0 | S(\infty, 0) S(0, -\infty) | \Phi_0 \rangle$ may have an ill-defined phase, this is, however, canceled by a similar phase-factor arising from the numerator of the definition of the time-ordered Green function:

$$G(x, t; x', t') = -i \frac{\langle \Phi_0 | T\{ S(\infty, -\infty) \hat{\psi}(x, t) \hat{\psi}^\dagger(x', t') \} | \Phi_0 \rangle}{\langle \Phi_0 | S(\infty, -\infty) | \Phi_0 \rangle} \ . \tag{8}$$

This important result generates the systematic perturbation scheme for the Green function. The calculation proceeds by expanding the S-matrix (both in the numerator and in the denominator) in $\hat{V}(t)$:

$$S(\infty, -\infty) = \sum_{n=0}^{\infty} \frac{(-i)^{n+1}}{n!} \int_{-\infty}^{+\infty} dt_1 \cdots dt_n T\{ \hat{V}(t_1) \cdots \hat{V}(t_n) \} \ , \tag{9}$$

Since each $\hat{V}$ contains three or four field operators, we need a device for evaluating expectation values such as

$$\langle \Phi_0 | T\{ \hat{\psi}(t) \hat{\psi}^\dagger(t') \hat{\psi}^\dagger(t_1) \hat{\psi}^\dagger(t_2) \hat{\psi}(t_2) \hat{\psi}(t_1) \} | \Phi_0 \rangle \ , \tag{10}$$

and higher order similar terms. These expressions are evaluated with Wick's theorem, which says that the result of (10) is the sum of all pairwise contractions. Thus (10) gives rise to six terms: for example, $\hat{\psi}(t)$ can be paired with $\hat{\psi}^\dagger(t')$, and the remaining 4 operators can be paired in two different ways. Thus one gets $3 \times 2 = 6$ terms. These terms are most easily expressed in terms of Feynman diagrams.

The various diagrams have quite distinct properties. Some of them are disconnected diagrams. These are exactly canceled by the denominator in (8). This is good because disconnected diagrams often diverge! After some combinatorics (see Sect. 12.3.3 in [2]), one finds that

$$G(x, t; x', t') = -i \sum_{n=0}^{\infty} (-i)^n \int_{-\infty}^{+\infty} dt_1 \cdots dt_n \langle \Phi_0 | T \hat{\psi}(x, t) \hat{\psi}^\dagger(x', t') \hat{V}(t_1) \cdots \hat{V}(t_n) | \Phi_0 \rangle_{\text{conn}} \ , \tag{11}$$

where the summation only includes topologically different connected diagrams. (11) is the desired perturbation expansion for the Green function, and it forms the starting point for many calculations.

III.   CONTOUR ORDERED GREEN FUNCTIONS

The central quantity in constructing the perturbation theory for Green functions is the S-matrix $S(\infty, -\infty)$. In nonequilibrium there is no guarantee that the system returns to its initial state for asymptotically large times. In fact, often it does not. Consider, for example, an important problem in surface physics, where atoms or molecules impinging on a surface exchange charge with the surface, and hence the initial state at $t = -\infty$ is very different from the final state at $t = +\infty$. Thus, one should avoid any reference to the asymptotically large times in the nonequilibrium theory. The general formulation of the theory is slightly more complicated than in the equilibrium case. As we shall see, however, the abstract structure of the theory bears a close resemblance to the equilibrium theory.

The nonequilibrium problem is formulated as follows. We consider a system evolving under the Hamiltonian

$$H = h + H'(t) \ . \tag{12}$$

Here the time-independent part of the Hamiltonian h is split in two parts: $h = H_0 + H_i$, where H_0 is "simple" (in the sense that it can be diagonalized, and hence Wick's theorem applies) and H_i is "complicated" (in the sense that it contains the many-body aspects of the problem, and hence requires a special treatment). It is further assumed that the nonequilibrium part vanishes for times $t < t_0$. The nonequilibrium part could be, e.g., an electric field, an light excitation pulse, or a coupling to contacts at differing (electro) chemical potentials.

One often lets $t_0 \to -\infty$ at a suitable point. This procedure simplifies the treatment, and in order to display the structure of the nonequilibrium theory as concisely as possible, we take this limit. However, in doing so the discussion of transient phenomena is excluded, and must be treated separately.
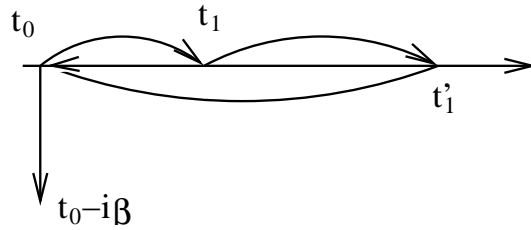
FIG. 1: Contour C_v

Before the perturbation is turned on, the system is described by the thermal equilibrium density matrix,

$$\varrho(h) = \frac{\exp(-\beta h)}{\text{Tr}[\exp(-\beta h)]} \ . \tag{13}$$

The task is to calculate the expectation value of a given observable, to which one associates a quantum mechanical operator O, for times $t \geq t_0$:

$$\langle O(t) \rangle = \text{Tr}[\varrho(h) O_H(t)] \ . \tag{14}$$

The subscript H indicates that the time-dependence is governed by the full Hamiltonian, i.e., O is written in the Heisenberg picture. The definition (14) can be generalized to two-time (or n-time) quantities (Green functions, correlation functions) in an obvious fashion.

One should note that we use an equilibrium density matrix $\varrho(h)$ in (14), and not some time-dependent ϱ. Physically this means that the thermodynamic degrees of freedom, contained in h, do not follow instantaneously the rapid variations contained in $H'(t)$. Other choices may be possible, but we make this choice here because of the difficulties related to other choices [see the discussion on pp. 214–216 in[4].

The general plan of attack is similar to the equilibrium case. We transform the "hopelessly complicated" time-dependence of O_H to a simpler form, namely to that of O_{H_0}. Since there are two operators to be eliminated, i.e., the time-dependent external perturbation $H'(t)$, and the "complicated" interaction term H_i, we expect to meet more complicated transformations than in the equilibrium case. However, with suitable generalizations, it can be shown that the nonequilibrium and equilibrium formalisms can be made *structurally* equivalent.

We skip here the technical details of these transformations because the final result is intuitive; an interested reader may consult [1]. Instead of the time-ordering operator used in equilibrium theory, we now introduce the contour-ordering operator, which orders the time-labels according to their order on the (Keldysh) contour. With this generalization, the topological structure of the perturbation theory is identical to the equilibrium theory. Thus, the contour-ordered Green function, defined as

$$G(1,1') \equiv -i \langle T_{C_v}[\psi_H(1)\psi_H^\dagger(1')] \rangle \ , \tag{15}$$

satisfies the same Dyson equation as the equilibrium function:

$$G(1,1') = G_0(1,1') + \int d^3x_2 \int_{C_v} d\tau_2 G_0(1,2) U(2) G(2,1') + \int d^3x_2 \int d3x_3 \int_{C_v} d\tau_2 \int_{C_v} d\tau_3 G_0(1,2) \Sigma(2,3) G(3,1') \ , \tag{16}$$

where all the time-labels now reside on the contour shown in Fig.1. In writing (16), we assume that the nonequilibrium term in the Hamiltonian can be represented by a one-body external potential U. The interactions are contained in the (irreducible) self-energy $\Sigma[G]$. The contour representation is rather impractical in calculations, and we want to replace the contour by real time integrals. This procedure is called the analytic continuation.

As mentioned above, a simplification occurs if we can set $t_0 \rightarrow -\infty$. If the interactions are coupled adiabatically, the contribution from the $[t_0, t_0 - i\beta]$ piece vanishes. The information lost by this procedure is related to initial correlations. In many physical situations, for example, in steady state transport, it appears plausible that the initial correlations have been washed out by the interactions when one reaches the steady state. On the contrary, if one studies transient response, the role of initial correlations can be important. This represents an interesting, and rather open problem. Here we consider the $t_0 \rightarrow -\infty$ limit. The contour thus consists of two parts, from $-\infty$ to ∞, and from ∞ to $-\infty$. Any time residing on the first part (call this C_1) is earlier in the contour sense to any time residing on the latter part C_2. The contour-ordered Green function thus contains four different functions:

$$G(1,1') = \begin{cases} G_c(1,1') & t_1, t_{1'} \in C_1 \\ G^>(1,1') & t_1 \in C_2, t_{1'} \in C_1 \\ G^<(1,1') & t_1 \in C_1, t_{1'} \in C_2 \\ G_{\bar{c}}(1,1') & t_1, t_{1'} \in C_2 \end{cases} \ . \tag{17}$$

Here we have introduced the *causal*, or *time-ordered* Green function G_c,

$$
\begin{aligned}
G_c(1,1') &= -i\langle T[\psi_H(1)\psi_H^\dagger(1')]\rangle \\
&= -i\theta(t_1 - t_{1'})\langle\psi_H(1)\psi_H^\dagger(1')\rangle + i\theta(t_{1'} - t_1)\langle\psi_H^\dagger(1')\psi_H(1)\rangle \,,
\end{aligned}
\tag{18}
$$

the *"greater"* function $G^>$,

$$
G^>(1,1') = -i\langle\psi_H(1)\psi_H^\dagger(1')\rangle \,,
\tag{19}
$$

the *"lesser"* function $G^<$,

$$
G^<(1,1') = +i\langle\psi_H^\dagger(1')\psi_H(1)\rangle \,,
\tag{20}
$$

and the *antitime-ordered* Green function $G_{\tilde{c}}$,

$$
\begin{aligned}
G_{\tilde{c}}(1,1') &= -i\langle\tilde{T}[\psi_H(1)\psi_H^\dagger(1')]\rangle \\
&= -i\theta(t_{1'} - t_1)\langle\psi_H(1)\psi_H^\dagger(1')\rangle + i\theta(t_1 - t_{1'})\langle\psi_H^\dagger(1')\psi_H(1)\rangle \,.
\end{aligned}
\tag{21}
$$

Since $G_c + G_{\tilde{c}} = G^< + G^>$, there are only three linearly independent functions. This freedom of choice reflects itself in the literature, where a number of different conventions can be found. For our purposes the most suitable functions are the functions $G^{>,<}$ (which are often also denoted by a common name, "correlation function"), and the advanced and retarded functions defined as

$$
\begin{aligned}
G^a(1,1') &= i\theta(t_{1'} - t_1)\langle\{\psi_H(1), \psi_H^\dagger(1')\}\rangle \\
&= \theta(t_{1'} - t_1)[G^<(1,1') - G^>(1,1')] \,,
\end{aligned}
\tag{22}
$$

and

$$
\begin{aligned}
G^r(1,1') &= -i\theta(t_1 - t_{1'})\langle\{\psi_H(1), \psi_H^\dagger(1')\}\rangle \\
&= \theta(t_1 - t_{1'})[G^>(1,1') - G^<(1,1')] \,.
\end{aligned}
\tag{23}
$$

Here curly brackets denote an anticommutator. We observe that $G^r - G^a = G^> - G^<$.

The main technical trick needed in the analytic continuation is included in the following theorem.

Langreth Theorem. In considering the Dyson equation (16) we encounter terms with the structure $C = AB$, or, explicitly,

$$
C(t_1, t_{1'}) = \int_C d\tau\, A(t_1, \tau) B(\tau, t_{1'}) \,,
\tag{24}
$$

and their generalizations involving products of three (or more) terms. Since we are presently only concerned with temporal variables, we suppress all other variables (spatial, spin, etc.), which have an obvious matrix structure. To evaluate (24) let us assume for definiteness that t_1 is on the first half of the contour ("on the way out"), and that $t_{1'}$ is on the latter half ("on the way back"). In view of our discussion in connection with (18)–(23), we are thus analyzing a "lesser" function.

The next step is to deform the contour as indicated in Fig. 2. Thus (24) becomes

$$
C^<(t_1, t_{1'}) = \int_{C_1} d\tau\, A(t_1, \tau) B^<(\tau, t_{1'}) + \int_{C_1'} d\tau\, A^<(t_1, \tau) B(\tau, t_{1'}) \,.
\tag{25}
$$

Here, in appending the sign $<$ to the function B in the first term, we made use of the fact that as long as the integration variable τ is confined on the contour C_1 it is less than (in the contour sense) $t_{1'}$. A similar argument applies to the second term. Now consider the first term in (25), and split the integration into two parts:

$$
\begin{aligned}
\int_{C_1} d\tau\, A(t_1, \tau) B^<(\tau, t_{1'}) &= \int_{-\infty}^{t_1} dt\, A^>(t_1, t) B^<(t, t_{1'}) + \int_{t_1}^{-\infty} dt\, A^<(t_1, t) B^<(t, t_{1'}) \\
&\equiv \int_{-\infty}^{\infty} dt\, A^r(t_1, t) B^<(t, t_{1'}) \,,
\end{aligned}
\tag{26}
$$
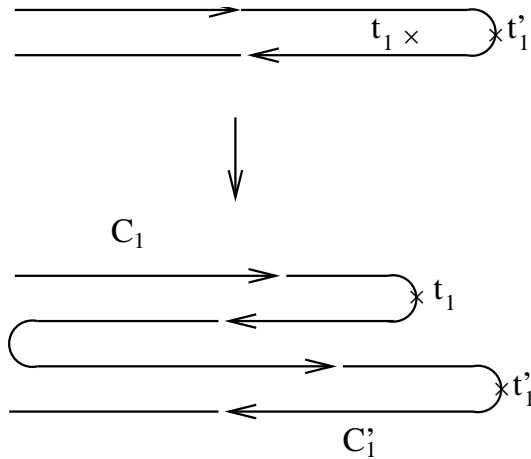
FIG. 2: Deformation of contour C

where we used the definition of the retarded function (23). A similar analysis can be applied to the second term involving contour C_1'; this time the advanced function is generated. Putting the two terms together, we have the first of Langreth's results:

$$C^<(t_1, t_{1'}) = \int_{-\infty}^{\infty} dt[A^r(t_1,t)B^<(t,t_{1'}) + A^<(t_1,t)B^a(t,t_{1'})] \ . \tag{27}$$

The same result applies for the "greater" function: one just replaces all $<$'s by $>$'s.

It is easy to generalize the result (27) for a (matrix) product of three functions: If $D = ABC$ on the contour, then, on the real axis, one has

$$D^< = A^r B^r C^< + A^r B^< C^a + A^< B^a C^a \ . \tag{28}$$

Once again a similar equation holds for the "greater" functions.

One often needs the retarded (or advanced) component of a product of functions defined on the contour. The required expression is derived by repeated use of the definitions (18)–(23), and the result (27):

$$
\begin{aligned}
C^r(t_1, t_{1'}) &= \theta(t_1 - t_{1'})[C^>(t_1, t_{1'}) - C^<(t_1, t_{1'})] \\
&= \theta(t_1 - t_{1'}) \int_{-\infty}^{\infty} dt[A^r(B^> - B^<) + (A^> - A^<)B^a] \\
&= \theta(t_1 - t_{1'}) \left[\int_{-\infty}^{t_1} dt(A^> - A^<)(B^> - B^<) \right. \\
&\qquad\qquad \left. + \int_{-\infty}^{t_{1'}} dt(A^> - A^<)(B^< - B^>) \right] \\
&= \int_{t_{1'}}^{t_1} dt A^r(t_1,t) B^r(t,t_{1'}) \ .
\end{aligned} \tag{29}
$$

In our compact notation this relation is expressed as $C^r = A^r B^r$.

When considering the various terms in the diagrammatic perturbation series one may also encounter terms where two Green function lines run (anti)parallel [this is the case, for example, of a polarization or electron-phonon self-energy (parallel Fermion and Boson Green functions)]. In this case one needs the "lesser" and/or retarded/advanced components of structures like

$$
\begin{aligned}
C(\tau, \tau') &= A(\tau, \tau')B(\tau, \tau') \ , \\
D(\tau, \tau') &= A(\tau, \tau')B(\tau', \tau) \ ,
\end{aligned} \tag{30}
$$

where τ and τ' are contour variables. The derivation of the required formulae is similar to the analysis presented above, and is left for an exercise. One finds

$$
\begin{aligned}
C^<(t, t') &= A^<(t, t')B^<(t, t') \ , \\
D^<(t, t') &= A^<(t, t')B^>(t', t) \ ,
\end{aligned} \tag{31}
$$

TABLE I: Rules for analytic continuation

Contour	Real axis
$C = \int_C AB$	$C^< = \int_t [A^r B^< + A^< B^a]$
	$C^r = \int_t A^r B^r$
$D = \int_C ABC$	$D^< = \int_t [A^r B^r C^< + A^r B^< C^a + A^< B^a C^a]$
	$D^r = \int_t A^r B^r C^r$
$C(\tau,\tau') = A(\tau,\tau')B(\tau,\tau')$	$C^<(t,t') = A^<(t,t')B^<(t,t')$
	$C^r(t,t') = A^<(t,t')B^r(t,t') + A^r(t,t')B^<(t,t')$
	$\qquad + A^r(t,t')B^r(t,t')$
$D(\tau,\tau') = A(\tau,\tau')B(\tau',\tau)$	$D^<(t,t') = A^<(t,t')B^>(t',t)$
	$D^r(t,t') = A^<(t,t')B^a(t',t) + A^r(t,t')B^<(t',t)$

and

$$
\begin{aligned}
C^r(t,t') &= A^<(t,t')B^r(t,t') + A^r(t,t')B^<(t,t') + A^r(t,t')B^r(t,t') \, , \\
D^r(t,t') &= A^r(t,t')B^<(t',t) + A^<(t,t')B^a(t',t) \\
&= A^<(t,t')B^a(t',t) + A^r(t,t')B^<(t',t) \, .
\end{aligned}
$$
(32)

As earlier, the relations (31) can immediately be generalized to "greater" functions. For a quick reference, we have collected the rules provided by the Langreth theorem in Table 4.1.

Equilibrium Electron-Phonon Self-Energy.

The retarded electron-phonon self-energy Σ_{ph}^r is a central object in the analysis of many physical properties of metals and semiconductors. At finite temperatures one conventionally uses the Matsubara technique to perform the analytic continuation [for an extended discussion, see [4]. The Langreth theorem can be used to give a very compact derivation of Σ_{ph}^r. In lowest order in the electron-phonon matrix element M_q we have

$$
\Sigma_{\mathrm{ph}}(k,\tau,\tau') = i\sum_q |M_q|^2 G(k-q,\tau,\tau')D(q,\tau,\tau') \, .
$$
(33)

Here G is the free-electron Green function while D is the free-phonon Green function. Equation (33) is in a form where we can apply (32). In equilibrium all quantities depend on time only through the difference of the two time-labels, and it is advantageous to work in frequency space. Performing the Fourier transform gives

$$
\Sigma_{\mathrm{ph}}^r(k,\omega) = i\int \frac{d\varepsilon}{2\pi} \sum_q |M_q|^2 [G^<(k-q,\omega-\varepsilon)D^r(q,\varepsilon) + G^r(k-q,\omega-\varepsilon)D^<(q,\varepsilon) + G^r(k-q,\omega-\varepsilon)D^r(q,\varepsilon)] \, .
$$
(34)

The expressions for the free equilibrium Green functions are (the reader is urged to verify these relations!):

$$
\begin{aligned}
D^<(q,\omega) &= -2\pi i[(N_q+1)\delta(\omega+\omega_q) + N_q\delta(\omega-\omega_q)] \, , \\
D^r(q,\omega) &= \frac{1}{\omega - \omega_q + i\eta} - \frac{1}{\omega + \omega_q + i\eta} \, , \\
G^<(k,\omega) &= 2\pi i n_{\mathrm{F}}(\omega)\delta(\omega - \varepsilon_k) \, , \\
G^r(k,\omega) &= \frac{1}{\omega - \varepsilon_k + i\eta} \, .
\end{aligned}
$$
(35)

Substituting these expressions in (34), one finds after some straightforward algebra

$$
\Sigma_{\mathrm{ph}}^r(k,\omega) = \sum_q M_q^2 \left[\frac{N_q - n_{\mathrm{F}}(\varepsilon_{k-q}) + 1}{\omega - \omega_q - \varepsilon_{k-q} + i\eta} + \frac{N_q + n_{\mathrm{F}}(\varepsilon_{k-q})}{\omega + \omega_q - \varepsilon_{k-q} + i\eta} \right] \, .
$$
(36)

The shortness of this derivation, as compared to the standard one, nicely illustrates the formal power embedded in the Langreth theorem.

IV.   KELDYSH FORMULATION

We now derive the Keldysh integral equation for the correlation function $G^<$, by applying the analytic continuation rules on the complex time Dyson equation. Thus, applying the rule (28) on (16)[10] yields

$$G^< = G_0^< + G_0^r \Sigma^r G^< + G_0^r \Sigma^< G^a + G_0^< \Sigma^a G^a \ . \tag{37}$$

We proceed by iteration with respect to $G^<$. Iterating once, and regrouping the terms we obtain

$$\begin{aligned} G^< = (1 + G_0^r \Sigma^r) G_0^< (1 \ + \ \Sigma^a G^a) + (G_0^r + G_0^r \Sigma^r G_0^r) \Sigma^< G^a \\ + \ G_0^r \Sigma^r G_0^r \Sigma^r G^< \ . \end{aligned} \tag{38}$$

The form of (38) is very suggestive, and it easy to convince oneself that the infinite order iterate is

$$G^< = (1 + G^r \Sigma^r) G_0^< (1 + \Sigma^a G^a) + G^r \Sigma^< G^a \ . \tag{39}$$

One can show, using the Dyson equation for the retarded Green function, that the first term in (39) vanishes for steady state systems, if the system was in a noninteracting state in infinite past. Thus, in many applications (also as is done below) it is sufficient to only keep the second term. Despite of its simple appearance, one should note that the Keldysh equation is an integral equation for the correlation function $G^<$, because usually $\Sigma^<$ is a functional of $G^<$.

V.   NONEQUILIBRIUM TECHNIQUES IN MESOSCOPIC TUNNELING STRUCTURES

Let us now examine how the techniques discussed above can be used to derive a perturbation scheme for mesoscopic systems far from equilibrium. We once again recall that the basic difference between construction of equilibrium and nonequilibrium perturbation schemes is that in nonequilibrium one cannot assume that the system returns to its ground state (or a thermodynamic equilibrium state at finite temperatures) as $t \to +\infty$. Irreversible effects break the symmetry between $t = -\infty$ and $t = +\infty$, and this symmetry was heavily exploited in the derivation of the equilibrium perturbation expansion. In nonequilibrium situations one can circumvent this problem by allowing the system to evolve from $-\infty$ to the moment of interest (for definiteness, let us call this instant t_0), and then continues the time evolvement from $t = t_0$ back to $t = -\infty$. The advantage of this procedure is that all expectation values are defined with respect to a well-defined state, i.e., the state in which the system was prepared in the remote past. The price is that one must treat the two time branches on an equal footing.

In the context of tunneling problems the nonequilibrium formalism works as follows. In the remote past the contacts (i.e., the left and right lead) and the central region are decoupled, and each region is in thermal equilibrium. The equilibrium distribution functions for the three regions are characterized by their respective chemical potentials; these do not have to coincide nor are the differences between the chemical potentials necessarily small. The couplings between the different regions are then established and treated as perturbations via the standard techniques of perturbation theory, albeit on the two-branch time contour. It is important to notice that the couplings do not have to be small, e.g., with respect level to spacings or $k_B T$, and typically must be treated to all orders.

VI.   MODEL HAMILTONIAN

We split the total Hamiltonian in three pieces: $H = H_c + H_T + H_{\text{cen}}$, where H_c describes the contacts, H_T is the tunneling coupling between contacts and the interacting region, and H_{cen} models the interacting central region, respectively. Below we discuss each of these terms.

Guided by the typical experimental geometry in which the leads rapidly broaden into metallic contacts, we view electrons in the leads as non-interacting except for an overall self-consistent potential. Thus, the contact Hamiltonian is

$$H_c = \sum_{k, \alpha \in L, R} \varepsilon_{k\alpha} \mathbf{c}_{k\alpha}^\dagger \mathbf{c}_{k\alpha} \ , \tag{40}$$

and the Green functions in the leads for the uncoupled system are:

$$\begin{aligned} g_{k\alpha}^<(t - t') \ &= \ i \langle \mathbf{c}_{k\alpha}^\dagger (t') \mathbf{c}_{k\alpha}(t) \rangle = i f(\varepsilon_{k\alpha}^0) \exp \left[-i \varepsilon_{k\alpha}(t - t') \right] , \tag{41} \\ g_{k\alpha}^{r,a}(t - t') \ &= \ \mp i \theta(\pm t \mp t') \langle \{ \mathbf{c}_{k\alpha}(t), \mathbf{c}_{k\alpha}^\dagger (t') \} \rangle = \mp i \theta(\pm t \mp t') \exp \left[-i \varepsilon_{k\alpha}(t - t') \right] . \tag{42} \end{aligned}$$

Here $f(\varepsilon_{k\alpha}) = \left[\exp[(\varepsilon_{k\alpha} - \mu_\alpha)/k_B T] + 1\right]^{-1}$ is the equilibrium distribution in a given lead.

The coupling constants between the leads and the central (interacting) region depend, in principle, on the actual charge densities (accumulation and depletion regions, charge build-up in the central region, etc.), and they should be determined via a self-consistent calculation. We do not attempt to perform such an analysis, and assume that these parameters are known. Thus we write

$$H_T = \sum_{\substack{k,\alpha \in L, R \\ n}} [V_{k\alpha,n} \mathbf{c}_{k\alpha}^\dagger \mathbf{d}_n + \text{h.c.}] \ . \tag{43}$$

Here, $\{\mathbf{d}_n^\dagger\}$ and $\{\mathbf{d}_n\}$ are the single-electron creation and annihilation operators for the complete and orthonormal set of the states $|n\rangle$ in the interacting region.

The form chosen for the central region Hamiltonian H_{cen} depends on geometry and on the physical behavior being investigated. We will discuss three particular examples in detail. In the first, the central region is taken to consist of non-interacting levels,

$$H_{\text{cen}} = \sum_m \varepsilon_m \mathbf{d}_m^\dagger \mathbf{d}_m \ . \tag{44}$$

Here, $\mathbf{d}_m^\dagger(\mathbf{d}_m)$ creates (destroys) an electron in state m. The choice (44) represents a simple model for resonant tunneling. Below we shall present general results for an arbitrary number of levels, and analyze the case of a single level, which is exactly solvable in detail.

A second example of interest is resonant tunneling with electron-phonon interaction:

$$H_{\text{cen}}^{\text{el}-\text{ph}} = \varepsilon_0 \mathbf{d}^\dagger \mathbf{d} + \mathbf{d}^\dagger \mathbf{d} \sum_{\vec{q}} M_{\vec{q}} [\mathbf{a}_{\vec{q}}^\dagger + \mathbf{a}_{-\vec{q}}] \ . \tag{45}$$

Here, the first term represents a single site, while the second term represents interaction of an electron on the site with phonons: $\mathbf{a}_{\vec{q}}^\dagger(\mathbf{a}_{\vec{q}})$ creates (destroys) a phonon in mode $\vec{q}$, and $M_{\vec{q}}$ is the interaction matrix element. The full Hamiltonian of the system must also include the free-phonon contribution $H_{\text{ph}} = \sum_{\vec{q}} \hbar\omega_{\vec{q}} \mathbf{a}_{\vec{q}}^\dagger \mathbf{a}_{\vec{q}}$. This example, while not exactly solvable, is helpful to show how interactions influence the current. This model is presently under intense study because of its relevance to inelastic effects in molecular electronics. A simple discussion is available in Ref.[1].

The final example consists of an Anderson-type model for electron-electron interactions in the central region:

$$H_{\text{cen}} = \sum_\sigma \varepsilon_0 \mathbf{d}_\sigma^\dagger \mathbf{d}_\sigma + U n_\uparrow n_\downarrow \ . \tag{46}$$

Here σ is a spin-label, n_σ is the occupation number operator of spin-state σ, and U describes the on-site Coulombic repulsion. This model has been the topic of intense study because of the very rich (and complicated) physics that it describes. For example, in the low temperature limit it exhibits Kondo behavior. In the high temperature limit the equation-of-motion technique allows a relatively simple analysis, see [1].

VII.   GENERAL EXPRESSION FOR THE CURRENT

The current from the left contact through left barrier to the central region can be calculated from the time evolution of the occupation number operator of the left contact:

$$J_L = -e\langle \dot{N}_L \rangle = -\frac{ie}{\hbar} \langle [H, N_L] \rangle \ , \tag{47}$$

where $N_L = \sum_{k,\alpha \in L} \mathbf{c}_{k\alpha}^\dagger \mathbf{c}_{k\alpha}$ and $H = H_c + H_T + H_{\text{cen}}$. Since H_c and H_{cen} commute with N_L, one readily finds:

$$J_L = \frac{ie}{\hbar} \sum_{\substack{k,\alpha \in L \\ n}} [V_{k\alpha,n} \langle \mathbf{c}_{k\alpha}^\dagger \mathbf{d}_n \rangle - V_{k\alpha,n}^* \langle \mathbf{d}_n^\dagger \mathbf{c}_{k\alpha} \rangle] \ . \tag{48}$$

Now define two new Green functions (we set $\hbar = 1$, and reintroduce it in the final expression for the current):

$$\begin{aligned}
G_{n,k\alpha}^<(t - t') &\equiv i\langle \mathbf{c}_{k\alpha}^\dagger(t') \mathbf{d}_n(t) \rangle \ , \\
G_{k\alpha,n}^<(t - t') &\equiv i\langle \mathbf{d}_n^\dagger(t') \mathbf{c}_{k\alpha}(t) \rangle \ .
\end{aligned} \tag{49}$$

We see that the current is given by the time-diagonal components of the Green functions defined in (49). These functions have the property $G^<_{k\alpha,n}(t,t) = -\left[G^<_{n,k\alpha}(t,t)\right]^*$, and inserting the time-labels, the current can be expressed as

$$J_L = \frac{2e}{\hbar}\mathrm{Re}\Big\{\sum_{\substack{k,\alpha\in L\\n}} V_{k\alpha,n}G^<_{n,k\alpha}(t,t)\Big\} . \tag{50}$$

Next, one needs an expression for $G^<_{n,k\alpha}(t-t')$. For the present case, with non-interacting leads, a general relation for the contour-ordered Green function $G_{n,k\alpha}(\tau,\tau')$ can be derived rather easily with the equation-of-motion technique. Since the nonequilibrium theory is structurally equivalent to equilibrium theory, it is sufficient to consider the $T=0$ equation-of-motion for the time-ordered Green function $G^t_{n,k\alpha}$:

$$-i\frac{\partial}{\partial t'}G^t_{n,k\alpha}(t-t') = \varepsilon_k G^t_{n,k\alpha}(t-t') + \sum_m G^t_{nm}(t-t')V^*_{k\alpha,m} , \tag{51}$$

where we defined the central region time-ordered Green function function $G^t_{nm}(t-t') = -i\langle T\{\mathbf{d}^\dagger_m(t')\mathbf{d}_n(t)\}\rangle$. Note that it is crucial that the leads be non-interacting; had we allowed interactions in the leads, the equation-of-motion technique would have generated higher order Green functions in (51), and we would not have a closed set of equations.

We can interpret the factors multiplying $G^t_{n,k\alpha}(t-t')$ as the inverse of the contact Green function operator, and introduce a short-hand notation: $G^t_{n,k\alpha}g^{-1}_{k\alpha} = \sum_m G^t_{nm}V^*_{k\alpha,m}$. By operating with $g^t_{k\alpha}$ from right, we arrive at

$$G^t_{n,k\alpha}(t-t') = \sum_m \int dt_1 G^t_{nm}(t-t_1)V^*_{k\alpha,m}g^t_{k\alpha}(t_1-t') . \tag{52}$$

Since the equilibrium and nonequilibrium theories are topologically equivalent, this equation has in nonequilibrium precisely the same form, except that the intermediate time integration runs on the complex contour:

$$G_{n,k\alpha}(\tau,\tau') = \sum_m \int d\tau_1 G_{nm}(\tau,\tau_1)V^*_{k\alpha,m}g_{k\alpha}(\tau_1,\tau') . \tag{53}$$

Here $G_{nm}(\tau,\tau_1)$ is the contour-ordered Green function for the central region. The analytic continuation rules of Table 1 can now be applied, and we find

$$G^<_{n,k\alpha}(t-t') = \sum_m \int dt_1 V^*_{k\alpha,m}[G^r_{nm}(t-t_1)g^<_{k\alpha}(t_1-t') + G^<_{nm}(t-t_1)g^a_{k\alpha}(t_1-t')] , \tag{54}$$

where the Green functions $g^{<,a}$ for the leads are defined in (41),(42). The Fourier transform of (54) is

$$G^<_{n,k\alpha}(\varepsilon) = \sum_m V^*_{k\alpha,m}[G^r_{nm}(\varepsilon)g^<_{k\alpha}(\varepsilon) + G^<_{nm}(\varepsilon)g^a_{k\alpha}(\varepsilon)] , \tag{55}$$

whereby the current (50) becomes

$$J_L = \frac{2e}{\hbar}\int\frac{d\varepsilon}{2\pi}\mathrm{Re}\Big\{\sum_{\substack{k,\alpha\in L\\n,m}} V_{k\alpha,n}V^*_{k\alpha,m}[G^r_{nm}(\varepsilon)g^<_{k\alpha}(\varepsilon) + G^<_{nm}(\varepsilon)g^a_{k\alpha}(\varepsilon)]\Big\} . \tag{56}$$

At this juncture it is useful to convert the momentum summations to energy integration and define a level-width function:

$$\left[\Gamma^L(\varepsilon_k)\right]_{mn} = 2\pi\sum_{\alpha\in L}\varrho_\alpha(\varepsilon_k)V_{\alpha,n}(\varepsilon_k)V^*_{\alpha,m}(\varepsilon_k) , \tag{57}$$

where $\varrho_\alpha(\varepsilon)$ is the density of states. There are two terms in the current expression (56). Consider, for example, the piece involving G^r_{mn}, which we evaluate as [11]

$$\begin{aligned}
\frac{2e}{\hbar}\int\frac{d\varepsilon}{2\pi}\int d\varepsilon_k\Gamma^L(\varepsilon_k)\mathrm{Re}\big[G^r(\varepsilon)i\delta(\varepsilon-\varepsilon_k)f_L(\varepsilon)\big] &= \frac{2e}{\hbar}\int\frac{d\varepsilon}{2\pi}f_L(\varepsilon)\Gamma^L(\varepsilon)\mathrm{Re}\big[iG^r(\varepsilon)\big] \\
&= -\frac{2e}{\hbar}\int\frac{d\varepsilon}{2\pi}f_L(\varepsilon)\Gamma^L(\varepsilon)\mathrm{Im}\big[G^r(\varepsilon)\big] \\
&= \frac{ie}{\hbar}\int\frac{d\varepsilon}{2\pi}\Gamma^L(\varepsilon)f_L(\varepsilon)[G^r(\varepsilon)-G^a(\varepsilon)] . \tag{58}
\end{aligned}$$

Similar manipulations can be applied to the other term, and the current from left (right) contact to central region becomes

$$J_{L(R)} = \frac{ie}{\hbar} \int \frac{d\varepsilon}{2\pi} \mathrm{Tr}\left(\mathbf{\Gamma}^{L(R)}(\varepsilon) \left\{ \mathbf{G}^<(\varepsilon) + f_{L(R)}(\varepsilon)\left[\mathbf{G}^r(\varepsilon) - \mathbf{G}^a(\varepsilon) \right] \right\} \right) . \tag{59}$$

Here, the boldface notation indicates that the level-width function $\mathbf{\Gamma}$ and the central-region Green functions $\mathbf{G}^{<,r}$ are matrices in the central-region indices m, n. In steady state, the current will be uniform, so that $J = J_L = -J_R$, and one can symmetrize the current: $J = (J_L + J_L)/2 = (J_L - J_R)/2$. Using (59) leads to the general expression for the d.c.-current:

$$J = \frac{ie}{2\hbar} \int \frac{d\varepsilon}{2\pi} \mathrm{Tr}\left\{ \left[\mathbf{\Gamma}^L(\varepsilon) - \mathbf{\Gamma}^R(\varepsilon) \right] \mathbf{G}^<(\varepsilon) + \left[f_L(\varepsilon)\mathbf{\Gamma}^L(\varepsilon) - f_R(\varepsilon)\mathbf{\Gamma}^R(\varepsilon) \right] \left[\mathbf{G}^r(\varepsilon) - \mathbf{G}^a(\varepsilon) \right] \right\} . \tag{60}$$

Often the energy-dependence of the level-width function is not very important, and further simplification can be achieved by making assumptions on this energy-dependence. In particular, if the left and right line-width functions are proportional to each other, i.e., $\mathbf{\Gamma}^L(\varepsilon) = \lambda\mathbf{\Gamma}^R(\varepsilon)$, a very simple final result can be be achieved. We observe that the current can be written as $J \equiv xJ_L - (1-x)J_R$, which gives, using (60):

$$J = \frac{ie}{\hbar} \int \frac{d\varepsilon}{2\pi} \mathrm{Tr}\left(\mathbf{\Gamma}^R(\varepsilon) \left\{ \left[\lambda x - (1-x) \right] \mathbf{G}^<(\varepsilon) + \left[\lambda x f_L - (1-x)f_R \right] \left[\mathbf{G}^r(\varepsilon) - \mathbf{G}^a(\varepsilon) \right] \right\} \right) . \tag{61}$$

The arbitrary parameter x is now fixed so that the first term vanishes, i.e., $x = 1/(1+\lambda)$, which results in

$$\begin{aligned}
J &= \frac{ie}{\hbar} \int \frac{d\varepsilon}{2\pi} [f_L(\varepsilon) - f_R(\varepsilon)]\mathcal{T}(\varepsilon) , \\
\mathcal{T}(\varepsilon) &= \mathrm{Tr}\left\{ \frac{\mathbf{\Gamma}^L(\varepsilon)\mathbf{\Gamma}^R(\varepsilon)}{\mathbf{\Gamma}^L(\varepsilon) + \mathbf{\Gamma}^R(\varepsilon)} \left[\mathbf{G}^r(\varepsilon) - \mathbf{G}^a(\varepsilon) \right] \right\} .
\end{aligned} \tag{62}$$

The ratio is well-defined because the $\mathbf{\Gamma}$-matrices are proportional. The difference between the retarded and advanced Green functions is essentially the density of states. Despite the apparent similarity of (62) to the Landauer formula, it is important to bear in mind that, in general, there is no immediate connection between the quantity $\mathcal{T}(\varepsilon)$ and the transmission coefficient $T(\varepsilon)$. In particular, when inelastic scattering is present, there is no such connection. In later sections, where we analyze a non-interacting central region, a connection with the transmission coefficient *can* be established. Further, it is possible to derive an analogous result for the average of the time-dependent current [1].

The results for the current derived in this section [(60) or (62)] form a starting point for many calculations. As such, they are powerful formal results, however, one must bear in mind that they involve both the full correlation function and the retarded Green functions *in the presence of tunneling*, and it is by no means obvious that these Green functions are easily calculable. The usefulness of (60),(62) depends on whether one is able to devise suitable calculation schemes for the Green functions. Below we shall see some examples of how this is done in practice.

VIII.   NON-INTERACTING RESONANT-LEVEL MODEL

In the non-interacting case, the Hamiltonian is $H = H_c + H_T + H_{\mathrm{cen}}$, where $H_{\mathrm{cen}} = \sum_n \varepsilon_n \mathbf{d}_n^\dagger \mathbf{d}_n$. It is straightforward to derive the Dyson equation for the retarded Green function:

$$\mathbf{G}^r(\varepsilon) = \mathbf{g}^r(\varepsilon) + \mathbf{g}^r(\varepsilon)\mathbf{\Sigma}^r(\varepsilon)\mathbf{G}^r(\varepsilon) , \tag{63}$$

where

$$\Sigma_{nn'}^r(\varepsilon) = \sum_{k\alpha \in L,R} V_{k\alpha,n}^* g_{k\alpha}^r(\varepsilon) V_{k\alpha,n'} , \tag{64}$$

and $g_{k\alpha}^r$ is given by (41). Since the lesser self-energy follows explicitly from (64) by analytic continuation, one can immediately write down an expression for the lesser function $G^<$ using the Keldysh equation (39) for $G^<$:

$$\mathbf{G}^<(\varepsilon) = \mathbf{G}^r(\varepsilon)\mathbf{\Sigma}^<(\varepsilon)\mathbf{G}^a(\varepsilon) . \tag{65}$$

In general, the Dyson equation for the retarded Green function requires matrix inversion. In the case of a single level, the scalar equations can be readily solved. The retarded (advanced) self-energy is

$$\Sigma^{r,a}(\varepsilon) = \sum_{k\alpha \in L,R} \frac{|V_{k\alpha}|^2}{\varepsilon - \varepsilon_{k\alpha} \pm i\eta} = \Lambda(\varepsilon) \mp \frac{i}{2}\Gamma(\varepsilon) , \tag{66}$$

where the real and imaginary parts contain "left" and "right" contributions: $\Lambda(\varepsilon) = \Lambda^L(\varepsilon) + \Lambda^R(\varepsilon)$ and $\Gamma(\varepsilon) = \Gamma^L(\varepsilon) + \Gamma^R(\varepsilon)$. The lesser self-energy is

$$\Sigma^<(\varepsilon) = \sum_{k\alpha \in L,R} |V_{k\alpha}|^2 g_{k\alpha}^<(\varepsilon) = i[\Gamma^L(\varepsilon)f_L(\varepsilon) + \Gamma^R(\varepsilon)f_R(\varepsilon)] . \tag{67}$$

Using the identity

$$G^r G^a = \frac{G^r - G^a}{(G^{a-1} - G^{r-1})} = \frac{A(\varepsilon)}{\Gamma(\varepsilon)} , \tag{68}$$

where $A(\varepsilon) = i[G^r(\varepsilon) - G^a(\varepsilon)]$ is the spectral function, one can write $G^<$ in a "pseudoequilibrium" form:

$$G^<(\varepsilon) = iA(\varepsilon)\bar{f}(\varepsilon) , \tag{69}$$

where

$$\bar{f}(\varepsilon) = \frac{\Gamma^L(\varepsilon)f_L(\varepsilon) + \Gamma^R(\varepsilon)f_R(\varepsilon)}{\Gamma(\varepsilon)} ,$$

$$A(\varepsilon) = \frac{\Gamma(\varepsilon)}{[\varepsilon - \varepsilon_0 - \Lambda(\varepsilon)]^2 + [\Gamma(\varepsilon)/2]^2} . \tag{70}$$

With these expressions the evaluation of the current (60) is straightforward:

$$\begin{aligned} J &= -\frac{e}{2\hbar} \int \frac{d\varepsilon}{2\pi} A(\varepsilon) \Big\{ \big[\Gamma^L(\varepsilon) - \Gamma^R(\varepsilon)\big]\bar{f}(\varepsilon) - \big[f_L(\varepsilon)\Gamma^L(\varepsilon) - f_R(\varepsilon)\Gamma^R(\varepsilon)\big] \Big\} \\ &= \frac{e}{\hbar} \int \frac{d\varepsilon}{2\pi} \frac{\Gamma^L(\varepsilon)\Gamma^R(\varepsilon)}{[\varepsilon - \varepsilon_0 - \Lambda(\varepsilon)]^2 + [\Gamma(\varepsilon)/2]^2} [f_L(\varepsilon) - f_R(\varepsilon)] . \end{aligned} \tag{71}$$

The factor multiplying the difference of the Fermi functions is the elastic transmission coefficient $T(\varepsilon)$. (Can you prove this?) It is important to understand the difference between this result and the result obtained in the previous section (despite the similarity of appearance): There, (62) gives the current for a fully interacting system, and the evaluation of the retarded and advanced Green functions requires a consideration of interactions (e.g., electron-electron, electron-phonon, and spin-flip) in addition to tunneling back and forth to the contacts. To further emphasize the difference, let us now suppose that the Green function for the interacting central region can be solved: $G^{r,a}(\varepsilon) = [\varepsilon - \varepsilon_0 - \lambda(\varepsilon) \pm i\gamma(\varepsilon)/2]^{-1}$, where λ and $\gamma/2$ are the real and imaginary parts of the self-energy (including interactions *and* tunneling). Then the interacting result for proportionate coupling (62) becomes

$$J = \frac{e}{\hbar} \int \frac{d\varepsilon}{2\pi} [f_L(\varepsilon) - f_R(\varepsilon)] \frac{\Gamma^L(\varepsilon)\Gamma^R(\varepsilon)}{\Gamma^L(\varepsilon) + \Gamma^R(\varepsilon)} \frac{\gamma(\varepsilon)}{[\varepsilon - \varepsilon_0 - \lambda(\varepsilon)]^2 + [\gamma(\varepsilon)/2]^2} . \tag{72}$$

This result coincides with the non-interacting current expression (71) if $\lambda(\varepsilon) \to \Lambda(\varepsilon)$ and $\gamma(\varepsilon) \to \Gamma(\varepsilon) = \Gamma^R(\varepsilon) + \Gamma^L(\varepsilon)$.

IX. MASTER EQUATION APPROACH FOR RESONANT TUNNELLING

The Master Equation (ME) approach is often a quick (and dirty) way of getting to results. In the present, exactly solvable case the results of the Keldysh approach and the ME, should of course agree. Let us verify this. In ME, on operates with the occupation probabilities of a given state, P_n. In the present case, the two possible states are "an empty state" and "a filled state", P_0 and P_1, respectively. Naturally, $P_0 + P_1 = 1$. To form a link to the Green function formulation, we note

$$P_1(t) = \langle d^\dagger(t)d(t) \rangle = -iG^<(t,t) = \int \frac{d\epsilon}{2\pi i} G^<(\epsilon). \tag{73}$$

Using (69), we calculate as follows (from this on, we work in a so-called Wide-Band Limit (WBL), which means that (i) the real part of the self-energy is set to zero, and (ii) the imaginary part, i.e., the Γ's, are assumed to be energy

independent):

$$
\begin{aligned}
P_1 &= \int \frac{d\epsilon}{2\pi} \frac{[\Gamma^L f_L(\epsilon) + \Gamma^R f_R(\epsilon)]}{(\epsilon - \epsilon_0)^2 + (\Gamma/2)^2} \times \left(\frac{\Gamma}{\Gamma} \right) \\
&\to \int d\epsilon \frac{[\Gamma^L f_L(\epsilon) + \Gamma^R f_R(\epsilon)]}{\Gamma} \delta(\epsilon - \epsilon_0) \\
&= \frac{[\Gamma^L f_L(\epsilon_0) + \Gamma^R f_R(\epsilon_0)]}{\Gamma}.
\end{aligned}
\tag{74}
$$

In the second line the limit means that we are concerned with the weak coupling limit; this is necessary because the ME is inherently low-order perturbation approach (Fermi Golden Rule). Nevertheless, (**??**) is a bit intriguing result, because it does not depend on the absolute value of the couplings, only on their *relative* strength.

Now let us the same using ME approach. Now we simply write down rate-equations for the occupations, using "common sense":

$$
\begin{aligned}
\dot{P}_1 &= \Gamma_{0\to1} P_0 - \Gamma_{1\to0} P_1 \\
\dot{P}_0 &= \Gamma_{1\to0} P_1 - \Gamma_{0\to1} P_0 \\
1 &= P_1 + P_0,
\end{aligned}
\tag{75}
$$

where (note that Golden Rule based Γ's in the ME are *rates*, not energies as in the GF formulation)

$$
\begin{aligned}
\hbar \Gamma_{0\to1} &= \Gamma^L f_L + \Gamma^R f_R \\
\hbar \Gamma_{1\to0} &= \Gamma^L (1 - f_L) + \Gamma^R (1 - f_R).
\end{aligned}
\tag{76}
$$

The reader is urged to make sure that she understands the reasoning behind these rates! In the stationary case, $\dot{P}_0 = \dot{P}_1 = 0$, one readily finds

$$
\begin{aligned}
P_1 &= \frac{\Gamma_{0\to1}}{\Gamma_{0\to1} + \Gamma_{1\to0}} = \frac{\Gamma^L f_L + \Gamma^R f_R}{\Gamma^L + \Gamma^R} \\
P_0 &= 1 - P_1 = \frac{\Gamma^L (1 - f_L) + \Gamma^R (1 - f_R)}{\Gamma^L + \Gamma^R},
\end{aligned}
\tag{77}
$$

in agreement with Eq.(74).

We can also evaluate the current. In the GF language we had

$$
\begin{aligned}
I &= \frac{e}{\hbar} \int \frac{d\epsilon}{2\pi} \frac{\Gamma^L \Gamma^R}{(\epsilon - \epsilon_0)^2 + (\Gamma/2)^2} [f_L(\epsilon) - f_R(\epsilon)] \\
&\to \frac{e}{\hbar} \frac{\Gamma^R \Gamma^L}{\Gamma} [f_L(\epsilon_0) - f_R(\epsilon_0)]
\end{aligned}
\tag{78}
$$

In ME, we calculate

$$
\begin{aligned}
I &= e[P_0 \Gamma^L_{0\to1} - P_1 \Gamma^L_{1\to0}] \\
&= \frac{e}{\hbar} \frac{1}{\Gamma} \{ [\Gamma^L (1 - f_L) + \Gamma^R (1 - f_R)] \Gamma^L f_L - (\Gamma^L f_L + \Gamma^R f_R) \Gamma^L (1 - f_L)] \} \\
&= \frac{e}{\hbar} \frac{\Gamma^R \Gamma^L}{\Gamma} [(1 - f_R) f_L - f_R (1 - f_L)] = \frac{e}{\hbar} \frac{\Gamma^R \Gamma^L}{\Gamma} (f_L - f_R),
\end{aligned}
\tag{79}
$$

in agreement with the GF result. (Again, do you understand the first line in this calculation?)

Finally, it may be of interest to inquire whether one can *derive* the ME from the GF formalism. The answer should be "yes", but I'm not aware of any elegant demonstrations. The argument could go roughly as given below, but there are several places where yellow warning lamps are blinking. You are encouraged to reflect upon them! I leave for you the pleasure of finding them.

For completeness, I give quite a few details. The hamiltonian is

$$
H = \sum \epsilon_{k\alpha} c^\dagger_{k\alpha} c_{k\alpha} + \epsilon_0 d^\dagger d + \sum (V_{k\alpha} c^\dagger_{k\alpha} d + V^*_{k\alpha} d^\dagger c_{k\alpha}).
\tag{80}
$$

In the equation-of-motion technique we need the following commutators:

$$[d, H] = \sum V_{k\alpha}^* c_{k\alpha} + \epsilon_0 d$$
$$[d^\dagger, H] = -(\sum V_{k\alpha} c_{k\alpha}^\dagger + \epsilon_0 d^\dagger)$$
$$[c_{k\alpha}, H] = \epsilon_{k\alpha} c_{k\alpha} + V_{k\alpha} d \tag{81}$$
$$[c_{k\alpha}^\dagger, H] = -(\epsilon_{k\alpha} c_{k\alpha}^\dagger + V_{k\alpha}^* d^\dagger)$$

The equation-of-motion for P_1 is

$$i\frac{\partial P_1}{\partial t} = \langle [d^\dagger, H] d \rangle + \langle d^\dagger [d, H] \rangle \tag{82}$$
$$= -\sum V_{k\alpha} \langle c_{k\alpha}^\dagger d \rangle + \sum V_{k\alpha}^* \langle d^\dagger c_{k\alpha} \rangle. \tag{83}$$

The hybrid functions have the following equations of motion:

$$i\frac{\partial}{\partial t} \langle c_{k\alpha}^\dagger d \rangle = -\epsilon_{k\alpha} \langle c_{k\alpha}^\dagger d \rangle - V_{k\alpha}^* \langle d^\dagger d \rangle + \sum V_{k'\alpha'}^* \langle c_{k\alpha}^\dagger c_{k'\alpha'} \rangle + \epsilon_0 \langle c_{k\alpha}^\dagger d \rangle \tag{84}$$

$$i\frac{\partial}{\partial t} \langle d^\dagger c_{k\alpha} \rangle = \epsilon_{k\alpha} \langle d^\dagger c_{k\alpha} \rangle + V_{k\alpha} \langle d^\dagger d \rangle - \sum V_{k'\alpha'} \langle c_{k'\alpha'}^\dagger c_{k\alpha} \rangle - \epsilon_0 \langle d^\dagger c_{k\alpha} \rangle, \tag{85}$$

or, in Fourier space,

$$[\omega - (\epsilon_0 - \epsilon_{k\alpha})] \langle c_{k\alpha}^\dagger d \rangle_\omega = -V_{k\alpha}^* \langle d^\dagger d \rangle_\omega + V_{k\alpha}^* 2\pi\delta(\omega) f_\alpha(\epsilon_{k\alpha}) \tag{86}$$
$$[\omega - (\epsilon_{k\alpha} - \epsilon_0)] \langle d^\dagger c_{k\alpha} \rangle_\omega = V_{k\alpha} \langle d^\dagger d \rangle_\omega - V_{k\alpha} 2\pi\delta(\omega) f_\alpha(\epsilon_{k\alpha}). \tag{87}$$

Here we used the fact that the contacts are noninteracting and in equilibrium, in order to write $\langle c_{k\alpha}^\dagger c_{k'\alpha'} \rangle = \delta_{kk'}\delta_{\alpha,\alpha'} f_\alpha(\epsilon_{k\alpha})$. Substituting these in the Fourier-transform of (83) gives

$$\omega \langle d^\dagger d \rangle_\omega = -\sum_{k\alpha} |V_{k\alpha}|^2 \left[2\pi\delta(\omega) f_\alpha(\epsilon_{k\alpha}) - \langle d^\dagger d \rangle_\omega \right] \left[\frac{1}{\omega + i\eta - (\epsilon_0 - \epsilon_{k\alpha})} + \frac{1}{\omega + i\eta - (\epsilon_{k\alpha} - \epsilon_o)} \right], \tag{88}$$

where we by hand set $\omega \to \omega + i\eta$. We try to proceed within the spirit of WBL. Consider first the term proportional to $f_\alpha(\epsilon_{k\alpha})$ (call this (1)). Because of $\delta(\omega)$, the principal value contributions cancel and we find

$$(1) \to -2\pi\delta(\omega) \sum_{k\alpha} |V_{k\alpha}|^2 f_\alpha(\epsilon_{k\alpha})(-2i\pi)\delta(\epsilon_0 - \epsilon_{k\alpha}) = 2\pi i \delta(\omega) \sum_\alpha \Gamma^\alpha f_\alpha(\epsilon_0), \tag{89}$$

where we identified $\Gamma^\alpha = \sum_k 2\pi |V_{k\alpha}|^2 \delta(\epsilon_0 - \epsilon_{k\alpha})$. The second term is evaluated in a similar fashion:

$$(2) \to \langle d^\dagger d \rangle_\omega \sum_{k\alpha} |V_{k\alpha}|^2 \left[\frac{1}{\omega + i\eta - (\epsilon_0 - \epsilon_{k\alpha})} + \frac{1}{\omega + i\eta - (\epsilon_{k\alpha} - \epsilon_o)} \right] = -i \langle d^\dagger d \rangle_\omega \sum_\alpha \Gamma^\alpha, \tag{90}$$

where we again used the WBL to suppress the principal value parts, and to ignore the energy-dependence of the Γ's. Putting the pieces together, we have arrived at

$$\omega \langle d^\dagger d \rangle_\omega = i \sum_\alpha \Gamma^\alpha [2\pi\delta(\omega) f_\alpha(\epsilon_0) - \langle d^\dagger d \rangle_\omega]. \tag{91}$$

Going back to time-domain with $\int d\omega/(2\pi) \exp(-i\omega t)$, introducing the P's, and recalling that $P_0 + P_1 = 1$, allows us to write

$$\frac{\partial P_1}{\partial t} = \sum_\alpha \Gamma^\alpha [f_\alpha(\epsilon_0)(P_0 + P_1) - P_1]$$
$$= \sum_\alpha \Gamma^\alpha f_\alpha(\epsilon_0) P_0 - \sum_\alpha \Gamma^\alpha (1 - f_\alpha(\epsilon_0)) P_1, \tag{92}$$

in perfect agreement with the ME.

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[9] In what follows we distinguish wavefunctions and operators in the interaction picture with a caret.

[10] For simplicity we suppress the single-body potential: it can, with a suitable redefinition, be absorbed in the free Green function. The reader is urged to check how this works out in practice.

[11] In the calculation leading to (58) we treat $\Gamma_{mn}(\varepsilon)$ as real and suppressed the indices mn. The above result, however, carries over to the general case, and the reader is urged to check this.