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Supriyo Datta

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GENERALIZED 'PROBE' MODEL FOR ARBITRARY DEPHASING MECHANISMS

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ABSTRACT

It has been shown earlier that in the linear response regime, dephasing by point scatterers (within the self-consistent Born approximation) can be visualized in terms of point voltage probes attached to each space and energy coordinate \((r,E)\). In this paper we derive a generalized linear response equation starting from the non-equilibrium Green function formalism that can be used to describe any dephasing process in any approximation. The dephasing is characterized by a 'reservoir function' which can be evaluated from the self-energy. The linear response equation can be visualized in terms of voltage probes but with individual probes connected to each pair of spatial coordinates and to each energy \((r,r',E)\). Unlike point scatterers, this generalized 'probe' model allows us to introduce phase relaxation without necessarily introducing momentum relaxation. We obtain explicit expressions for the transmission \(T_{ij}\) from terminal \(j\) to terminal \(i\) by eliminating the 'floating probes' inside the device. These expressions for \(T_{ij}\) clearly show the role of the exclusion principle in determining the transmission. Proof of reciprocity in multiterminal conductors is provided. We also present a simple illustrative example calculating \(T_{ij}\) for a short single-moded electron waveguide with electron-phonon interactions. An important difference between the present formulation and usual linear response theory is that the electrochemical potential difference is treated as the driving force; however, we do not neglect the self-consistent fields that appear in an interacting system when a small bias is applied.
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1. Introduction

The non-equilibrium Green function formalism developed by Keldysh\(^{(1)}\) and by Kadanoff and Baym\(^{(2)}\) provides a general framework for including phase-breaking processes into transport problems. This approach was originally applied primarily to homogeneous systems and several excellent reviews are available\(^{-7}\). In homogeneous systems it is customary to make the so-called 'gradient expansion' which is inapplicable to mesoscopic devices with rapid spatial variations in the potential. However, the basic formalism is quite general and has been applied to tunneling devices\(^{(8)}\), to current fluctuations in mesoscopic devices\(^{(9,10)}\), to resonant tunneling diodes\(^{(11,12)}\) and to single electron charging effects\(^{(13)}\).

Starting from this formalism we have earlier derived the following linear response equation assuming that the phase-breaking is caused by point scatterers\(^{(14)}\) which are treated in the self-consistent Born approximation.

\[
I(r_1,E_1) = \frac{e}{h} \int dr_2 \int dE_2 T(r_1,E_1;r_2,E_2) \left[ \mu(r_1,E_1) - \mu(r_2,E_2) \right] \tag{1.1}
\]

The energy-dependent potential \(\mu(r,E)\) was defined as follows

\[
f(r,E) = \frac{n(r,E)}{N(r,E)} = \frac{1}{e^{(E-\mu(r,E))/k_B T} + 1} \tag{1.2}
\]

Here \(n(r,E)\) is the electron density per unit energy and \(N(r,E)\) is the local density of states. Note that this definition involves no loss of generality – any function \(f(r,E)\) can be expressed in this form. If \(f(r,E)\) is a Fermi-Dirac function then \(\mu(r,E)\) is independent of energy \((E)\) and we can reduce Eq. (1.1) to the form\(^{(15)}\)

\[
\tilde{I}(r_1) = \frac{e}{h} \int dr_2 \tilde{T}(r_1,r_2) \left[ \mu(r_1) - \mu(r_2) \right] \tag{1.3}
\]

For a given device structure (such as the one shown in Fig. 1) Eq. (1.1) or (1.3) can be solved by first computing \(\mu(r,E)\) for points \(r\) lying within the device (where \(I(r,E) = 0\)) assuming the boundary condition that \(\mu(r,E) = \mu_i\) in contact 'i'. We then compute \(I(r,E)\) in the contacts and integrate it over each contact 'i' over all energy to obtain the corresponding terminal
Fig. 1: Sketch of a generic multiterminal device showing the terminal currents and potentials.
current $I_i$:

$$I_i = \int_{r \in \text{contact } i} dr \int dE \ I(r,E)$$  \hspace{1cm} (1.4)

It should be mentioned that the assumption of a constant electrochemical potential inside the contacts can only be justified if we **assume** that the contacts are **infinitely** conductive regions in zero magnetic field. Consequently there appears a contact resistance of $(2e^2/h)M$ ($M$: number of transverse modes in the leads) at the device-contact interfaces just as it does when using the **Landauer formula**\(^{(16)}\): $G = (e^2/h)T$.

**'Probe' model**

Eq. (1.3) looks like Büttiker's multiprobe formula\(^{(17)}\)

$$I_i = \frac{e}{h} \sum_j \tilde{T}_{ij} \left[\mu_i - \mu_j\right]$$  \hspace{1cm} (1.5)

extended to a continuous distribution of probes. This suggests that phase-breaking by point scatterers can be simulated using point-like floating probes with the appropriate coupling, in agreement with the phenomenological approach pioneered by Büttiker\(^{(18-20)}\). This result has also been derived from linear response theory assuming zero temperature and elastic scattering\(^{(21)}\).

Eq. (1.1) too can be visualized in terms of the 'probe' model, but with a floating probe connected to each space and energy coordinate $r$ and $E$. If the probes at a point $r$ for different energies $E$ float to a common potential $\mu(r)$ then Eq. (1.1) reduces to (1.3). This could happen if the inelastic scattering were strong enough to 'short' out the probes at different energies, so that any imbalance in the potential would cause large 'vertical' currents to flow from one energy to another. However, even if there is no inelastic scattering the potential $\mu(r,E)$ could be nearly independent of energy if the temperature is low enough that transport occurs in a very small range of energies. If the transmission characteristics are nearly uniform over this energy range then different energy channels will tend to stay in equilibrium automatically, at least to
first-order in $eV_A/k_BT$ ($V_A$: applied bias). Low temperature mesoscopic experiments possibly belong to this category, so that Eq. (1.3) can be used instead of Eq. (1.1). However, it is likely that in smaller structures interesting quantum effects will be observed at higher temperatures where different energy channels are significantly out of equilibrium and Eq. (1.3) cannot be used in place of (1.1).

Eq. (1.3) has been used to study the effect of dephasing on transport in mesoscopic systems\textsuperscript{(20,22)}. It has also been shown that it reduces to the diffusion equation in the macroscopic limit and yields the correct values for the diffusion coefficient\textsuperscript{(22a,23)}. However one major limitation of this point scatterer model is that phase relaxation is always accompanied by momentum relaxation. It is desirable to have a model for which the phase-breaking time ($\tau_\phi$) and the momentum relaxation time ($\tau_m$) are not necessarily equal, since it is well-known that at low temperatures $\tau_\phi \neq \tau_m$. This requires us to go beyond point scatterers.

Beyond point scatterers

The basic quantities one calculates (at steady-state) in the Keldysh formalism are the correlation function $-iG^\omega(r,r';E)$ and the spectral function $A(r,r',E)$. The simplicity of the point scatterer model arises from the fact that one can describe transport solely in terms of the diagonal elements of these functions which can be identified with the electron density per unit energy $n(r,E)$ and the local density of states $N(r,E)$.

$$2\pi n(r,E) = -i \, G^\omega(r,r,E) \tag{1.6a}$$
$$2\pi N(r,E) = A(r,r,E) \tag{1.6b}$$

One can then define a 'potential' $\mu(r,E)$ (see Eq. 1.2)) and the linear response equation, Eq. (1.1), is obtained by linearizing the kinetic equation about the equilibrium solution: $I(r,E) = 0$ and $\mu(r,E) = \mu_{eq}$ (constant).

As we go beyond the point scatterer model, we cannot describe transport in terms of the diagonal elements any more: the kinetic equation involves the full correlation function
We can now define a ‘potential’ \( \mu(r, r'; E) \) by analogy with Eq. (1.2):

\[
f(r, r', E) = \frac{-iG^<(r, r', E)}{A(r, r', E)} \frac{1}{e^{(E-\mu(r, r', E))/k_B T} + 1}
\]

(1.7)

Note that the functions \( f(r, r', E) \) and \( \mu(r, r', E) \) are in general complex. However, they are Hermitian, that is,

\[
f(r, r', E) = f(r', r, E)^* \quad \text{(1.8a)}
\]

\[
\mu(r, r', E) = \mu(r', r, E)^* \quad \text{(1.8b)}
\]

This is because the functions \(-iG^<\) and \( A \) are Hermitian.

In the linear response regime we can expect the external current to depend linearly on the potentials, in analogy with Eq. (1.1).

\[
I(\rho_1, E_1) = \frac{e}{h} \int d\rho_2 \int dE_2 \ X(\rho_1, E_1; \rho_2, E_2) \left[ \mu(\rho_1, E_1) - \mu(\rho_2, E_2) \right]
\]

(1.9)

where \( \rho_1 = (r_1, r'_1) \) and \( \rho_2 = (r_2, r'_2) \). Indeed in this paper, we will derive Eq. (1.9) by linearizing the kinetic equation, without invoking any specific model for the phase-breaking processes within the device. We obtain an explicit expression for the kernel \( T(\rho_1, E_1; \rho_2, E_2) \) in terms of a reservoir conductance function \( g_R(\rho_1, E_1; \rho_2, E_2) \) which can be evaluated in a straightforward manner from the self-energy function for any dephasing process in any approximation. Example calculations of \( g_R \) are provided for electron-phonon and electron-electron interactions in the self-consistent Born approximation (see Appendix B).

Eq. (1.9) can be solved for a given device structure (Fig. 1) in much the same way as we solve Eq. (1.1) or (1.3). We first obtain \( \mu(\rho, E) \) everywhere within the device (where \( I(\rho, E) = 0 \)) assuming that \( \mu(\rho, E) = \mu_i \), if the pair of points \( \rho = (r, r') \) both lie inside the same contact ‘i’.

Once we have computed \( \mu(\rho, E) \) inside the device, we can calculate \( I(\rho, E) \) in the contacts and integrate over each contact ‘i’ and over all energy to obtain the terminal current \( I_i \).

Actually (see Appendix C) we find an additional component to the terminal current which could be non-zero if the dephasing processes in the contacts are non-local. However, this
component vanishes if we assume that the phase-breaking is caused by point scatterers with the **contacts**. This assumption also leads to conceptual and practical simplifications since 'mixed' points $\mathbf{r} = (\mathbf{r}, \mathbf{r}')$, with $\mathbf{r}$ inside one contact and $\mathbf{r}'$ inside the device or another contact, get decoupled from Eq. (1.9). It seems that no essential physics is lost by making this assumption since the contacts are idealized regions (with infinite conductivity and zero magnetic field) sufficiently removed from the interesting part of the device. Non-local dephasing processes in the contacts blur the demarcation between device and contact and lead to conceptual complications as discussed above. We leave it to future work to resolve the interesting questions raised by contacts with non-local dephasing processes.

**Special Cases**

Eq. (1.9) can be simplified in special circumstances. For example, if the dephasing processes are purely elastic, then it can be shown that the kernel has the form

$$T(\rho_1, \rho_2; E) \Rightarrow \left\{ \frac{\partial f_{\text{eq}}(E)}{\partial E} \right\} T(\rho_1, \rho_2; E) \delta(E_1 - E_2)$$

where $f_{\text{eq}}(E)$ is the equilibrium Fermi-Dirac function. Eq. (1.9) then simplifies to

$$I(\rho_1, E) = \frac{e}{h} \left\{ \frac{\partial f_{\text{eq}}(E)}{\partial E} \right\} \int d\rho_2 \ T(\rho_1, \rho_2; E) [\mu(\rho_1, E) - \mu(\rho_2, E)] \quad (1.10)$$

In this case each energy $E$ acts as an independent channel and the conductance can be expressed in the form $G = \int dE (-\partial f_{\text{eq}}(E)/\partial E) G(E)$.

If the temperature is low enough such that the propagation characteristics of the electrons is nearly uniform over the range of energies $(E_F \pm \text{a few } k_B T)$ where transport takes place then it can be shown that the kernel has the form

$$T(\rho_1, E_1; \rho_2, E_2) = \tilde{T}(\rho_1, \rho_2) \delta(E_1 - E_2) \delta(E_2 - E_F)$$

Eq. (1.9) then simplifies to a form analogous to Eq. (1.3):
\[ \tilde{I}(\rho_1) = \frac{e}{h} \int d\rho_2 \tilde{T}(\rho_1, \rho_2)(\mu(\rho_1) - \mu(\rho_2)) \]  

(1.11)

This \textbf{form} is also valid at high temperatures if the inelastic scattering is strong enough to maintain different energy channels in \textbf{equilibrium} such that the potential \( \mu(\rho, E) \) is independent of energy.

\textit{Biittiker} formula

It has been shown earlier that both Eq. (1.1) and Eq. (1.3) can be reduced to the \textit{Biittiker formula}, Eq. (1.5), by eliminating the floating probes within the device. This yields an expression for the transmission \( \tilde{T}_{ij} \) from contact 'j' to contact 'i' in the form of an infinite series whose \( n \)th term represents the transmission \( \tilde{T}_{ij}^{(n)} \) after suffering 'n' phase-breaking processes with the device. Eqs. (1.9) and (1.11) can also be reduced to the \textit{Biittiker} formula using much the same procedure to obtain explicit expressions for \( \tilde{T}_{ij} \). These expressions clearly show the role of the exclusion principle in determining the transmission. It will also be shown that the coefficients \( \tilde{T}_{ij} \) in multiterminal conductors obey reciprocity.

\textit{Outline} of paper

The outline of this paper is depicted in Fig. 2. We start with a \textbf{brief} review of the \textbf{non-equilibrium} Green function formalism (Section 2). We then linearize the kinetic equation about the \textbf{equilibrium} solution (Section 3) and calculate the terminal current (Section 4) to obtain Eq. (1.9) with an explicit expression for \( T(\rho_1, E_1; \rho_2, E_2) \). Next we derive the 'zero' temperature linear response equation, Eq. (1.11) and obtain an expression for \( \tilde{T}(\rho_1, \rho_2) \) (Section 5). Finally we reduce the linear response equation to the \textit{Biittiker formula} and obtain expressions for the transmission \( \tilde{T}_{ij} \) (Section 6). We then present a simple illustrative example with an actual calculation of \( \tilde{T}_{ij} \) for a short single-moded electron waveguide with electron-phonon interactions (Section 7). We conclude with a \textbf{brief} summary of the main results (Section 8).
Section 2

Non-equilibrium Green function formalism (Steady-state)

Section 3

Linearize about the equilibrium solution

Section 4

Treat contacts explicitly to obtain terminal currents: Eq. (1.9)

Section 5

Simplify for 'zero' temperature: Eq. (1.11)

Section 6

Eliminate internal variables to obtain Biittiker formula with an explicit expression for $T_{ij}$: non-zero as well as 'zero' temperature

Section 7

Simple illustrative example: actual calculation of $T_{ij}$ for a short single-noded electron waveguide with electron-phonon interactions

Fig. 2: Outline of the paper.
2. **Non-equilibrium Green function** formalism

In this section we will briefly review the **non-equilibrium** Green function formalism as applied to **steady-state** transport (the time variable does not appear in this description).

**Notation**

There are four different Green functions $G^c$, $G^>$, $G^\Sigma$, $G^\Sigma^*$ and four self-energy functions $\Sigma^c$, $\Sigma^>$, $\Sigma^R$, $\Sigma^A$ appearing in the Keldysh formalism. We will introduce the following notation in this paper:

$$
-iG^c(r,r',E) = G_n(r,r',E) \\
+iG^>(r,r',E) = G_p(r,r',E) \\
-i\Sigma^c(r,r',E) = \Gamma_i(r,r',E) \\
+i\Sigma^>(r,r',E) = \Gamma_0(r,r',E)
$$

(2.1a) (2.1b) (2.1c) (2.1d)

This notation is motivated by the fact that the diagonal elements of $-iG^c$ give us the electron density $n(r,E)$ (see Eq. (1.6a)), suggesting that we view $G_n$ as a generalized electron density. Similarly $G_p$ is like a generalized hole density $p(r,E)$. The function $-i\Sigma^c$ and $+i\Sigma^>$ play the roles of in-scattering and out-scattering functions respectively – this motivates our choice of the notation $\Gamma_i$ and $\Gamma_0$. Note that each of these quantities, like $G_n(r,r',E)$, can be viewed as the position representation of corresponding operators like $G_n(E)$. These operators are Hermitian:

$$
G_n(r,r',E) = G_n(r',r,E)^* \\
G_p(r,r',E) = G_p(r',r,E)^* \\
\Gamma_i(r,r',E) = \Gamma_i(r',r,E)^* \\
\Gamma_0(r,r',E) = \Gamma_0(r',r,E)^*
$$

(2.2a) (2.2b) (2.2c) (2.2d)

The operators $G^R$, $G^A$, $\Sigma^R$, $\Sigma^A$, however, are not Hermitian. The advanced functions ($G^A$, $\Sigma^A$) are Hermitian conjugates of the retarded functions ($G^R$, $\Sigma^R$).
\[
G^R(r,r',E) = G^A(r',r,E)^* \\
\Sigma^R(r,r',E) = \Sigma^A(r',r,E)^*
\]

We can **define** Hermitian quantities \(A\) and \(\Gamma\) as follows:

\[
A(r,r',E) = i \left[ G^R(r,r',E) - G^A(r,r',E) \right] = G_n(r,r',E) + G_p(r,r',E)
\]

\[
\Gamma(r,r',E) = i \left[ \Sigma^R(r,r',E) - \Sigma^A(r,r',E) \right] = \Gamma_1(r,r',E) + \Gamma_0(r,r',E)
\]

A is the spectral function whose diagonal elements give the local density of states \(N(r,E)\) (see Eq. (1.6b)).

**Basic equations**

To apply this formalism to a specific problem we need to solve two equations self-consistently\(^{(24)}\)

\[
(E - H_0 - \Sigma^R(E)) G^R(E) = 1
\]

and

\[
G_n(E) = G^R(E) \Gamma_1(E) G^A(E)
\]

Here \(H_0 = (i\hbar \nabla + eA)^2/2m + V\) is a one-electron effective mass Hamiltonian, where the scalar potential \(V\) includes all static fields such as those due to boundaries, space-charge or applied bias. A self-consistent solution of Eqs. (2.6) and (2.7) is required because the self-energy functions \(\Sigma^R, \Gamma_1, \Gamma_0\) are all related to the Green functions \(G^R, G_n, G_p\). The functional form of this relationship is determined by the specific model we adopt for the interactions between the one-electron system and the surroundings. For example, if we treat phonon scattering in the Born approximation then

\[
\Gamma_1(r,r',E) \Rightarrow \int d(\hbar \omega) D(r,r',\hbar \omega) G_n(r,r',E - \hbar \omega)
\]

where the function \(D\) describes the spatial correlation and spectrum of the phonons. In this paper we will derive general results valid in the linear response regime without adopting any
specific relationship between the self-energies and the Green functions. For higher order processes and for electron-electron interactions the relation between $\Gamma$ and $G$ is complicated and non-linear. However, in the linear response regime close to equilibrium, the relationship can still be characterized by a single function which can be evaluated once we adopt a specific model for the interactions. Our results can thus be applied to arbitrary phase-breaking processes using the appropriate 'reservoir function'.

3. Linear response equation

In this Section we will linearize the transport equation, Eq. (2.7) about the equilibrium solution to obtain the linear response equation, Eq. (1.9).

Equilibrium solution

At equilibrium,

$$G_n(E) = \Lambda(E) f_{eq}(E)$$  \hspace{1cm} (3.1a)

$$\Gamma_1(E) = \Gamma(E) f_{eq}(E)$$  \hspace{1cm} (3.1b)

where $f_{eq}(E)$ is the Fermi-Dirac function with a constant electrochemical potential $\mu_{eq}$.

$$f_{eq}(E) = \frac{1}{e^{(E-\mu_{eq})/k_B T} + 1}$$  \hspace{1cm} (3.2)

The equilibrium solution in Eqs. (3.1a,b) satisfies the transport equation, Eq. (2.7) because of the following identity which is always valid, even away from equilibrium (see Appendix A).

$$\Lambda(E) = G^R(E) \Gamma(E) G^A(E)$$  \hspace{1cm} (3.3)

Non-equilibrium potentials

The equilibrium solution, Eqs. (3.1a,b), motivates us to define a non-equilibrium distribution function $f(r,r',E)$ and a non-equilibrium potential $\mu(r,r',E)$ as follows.
At equilibrium $\mu(r, r', E) = \mu_{eq}$ (constant). Away from equilibrium the potentials $\mu(r, r', E)$ are in general complex numbers. However, as we mentioned in Section 1,

$$\mu(r, r', E) = \mu(r', r, E)^*$$

so that the diagonal elements $\mu(r, r, E)$ are always real.

**Linearization of Eq. (2.7)**

The transport equation, Eq. (2.7), in position representation, reads

$$G_n(r_1, r_1', E) = \int dr_2 dr_2' G^R(r_1, r_2, E) \Gamma_i(r_2, r_2', E) G^A(r_2', r_1', E)$$

Using Eqs. (3.4) and (2.3a) we rewrite Eq. (3.6) as

$$f(\alpha_1) = \int d\alpha_2 P(\alpha_1, \alpha_2) f_\Gamma(\alpha_2)$$

where $\alpha_1$ stands for $(r_1, r_1', E_1)$ and $\alpha_2$ stands for $(r_2, r_2', E_2)$. Also,

$$f_\Gamma(\alpha_2) \equiv \frac{\Gamma_i(\alpha_2)}{\Gamma(\alpha_2)} = \frac{\Gamma_i(\alpha_2)}{\Gamma_i(\alpha_2) + \Gamma_0(\alpha_2)}$$

$$P(\alpha_1, \alpha_2) \equiv g(\alpha_1, \alpha_2) \frac{\Gamma(\alpha_2)}{A(\alpha_1)}$$

$$g(r_1, r_1', E_1; r_2, r_2', E_2) \equiv G^R(r_1, r_2, E_1) G^R(r_1', r_2', E_1)^* \delta(E_1 - E_2)$$

At equilibrium (see Eqs. (3.1a,b)) both $f(\alpha)$ and $f_\Gamma(\alpha)$ are equal to $f_{eq}(E)$ and Eq. (3.7) is satisfied. This is because the identity stated in Eq. (3.3) ensures that

$$\int d\alpha_2 P(\alpha_1, \alpha_2) F(E_2) = F(E_1)$$

where $F(E)$ is any function of energy.

Expanding about the equilibrium solution we obtain from Eq. (3.7)
where the subscript 'eq' denotes that the function is evaluated at equilibrium. Note that in writing Eq. (3.12) we are not neglecting $\delta P/\delta \mu$. Terms involving $\delta P/\delta \mu$ cancel out because of the result stated in Eq. (3.11).

$$\int d\alpha_2 \int d\alpha_3 \frac{\delta P(\alpha_1, \alpha_2)}{\delta \mu(\alpha_3)} f_{eq}(E_2) = \int d\alpha_3 \frac{\delta}{\delta \mu(\alpha_3)} \int d\alpha_2 P(\alpha_1, \alpha_2) f_{eq}(E_2) = 0$$

This is an important point because the self-energy functions $\Sigma^R, \Gamma$ (and hence the Green function $G^R$ and the spectral function $A$) do change under bias. Consequently $\delta P/\delta \mu$ cannot be neglected a priori.

It can be shown that

$$\left[ \int d\alpha_3 \frac{\delta f_\Gamma(\alpha_2)}{\delta \mu(\alpha_3)} \right]_{eq} = \left[ \frac{-\partial f_{eq}(E_2)}{\partial E_2} \right]_{eq}$$

To show this we note that if we change $\mu(\alpha)$ by a constant $\Delta \mu$ for all $\alpha$, then we go from the equilibrium state with $\mu = \mu_{eq}$ to another equilibrium state with $\mu = \mu_{eq} + \Delta \mu$. Hence the function $f_\Gamma$ simply changes from $f_{eq}(E)$ to $f_{eq}(E - \Delta \mu)$.

Using Eqs. (3.11) and (3.13) we obtain

$$\int d\alpha_2 \int d\alpha_3 P_{eq}(\alpha_1, \alpha_2) \frac{\delta f_\Gamma(\alpha_2)}{\delta \mu(\alpha_3)} \left|_{eq} \right. = \left[ \frac{-\partial f_{eq}(E_1)}{\partial E_1} \right]_{eq}$$

This identify allows us to rewrite the linear response equation, Eq. (3.12) as

$$0 = \int d\alpha_2 \int d\alpha_3 P_{eq}(\alpha_1, \alpha_2) \frac{\delta f_\Gamma(\alpha_2)}{\delta \mu(\alpha_3)} \left|_{eq} \right. \left[ \mu(\alpha_1) - \mu(\alpha_3) \right]$$
Reservoir conductance function

The function $\delta f_{\tau}(\alpha_1) / \delta \mu(\alpha_2)$ appearing in Eq. (3.15) describes the change in the scattering at $\alpha_1 \equiv (r_1, r_1', E_1)$ due to a change in the potential at $\alpha_2 \equiv (r_2, r_2', E_2)$. We can define a related quantity $g_R(\alpha_1, \alpha_2)$ which we will call the reservoir conductance function:

$$g_R(\alpha_1, \alpha_2) \equiv \frac{e}{h} \Gamma_{eq}(\alpha_1) A_{eq}^*[\alpha_1] \left. \frac{\delta f_{\tau}(\alpha_1)}{\delta \mu(\alpha_2)} \right|_{eq} \tag{3.16}$$

This function has a simple interpretation as we describe below.

Consider the quantity

$$i(\alpha) = \frac{e}{h} \left[ \Gamma_1(\alpha) G_p^*(\alpha) - \Gamma_0(\alpha) G_n^*(\alpha) \right] \tag{3.17}$$

We can interpret (the real part of) $\Gamma_1 G_p^*$ as the in-scattering into 'a' and $\Gamma_0 G_n^*$ as the out-scattering from 'a'. Their difference 'i' thus represents the net in-scattering which, as we might expect, is zero at equilibrium (see equilibrium solution, Eqs. (3.1a,b)). We can show that (see Appendix B)

$$\left. \frac{\delta i(\alpha_1)}{\delta \mu(\alpha_2)} \right|_{eq} = -I_{eq}(\alpha_1) \delta(\alpha_1 - \alpha_2) + g_R(\alpha_1, \alpha_2) \tag{3.18}$$

where

$$I_{eq}(\alpha_1) \equiv \frac{e}{h} \Gamma_{eq}(\alpha_1) A_{eq}^*[\alpha_1] \left[ - \frac{\partial f_{eq}(E_1)}{\partial E_1} \right] \tag{3.19}$$

and $\alpha_1 \equiv (r_1', E_1)$. Note that from Eqs. (3.13), (3.16) and (3.19)

$$\int d\alpha_2 \ g_R(\alpha_1, \alpha_2) = I_{eq}(\alpha_1) \tag{3.20}$$

We can rewrite the linear response equation, Eq. (3.15) in terms of the reservoir conductance function defined above. To obtain this new form we multiply Eq. (3.15) by $(e/h) A_{eq}(\alpha_1)$ $\Gamma_{eq}^*[\alpha_1]$ and write
The kernel $T$ is given by

$$0 = \frac{e}{\hbar} \int d\alpha_3 \ T(\alpha_1, \alpha_3) \ [\tilde{\mu}(\alpha_1) - \mu(\alpha_3)]$$

(3.21)

The reservoir conductance function can be evaluated once we write down the in-scattering and out-scattering functions $T_i$ and $T_o$ assuming a specific model for the dephasing process. Explicit expressions for $g_R$ are derived in Appendix B for electron-phonon and electron-electron interactions in the self-consistent Born approximation.

4. Terminal current

For a given device structure such as the one shown in Fig. 1 we can solve the linear response equation, Eq. (3.21) subject to the boundary condition that $\mu(\mathbf{r}, \mathbf{r}', E) = \mu_i$ if $\mathbf{r}, \mathbf{r}' \in$ contact 'i'. Once we have computed $\mu(\mathbf{r})$ from Eq. (3.21), we can compute the full correlation function $\langle \mathbf{r}, \mathbf{r}; E \rangle$ from which the current density $J(\mathbf{r}, E)$ can be computed. Integrating the flux $J \cdot dS_i$ over a device-contact interface we could obtain the terminal current $I_i$. This is the straight-forward procedure. However, one can obtain the terminal current using a simpler procedure which we describe below. The proof of the equivalence of the two approaches is described in Appendix C.

The key point to realize is that Eq. (3.21) is actually not satisfied within the contacts where we impose the boundary condition on $\mu(\mathbf{r})$ instead of solving for it. This can be understood by considering a simple analogy. If we solve the diffusion equation in 1-D ($d^2 \mu/dz^2 = 0$) subject to the boundary condition that $\mu = 0$ for $z<0$ and $\mu = \mu_0$ for $z>L$ then we obtain, $\mu = \mu_0 z/L$ for $0<z<L$. It is easy to see that $d^2 \mu/dz^2 = (\mu_0/L)[\delta(z) - \delta(z-L)]$ so that the equation that we are
solving \((d^2 \mu/dz^2 = 0)\) is not satisfied at the points \(z=0\) and at \(z=L\). Similarly when we solve the integral equation, Eq. (3.21), subject to boundary conditions on \(\mu(\alpha)\) at the contacts we find that Eq. (3.21) is not satisfied for a short distance into the contacts near the device – contact interface; this distance is determined by the spatial extent of the kernel which can be identified with the phase-breaking length \(L_\phi\). The terminal current \(I_i\) can be obtained from the following relation:

\[
I_i = \int dE \int_{r, r' \in \text{contact}} dr' I(r, r', E)
\]  

(4.1)

where \(I(\alpha)\) is equal to the difference between the two sides in Eq. (3.21) (it is non-zero only for points \((r, r')\) lying within one of the contacts).

\[
I(\alpha_1) = \frac{e}{h} \int d\alpha_3 T(\alpha_1, \alpha_3)[\mu(\alpha_1) - \mu(\alpha_3)]
\]  

(4.2)

Using Eqs. (3.20) and (3.19) we can show that

\[
\frac{e}{h} \int d\alpha_3 T(\alpha_1, \alpha_3) = I_{eq}^*(\alpha_1)
\]  

(4.3)

This relation allows us to write Eq. (4.2) alternatively in the form

\[
I(\alpha_1) = I_{eq}^*(\alpha_1) \mu(\alpha_1) - \frac{e}{h} \int d\alpha_3 T(\alpha_1, \alpha_3) \mu(\alpha_3)
\]  

(4.4)

The above approach allows us to compute the terminal current \(I_i\) without explicitly computing the current density \(J(r, E)\). However, we could compute the detailed current density if we are interested and an explicit expression for the linear response current density is derived in Appendix C. Integrating the flux over the device-contact interface yields results identical to those obtained from Eq. (4.4).
5. 'Zero' temperature

The reservoir function $g_R(\alpha_1, \alpha_2)$ is non-zero only if $E_1$ and $E_2$ lie within a few $k_B T$ of the Fermi energy $E_F$. This is because $g_R(\alpha_1, \alpha_2)$ represents the change in the net in-scattering $\delta n(\alpha_1)$ in response to a change in the potential $\delta \mu(\alpha_2)$. Deep inside the Fermi sea or high above the Fermi sea, a change in the potential $\delta \mu(\alpha)$ has no effect on the distribution function $f(\alpha)$ (see definition, Eq. (3.4)) and hence no change in the scattering rates; consequently, $g_R \to 0$. Assuming that the functions $G^R$, $\Gamma$ and $A$ are nearly independent of energy within this range of energies ($-E_F \pm$ a few $k_B T$) we could write $g_R$ in the form [Note: $\rho \equiv (r, r')$]:

$$g_R(\rho_1 E_1, \rho_2 E_2) = \tilde{g}_R(\rho_1, \rho_2) \delta(E_1-E_2) \delta(E_2-E_F)$$

(5.1)

From Eqs. (3.22), (3.23) and (3.10)

$$T(\rho_1 E_1, \rho_3 E_3) = \tilde{T}(\rho_1, \rho_3) \delta(E_1-E_3) \delta(E_3-E_F)$$

(5.2)

where

$$\tilde{T}(\rho_1, \rho_3) = \int d\rho_2 \tilde{P}_{eq}(\rho_1, \rho_2) \tilde{g}_R(\rho_2, \rho_3)$$

(5.3)

$$\tilde{P}_{eq}(\rho_1, \rho_2) = \tilde{\Gamma}(\rho_1)^* \tilde{g}_{eq}(\rho_1, \rho_2) / \tilde{A}(\rho_2)^*$$

(5.4)

$$\tilde{g}_{eq}(\rho_1, \rho_2) = G^R_{eq}(r_1, r_2; E_F) G^R_{eq}(r_1', r_2'; E_F)^*$$

(5.5)

$$\tilde{\Gamma}_{eq}(\rho_1) = \Gamma_{eq}(\rho_1, E_F)$$

(5.6)

$$\tilde{A}_{eq}(\rho_1) = A_{eq}(\rho_1, E_F)$$

(5.7)

Using Eqs. (3.19) and (3.20) we can show that (assuming $-\partial f/\partial E = \delta(E-E_F)$)

$$\int d\rho_2 \tilde{g}_R(\rho_1, \rho_2) = \frac{e}{\hbar} \tilde{\Gamma}(\rho_1) \tilde{A}(\rho_1)^* = \tilde{I}_{eq}(\rho_1)$$

(5.8)

Also, from Eq. (4.3) we obtain

$$\frac{e}{\hbar} \int d\rho_3 \tilde{T}(\rho_1, \rho_3) = \tilde{I}_{eq}(\rho_1)$$

(5.9)
Using Eq. (5.2) we obtain the ‘zero’ temperature version of Eq. (4.2):

$$\tilde{I}(\rho_1) = \frac{e}{\hbar} \int dp_3 \tilde{\mathcal{T}}(\rho_1, \rho_3)[\mu(\rho_1) - \mu(\rho_3)]$$  \hspace{1cm} (5.10)

where $\tilde{I}(\rho_1) = \int dE_1 I(\rho_1, E_1)$.

6. **Büttiker formula**

The linear response equation, Eq. (4.2), can be reduced to the Büttiker formula, Eq. (1.5), by eliminating the floating probes within the device. Within the device $I(\alpha) = 0$ so that Eq. (4.4) reduces to ($\alpha_1 \in \text{device}$)

$$\mu(\alpha_1) = \int d\alpha_3 \frac{e}{\hbar} \frac{T(\alpha_1, \alpha_3)}{\Gamma_{eq}(\alpha_1)} \mu(\alpha_3)$$  \hspace{1cm} (6.1)

Eq. (6.1) can be solved interatively to obtain a solution for $\mu(\alpha_1)$ in terms of the terminal potential $\mu_i$ in the form of an infinite series. Substituting this series back into Eq. (4.2) we obtain the Büttiker formula, Eq. (1.5) (see Appendix D), with an infinite series solution for the transmission $\tilde{T}_{ij}$

$$\tilde{T}_{ij} = \sum_{n=0}^{\infty} \tilde{T}_{ij}^{(n)}$$  \hspace{1cm} (6.2)

The nth order term represents the transmission after suffering ‘n’ phase-breaking processes within the device. The first three terms are depicted in Fig. 3. These diagrams are readily translated into analytical expressions as follows. ($\alpha_a \in \text{contact 'i'}, \alpha_b \in \text{contact 'j'}$)

$$\tilde{T}_{ij}^{(0)} = (1-\delta_{ij}) \int d\alpha_a \int d\alpha_b \frac{(1-f_{eq}(E_a))f_{eq}(E_b)}{k_B T} \frac{1}{\Gamma_{eq}(\alpha_a)\Gamma_{eq}(\alpha_b) g_{eq}(\alpha_a, \alpha_b)}$$  \hspace{1cm} (6.3)

$$\tilde{T}_{ij}^{(1)} = \int d\alpha_a \int d\alpha_b \int d\alpha_{1,2}^{a, \alpha_2 \in \text{Device}} \frac{(1-f_{eq}(E_a))f_{eq}(E_b)}{k_B T} \frac{1}{\Gamma_{eq}(\alpha_a)\Gamma_{eq}(\alpha_b)} g_{eq}(\alpha_a, \alpha_1) D_R(\alpha_1, \alpha_2) g_{eq}(\alpha_2, \alpha_b)$$  \hspace{1cm} (6.4)
Fig. 3: Successive terms \( n=0,1,2 \) representing the transmission \( \tilde{T}_{ij}^{(n)} \) with 'n' phase-breaking processes within the device (see Eqs. (6.3)-(6.5)).
\[ T_{ij}^{(2)} = \int d\alpha_a \int d\alpha_b \int d\alpha_c \int d\alpha_d \Gamma_{eq}(\alpha_a) \Gamma_{eq}(\alpha_b) \frac{(1-f_{eq}(E_a))f_{eq}(E_b)}{k_BT} \]

\[ g_{eq}(\alpha_a, \alpha_1) \mathcal{D}_R(\alpha_1, \alpha_2) g_{eq}(\alpha_2, \alpha_3) \mathcal{D}_R(\alpha_3, \alpha_4) g_{eq}(\alpha_4, \alpha_b) \]

and so on. The function \( \mathcal{D}_R \) is defined as

\[ \mathcal{D}_R(\alpha_1, \alpha_2) = \frac{h k_B T g_R(\alpha_1, \alpha_2)}{e \mathcal{A}_{eq}(\alpha_1) \mathcal{A}_{eq}(\alpha_2)f_{eq}(E_2)(1-f_{eq}(E_1))} \]

'Zero' temperature

At low temperatures we can write the reservoir function \( g_R \) in the form shown in Eq. (5.1) so that the reservoir coupling function \( \mathcal{D}_R \) can be written as

\[ \mathcal{D}_R(\alpha_1, \alpha_2) = \mathcal{D}_R(\rho_1, \rho_2) \delta(E_1 - E_2) \]

where

\[ \mathcal{D}_R(\rho_1, \rho_2) = \frac{h g_R(\rho_1, \rho_2)}{e \mathcal{A}_{eq}(\rho_1) \mathcal{A}_{eq}(\rho_2)} \]

This leads to a simplification in the expressions (Eqs. (6.3) - (6.5)) for the transmission. \( \rho_a \in \) contact 'i', \( \rho_b \in \) contact 'j'

\[ T_{ij}^{(0)} = (1-\delta_{ij}) \int dp_a \int dp_b \Gamma_{eq}(\rho_a) \Gamma_{eq}(\rho_b) g_{eq}(\rho_a, \rho_b) \]

\[ T_{ij}^{(1)} = \int dp_a \int dp_b \int dp_1 dp_2 \Gamma_{eq}(\rho_a) \Gamma_{eq}(\rho_1) g_{eq}(\rho_a, \rho_1) \mathcal{D}_R(\rho_1, \rho_2) g_{eq}(\rho_2, \rho_b) \]

\[ T_{ij}^{(2)} = \int dp_a \int dp_b \int dp_1 dp_2 dp_3 \Gamma_{eq}(\rho_a) \Gamma_{eq}(\rho_b) \mathcal{D}_R(\rho_1, \rho_2) \mathcal{D}_R(\rho_2, \rho_3) g_{eq}(\rho_4, \rho_b) \]

and so on. Eqs. (6.8) - (6.10) are depicted in Fig. 4.
'Zero' temperature

Fig. 4: Same as Fig. 3 but at low temperatures. All quantities are evaluated at the Fermi energy (see Eqs. (6.8) - (6.10)).
Reciprocity

We note that at equilibrium, $G^R(r,r',E)\bigg|_{+B} = G^R(r',r,E)\bigg|_{-B}$ (see Appendix A) so that from Eq. (3.10) we can write

$$g_{eq}(\alpha_1,\alpha_2)\bigg|_{+B} = g_{eq}(\alpha_2,\alpha_1)\bigg|_{-B}$$  \hspace{1cm} (6.11)

We assume that the reservoir is reciprocal so that

$$g_R(\alpha_1,\alpha_2)\bigg|_{+B} = g_R(\alpha_2,\alpha_1)\bigg|_{-B}$$  \hspace{1cm} (6.12)

This seems like a reasonable assumption and we can see from Appendix B that this relation is true for electron-phonon and electron-electron interactions in the self-consistent Born approximation. We are not sure if this result can be proved to be true in general. From Eqs. (6.6) and (6.12) we have

$$D_R(\alpha_1,\alpha_2)\bigg|_{+B} = D_R(\alpha_2,\alpha_1)\bigg|_{-B} = e^{(E_2-E_1)/\kappa_B T}$$  \hspace{1cm} (6.13)

Using Eqs. (6.11) and (6.13) we can show from Eqs. (6.3) - (6.5) that

$$T_{ij}^{(n)}\bigg|_{+B} = T_{ji}^{(n)}\bigg|_{-B}$$

noting that the contacts are assumed to be in zero magnetic field. We can prove this for the 'zero' temperature results (Eqs. (6.8) - (6.10)) as well, noting that

$$\tilde{g}_{eq}(\rho_1,\rho_2)\bigg|_{+B} = \tilde{g}_{eq}(\rho_2,\rho_1)\bigg|_{-B}$$  \hspace{1cm} (6.14)

$$\tilde{D}_R(\rho_1,\rho_2)\bigg|_{+B} = \tilde{D}_R(\rho_2,\rho_1)\bigg|_{-B}$$  \hspace{1cm} (6.15)

It is interesting to note that the kernel of the 'zero' temperature equation, Eq. (1.11), is reciprocal: $\tilde{T}(\rho_1,\rho_2)\bigg|_{+B} = \tilde{T}(\rho_2,\rho_1)\bigg|_{-B}$ while that of the general equation, Eq. (1.9) is not: $T(\rho_1,E_1;\rho_2,E_2)\bigg|_{+B} \neq T(\rho_2,E_2;\rho_1,E_1)\bigg|_{-B}$. Nonetheless, even in the latter case the transmission on $\tilde{T}_{ij}$ between two reservoirs in equilibrium does exhibit reciprocity as shown above.
7. A simple example

Our objective in this section is to calculate the transmission $\tilde{T}_{ij}$ explicitly for a short single-moded electron waveguide (Fig. 4) with electron-phonon interaction which we treat in the Born approximation. We will evaluate the transmission $\tilde{T}_{ij}$ from Eq. (6.4) to first-order in the interaction and show that the result agrees with what one would expect from the Golden rule.

**Reflectionless contacts**

It may seem surprising that the scattering function $\Gamma$ in the contacts enters the expression for $\tilde{T}_{ij}$ (see Eqs. (6.3)-(6.5), (6.8)-(6.10)). However, a larger $\Gamma$ within the contact causes the function $g_{eq}$ to damp out quickly so that on integration over the area of the contact the result is nearly independent of $\Gamma$. Indeed we can eliminate $\Gamma$ altogether from the expressions for $\tilde{T}_{ij}$ if we neglect any reflections at the contacts and treat the contacts simply as an extension of the device (as shown by the dotted lines in Fig. 1). For a one-dimensional waveguide (Fig. 5) the Green function within the contact can be written as

$$G^R(z, z', E) = \frac{i}{\hbar v} e^{ik|z-z'|} e^{-\Gamma_c(E)|z-z'|/2\hbar v}$$

where $k = \sqrt{2mE/\hbar^2}, v = \sqrt{2E/m}$ and the scattering function is assumed to be local inside the contacts: $\Gamma(z, z', E) \Rightarrow \Gamma_c(E)\delta(z-z')$. This allows us to write

$$G^R(z_{ic}, z_1, E) = G^R(z_1, z_{1c}, E)e^{ik|z_1-z_{1c}|} e^{-\Gamma_c(E)|z_1-z_{1c}|/2\hbar v}$$

where $z_{1c}$ is a point within the device, $z_i$ is located at the interface between the device and contact 'i' and $z_{ic}$ is a point inside contact 'i.' Using this result (and Eq. (3.10) for $g$) we obtain from Eqs. (6.3) and (6.4)
Fig. 5: A single-moded waveguide with phonon scattering. The initial energy and wave vector are $E_j, k_j$. Phonon absorption leads to a forward scattered wave with wave vector $k^+$ and a backscattered wave with wave vector $-k^+$. 
\[ T_{ij}^{(0)} = \int dE_1 \frac{f_1(1-f_1)}{k_B T} \hbar^2 v_1^2 \left| G^R(z_i,z_1;E_j) \right|^2 \]  
(7.1)

\[ T_{ij}^{(1)} = \int dE_1 \int dE_2 \frac{f_2(1-f_1)}{k_B T} \hbar^2 v_1 v_2 \int \int \int \int \int L d\zeta_1 \int d\zeta_2 \right| G^R(z_i,z_1;E_1) \right| G^R(z_j,z_2;E_2) \right| G^R(z_2,z_j;E_2) \left| \right|^2 \]  
(7.2)

where \( z_i \) and \( z_j \) are points located right at the interfaces between the device and contacts 'i' and 'j' respectively. We have used \( f_1 \) and \( f_2 \) to denote \( f_{eq}(E_1) \) and \( f_{eq}(E_2) \) respectively. In this section, we will generally drop the subscript 'eq' for convenience. Note the similarity of Eq. (7.1) to the formula derived by Fisher and Lee for coherent transport\(^{25}\). However, Eq. (7.1) does not assume coherent transport; it gives us the coherent part of the transmission in the presence of dephasing.

Next we note that for a single-mode waveguide without any scattering \( k = \sqrt{2mE/\hbar} \),

\[ v = \sqrt{2E/m} \),

\[ G^R(z,z';E) = -\frac{i}{\hbar v} e^{ik|z-z'|} \]  
(7.3)

Since we are interested in calculating \( \tilde{T}_{ij} \) only to first-order in the scattering, we use the unperturbed Green function to evaluate \( \tilde{T}_{ij}^{(1)} \). Using Eq. (7.3) for \( G^R \) we can write the spectral function \( A \) (see Eq. (2.4a)) as

\[ A(z,z',E) = \frac{e^{ik|z-z'|} + e^{-ik|z-z'|}}{\hbar v} - \frac{e^{ik(z-z')} + e^{-ik(z-z')}}{\hbar v} \]

We can write

\[ A(z,z',E) = A^+(z,z',E) + A^-(z,z',E) \]  
(7.4)

where

\[ A^+(z,z',E) \equiv e^{ik(z-z')/\hbar v} \]  
(7.5)
Using Eqs. (7.3) - (7.5) we rewrite \( T_{ij}^{(1)} \) as

\[
T_{ij}^{(1)} = \int dE_1 \, dE_2 \, \frac{(1-f_1)f_2}{k_B T} \int dz_1 \int dz_2 \int dz_1' \int dz_2' \left[ A^+(z_1z_1' E_1) \right]^* D_R(z_1z_1';z_2z_2' E_2) A^+(z_2z_2' E_2)
\] (7.6)

where the positive sign is used for transmission \( (i \neq j) \) and the negative sign for reflection \( (i = j) \).

To proceed further we need to substitute a specific expression for the reservoir coupling \( D_R \).

**Electron-phonon interaction**

Using Eq. (B.6) for the reservoir coupling \( D_R \) we obtain from Eq. (7.6) for the transmission \( (i \neq j) \) and the reflection \( (i = j) \).

\[
\tilde{T}_{ij}^{(1)} = \int \frac{dE}{k_B T} \, f_{eq}(E) \int \frac{d(\hbar \omega)}{2\pi \hbar v^+} \frac{1-f^+}{2\pi \hbar v^+} \times \frac{2\pi L}{\hbar v} \int dz_1 \int dz_1' \, D(z_1,z_1';\hbar \omega) \, e^{ik^+(z_1-z_1')}
\] (7.7)

\[
\tilde{T}_{ij}^{(1)} = \int \frac{dE}{k_B T} \, f_{eq}(E) \int \frac{d(\hbar \omega)}{2\pi \hbar v^+} \frac{1-f^+}{2\pi \hbar v^+} \times \frac{2\pi L}{\hbar v} \int dz_1 \int dz_1' \, D(z_1,z_1';\hbar \omega) \, e^{ik^+(z_1-z_1')}
\] (7.8)

where \( E^+ = E + \hbar \omega, f^+ = f_{eq}(E^+), k^+ = \sqrt{2mE^+}/\hbar \). Note that the integration over \( \hbar \omega \) includes negative frequencies as well which correspond to emission. Although we show only absorption processes (Fig. 4), emission processes are also included implicitly.

If we neglect end effects and assume that the phonon function \( D(z,z';\hbar \omega) \) depends only on the difference coordinate \( (z-z') \) then we obtain from Eqs. (7.7) and (7.8)

\[
\tilde{T}_{ij}^{(1)} \Rightarrow \int \frac{dE}{k_B T} \, f_{eq}(E) \int \frac{d(\hbar \omega)}{2\pi \hbar v^+} \frac{1-f^+}{2\pi \hbar v^+} \times \frac{2\pi L}{\hbar v} \, D(k+k^+;\hbar \omega)
\]

\[
\tilde{T}_{ij}^{(1)} \Rightarrow \int \frac{dE}{k_B T} \, f_{eq}(E) \int \frac{d(\hbar \omega)}{2\pi \hbar v^+} \frac{1-f^+}{2\pi \hbar v^+} \times \frac{2\pi L}{\hbar v} \, D(k-k^+;\hbar \omega)
\]

where \( D(q;\hbar \omega) \) is the spatial Fourier Transform of \( D(z-z';\hbar \omega) \). This is similar to what we would obtain from the Golden rule, noting that \( (2\pi \hbar v^+)^{-1} \) is the final density of states and \((L/\nu)\)
is the transit time. If the phonon function $D(q, \omega)$ is peaked around small wave numbers $q$ then $
abla (1) \nabla (1) T_{ij} < \nabla (1) T_{ij}$ indicating phase-relaxation with minimal momentum relaxation. But for point scatterers $D(q, \omega)$ is independent of $q$, so that $\nabla (1) T_{ij} = \nabla (1) T_{ij}$ as obtained in Ref. 14.

The simple example presented above is intended to illustrate how our results can be applied to a concrete problem. It should be possible to apply these results to more difficult problems involving multiple modes, multiple scatterings and higher order dephasing processes. We leave this for future work.

8. Summary and conclusions

To summarize, we have derived a linear response equation $(\alpha \equiv r, r', E)$:

$$I(\alpha_1) = \frac{e}{h} \int d\alpha_3 \ n(\alpha_1, \alpha_3) \left[ \mu(\alpha_1) - \mu(\alpha_3) \right]$$  \hspace{1cm} (8.1)

for arbitrary phase-breaking processes. The kernel $T$ is given by

$$T(\alpha_1, \alpha_3) = \int d\alpha_2 \ P_{eq}^{\prime}(\alpha_1, \alpha_2) \ g_R(\alpha_2, \alpha_3)$$  \hspace{1cm} (8.2)

where

$$P_{eq}^{\prime}(\alpha_1, \alpha_2) = \frac{\Gamma_{eq}^{\ast}(\alpha_1) g_{eq}(\alpha_1, \alpha_2)}{A_{eq}(\alpha_2)}$$  \hspace{1cm} (8.3)

$$g_{eq}(\alpha_1, \alpha_2) = G_{eq}(r_1, r_2, E_1) G_{eq}(r_1, r_2, E_1)^* \delta(E_1 - E_2)$$  \hspace{1cm} (8.4)

$$g_R(\alpha_2, \alpha_3) = I_{eq}(\alpha_2) \delta(\alpha_2 - \alpha_3) + \frac{e}{h} \left[ \frac{\delta}{\delta \mu(\alpha_3)} \left[ \Gamma_0(\alpha_2) G_n^{\ast}(\alpha_2) - \Gamma_0(\alpha_2) G_n^{\ast}(\alpha_2) \right] \right]$$  \hspace{1cm} (8.5)

Eq. (8.1) can be reduced to the Büttiker formula. The first three terms in the resulting expression for the transmission $\nabla (1) I_{ij}$ are depicted diagrammatically in Fig. 3a, where

$$D_R(\alpha_1, \alpha_2) = \frac{\hbar k_B T g_R(\alpha_1, \alpha_2)}{e A_{eq}^{\ast}(\alpha_1) A_{eq}(\alpha_2) f_{eq}(E_2)(1 - f_{eq}(E_1))}$$  \hspace{1cm} (8.6)
At low temperatures, Eq. (8.1) simplifies to \( p \equiv r, r' \):

\[
\tilde{T}(\rho_1, \rho_3) = \frac{e}{\hbar} \int dp_3 \tilde{T}(\rho_1, \rho_3) \left[ \mu(\rho_1) - \mu(\rho_3) \right]
\] (8.7)

The kernel \( \tilde{T} \) is given by

\[
\tilde{T}(\rho_1, \rho_3) = \int dp_2 \int \tilde{P}' \tilde{g}_R(\rho_1, \rho_2) \tilde{g}_R(\rho_2, \rho_3)
\] (8.8)

where

\[
\tilde{g}_R(\rho_2, \rho_3) = \int dE_2 \int dE_3 g_R(\rho_2, E_2; \rho_3, E_3)
\] (8.9)

\[
\tilde{P}'(\rho_1, \rho_2) = \tilde{g}_eq(\rho_1, \rho_2)^* \tilde{g}_eq(\rho_1, \rho_2)/\tilde{A}_eq(\rho_2)
\] (8.10)

\[
\tilde{g}_eq(\rho_1, \rho_2) = G_{eq}^R(r_1, r_2; E_F) G_{eq}^R(r_1, r_2; E_F)^*
\] (8.11)

\( \tilde{g}_eq(\rho) \) and \( \tilde{A}_eq(\rho) \) denote \( \Gamma_{eq}(\rho, E_F) \) and \( A_{eq}(\rho, E_F) \) respectively. The first three terms in the expression for \( \tilde{T}_{ij} \), obtained by reducing Eq. (8.7) to the Büttiker formula, are depicted in Fig. 3b. The function \( \tilde{D}_R \) is given by

\[
\tilde{D}_R(\rho_1, \rho_2) = h \tilde{g}_R(\rho_1, \rho_2)/e \tilde{A}(\rho_1)^* \tilde{A}(\rho_2)
\] (8.12)

Normalization

The reservoir conductance function obeys the following normalization conditions:

\[
\int d\alpha_2 g_R(\alpha_1, \alpha_2) = \frac{e}{\hbar} \Gamma_{eq}(\alpha_1) A_{eq}^*(\alpha_1) \left[ \frac{\partial f_{eq}(E_1)}{\partial E_1} \right]
\] (8.13a)

\[
\int dp_2 \tilde{g}_R(\rho_1, \rho_2) = \frac{e}{\hbar} \tilde{T}_{eq}(\rho_1) \tilde{A}_{eq}(\rho_1)
\] (8.13b)

The kernels \( T(\alpha_1, \alpha_2) \) and \( \tilde{T}(\rho_1, \rho_2) \) in Eqs. (8.1) and (8.7) obey the relations:
Electron-phonon interaction

Note that the above results are obtained without invoking any specific model for the phase-breaking processes. Thus these results are perfectly general and can be applied to arbitrary dephasing mechanisms. Of course, for any concrete calculation one has to assume some model in order to evaluate the reservoir conductance function $g_R$ or the reservoir coupling function $D_R$. In Appendix B the reservoir functions are evaluated for electron-phonon and electron-electron interactions in the Born approximation. The results for electron-phonon interaction (see Eqs. (B.5), (B.6)) are stated below ($p \equiv r, r'$):

$$g_R(p_1E_1;p_2E_2) = \frac{e}{h} \frac{(1-f_{eq}(E_1))f_{eq}(E_2)}{k_B T} A_{eq}(p_1,E_1)A_{eq}(p_1,E_2)D(p_1,E_1-E_2) \quad (8.15a)$$

$$D_R(p_1E_1,p_2E_2) = \delta(p_1-p_2)D(p_1,E_1-E_2) \quad (8.15b)$$

where $D(r, r', \hbar\omega)$ is a function describing the spatial correlation and spectrum of the phonons. If $M_q$ is the coupling strength of a phonon of wavevector $'q'$ then

$$D(r, r', \hbar\omega) = |M_q|^2 e^{i\hbar q \cdot (r-r')} \delta(\omega-\omega_q) N_{\omega} , \hbar\omega > 0 \quad (8.16a)$$

$$N_{\omega} + 1, \hbar\omega < 0 \quad (8.16b)$$

where $N_{\omega}$ is the Bose-Einstein factor describing the equilibrium number of phonons with frequency $\omega$.

Using $g_R$ from Eq. (8.15a) we can write down an explicit expression for the kernel $T$ appearing in Eq. (8.1):

$$\int d\alpha_2 T(\alpha_1, \alpha_2) = \frac{e}{h} \Gamma_{eq}(\alpha_1) A_{eq}(\alpha_1) \left( \frac{\partial f_{eq}(E_1)}{\partial E_1} \right) \quad (8.14a)$$

$$\int dp_2 \tilde{T}(p_1, p_2) = \frac{e}{h} \Gamma_{eq}(p_1) \tilde{A}_{eq}(p_1) \quad (8.14b)$$

where $D(r, r', \hbar\omega)$ is a function describing the spatial correlation and spectrum of the phonons. If $M_q$ is the coupling strength of a phonon of wavevector $'q'$ then

$$D(r, r', \hbar\omega) = |M_q|^2 e^{i\hbar q \cdot (r-r')} \delta(\omega-\omega_q) N_{\omega} , \hbar\omega > 0 \quad (8.16a)$$

$$N_{\omega} + 1, \hbar\omega < 0 \quad (8.16b)$$

where $N_{\omega}$ is the Bose-Einstein factor describing the equilibrium number of phonons with frequency $\omega$.
For point scatterers $D(\rho; E_1 - E_2)$ reduces to $F(r; E_1 - E_2)$ and Eq. (8.17) reduces to our earlier result (see Eq. (5) of Ref. 14a). Similarly we obtain for the kernel $\tilde{T}$ appearing in the 'zero' temperature equation, Eq. (8.7),

$$\tilde{T}(\rho_1, \rho_2) = \Gamma_{eq}(\rho_1) G_{eq}(r_1, r_2; E_F) G_{eq}(r_1, r_2; E_F) \Gamma_{eq}(\rho_2)$$  \hspace{1cm} (8.18)

Once again for point scatterers we recover our earlier result\textsuperscript{15,22}

$$\tilde{T}(r_1, r_2) = \hbar^2 |G_{eq}(r_1, r_2; E_F)|^2 / \tau\phi(r_1, E_F) \tau\phi(r_2, E_F)$$

**Concluding remarks**

In this paper we have presented a linear response formulation of the non-equilibrium Green function formalism in real space which we believe is suitable for mesoscopic systems. An important difference between the present formulation and usual linear response theory\textsuperscript{(26)} is that the electrochemical potential difference is treated as the driving force. However, we do not neglect the self-consistent fields that arise in an interacting system under bias. These fields do not appear in the linearized equation because terms involving $\delta F / \delta \mu$ cancel out, as explained following Eq. (3.12).

The derivation presented in this paper generalizes our earlier results\textsuperscript{(14)} which were derived assuming point scatterers. One limitation of the point scatterer model is that phase relaxation is always accompanied by momentum relaxation ($\tau_m = \tau\phi$). Consequently, one goes from quantum ballistic transport (long $\tau\phi, \tau_m$) to semiclassical diffusive transport (short $\tau\phi, \tau_m$) as the scattering is increased; but it is difficult to simulate the semiclassical ballistic regime (short $\tau\phi$, long $\tau_m$) with the point scatterer model. The generalized 'probe' model presented in this paper allows us to overcome this limitation, as illustrated by the simple example involving a short electron waveguide with electron-phonon interactions.
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Appendix A: Some useful properties of $G^R$

Eq. (3.3)

We start from an alternative form of Eq. (2.6) (see Eq. (24), Ref. 6)

\[ G^R (E - H_0 - \Sigma^R) = 1 \]  \hspace{1cm} (A.1a)

and its Hermitian conjugate,

\[ (E - H_0 - \Sigma^A) G^A = 1 \]  \hspace{1cm} (A.1b)

Post-multiplying Eq. (A.1a) by $G^A$ and pre-multiplying Eq. (A.1b) by $G^R$ we obtain

\[ G^R (E - H_0 - \Sigma^R) G^A = G^A \]  \hspace{1cm} (A.2a)

\[ G^R (E - H_0 - \Sigma^A) G^A = G^R \]  \hspace{1cm} (A.2b)

Subtracting Eq. (A.2b) from Eq. (A.2a),

\[ G^R (\Sigma^A - \Sigma^R) G^A = G^A - G^R \]  \hspace{1cm} (A.3)

Using Eqs. (2.4a,b) we obtain our desired result (Eq. (3.3)). Note that if we start from Eq. (2.6)

\[ (E - H_0 - \Sigma^R) G^R = 1 \]

then we obtain a slightly different version of Eq. (3.3): $G^A \Gamma G^R = A$.

Reciprocity

The reciprocity relation $G^R(r, r', E) \big|_B = G^R(r', r, E) \big|_-B$ can be proved using the eigenfunction expansion for $G^R$. However, it should be noted that since $\Sigma^R$ is non-Hermitian, we need the set of bi-orthonormal eigenfunctions $\phi_m(r, E)$ and $\psi_n(r, E)$ defined as follows:\textsuperscript{27,28}:

\[ H_0(r) \phi_m(r, E) + \int dr' \Sigma^R(r, r', E) \phi_m(r', E) = \epsilon_m(E) \phi_m(r, E) \]  \hspace{1cm} (A.4a)

\[ H_0(r) \psi_n(r, E) + \int dr' \Sigma^A(r, r', E) \psi_n(r', E) = \epsilon_n^*(E) \psi_n(r, E) \]  \hspace{1cm} (A.4b)

The retarded Green function is given by
Next, we note that

\[ H_0(r) \bigg|_B = H_0(r) \bigg|_{-B} \]  \hspace{1cm} \text{(A.6)}

Also, let us assume that

\[ \Sigma^R(r, r', E) \bigg|_B = \Sigma^R(r', r, E) \bigg|_{-B} \]  \hspace{1cm} \text{(A.7)}

We will verify this assumption later. Using Eqs. (A.6) and (A.7) we can show that

\[ \phi_m(r, E) \bigg|_B = \psi_m^*(r, E) \bigg|_{-B} \]  \hspace{1cm} \text{(A.8)}

From Eqs. (A.5) and (A.8) we obtain the reciprocity relation

\[ G^R(r, r', E) \bigg|_B = G^R(r', r, E) \bigg|_{-B} \]  \hspace{1cm} \text{(A.9)}

To complete the proof we need to verify our assumption in Eq. (A.7). We note from Eq. (A.9) that (see Eq. (2.4))

\[ A(r, r', E) \bigg|_B = A(r', r, E) \bigg|_{-B} \]  \hspace{1cm} \text{(A.10)}

Using Eqs. (A.9) and (A.10) we can show from Eq. (3.3) that

\[ \Gamma(r, r', E) \bigg|_B = \Gamma(r', r, E) \bigg|_{-B} \]  \hspace{1cm} \text{(A.11)}

Now, \( \Sigma = \Sigma_{HF} + (\Gamma' - i\Gamma)/2 \) where \( \Gamma' \) is the Hilbert transformation of \( \Gamma \). Eq. (A.11) states that reversing the magnetic field has the effect of interchanging \( r \) and \( r' \) in \( \Gamma \) and hence in \( \Gamma^R \). The **Hartree-Fock** self-energy \( \Sigma_{HF}(r, r') \) depends on \( G_0(r, r', E) \). At equilibrium, Eq. (A.10) implies that
\[ G_n(r, r', E) \bigg|_B = G_n(r', r, E) \bigg|_{-B} \]  \hspace{1cm} (A.12)

Since \( G_n(E) = f_{eq}(E)A(E) \). Hence, at equilibrium, reversing the magnetic field has the effect of interchanging \( r \) and \( r' \) in \( \Sigma_{HF} \). Since this is true of \( \Gamma' \) and \( \Gamma \) as well, it is true of \( \Sigma^R \) as stated in Eq. (A.7) (at equilibrium).
Appendix B: Reservoir function

Eq. (3.18)

We start by rewriting Eq. (3.17) using Eqs. (3.4), (2.4) and (2.5):

\[ i(\alpha) = \frac{e}{\hbar} \left[ \Gamma_i(\alpha) A^*(\alpha) - \Gamma(\alpha) A^*(\alpha) f^*(\alpha) \right] \]

\[ = \frac{e}{\hbar} \Gamma(\alpha) A^*(\alpha) \left[ f_\Gamma(\alpha) - f(\alpha) \right] \]

where \( \alpha \equiv (r',r,E) \) and we have used the relation \( f(\alpha) = f^*(\alpha) \) (see Eq. (1.8a)). Taking the functional derivative around the equilibrium solution \( (f(\alpha) = f_\Gamma(\alpha) = f_{eq}(E)) \), we obtain Eq. (3.18),

\[ \frac{\delta i(\alpha_1)}{\delta \mu(\alpha_2)} = \frac{e}{\hbar} \Gamma_{eq}(\alpha_1) A_{eq}^*(\alpha_1) \left[ \frac{\delta f_\Gamma(\alpha_1)}{\delta \mu(\alpha_2)} - \left[ - \frac{\delta f_{eq}(E_1)}{\delta E_1} \right] \delta(\alpha_1 - \alpha_2) \right] \]

\[ = g_R(\alpha_1, \alpha_2) - I_{eq}(\alpha_1) \delta(\alpha_1 - \alpha_2) \]

where we have made use of Eqs. (3.16) and (3.19). Next we will evaluate the reservoir functions \( g_R \) and \( D_R \) for electron-phonon and electron-electron interactions in the self-consistent Born approximation.

**Electron-phonon** interaction

For electron-phonon interaction we can write in the self-consistent Born approximation (5),

\[ \Gamma_i(\rho_1, E_1) = \int dE_2 D(\rho_1, E_1 - E_2) G_n(\rho_1, E_2) \]  \hspace{1cm} (B.1a)

\[ \Gamma_0(\rho_1, E_1) = \int dE_2 D(\rho_1, E_2 - E_1) G_p(\rho_1, E_2) \]  \hspace{1cm} (B.1b)

where \( p \) stands for a pair of points \((r,r')\) and \( D(\rho, \hbar \omega) \) describes the spatial correlation and frequency spectrum of the phonons. Using Eqs. (B.1a,b) we can write,
\begin{align*}
i(\rho_1 E_1) &= \frac{e}{\hbar} \left[ \Gamma_{\uparrow}(\rho_1 E_1) G_p^\uparrow(\rho_1 E_1) - \Gamma_0(\rho_1 E_1) G_p^\downarrow(\rho_1 E_1) \right] \\
&= \frac{e}{\hbar} \int dE_2 \ D(\rho_1, E_1 - E_2) G_p^\uparrow(\rho_1, E_1) G_n(\rho_1, E_2) \left[ 1 - e^{(\mu(\rho_1, E_1) - \mu(\rho_1, E_2))/k_B T} \right] \tag{B.2}
\end{align*}

Here we have made use of the definition of the non-equilibrium potential $\mu$ (see Eq. (3.4)) and the relation

\[ D(\rho_1, E_2 - E_1) = D(\rho_1, E_1 - E_2) e^{(E_2 - E_1)/k_B T} \tag{B.3} \]

Taking the functional derivative we obtain from Eq. (B.2),

\[
\frac{\delta i(\rho_1, E_1)}{\delta \mu(\rho_2, E_2)} = \delta(\rho_1 - \rho_2) \left. \frac{e}{\hbar k_B T} D(\rho_1, E_1 - E_2) G_p^\uparrow(\rho_1, E_1) G_n(\rho_1, E_2) \right|_{\text{eq}} \\
- \delta\rho_1 - \rho_2 \delta(\rho_2, E_2) \left. \frac{e}{\hbar k_B T} \Gamma_{\uparrow}(\rho_1, E_1) G_p^\uparrow(\rho_1, E_1) \right|_{\text{eq}} \tag{B.4}
\]

At equilibrium

\[ \Gamma_{\uparrow}(\rho_1, E_1) G_p^\uparrow(\rho_1, E_1) = \Gamma_{\text{eq}}(\rho_1, E_1) A_{\text{eq}}^\uparrow(\rho_1, E_1) f_{\text{eq}}(E_1)(1 - f_{\text{eq}}(E_1)) \]

so that the second term in Eq. (B.4) can be written as $\delta(\rho_1 - \rho_2) \delta(E_1 - E_2) I_{\text{eq}}(\rho_1, E_1)$ (using Eq. (3.19)). Hence, from Eqs. (B.4) and (8.5),

\[ g_R(\rho_1, E_1; \rho_2, E_2) = \delta(\rho_1 - \rho_2) \left. \frac{e}{\hbar k_B T} D(\rho_1, E_1 - E_2) G_p^\uparrow(\rho_1, E_1) G_n(\rho_1, E_2) \right|_{\text{eq}} \tag{B.5} \]

It is interesting to note that $g_R$ is proportional to the scattering rate from $(\rho_2, E_2)$ to $(\rho_1, E_1)$ at equilibrium which is, of course, balanced by an equal and opposite scattering from $(\rho_2, E_2)$ to $(\rho_1, E_1)$. This is possibly a general feature true of other dephasing mechanisms as well. It is reminiscent of the linear conductance of a diode $(I_0/k_B T)$ where $I_0$ is the 'equilibrium current'. Using Eq. (8.6) we obtain the result stated in Eq. (8.15).

\[ D_R(\rho_1 E_1; \rho_2 E_2) = \delta(\rho_1 - \rho_2) D(\rho_1, E_1 - E_2) \tag{B.6} \]
Electron-electron interaction

For electron-electron interaction we can write in the self-consistent Born approximation (direct, not exchange)

\[ \Gamma_1(p_1 E_1) = \int dp_3 dE_3 dE_4 v(r_1-r_3) v(r'_1-r'_3) G_n(p_1, E_1-E_3+E_4) G_n(p_3 E_3) G_p(\bar{p}_3 E_4) \]  \hspace{1cm} (B.7a)

\[ \Gamma_0(p_1 E_1) = \int dp_3 dE_3 dE_4 v(r_1-r_3) v(r'_1-r'_3) G_p(p_1, E_1-E_3+E_4) G_p(p_3 E_3) G_n(\bar{p}_3 E_4) \]  \hspace{1cm} (B.7b)

Here \( \mathbf{p} \) stands for \((r,r')\) and \( \bar{\mathbf{p}} \) for \((r',r)\); also, \( v(r_1-r_2) \) is the Coulomb interaction potential between electrons at \( r_1 \) and \( r_2 \).

Using Eqs. (B.7a,b) we can write

\[ i(p_1 E_1) = \frac{e}{\hbar} \left[ \Gamma_1(p_1 E_1) G_p^*(p_1 E_1) - \Gamma_0(p_1 E_1) G_n^*(p_1 E_1) \right] \]

\[ = \frac{e}{\hbar} \int dp_3 dE_3 dE_4 V(p_1 p_3) G_p^*(p_1 E_1) G_n(p_1, E_1-E_3+E_4) G_n(p_3 E_3) G_p(\bar{p}_3 E_4) \]

\[ \left[ 1 - \exp \left( \frac{\mu(p_1 E_1)^* - \mu(p_1, E_1-E_3+E_4) - \mu(p_3 E_3) + \mu(\bar{p}_3 E_4)}{k_B T} \right) \right] \]  \hspace{1cm} (B.8)

where \( V(p_1, p_3) \equiv v(r_1-r_3) v(r'_1-r'_3) \). Taking the functional derivative we obtain from Eq. (B.8),

\[ \frac{\delta i(p_1 E_1)}{\delta \mu(p_2 E_2)} = -\frac{e}{\hbar k_B T} \int dp_3 dE_3 dE_4 V(p_1 p_3) G_p^*(p_1 E_1) G_n(p_1, E_1-E_3+E_4) G_n(p_3 E_3) G_p(\bar{p}_3 E_4) \]

\[ \left[ -\delta(p_1-p_2) \delta(E_1-E_2) + \delta(p_1-p_2) \delta(E_1-E_3+E_4-E_2) + \delta(p_3-p_2) \delta(E_3-E_2) - \delta(p_3-p_2) \delta(E_4-E_2) \right] \]

\hspace{1cm} (B.9)

The first Gfunction in Eq. (B.9) yields the term \(-I_{eq}(p_1 E_1) \delta(p_1-p_2) \delta(E_1-E_2)\), so that from Eq. (8.5a),
Using Eq. (8.6) we obtain the reservoir coupling function \( D_R \).

\[
\frac{\hbar k_B T}{e} \delta_R(\rho_1, \rho_2) = \\
\delta(\rho_1 - \rho_2) \int d\rho_3 dE_3 \quad V(\rho_1, \rho_3) G_n(\rho_1, E_2) G_n(\rho_3, E_3) G_p(\rho_3, E_3 + E_2 - E_1) \left|_{\text{eq}} \right.
\]
\[
+ V(\rho_1, \rho_2) \int dE_3 \quad G_p(\rho_1, E_1) G_n(\rho_1, E_1 - E_2 + E_3) G_n(\rho_2, E_2) G_p(\rho_2, E_3) \left|_{\text{eq}} \right.
\]
\[
- V(\rho_1, \rho_2) \int dE_3 \quad G_p(\rho_1, E_1) G_n(\rho_1, E_1 + E_2 - E_3) G_n(\rho_2, E_3) G_p(\rho_2, E_2) \left|_{\text{eq}} \right.	ag{B.10}
\]

(B.10)

Using Eq. (8.6) we obtain the reservoir coupling function \( D_R \).

\[
D_R(\rho_1, \rho_2) = \delta(\rho_1 - \rho_2) \int d\rho_3 dE_3 \quad V(\rho_1, \rho_3) G_n(\rho_3, E_3) G_p(\rho_3, E_3 + E_2 - E_1) \left|_{\text{eq}} \right.
\]
\[
+ V(\rho_1, \rho_2) \int dE_3 \quad G_n(\rho_1, E_1 - E_2 + E_3) G_p(\rho_2, E_3) \left|_{\text{eq}} \right.
\]
\[
- \frac{1 - f_2}{f_2} V(\rho_1, \rho_2) \int dE_3 \quad G_n(\rho_1, E_1 + E_2 - E_3) G_n(\rho_2, E_3) \left|_{\text{eq}} \right. \tag{B.11}
\]

(B.11)

where \( f_2 \) stands for \( f_{\text{eq}}(E_2) \).
Appendix C: Terminal current

The current density \( J(r, E) \) is obtained from the correlation function \( G_n(r, r', E) \) using the relation

\[
2\pi J(r, E) = -\frac{i\hbar}{2m} \left( \nabla - \nabla' \right) G_n(r, r', E) \bigg|_{r' = r} - \frac{e^2}{m} A(r) G_n(r, r, E) \tag{C.1}
\]

Note that here we are using \( A \) to denote the vector potential and not the spectral function as we have done throughout the paper. Substituting for \( G_n \) from Eq. (3.6) into Eq. (C.1),

\[
2\pi J(r, E) = \int d\rho_1 \, K_j(r, \rho_1, E) \Gamma_1(\rho_1, E) \tag{C.2}
\]

where \( \rho_1 = (r_1, r_1') \) and \( K_j \) is given by

\[
K_j(r, \rho_1, E) = -\frac{i\hbar}{2m} \left[ G^R(r, r_1', E)^* \nabla G^R(r, r_1, E) - G^R(r, r_1, E) \nabla G^R(r, r_1', E)^* \right] - \frac{e^2}{m} A(r) G^R(r, r_1, E) G^R(r, r_1', E)^* \tag{C.3}
\]

The terminal current \( I_i \) at contact 'i' is obtained by integrating the flux \( J \cdot dS_i \) over the device-contact interface. There is no current flow deep inside the contact far away from the device since we have assumed it to be in equilibrium. This allows us to replace the integral over the device-contact interface by an integral over a closed surface enclosing contact 'i' and then to use the divergence theorem to obtain

\[
I_i = \int dE \oint J(r, E) \cdot dS_i = \int dE \int_{r \in \text{contact 'i'}} dr \nabla \cdot J(r, E) \tag{C.4}
\]

Note that the divergence of the current density integrated over all energy (\( \int dE \nabla \cdot J(r, E) \)) is zero everywhere except in the contacts within a region of the order of a phase-breaking length from the device-contact interface. This non-zero divergence integrated over the contact gives us the net current flowing into the device from the contact as indicated in Eq. (C.4).

From Eq. (C.2) we can write
\[ \mathbf{V} \cdot \mathbf{J}(r, E) = \int d\rho_1 \left[ \frac{\mathbf{V} \cdot \mathbf{K}_J(r, \rho_1, E)}{2\pi} \right] \Gamma_1(r, E) \]  

(C.5)

We now note that

\[ \frac{1}{2\pi} \mathbf{V} \cdot \mathbf{K}_J(r, \rho_1, E) = \frac{ie}{\hbar} \left[ G^R(r, r'_1, E)^* (H_0(r) G^R(r, r_1, E)) - G^R(r, r_1, E)(H_0(r) G^R(r, r'_1, E))^* \right] \]

(C.6)

where \( H_0 = (i\hbar \nabla + eA)^2/2m + V \) is the one-electron effective mass Hamiltonian. Substituting for \( H_0 G^R \) from Eq. (2.6) we obtain the identity

\[ \frac{1}{2\pi} \mathbf{V} \cdot \mathbf{K}_J(r, \rho_1, E) = \frac{ie}{\hbar} \left[ \delta(r-r'_1) G^R(r, r_1, E) - \delta(r-r_1) G^R(r, r'_1, E)^* \right. \]

\[ + G^R(r, r_1, E) \int dr' \Sigma^R(r, r', E)^* G^R(r', r'_1, E)^* \]

\[ - G^R(r, r'_1, E)^* \int dr' \Sigma^R(r, r', E) G^R(r', r_1, E) \]  

(C.7)

From Eqs. (C.4), (C.5) and (C.7) we can write

\[ I_i = \int dE \int dr \int_{\text{contact 'i'}} dr' \frac{ie}{\hbar} \left[ \Gamma_1(\alpha)^* G^R(\alpha) + \Sigma^R(\alpha)^* G_n(\alpha) + \Sigma^R(\alpha) Y(\alpha)^* \right. \]

\[ - \text{complex conjugate} \]  

(C.8)

Note that \( \alpha \) stands for \( (r, r', E) \) and \( Y \) stands for the quantity

\[ Y(E) = G_n(E) - G^R(E) \Gamma_1(E) G^A(E) \]  

(C.9)

From Eq. (2.7) we would expect \( Y \) to be identically zero. However, \( Y(r, r', E) \) is not necessarily zero when \( r \) and \( r' \) both lie within the same contact. This is because for \( (r, r') \in \text{contact 'i'} \), we impose a boundary condition on \( G_n(r, r', E) \) instead of solving Eq. (2.7) for it. For all other pairs of points we actually solve Eq. (2.7) thus ensuring that \( Y(r, r', E) = 0 \).

We can write the terminal current \( I_i \) as a sum of two parts \( I_i' \) and \( I_i'' \)
which are given by

\[ I_i' = \int dE \int dr \int dr' \frac{ie}{\hbar} \left[ \Gamma_i(\alpha)^* G^R(\alpha) + \Sigma^R(\alpha)^* G_n(\alpha) + \Sigma^R(\alpha) Y(\alpha)^* \right] - \text{complex conjugate} \]  
\[ I_i'' = \int dE \int dr \int dr' \frac{ie}{\hbar} \left[ \Gamma_i(\alpha)^* G^R(\alpha) + \Sigma^R(\alpha)^* G_n(\alpha) - \text{complex conjugate} \right] \]

The expression for \( I_i' \) can be simplified by noting that the contacts are assumed to be equilibrium regions in zero magnetic field so that the functions \( \Gamma_i, \Gamma, G_n, Y \) are all real. Also \( \Gamma_i(\alpha)/\Gamma(\alpha) = G_n(\alpha)/A(\alpha) \). Using these relations we can write

\[ I_i' = \int dE \int dr \int dr' I(r, r', E) \text{amt contact 'i'} \]

where (using Eq. (C.9) to substitute for \( Y(E) \))

\[ I(r_1, r'_1, E) = \frac{e}{\hbar} I^*(r_1, r'_1, E) [G_n(r_1, r'_1, E) - \int dr_2 dr'_2 G^R(r_1, r_2, E) G^R(r'_1, r'_2, E)^* \Gamma_i(r_2, r'_2, E)] \]  
\[ \text{(C.13)} \]

Note that \( I(r, r', E) \) is non-zero only when both \( r \) and \( r' \) lie within the same contact. These are the points for which we impose boundary conditions. For all other points \( I(r, r', E) = 0 \) and Eq. (C.13) reduces to Eq. (3.6).

Eq. (C.13) can be rewritten in the form

\[ I(\alpha_1) = \frac{e}{\hbar} \Gamma(\alpha_1)^* A(\alpha_1) \left[ f(\alpha_1) - \int d\alpha_2 P(\alpha_1, \alpha_2) f_1(\alpha_2) \right] \]  
\[ \text{(C.14)} \]

where \( \alpha_1 \equiv (r_1, r'_1, E_1) \) and \( \alpha_2 = (r_2, r'_2, E_2) \). Note the similarity with Eq. (3.7). At equilibrium the quantity within parenthesis is zero and there is no terminal current: \( I(\alpha) = 0 \). For small deviations from this equilibrium state we can write
The functional derivative is now evaluated exactly as we did in Section 3 to obtain instead of Eq. (3.21):

\[
I(\alpha) = \frac{e}{\hbar} \Gamma_{eq}(\alpha_1) A_{eq}(\alpha_1) \int d\alpha_3 \left[ \mu(\alpha_3) - \mu_{eq} \right] \frac{\delta}{\delta \mu(\alpha_3)} \left[ f(\alpha_1) - \int d\alpha_2 P(\alpha_1, \alpha_2) f_\Gamma(\alpha_2) \right]
\]

(C. 15)

If \( I(\alpha) = 0 \), then Eq. (C.13) reduces to Eq. (3.21). But inside the contacts \( I(\alpha) \) is non-zero for a short distance (~\( L_0 \)) near the device-contact interface. Integrating over the contact we obtain the terminal current as indicated in Eq. (C.12) Note, however, that there is another component of the terminal current \( I''_1 \) (see Eq. (C.11b)). This component is zero for point scatterers and we will not consider it further in this paper.

**Current Density**

The above approach allows us to compute the terminal current \( I_1 \) without explicitly computing the current density \( J(\mathbf{r}, E) \). However, we could compute the linear response current density if we are interested. We write Eq. (C.2) in the form \((\mathbf{p}_1 = \mathbf{r}_1, \mathbf{r}_1')\)

\[
J(\mathbf{r}, E) = \int d\mathbf{p}_1 P_J(\mathbf{r}, \mathbf{p}_1, E) f_\Gamma(\mathbf{p}_1, E)
\]

(C.16)

where

\[
P_J(\mathbf{r}, \mathbf{p}_1, E) \equiv K_J(\mathbf{r}, \mathbf{p}_1, E) \Gamma(\mathbf{p}_1, E)/2\pi
\]

(C.17)

The current density is not necessarily zero at equilibrium when a magnetic field is present. We can write the change \( \delta J(\mathbf{r}, E) \) due to a change \( \delta \mu(\rho_2, E_2) \) as

\[
\frac{\delta J(\mathbf{r}, E)}{\delta \mu(\rho_2, E_2)} = \int d\mathbf{p} P_J(\mathbf{r}, \mathbf{p}_1, E) \left| \frac{\delta f_\Gamma(\mathbf{p}_1, E)}{\delta \mu(\rho_2, E_2)} \right|_{\text{eq}} + \int d\mathbf{p}_1 \frac{\delta P_J(\mathbf{r}, \mathbf{p}_1, E)}{\delta \mu(\rho_2, E_2)} \left| f_\text{eq}(E) \right|_{\text{eq}}
\]

(C.18a)

The net change \( \delta J(\mathbf{r}, E) \) is given by
\[ \delta J(r, E) = \int d\rho_2 \, dE_2 \left. \frac{\delta J(r, E)}{\delta \mu(\rho_2, E_2)} \right|_{eq} (\mu(\rho_2, E_2) - \mu_{eq}) \]  

(C.18b)

which can be evaluated once the potential \( \mu(\rho_2, E_2) \) has been computed everywhere by solving Eq. (3.21) subject to the boundary conditions at the contacts.

Once \( \delta J(r, E) \) has been obtained one could calculate the terminal current \( I_i \) by integrating the flux across the device-contact interface \( S_i \)

\[ I_i = \int dE \int \delta J(r, E) \cdot dS_i \]  

(C.19)

It can be shown that only the first term in Eq. (C.18a) contributes to the terminal current; the second term gives a net current of zero when integrated over the interface.
Appendix D: Büttiker formula

We start by rewriting Eq. (6.1) as

\[ \mu(\alpha_1) = \sum_j \mu_j \left[ \int \! \! \int d\alpha_j \frac{eT(\alpha_1, \alpha_j)}{h \lambda^*_e(\alpha_1)} \right] + \int \! \! \int d\alpha_3 \frac{eT(\alpha_1, \alpha_3)}{h \lambda^*_e(\alpha_1)} \mu(\alpha_3) \]  \hspace{1cm} (D.1)

It is implied that the integration over \( \alpha_j \) is carried out for spatial coordinates lying within contact 'j'. We can solve Eq. (D.1) iteratively to obtain

\[ \mu(\alpha_1) = \sum_j \mu_j \left[ \int \! \! \int d\alpha_j \frac{eT(\alpha_1, \alpha_j)}{h \lambda^*_e(\alpha_1)} + \int \! \! \int d\alpha_3 \frac{eT(\alpha_1, \alpha_3)}{h \lambda^*_e(\alpha_1)} \mu(\alpha_3) \right] + \ldots \]  \hspace{1cm} (D.2)

To obtain the terminal current we combine Eqs. (4.1) and (4.4) to write \((\alpha \in \text{contact } 'i')\)

\[ I_i = \mu_i \int \! \! \int d\alpha I^*_e(\alpha) - \frac{e}{h} \sum_j \mu_j \int \! \! \int d\alpha d\alpha_j T(\alpha, \alpha_j) - \frac{e}{h} \int \! \! \int d\alpha d\alpha_2 T(\alpha, \alpha_2) \mu(\alpha_2) \]  \hspace{1cm} (D.3)

Substituting for \( \mu(\alpha_1) \) from Eq. (D.2) we obtain \((\alpha \in \text{contact } 'i')\)

\[ I_i = \mu_i \int \! \! \int d\alpha I^*_e(\alpha) - \frac{e}{h} \sum_j \mu_j \left[ \int \! \! \int d\alpha d\alpha_j T(\alpha, \alpha_j) + \int \! \! \int d\alpha d\alpha_2 d\alpha_j T(\alpha, \alpha_2) \frac{eT(\alpha_2, \alpha_j)}{h \lambda^*_e(\alpha_2)} \right] 

+ \int \! \! \int d\alpha d\alpha_2 d\alpha_4 d\alpha_j T(\alpha, \alpha_1) \frac{eT(\alpha_2, \alpha_4)}{h \lambda^*_e(\alpha_2)} \frac{eT(\alpha_4, \alpha_j)}{h \lambda^*_e(\alpha_4)} + \ldots \]  \hspace{1cm} (D.4)

Eq. (D.4) can be written in the form

\[ I_i = \frac{e}{h} \left[ \tilde{M}_i \mu_i - \sum_j \tilde{T}_{ij} \mu_j \right] \]  \hspace{1cm} (D.5a)

where

\[ \tilde{M}_i = \int \! \! \int d\alpha \sum_{\alpha \in \text{contact } 'i'} [I^*_e(\alpha) - \int \! \! \int d\alpha T(\alpha, \alpha_i)] \]  \hspace{1cm} (D.5b)

Since the current \( I_i \) is zero when all the potentials \( \mu_j \) are equal, \( \tilde{M}_i = \sum_j \tilde{T}_{ij} \) and Eq. (D.5a) can be rewritten as Eq. (1.5). The transmission \( \tilde{T}_{ij} \) is given by an infinite series whose successive terms are \((\alpha \in \text{contact } 'i')\):
\[
\tilde{T}_{ij}^{(0)} = (1-\delta_{ij}) \int d\alpha d\alpha' T(\alpha, \alpha') \tag{D.6}
\]
\[
\tilde{T}_{ij}^{(1)} = \int d\alpha d\alpha_2 d\alpha_j T(\alpha, \alpha_2) \frac{eT(\alpha_2, \alpha_j)}{h \Omega_{eq}(\alpha_2)} \tag{D.7}
\]
\[
\tilde{T}_{ij}^{(2)} = \int d\alpha d\alpha_2 d\alpha_4 d\alpha_j T(\alpha, \alpha_2) \frac{eT(\alpha_2, \alpha_4)}{h \Omega_{eq}(\alpha_2)} \frac{eT(\alpha_4, \alpha_j)}{h \Omega_{eq}(\alpha_4)} \tag{D.8}
\]

In Eq. (D.5), \(\delta_{ij}\) stands for the Kronecker delta. We now make use of Eq. (3.22) to rewrite Eqs. (D.6) - (D.8) as \((\alpha_i \in \text{contact 'i'}, \alpha_b \in \text{contact 'i'}, \alpha_2, \alpha_4 \in \text{device}, \alpha_1, \alpha_3, \alpha_5 \text{ unrestricted})\)

\[
\tilde{T}_{ij}^{(0)} = (1-\delta_{ij}) \int d\alpha d\alpha_b \frac{h \Omega_{eq}(\alpha, \alpha_1)}{e} g_R(\alpha_1, \alpha_b) \tag{D.9}
\]
\[
\tilde{T}_{ij}^{(1)} = \int d\alpha d\alpha_b d\alpha_1 d\alpha_2 \frac{h \Omega_{eq}(\alpha, \alpha_1)}{e} \frac{P_{eq}(\alpha_2, \alpha_3)}{I_{eq}(\alpha_2)} g_R(\alpha_3, \alpha_b) \tag{D.10}
\]
\[
\tilde{T}_{ij}^{(2)} = \int d\alpha d\alpha_b d\alpha_1 d\alpha_2 d\alpha_3 d\alpha_4 \frac{h \Omega_{eq}(\alpha, \alpha_1)}{e} \frac{P_{eq}(\alpha_2, \alpha_3)}{I_{eq}(\alpha_2)} \frac{P_{eq}(\alpha_4, \alpha_5)}{I_{eq}(\alpha_4)} g_R(\alpha_5, \alpha_b) \tag{D.11}
\]

We now make use of our assumption that the dephasing processes are local within the contacts. Consequently the reservoir function \(g_R(\alpha_1, \alpha_2)\) is zero if \(\alpha_1 \in \text{contact and } \alpha_2 \in \text{device or vice versa}. Substituting for \(P'_{eq}\) from Eq. (3.23) and making use of Eq. (3.20) we obtain \((\alpha_i \in \text{contact 'i'}, \alpha_b \in \text{contact 'i')}\)

\[
\tilde{T}_{ij}^{(0)} = (1-\delta_{ij}) \int d\alpha d\alpha_b \frac{h \Omega_{eq}(\alpha, \alpha_1) g_{eq}(\alpha, \alpha_b)}{e A_{eq}(\alpha_b)} I_{eq}(\alpha_b) \tag{D.12}
\]
Substituting for \( \Gamma_{eq} \) from Eq. (3.19), rearranging and making use of Eq. (6.6) we obtain the forms stated earlier (Eqs. (6.3) - (6.5)). We also make use of the fact that 
\( g_{eq}(\alpha_1, \alpha_2) = \delta(E_1 - E_2) \) and that \( \Gamma_{eq} \) is real inside the contacts.