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A simple kinetic equation for steady-state quantum transport

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Abstract. An important problem in quantum transport is to understand the role of dissipative processes. In this paper we assume a model in which phase-breaking and dissipation are caused by the interaction of electrons with a reservoir of oscillators through a delta potential. In our model the self-energy is a delta function in space, leading to a kinetic equation with a simple physical interpretation. A novel treatment of the contacts is used to introduce the external current into the kinetic equation. On specializing to linear response we obtain an integral equation that looks like the Büttiker formula extended to a continuous distribution of probes. We show that this equation with a continuous distribution of probes can be reduced to the usual Büttiker formula which involves only the actual physical probes. The effect of dissipation is to modify the transmission coefficients, and we present explicit expressions derived from our model. Also, in a homogeneous medium the integral equation reduces to the diffusion equation, if the electrochemical potential is assumed to vary slowly. This paper serves to establish a bridge between the quantum kinetic approach which rigorously accounts for the exclusion principle and the one-particle approach which is intuitively appealing. We believe that this work can be extended to more sophisticated models where the self-energy is not a delta function.

Contents

1. Introduction
 2. Microscopic model
 3. Kinetic equation
 4. Low-bias conditions
 5. Linear response
 6. Summary
 7. References
- Appendix A. Derivation of self-energy functions
 - Appendix B. Derivation of the kinetic equation
 - Appendix C. Derivation of some useful properties of Green Functions
 - Appendix D. Derivation of the diffusion equation from the linearised kinetic equation

1. Introduction

Much of the current theoretical work on mesoscopic structures is based on the Landauer approach [1]. In particular, the Büttiker formula relating the currents I_i at the probes i to the electrochemical potentials μ_j at the probes j has found widespread use [2].

$$I_i = \frac{e^2}{h} \left(\bar{T}_i \mu_i - \sum_j T_{ij} \mu_j \right) \quad (1.1)$$

where

$$\bar{T}_i = \sum_j T_{ij} = \sum_j T_{ji} \quad (1.2)$$

$$T_{ij}(B) = T_{ji}(-B) \quad (1.3)$$

B being the magnetic field. Equation (1.1) has been related to linear response theory [3] and has been very successful in explaining many experimental observations [4]. However, there are a number of unanswered questions:

(1) How can we compute the transmission coefficients T_{ij} in the presence of phase-breaking scattering processes within the device? Usually the coefficients T_{ij} are computed from the one-electron Schrödinger equation assuming that transport through the device is phase-coherent.

(2) How can we describe harmonic generation [5] and large signal response [6] including phase-breaking processes? Equation (1.1) describes linear response only.

(3) How can we compute the electron density in the device so that the electrostatic potential can be determined self-consistently from the Poisson equation? In linear response only the equilibrium electron density is needed. This can, in principle, be computed by multiplying the local density of states $N_0(\mathbf{r}; E)$ with the Fermi factor $f_0(E)$; thus no new theory is necessary. However, for larger bias, we need the electron density under conditions far from equilibrium and a transport equation that accounts for phase-breaking processes is desirable. It would also be instructive to compute quantities like the current density inside the structure.

This paper represents an attempt to provide answers to these questions assuming a specific model for the phase-breaking scattering processes [7, 8]. A quantum kinetic approach is adopted so that the exclusion principle is rigorously accounted for. This paper thus also serves to establish a bridge between the one-electron approach commonly used to derive (1.1) and the quantum kinetic approach.

The role of the distribution function in semiclassical transport theory is played by the correlation function $G^<$ (or the related Wigner function) in quantum transport theory [9–15].

$$G^<(\mathbf{r}_1, \mathbf{r}_2; t_1, t_2) = (i/\hbar) \langle \psi^+(\mathbf{r}_2, t_2) \psi(\mathbf{r}_1, t_1) \rangle \quad (1.4)$$

where $\psi(\mathbf{r}, t)$ is the electron field operator. It is common to transform to centre of mass

$$\mathbf{r} = (\mathbf{r}_1 + \mathbf{r}_2)/2 \quad t = (t_1 + t_2)/2 \quad (1.5)$$

and relative coordinates, and then Fourier transform with respect to the relative coordinate

$$\mathbf{r}_1 - \mathbf{r}_2 \rightarrow \mathbf{k} \quad t_1 - t_2 \rightarrow E \quad (1.6)$$

to obtain $G^<(\mathbf{r}; \mathbf{k}; E; t)$. Quantum kinetic equations have been derived that can, in principle, be solved to obtain $G^<$. Various quantities of interest such as the electron density and the current density can all be computed, once $G^<$ is known. In practice, the large number of independent variables $(\mathbf{r}; \mathbf{k}; E; t)$ often make it difficult to solve the kinetic equation.

The kinetic equation we derive involves only the electron density per unit energy $n(\mathbf{r}; E)$ which is obtained by integrating the correlation function over \mathbf{k} or equivalently by setting $\mathbf{r}_1 = \mathbf{r}_2 = \mathbf{r}$:

$$2\pi n(\mathbf{r}; E) = -i \int \frac{d\mathbf{k}}{(2\pi)^3} G^<(\mathbf{r}; \mathbf{k}; E) = -i G^<(\mathbf{r}_1, \mathbf{r}_2; E)|_{\mathbf{r}_1 = \mathbf{r}_2 = \mathbf{r}} \quad (1.7)$$

The time variable $t = (t_1 + t_2)/2$ does not appear because of our restriction to steady-state. The averaging over \mathbf{k} is made possible by assuming a special form for the phase-breaking scatterers. We assume that the scattering is caused by a distribution of independent oscillators, each of which interacts with the electrons through a delta potential. We also assume that the phase-breaking processes are weak and infrequent, just as one does in deriving Fermi's golden rule (however, *the elastic scattering processes are treated exactly*). In the 'golden rule' approximation, each scatterer acts independently. Since we have assumed a delta interaction potential, a phase-breaking event only involves the wavefunction at a particular point and is insensitive to spatial correlations. This allows us to write a transport equation that only involves the diagonal elements $G^<(\mathbf{r}, \mathbf{r}; E)$ of the correlation function which represent the electron density $n(\mathbf{r}; E)$ (see equation (1.7)). Spatial correlations of the field represented by the off-diagonal elements $G^<(\mathbf{r}_1, \mathbf{r}_2; E)$, $\mathbf{r}_1 \neq \mathbf{r}_2$ do not appear in this equation. However, once we have solved this equation for the diagonal elements, we can also compute the full correlation function $G^<(\mathbf{r}_1, \mathbf{r}_2; E)$ including the off-diagonal elements in a straightforward manner. Other quantities of interest such as the current density $\mathbf{J}(\mathbf{r}; E)$ can then be computed. It will be noted that $G^<(\mathbf{r}; \mathbf{k}; E)$ is in general a complex quantity. However, the electron density per unit energy $n(\mathbf{r}; E)$ obtained by integrating over \mathbf{k} is positive definite. We believe that this is related to the fact that the simultaneous use of \mathbf{r} and \mathbf{k} violates the uncertainty principle but the simultaneous use of \mathbf{r} and E does not.

An obvious question to ask is whether our model for the phase-breaking scatterers is realistic. It closely approximates a laboratory sample with magnetic impurities or impurities having internal degrees of freedom. For other types of phase-breaking scattering processes, the model may not be accurate; however, it may still be possible to describe much of the essential physics of dissipation in quantum transport. *At the very least*, we have a well-defined microscopic model whose predictions can be worked out numerically for realistic structures and compared with experiment. This should enable us to identify new phenomena arising from spatially correlated inelastic scattering processes and many-body effects that are neglected in our model.

The kinetic equation is further simplified by assuming that there is no carrier heating so that the energy distribution of carriers at any point \mathbf{r} can be expressed in terms of a local electrochemical potential $\mu(\mathbf{r})$ as shown in (2.11). Specializing to linear response

we obtain an equation for $\mu(\mathbf{r})$ that looks like (1.1) generalized to include a continuous distribution of probes. This can be understood easily following the approach used by Büttiker to simulate phase-breaking processes [16]. Since the phase-breaking scattering process in our model is purely local, it can be viewed as an exit into a reservoir followed by reinjection into the main structure. From this point of view it would seem that distributed inelastic scattering processes can be simulated by connecting a continuous distribution of reservoirs throughout a structure [17, 18]. A direct generalization of (1.1), however, would appear to be a phenomenological approach to simulating phase-breaking scattering. This paper provides the rigorous justification for such an approach, by deriving the kinetic equation directly from a model Hamiltonian making certain well-defined assumptions; it also provides quantitative expressions for the transmission coefficients and allows us to compute the full correlation function (or the Wigner function) from which other quantities of interest such as the electron density and the current density can be obtained.

The outline of this paper is as follows. In section 2 we describe the microscopic model that we assume and derive the self-energy functions. In section 3 we discuss the general kinetic equation—its physical interpretation and how it can be solved numerically. A novel treatment of the contacts is then used to introduce the external current into the kinetic equation. In section 4 we simplify the kinetic equation assuming that the energy distribution of carriers at any point is described by a Fermi factor with a local electrochemical potential. We believe that this simplified equation can be used to describe linear and non-linear response at low bias voltages. In section 5 we specialize to linear response and obtain an equation that looks like (1.1) generalized to a continuous distribution of probes. We also show that this equation can be reduced to (1.1) and obtain an explicit expression for T_{ij} . Also we show that in a homogeneous medium with a slowly varying electrochemical potential this equation reduces to the familiar diffusion equation. We also address the question of whether $\mu(\mathbf{r})$ can be measured by a weakly coupled non-invasive probe. It is shown in section 5 that such a probe measures a weighted average of $\mu(\mathbf{r})$ within a region of the order of a phase-breaking length. The weighting function is characteristic of the probe geometry and construction. Finally we conclude in section 6 by summarizing the key results. In the main paper we have tried to emphasize the physical interpretation of the results, relegating the mathematical details to Appendices A to D.

2. Microscopic model

We consider any arbitrary structure in which the propagation of electrons is described by a one-electron effective mass Hamiltonian of the form

$$H_0 = (\mathbf{p} - e\mathbf{A}(\mathbf{r}))^2/2m^* + eV(\mathbf{r}) \quad (2.1)$$

where m^* is the effective mass. The scalar potential $V(\mathbf{r})$ contains the Hartree potential obtained from a self-consistent solution of the Poisson equation. It includes band-bending due to space charge and external bias, band discontinuities due to heterojunctions, as well as all sources of elastic scattering such as impurities, defects and boundaries. This part of the Hamiltonian (H_0) will be treated exactly.

The phase-breaking scattering is assumed to be due to a reservoir of independent oscillators labeled by the index m ,

$$H_R = \sum_m \hbar\omega_m (a_m^\dagger a_m + \frac{1}{2}) \tag{2.2}$$

where a_m^\dagger and a_m are the creation and annihilation operators for oscillation m . We assume that each oscillator interacts with the electrons through a delta-potential, so that the interaction Hamiltonian H' can be written as

$$H' = \sum_m U\delta(\mathbf{r} - \mathbf{r}_m)(a_m^\dagger + a_m). \tag{2.3}$$

Note that we have assumed the interaction strength U to be constant. There is no loss of generality since the strength of the scattering can be adjusted through the density of scatterers per unit volume per unit energy, described by some function $J_0(\mathbf{r}; \hbar\omega)$. The summation over m is eventually replaced by an integral.

$$\sum_m \rightarrow \int d\mathbf{r} \int d(\hbar\omega) J_0(\mathbf{r}; \hbar\omega). \tag{2.4}$$

A phase-breaking scattering process is usually defined as one in which the scatterer changes its internal state. It is well-known that phase-breaking processes are not necessarily inelastic or dissipative since the final state of the scatterer could have the same energy as the initial state. Such elastic phase-breaking processes are included in our model as a special case when the oscillator frequency $\hbar\omega \rightarrow 0$. Since the spectral distribution of the oscillators $J_0(\mathbf{r}; \hbar\omega)$ in equation (2.4) is completely arbitrary, there is considerable latitude in simulating different scattering mechanisms. In our discussion we will not distinguish the phase-breaking elastic processes from the inelastic ones; we will generally refer to all processes involving the oscillators as phase-breaking processes and the associated time constant as the phase-breaking time.

In calculating the self-energy we assume that the reservoir is in thermal equilibrium and restrict ourselves to one-phonon processes as one does in deriving Fermi's golden rule. With these assumptions, the self-energy function can be shown to be [18] (see appendix A, equations (A.10a, b))

$$\Sigma^>(\mathbf{r}, \mathbf{r}'; E) = \frac{-i\hbar}{\tau_n(\mathbf{r}; E)} \delta(\mathbf{r} - \mathbf{r}') \tag{2.5a}$$

$$\Sigma^<(\mathbf{r}, \mathbf{r}'; E) = \frac{i\hbar}{\tau_p(\mathbf{r}; E)} \delta(\mathbf{r} - \mathbf{r}') \tag{2.5b}$$

where

$$\frac{1}{\tau_n(\mathbf{r}; E)} = \frac{2\pi}{\hbar} \int dE' F(\mathbf{r}; E' - E)p(\mathbf{r}; E') \tag{2.6a}$$

$$\frac{1}{\tau_p(\mathbf{r}; E)} = \frac{2\pi}{\hbar} \int dE' F(\mathbf{r}; E - E')n(\mathbf{r}; E') \tag{2.6b}$$

$$F(\mathbf{r}; \varepsilon) = \begin{cases} U^2 J_0(\mathbf{r}; \varepsilon) N(\varepsilon) & \varepsilon > 0 \\ U^2 J_0(\mathbf{r}; |\varepsilon|) N(|\varepsilon|) e^{|\varepsilon|/k_B T} & \varepsilon < 0. \end{cases} \tag{2.7}$$

$n(\mathbf{r}; E)$ is the electron density per unit energy, while $p(\mathbf{r}; E)$ is the 'hole' density per unit

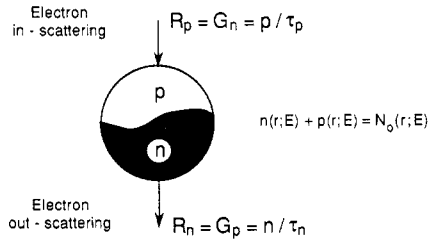


Figure 1. Out-scattering and in-scattering of electrons due to interaction with the reservoir of point oscillators.

energy. Note that the electron density and the hole density refer to the same band. Their sum is equal to the density of states $N_0(\mathbf{r}; E)$.

$$n(\mathbf{r}; E) + p(\mathbf{r}; E) = N_0(\mathbf{r}; E). \quad (2.8a)$$

The density of states is obtained from the imaginary part of the retarded Green function (to be discussed in section 3, see equation (3.2)).

$$N_0(\mathbf{r}; E) = -\text{Im}(G^R(\mathbf{r}, \mathbf{r}; E))/\pi. \quad (2.8b)$$

$N(\hbar\omega)$ is the average number of ‘phonons’ in an oscillator of frequency ω and is given by the Bose–Einstein factor

$$N(\hbar\omega) = 1/(e^{\hbar\omega/k_B T} - 1). \quad (2.9)$$

It is easy to see why the self-energy functions in our model are delta functions in space. Since we consider only one phonon processes, the electron interacts with the same oscillator at \mathbf{r} and \mathbf{r}' . But the interaction potential has been assumed to be a delta function at the location \mathbf{r}_m of the oscillator. Hence \mathbf{r} and \mathbf{r}' must both coincide with \mathbf{r}_m .

The similarity of (2.6a, b) to Fermi’s golden rule will be noted. However, unlike the usual golden rule we are not using energy eigenstates. We are using the position representation and a simple golden rule-like result is not valid in general. It is made possible by our assumption of independent point oscillators that only see the electron wavefunction at one point. In this model, the phase-breaking scattering process is a purely local affair that shuffles the energy E of the electrons at a fixed point \mathbf{r} . The rate R_n at which electrons are scattered out of energy E at the point \mathbf{r} (or the rate G_p at which holes are scattered in) is proportional to the imaginary part of $\Sigma^>(\mathbf{r}, \mathbf{r}; E)$ (equation (2.5a)).

$$R_n(\mathbf{r}; E) = n(\mathbf{r}; E)/\tau_n(\mathbf{r}; E) = G_p(\mathbf{r}; E). \quad (2.10a)$$

Similarly the rate R_p at which holes are scattered out (or the rate G_n at which electrons are scattered in) is proportional to the imaginary part of $\Sigma^<(\mathbf{r}, \mathbf{r}; E)$ (equation (2.5b)).

$$R_p(\mathbf{r}; E) = p(\mathbf{r}; E)/\tau_p(\mathbf{r}; E) = G_n(\mathbf{r}; E). \quad (2.10b)$$

The out-scattering and in-scattering of electrons is shown schematically in figure 1.

It will be noted that if the energy distribution of electrons is given by the Fermi-Dirac factor with some local electrochemical potential $\mu(\mathbf{r})$

$$n(\mathbf{r}; E)/N_0(\mathbf{r}; E) \equiv f(\mathbf{r}; E) = 1/(e^{(E - e\mu(\mathbf{r}))/k_B T} + 1) \tag{2.11}$$

then the out-scattering and in-scattering rates exactly balance each other.

$$n(\mathbf{r}; E)/\tau_n(\mathbf{r}; E) = p(\mathbf{r}; E)/\tau_p(\mathbf{r}; E). \tag{2.12}$$

This is shown in section 4.

3. Kinetic equation

The general steady-state quantum kinetic equation has the form [7, 14] (see appendix B, equations (B.14) and (A.21))

$$G^<(\mathbf{r}_1, \mathbf{r}_2; E) = \int d\mathbf{r}' \int d\mathbf{r}'' G^R(\mathbf{r}_1, \mathbf{r}'; E) G^R(\mathbf{r}_2, \mathbf{r}''; E)^* \Sigma^<(\mathbf{r}', \mathbf{r}''; E). \tag{3.1}$$

This is the kinetic equation one would solve in general to obtain the function $G^<(\mathbf{r}_1, \mathbf{r}_2; E)$ from which the electron density $n(\mathbf{r}; E)$ and the current density $\mathbf{J}(\mathbf{r}; E)$ can be computed. Because the self-energy is a delta function in our model we can solve a simpler equation involving only the diagonal elements $G^<(\mathbf{r}, \mathbf{r}; E) = 2\pi i n(\mathbf{r}; E)$. Using (2.5b) for $\Sigma^<$ and letting $\mathbf{r}_1 = \mathbf{r}_2 = \mathbf{r}$, (3.1) simplifies to

$$n(\mathbf{r}; E) = \frac{\hbar}{2\pi} \int d\mathbf{r}' \frac{|G^R(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_p(\mathbf{r}'; E)}. \tag{3.2}$$

Once the electron density $n(\mathbf{r}; E)$ has been obtained by solving (3.2) we can compute the full function $G^<(\mathbf{r}_1, \mathbf{r}_2; E)$ from (B.15). Various quantities of interest such as the current density per unit energy $\mathbf{J}(\mathbf{r}; E)$ can be obtained from $G^<$. Later in this section an explicit expression $\mathbf{J}(\mathbf{r}; E)$ will be presented.

The retarded Green function $G^R(\mathbf{r}, \mathbf{r}'; E)$ is obtained from the Schrödinger equation modified to include an 'optical potential' Σ^R (equation (B.13)). Because the self-energy is a delta function in space, Σ^R is a simple local potential (equations (A.18a, b)) which we write as $V_{op}(\mathbf{r}; E)$.

$$(E - H_0(\mathbf{r}) - V_{op}(\mathbf{r}; E))G^R(\mathbf{r}, \mathbf{r}'; E) = \delta(\mathbf{r} - \mathbf{r}') \tag{3.3a}$$

$$\text{Im}(V_{op}(\mathbf{r}; E)) = -\frac{\hbar}{2\tau_\phi(\mathbf{r}; E)} \tag{3.3b}$$

$$\text{Re}(V_{op}(\mathbf{r}; E)) = \frac{\hbar}{2\pi} \text{P} \int \frac{dE'}{(E - E')\tau_\phi(\mathbf{r}; E')} \tag{3.3c}$$

where P represents the principal value of the integral and τ_ϕ is given by the parallel combination of τ_n and τ_p .

$$1/\tau_\phi(\mathbf{r}; E) = 1/\tau_n(\mathbf{r}; E) + 1/\tau_p(\mathbf{r}; E). \tag{3.3d}$$

Note that the elastic processes described by H_0 (equation (2.1)) are treated exactly, while the phase-breaking processes due to H' (equation (2.3)) are treated approximately through the optical potential obtained from the lowest order self-energy function.

Equation (3.2) involves only positive definite quantities. All interference effects are contained in the function $G^R(\mathbf{r}, \mathbf{r}'; E)$ which is obtained from (3.3). The imaginary part of the optical potential ($-\hbar/2\tau_\phi$) causes these interference effects to decay. We can thus identify τ_ϕ as the phase-breaking time due to the interaction of the electrons with the bath of oscillators (this includes both elastic and inelastic processes as explained earlier in section 2).

It will be noted that $\tau_\phi(\mathbf{r}; E)$ in general is affected by the electron density $n(\mathbf{r}; E)$ and thus needs to be computed self-consistently. However, if the energies $\hbar\omega$ of the oscillators are much less than $k_B T$, then $F(\mathbf{r}; E' - E) \simeq F(\mathbf{r}; E - E')$ (see equation (2.7)); under this condition it can be shown from (3.3c), (2.6a, b) and (2.8) that $\tau_\phi(\mathbf{r}; E)$ depends on the total density of states $N_0(\mathbf{r}; E)$ and not on the electron density $n(\mathbf{r}; E)$. Consequently, a self-consistent calculation is not necessary.

It may appear surprising that the phase-breaking time is not simply the electron lifetime τ_n but is determined by the parallel combination of τ_n and τ_p (equation (3.3c)). This result follows rigorously from the quantum kinetic approach and could not be anticipated from a single-particle picture. Physically it can be understood following the discussion in section 4.4 of Kadanoff and Baym [9]. Phase-coherence of the one-particle Green function is lost if the additional electron disturbs the free evolution of the bath of oscillators. This can happen in one of two ways: (1) the electron can outscatter by interacting with the bath, or, (2) the electron can inhibit inscattering (that would otherwise have occurred due to interaction with the bath) through the exclusion principle. The former process occurs at the rate n/τ_n while the latter occurs at the rate n/τ_p —leading to an overall phase-breaking rate of n/τ_ϕ . In a dilute Boltzmann gas near equilibrium τ_n is much less than τ_p (since $n \ll p$, see equation (2.12)) so that the former process is dominant and $\tau_\phi \simeq \tau_n$, as one would expect from a one-electron picture.

Physical Interpretation: Physically (3.3a) describes the propagation of electron waves away from a point excitation source at \mathbf{r}' . If electrons are injected at a steady rate at the point \mathbf{r}' they will propagate outwards and establish an electron density distribution proportional to $|G^R(\mathbf{r}, \mathbf{r}'; E)|^2$ (figure 2). The imaginary part of the optical potential causes the wave to decay which corresponds to the loss of electrons from an initial energy E by phase-breaking scattering processes (it also includes the inhibited in-scattering as discussed earlier). The rate at which electrons are lost by scattering out of a volume $d\mathbf{r}$ is given by $|G^R(\mathbf{r}, \mathbf{r}'; E)|^2 d\mathbf{r}/\tau_\phi(\mathbf{r}; E)$. It can be shown that (see appendix C)

$$\int d\mathbf{r} \frac{|G^R(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_\phi(\mathbf{r}; E)} = \int d\mathbf{r} \frac{|G^R(\mathbf{r}', \mathbf{r}; E)|^2}{\tau_\phi(\mathbf{r}; E)} = \frac{2\pi}{\hbar} N_0(\mathbf{r}'; E). \quad (3.4)$$

Equation (3.4) shows that the total rate at which electrons are lost by scattering is equal to $2\pi N_0(\mathbf{r}'; E)/\hbar$. This must equal the rate at which electrons are injected at \mathbf{r}' as shown in figure 2. Thus we can write the probability $P(\mathbf{r}, \mathbf{r}'; E)$ that an electron having an energy E after suffering a phase-breaking process at \mathbf{r}' will suffer its next phase-breaking event at \mathbf{r} is given by

$$P(\mathbf{r}, \mathbf{r}'; E) = (\hbar/2\pi) |G^R(\mathbf{r}, \mathbf{r}'; E)|^2 / N_0(\mathbf{r}'; E) \tau_\phi(\mathbf{r}; E). \quad (3.5)$$

The relationship expressed by (3.4) ensures that the probability function $P(\mathbf{r}, \mathbf{r}'; E)$ is properly normalized:

$$\int d\mathbf{r} P(\mathbf{r}, \mathbf{r}'; E) = 1. \quad (3.6)$$

The range of $|\mathbf{r} - \mathbf{r}'|$ over which the probability function $P(\mathbf{r}, \mathbf{r}'; E)$ is significant defines

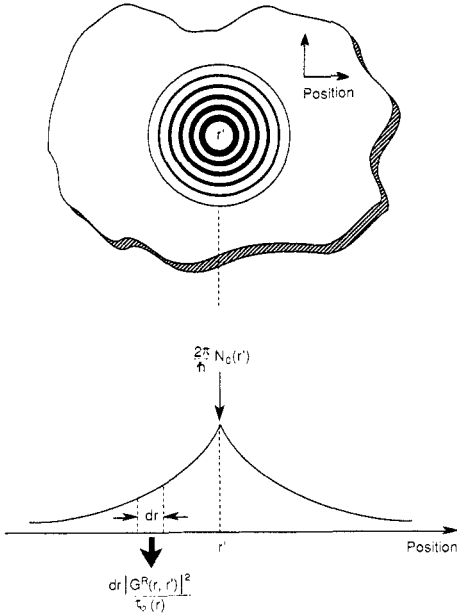


Figure 2. Propagation of electron waves away from a point excitation. The argument E has been suppressed for simplicity.

the *phase-breaking length*. The probability function can also be computed semiclassically using a Monte Carlo approach, and a comparison of the semiclassical result with the quantum mechanical result could be illuminating. In fact we believe that by replacing $|G^R|^2$ in (3.1) with the appropriate semiclassically computed quantity, it is possible to use the equations derived in this paper to describe semiclassical transport as well.

We now rewrite the kinetic equation (2.2) in the form

$$\frac{n(\mathbf{r}; E)}{\tau_\varphi(\mathbf{r}; E)} = \int d\mathbf{r}' P(\mathbf{r}, \mathbf{r}'; E) \frac{N_0(\mathbf{r}'; E)}{\tau_p(\mathbf{r}'; E)}. \tag{3.7}$$

Equation (3.7) is readily understood if the rate \tilde{G}_n of in-scattering of electrons per unit volume per unit energy is identified with

$$\tilde{G}_n(\mathbf{r}; E) = N_0(\mathbf{r}; E) / \tau_p(\mathbf{r}; E). \tag{3.8a}$$

Since $P(\mathbf{r}, \mathbf{r}'; E)$ is the fraction of electrons in-scattered at \mathbf{r}' that get out-scattered at \mathbf{r} , the right hand side must equal the out-scattering rate \tilde{R}_n per unit volume per unit energy at \mathbf{r} which we identify with

$$\tilde{R}_n(\mathbf{r}; E) = n(\mathbf{r}; E) / \tau_\varphi(\mathbf{r}; E). \tag{3.8b}$$

Note that \tilde{G}_n and \tilde{R}_n are larger than the in-scattering rate G_n and the out-scattering rate R_n discussed in section 2 [equation (2.10a, b)].

$$\tilde{G}_n(\mathbf{r}; E) - G_n(\mathbf{r}; E) = \tilde{R}_n(\mathbf{r}; E) - R_n(\mathbf{r}; E) = n(\mathbf{r}; E) / \tau_p(\mathbf{r}; E). \tag{3.9}$$

The excess scattering rate $(\tilde{R}_n - R_n)$ or $(\tilde{G}_n - G_n)$ is negligible for a dilute electron gas with $n(\mathbf{r}; E) \ll p(\mathbf{r}; E) \approx N_0(\mathbf{r}; E)$. But for a degenerate electron gas, n/τ_p represents the part of the in-scattering that is inhibited by the exclusion principle as discussed earlier. Equation (3.2) (which is rigorously derived in appendix B taking the exclusion principle into account) is thus consistent with a simple one-electron picture in which the

in-scattering is not inhibited but balanced by an equal amount of out-scattering; however, this result is difficult to anticipate from a one-electron picture.

Numerical Solution Procedure: We can rewrite (3.2) in the form of an integral equation for the electron density $n(\mathbf{r}; E)$, using (2.6b) to replace $\tau_p(\mathbf{r}; E)$.

$$n(\mathbf{r}; E) = \int d\mathbf{r}' \int dE' K_n(\mathbf{r}, \mathbf{r}'; E, E') n(\mathbf{r}'; E'). \quad (3.10)$$

The kernel K_n is given by

$$K_n(\mathbf{r}, \mathbf{r}'; E, E') = |G^R(\mathbf{r}, \mathbf{r}'; E)|^2 F(\mathbf{r}', E - E'). \quad (3.11)$$

Once the kernel has been computed from (3.3), we can solve (3.10) with the appropriate boundary conditions to obtain the electron density $n(\mathbf{r}; E)$ everywhere in a given structure. We assume that the structure contains two or more contact regions where the electron density is given by a Fermi distribution with a given local electrochemical potential μ (figure 3). We can then discretize the variables $(\mathbf{r}; E)$ into, say, N nodes over the rest of the structure (labelled 'device'). Equation (3.10) yields one equation at each node, leading to N equations for the N unknowns (values of $n(\mathbf{r}; E)$ at the N nodes). It will be noted that the kernel, in general, depends on the electron density $n(\mathbf{r}; E)$ and may have to be computed self-consistently. This is because $G^R(\mathbf{r}, \mathbf{r}'; E)$ depends on the Hartree potential. It also depends on $\tau_\varphi(\mathbf{r}; E)$ (equation (3.3)) which, in general, is affected by $n(\mathbf{r}; E)$; however, $\tau_\varphi(\mathbf{r}; E)$ is nearly independent of $n(\mathbf{r}; E)$ if the energies $\hbar\omega$ of the oscillators are much less the $k_B T$, as discussed earlier in section 3.

It can be shown that (3.10) is satisfied by the equilibrium solution $n(\mathbf{r}; E) = N_0(\mathbf{r}; E) f_0(E)$ where $f_0(E)$ is the Fermi distribution with a spatially constant electrochemical potential μ_0 . This is the solution we expect to obtain if we solve (3.10) assuming that all the contacts are at the same potential $\mu = \mu_0$.

The current density is obtained from the off-diagonal elements of the Green function $G^<(\mathbf{r}_1, \mathbf{r}_2; E)$ as described in appendix B (equations (B.21, 24)).

$$\mathbf{J}(\mathbf{r}; E) = \frac{\hbar}{2\pi} \int \frac{d\mathbf{r}'}{\tau_p(\mathbf{r}'; E)} \mathbf{J}_\delta(\mathbf{r}, \mathbf{r}'; E) \quad (3.12)$$

where

$$\mathbf{J}_\delta(\mathbf{r}, \mathbf{r}'; E) = |G^R(\mathbf{r}, \mathbf{r}'; E)|^2 (e/m^*) (\hbar \nabla \theta(\mathbf{r}, \mathbf{r}'; E) - e\mathbf{A}(\mathbf{r})) \quad (3.13)$$

and

$$G^R(\mathbf{r}, \mathbf{r}'; E) = |G^R(\mathbf{r}, \mathbf{r}'; E)| \exp(i\theta(\mathbf{r}, \mathbf{r}'; E)). \quad (3.14)$$

∇ denotes the gradient operation with respect to \mathbf{r} . It can be shown that this expression for the current density is gauge-invariant; that is, if we change the vector potential from $\mathbf{A}(\mathbf{r})$ to $\mathbf{A}(\mathbf{r}) + \nabla\chi(\mathbf{r})$, $\chi(\mathbf{r})$ being any scalar function, the current density is unchanged. Using (2.6b) for $\tau_p(\mathbf{r}'; E)$ we can write (3.12) in a form similar to (3.10).

$$\mathbf{J}(\mathbf{r}; E) = \int d\mathbf{r}' \int dE' K_j(\mathbf{r}, \mathbf{r}'; E, E') n(\mathbf{r}'; E') \quad (3.15)$$

The kernel K_j is given by

$$K_j(\mathbf{r}, \mathbf{r}'; E, E') = (e/m) K_n(\mathbf{r}, \mathbf{r}'; E, E') (\hbar \nabla \theta(\mathbf{r}, \mathbf{r}'; E) - e\mathbf{A}(\mathbf{r})). \quad (3.16)$$

Once the electron density $n(\mathbf{r}; E)$ has been obtained throughout the structure from

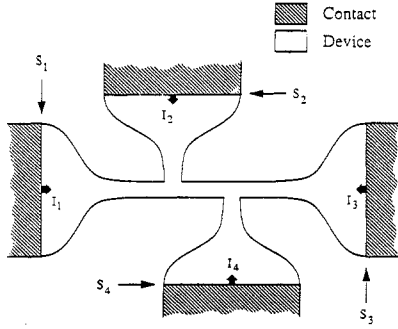


Figure 3. The structure is assumed to contain two or more contact regions (four shown in the figure) where the electron density $n(\mathbf{r}; E)$ is given by a Fermi distribution with a local electrochemical potential μ . The electron density is free to assume any form in the rest of the structure, labelled as 'device'. The four contacts supply currents I_1 , I_2 , I_3 and I_4 to the device through the surfaces S_1 , S_2 , S_3 and S_4 respectively.

(3.10), we can compute the current density $\mathbf{J}(\mathbf{r}; E)$ by performing the integral in (3.15). The external current I_i coming in from contact i is obtained by computing the flux passing through the surface S_i (figure 3).

$$I_i = \int dE \int \mathbf{J}(\mathbf{r}; E) \cdot d\mathbf{S}_i. \quad (3.17)$$

It will be noted that the current density is zero deep inside the contact since we have assumed the electrochemical potential to be constant over the entire contact. This is not what happens in a real contact where the electrochemical potential is not constant but varies linearly. Current flows into the contact from one end and out the other end into the device. But in our solution the potential is assumed constant and no current flows into the contact. Instead it appears magically inside the contact within a phase-breaking length of the device (where the divergence of the current density is non-zero) and flows into the device through S_i . For this reason, one should not attach any physical significance to the current density $\mathbf{J}(\mathbf{r}; E)$ that we compute inside the contact using the solution procedure described above. But we believe that this procedure yields the correct terminal current as well as the correct electron density and current density within the device (provided the contacts are conductive enough that the potential drop inside them is negligible over a phase-breaking length).

The solution procedure described above is similar to the procedure one would adopt if the structure shown in figure 3 were a classical resistor with a conductivity σ . First, one solves the diffusion equation $\nabla \cdot (\sigma \nabla \mu) = 0$ subject to the boundary condition $\mu = \mu_n$ at contact n ; this is analogous to solving (3.10) subject to the appropriate boundary condition for $n(\mathbf{r}; E)$. Next, one computes the current density from the relation $\mathbf{J}(\mathbf{r}) = -\sigma \nabla \mu(\mathbf{r})$, σ being the conductivity of the sample; this is analogous to computing $\mathbf{J}(\mathbf{r}; E)$ from (3.15). Finally, the terminal current at contact i is obtained by computing the flux through the surface S_i (cf. equation (3.17)). In this case too the current density is zero inside the contact and suddenly acquires a non-zero value inside the device; the divergence of the current density is thus non-zero at the device–contact interface.

External Current: If we are not interested in the detailed current distribution $\mathbf{J}(\mathbf{r}; E)$ within a device, then we can compute the external currents I_i in a simpler manner using the procedure described below. This alternative approach also helps establish a connection with the Buttiker formula in the linear response regime.

First we substitute (3.12) into (3.17) to write

$$I_i = \frac{\hbar}{2\pi} \int dE \int \frac{d\mathbf{r}'}{\tau_p(\mathbf{r}'; E)} \int \mathbf{J}_\delta(\mathbf{r}, \mathbf{r}'; E) \cdot d\mathbf{S}_i. \quad (3.18)$$

Next we use the following result (see appendix C, equations (C.15a, b)).

$$\int \mathbf{J}_\delta(\mathbf{r}, \mathbf{r}'; E) \cdot d\mathbf{S}_i = \begin{cases} -e \int_{r \in \Omega_i} d\mathbf{r} \frac{|G^R(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_\varphi(\mathbf{r}; E)} & \text{if } \mathbf{r}' \notin \Omega_i \\ e \int_{r \notin \Omega_i} d\mathbf{r} \frac{|G^R(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_\varphi(\mathbf{r}; E)} & \text{if } \mathbf{r}' \in \Omega_i. \end{cases} \quad (3.19)$$

Ω_i is the volume of contact i . Equation (3.19) is easy to understand physically. The left hand side represents the current crossing the surface S_i due to a delta function source at \mathbf{r}' . This must equal the rate at which electrons are lost by scattering (see discussion following (3.4)) on the side of S_i away from the source. Thus, if \mathbf{r}' lies outside the contact, we integrate $|G^R|^2/\tau_\varphi$ inside the contact and vice versa. Using (3.19) and (3.5) we can rewrite (3.18) as

$$I_n = \int dE \int_{r \in \Omega_i} d\mathbf{r} \int_{r' \notin \Omega_i} d\mathbf{r}' \left(P(\mathbf{r}', \mathbf{r}; E) \frac{eN_0(\mathbf{r}; E)}{\tau_p(\mathbf{r}; E)} - P(\mathbf{r}, \mathbf{r}'; E) \frac{eN_0(\mathbf{r}'; E)}{\tau_p(\mathbf{r}'; E)} \right). \quad (3.20)$$

Equation (3.20) is understood physically as follows. The rate at which electrons are in-scattered at \mathbf{r} is given by N_0/τ_p ; a fraction $P(\mathbf{r}', \mathbf{r}; E)$ of these electrons suffer their next scattering at \mathbf{r}' . The first term of the integrand in (3.20) thus represents the number of electrons per unit time that suffer a phase-breaking scattering at \mathbf{r} and their next phase-breaking scattering at \mathbf{r}' . Since \mathbf{r} lies within contact i and \mathbf{r}' lies outside contact i , we can view this as the current flowing out of contact i . Similarly the second term represents the current flowing into contact i . Their difference yields the net current flowing from contact i into the device.

We can remove the restriction over the range of integration for \mathbf{r}' in (3.20); this is because if both \mathbf{r} and \mathbf{r}' lie inside Ω_i then the integral vanishes:

$$I_i = \int dE \int_{r \in \Omega_i} d\mathbf{r} \int d\mathbf{r}' \left(P(\mathbf{r}', \mathbf{r}; E) \frac{eN_0(\mathbf{r}; E)}{\tau_p(\mathbf{r}; E)} - P(\mathbf{r}, \mathbf{r}'; E) \frac{eN_0(\mathbf{r}'; E)}{\tau_p(\mathbf{r}'; E)} \right). \quad (3.21)$$

Within the contacts the carriers are distributed in energy according to the Fermi distribution, so that $p/\tau_p = n/\tau_n$ (equation (2.12)); hence $N_0/\tau_p = n/\tau_\varphi$. Using this relation and the normalization condition for the probability function (equation (3.6)), we can write (3.21) as

$$I_i = \int dE \int_{r \in \Omega_i} d\mathbf{r} I(\mathbf{r}; E) \quad (3.22)$$

where

$$I(\mathbf{r}; E) = \frac{en(\mathbf{r}; E)}{\tau_\varphi(\mathbf{r}; E)} - \int d\mathbf{r}' P(\mathbf{r}, \mathbf{r}'; E) - \frac{eN_0(\mathbf{r}'; E)}{\tau_p(\mathbf{r}'; E)}. \quad (3.23)$$

Note that within the device $I(\mathbf{r}; E)$ is equal to zero, since the kinetic equation that we solve for the electron density $n(\mathbf{r}; E)$ requires the right-hand side to be zero (see equation (3.7)). But inside each contact, the kinetic equation is not satisfied, since we *impose* a boundary condition on $n(\mathbf{r}; E)$ rather than *solve* for it. It can be shown, however, that $I(\mathbf{r}; E)$ is zero deep inside the contact where the electrochemical potential is constant for all values of \mathbf{r}' for which the function $P(\mathbf{r}, \mathbf{r}'; E)$ is significant. But $I(\mathbf{r}; E)$ is non-zero inside the contact over a region lying within a phase-breaking length (that is, the range of $|\mathbf{r} - \mathbf{r}'|$ over which the probability of function $P(\mathbf{r}, \mathbf{r}'; E)$ is significant) of the

device. This is precisely the region where the current density diverges, as discussed earlier following (3.17). Indeed, the right hand side of (3.23) is equal to the divergence of the current density and by integrating it over the contact as indicated in (3.22) we obtain the net current flowing into the contact. As we discussed earlier, our imposed boundary condition with a constant electrochemical potential is not quite right—the actual potential has a small slope due to the finite conductivity of the contacts. If we make the contacts more conductive by making them wider, then our assumed contact boundary conditions become more accurate and we would expect $I(\mathbf{r}; E)$ to approach zero. However, at the same time the volume of integration Ω_i in (3.22) becomes larger and we believe that the terminal current I_i will approach a constant value. The same is true if we make the contacts more conductive by increasing τ_φ in these regions. Once again $I(\mathbf{r}; E)$ decreases but the volume of integration in (3.22) is effectively increased since the phase-breaking length increases.

We emphasize that the function $I(\mathbf{r}; E)$ should be viewed as one that yields the correct terminal current when integrated over the contact volume Ω_i (equation (3.22)), but no physical significance should be attached to its precise spatial form.

Using equations (2.6b) and (3.5) we can rewrite (3.23) in the form of an integral equation with a source term.

$$I(\mathbf{r}; E) = \frac{e(\mathbf{r}; E)}{\tau_\varphi(\mathbf{r}; E)} \left(n(\mathbf{r}; E) - \int d\mathbf{r}' \int dE' K_n(\mathbf{r}, \mathbf{r}'; E, E') n(\mathbf{r}'; E') \right). \quad (3.24)$$

The kernel K is given by (3.11). Within the device, $I(\mathbf{r}; E) = 0$, so that (3.24) is the same as (3.10) and can be solved numerically in the same way to obtain the electron density at all points. We can then compute $I(\mathbf{r}; E)$ in the contact regions from (3.24) and integrate it over each contact and over all energies (as indicated in equation (3.22)) to obtain the corresponding external current. We have thus included the external current by modifying the kinetic equation (3.10) into (3.24). Note that for the classical resistor too we could modify $\nabla \cdot (\sigma \nabla \mu) = 0$ into $\nabla \cdot (\sigma \nabla \mu) = I(\mathbf{r})$ and obtain the external current by integrating $I(\mathbf{r})$ over the device–contact interface region.

4. Low-bias conditions

We will now specialize to biasing conditions that are low enough that ‘carrier heating’ is insignificant. We assume that we can write the energy distribution of electrons everywhere in the form shown in (2.11) which we restate here for convenience:

$$n(\mathbf{r}; E)/N_0(\mathbf{r}, E) \equiv f(\mathbf{r}; E) = 1/(e^{(E - e\mu(\mathbf{r}))/k_B T} + 1). \quad (4.1)$$

It follows that

$$p(\mathbf{r}; E)/N_0(\mathbf{r}, E) = 1 - f(\mathbf{r}; E). \quad (4.2)$$

At equilibrium with no bias applied the electrochemical potential $\mu(\mathbf{r})$ is constant everywhere, and the *ansatz* in (4.1) is clearly valid. Preliminary numerical simulations suggest that (4.1) remains accurate as long as the potential drop over an inelastic scattering length is a small fraction of $k_B T$ and there are no sharp resonances in energy.

We leave it to future work to establish the precise criteria for the validity of this *ansatz* and to determine if this is a necessary condition for linear response.

It will be noted that although we are assuming that carriers at different energies are distributed according to the Fermi distribution, we are not making any assumption regarding the distribution of carriers among different current-carrying states at the same energy. It is apparent from (1.7) that the electron density $n(\mathbf{r}; E)$ is the total number of electrons integrated over all directions of the \mathbf{k} -vector. No assumption is being made regarding $G^<(\mathbf{r}; \mathbf{k}; E)$, that is, regarding the distribution of electrons along different directions in \mathbf{k} -space.

It is intuitively appealing to define two electrochemical potentials μ_L, μ_R for states carrying current to the left and to the right respectively [19]. The electrochemical potential defined by us corresponds to the average of the two and we do not wish to imply that $\mu_L = \mu_R$. To avoid this implication we will not refer to the above assumption (equation (4.1)) as 'local thermodynamic equilibrium' as we did in our earlier work [7, 8, 18].

We believe that the concept of μ_L and μ_R can only be defined in an average sense over a de Broglie wavelength while the total electrochemical potential $\mu(\mathbf{r})$ defined by us is a valid concept in a local sense. This is because if we compute the 'left-moving' electron density $n_L(\mathbf{r}; E)$ at a point by integrating $G^<(\mathbf{r}; \mathbf{k}; E)$ over $k_z > 0$, the result is not necessarily positive. Only by averaging over some volume (having dimensions \sim de Broglie wavelength) can we ensure a positive result. On the other hand, the total electron density $n(\mathbf{r}; E)$ obtained by integrating $G^<(\mathbf{r}; \mathbf{k}; E)$ over all \mathbf{k} is positive definite and can be used to define a local electrochemical potential $\mu(\mathbf{r})$.

We will first show that when the electron energy distribution is given by (4.1), the following relation is true:

$$1/\tau_p(\mathbf{r}; E) = f(\mathbf{r}; E)/\tau_\varphi(\mathbf{r}; E). \quad (4.3)$$

This relation will then be used to simplify (3.23). To obtain (4.3) we note that from (4.1) and (4.2)

$$n(\mathbf{r}; E)p(\mathbf{r}; E')/p(\mathbf{r}; E)n(\mathbf{r}; E') = e^{(E' - E)/k_B T}. \quad (4.4)$$

On the other hand from (2.7)

$$F(\mathbf{r}; E - E')/F(\mathbf{r}; E' - E) = e^{(E' - E)/k_B T} \quad (4.5)$$

Hence from (4.4) and (4.5),

$$n(\mathbf{r}; E)F(\mathbf{r}; E' - E)p(\mathbf{r}; E') = p(\mathbf{r}; E)F(\mathbf{r}; E - E')n(\mathbf{r}; E'). \quad (4.6)$$

Integrating both sides over E' and using (2.6a, b) we obtain (2.12) which is restated here for convenience:

$$n(\mathbf{r}; E)/\tau_n(\mathbf{r}; E) = p(\mathbf{r}; E)/\tau_p(\mathbf{r}; E). \quad (4.7)$$

Using (4.1) and (4.2) we can rewrite (4.7) as

$$f(\mathbf{r}; E)/\tau_n(\mathbf{r}; E) = (1 - f(\mathbf{r}; E))/\tau_p(\mathbf{r}; E). \quad (4.8)$$

Equation (4.3) follows from (4.8) noting that τ_φ is the parallel combination of τ_p and τ_n (equation (3.3c)).

Using (4.3) we can rewrite (3.23) as

$$I(\mathbf{r}; E) = \frac{e}{\hbar} \left(\bar{T}(\mathbf{r}; E) f(\mathbf{r}; E) - \int d\mathbf{r}' T(\mathbf{r}, \mathbf{r}'; E) f(\mathbf{r}'; E) \right) \quad (4.9)$$

where

$$T(\mathbf{r}, \mathbf{r}'; E) = \hbar^2 |G^R(\mathbf{r}, \mathbf{r}'; E)|^2 / \tau_\varphi(\mathbf{r}; E) \tau_\varphi(\mathbf{r}'; E) \quad (4.10)$$

$$\bar{T}(\mathbf{r}; E) = \hbar N_0(\mathbf{r}; E) / \tau_\varphi(\mathbf{r}; E). \quad (4.11)$$

Using (3.4) and the relation $G^R(\mathbf{r}, \mathbf{r}'; E)|_{\text{B}} = G^R(\mathbf{r}', \mathbf{r}; E)|_{-\text{B}}$ (see appendix C), it can be shown that the quantities $T(\mathbf{r}, \mathbf{r}'; E)$ and $\bar{T}(\mathbf{r}; E)$ obey relations very similar to (1.2) and (1.3) [18]:

$$\bar{T}(\mathbf{r}; E) = \int d\mathbf{r}' T(\mathbf{r}, \mathbf{r}'; E) = \int d\mathbf{r}' T(\mathbf{r}', \mathbf{r}; E) \quad (4.12)$$

$$T(\mathbf{r}, \mathbf{r}'; E)|_{\text{B}} = T(\mathbf{r}', \mathbf{r}; E)|_{-\text{B}}. \quad (4.13)$$

Note, however, that while (1.1) describes linear response only, (4.9) is capable of describing non-linear response as well. In (1.1) the coefficients T_{ij} are evaluated at equilibrium. But in (4.9) the coefficients $T(\mathbf{r}, \mathbf{r}'; E)$ are computed in the *presence of an applied bias*. Consequently $T(\mathbf{r}, \mathbf{r}'; E)$ can be different for positive and negative bias for asymmetric devices, and the current I for a positive bias V may have a very different magnitude compared to that for a negative bias, leading to the generation of even harmonics. By contrast the T_{ij} in (1.1) are equilibrium quantities independent of bias. Consequently the current response to an applied bias is precisely linear. In the next section we will specialize (4.9) to linear response.

The expression for the current density $\mathbf{J}(\mathbf{r}; E)$ (equation (3.12)) can also be simplified using (4.3).

$$\mathbf{J}(\mathbf{r}; E) = \frac{e}{\hbar} \int d\mathbf{r}' T_{\mathbf{J}}(\mathbf{r}, \mathbf{r}'; E) f(\mathbf{r}'; E) \quad (4.14)$$

where

$$T_{\mathbf{J}}(\mathbf{r}, \mathbf{r}'; E) = T(\mathbf{r}, \mathbf{r}'; E) \tau_\varphi(\mathbf{r}; E) (e\mathbf{A}(\mathbf{r}) + \hbar\nabla\theta(\mathbf{r}, \mathbf{r}'; E)) / m^*. \quad (4.15)$$

5. Linear response

Using the property expressed by (4.12) it can be shown that the distribution function

$$f(\mathbf{r}; E) = f_0(E) = 1 / (e^{(E - e\mu_0)/k_B T} + 1) \quad (5.1)$$

with a spatially constant electrochemical potential μ_0 satisfies (4.9) with $I(\mathbf{r}; E)$ set equal to zero. This is the equilibrium condition. In linear response theory it is assumed that the distribution function $f(\mathbf{r}; E)$ deviates only slightly from the equilibrium distribution

$f_0(E)$ so that we can expand $f(\mathbf{r}; E)$ in a Taylor series about $\mu = \mu_0$. Noting that $\partial/\partial\mu = -e\partial/\partial E$, we obtain

$$f(\mathbf{r}; E) = f_0(E) + (-\partial f_0/\partial E) e(\mu(\mathbf{r}) - \mu_0). \quad (5.2)$$

Substituting (5.2) into (4.9) and integrating over the energy E , we obtain

$$\tilde{I}(\mathbf{r}) = \frac{e^2}{h} \left(\bar{T}_0(\mathbf{r})\mu(\mathbf{r}) - \int d\mathbf{r}' T_0(\mathbf{r}, \mathbf{r}')\mu(\mathbf{r}') \right) \quad (5.3)$$

where

$$T_0(\mathbf{r}, \mathbf{r}') \equiv \int dE \left(-\frac{\partial f_0}{\partial E} \right) T^{(0)}(\mathbf{r}, \mathbf{r}'; E) \quad (5.4a)$$

$$\bar{T}_0(\mathbf{r}) \equiv \int dE \left(-\frac{\partial f_0}{\partial E} \right) \bar{T}^{(0)}(\mathbf{r}; E) \quad (5.4b)$$

$$\tilde{I}(\mathbf{r}) \equiv \int dE I(\mathbf{r}; E) \quad (5.4c)$$

The superscript 0 indicates that the quantities $T(\mathbf{r}, \mathbf{r}'; E)$ and $\bar{T}(\mathbf{r}; E)$ are evaluated under equilibrium conditions. It is evident that the quantities $T_0(\mathbf{r}, \mathbf{r}')$ and $\bar{T}_0(\mathbf{r})$ obey relations similar to (4.12) and (4.13).

$$\bar{T}_0(\mathbf{r}) = \int d\mathbf{r}' T_0(\mathbf{r}, \mathbf{r}') = \int d\mathbf{r}' T_0(\mathbf{r}', \mathbf{r}) \quad (5.5a)$$

$$T_0(\mathbf{r}, \mathbf{r}')|_{\text{B}} = T_0(\mathbf{r}', \mathbf{r})|_{-\text{B}}. \quad (5.5b)$$

It will be noted that under bias there is a change $\delta\varphi$ in the electrostatic potential which causes the coefficient T to change from its equilibrium value $T^{(0)}$. This leads to a first-order term of the form

$$\delta T_0(\mathbf{r})\mu_0 - \int d\mathbf{r}' \delta T_0(\mathbf{r}, \mathbf{r}')\mu_0$$

in (5.3); however, the relation (5.5a) ensures that this term is zero. Higher-order terms involving quantities like $\delta T_0 \delta\mu$ are neglected in the linear response regime. Equation (5.3) has the appearance of (1.1) extended to a continuous distribution of probes. The expression for the transmission coefficient $T(\mathbf{r}, \mathbf{r}'; E)$ from \mathbf{r}' to \mathbf{r} (equation (4.10)) is understood easily from this point of view. The probability of injection from the probe at \mathbf{r}' is proportional to $1/\tau_\varphi(\mathbf{r}'; E)$, that of propagation from \mathbf{r}' to \mathbf{r} is proportional to $|G^{\text{R}}(\mathbf{r}, \mathbf{r}'; E)|^2$ and that of ejection into the probe at \mathbf{r} is proportional to $1/\tau_\varphi(\mathbf{r}; E)$. In fact the same expression is obtained if we start from the Kubo formula for the non-local conductivity tensor $\sigma(\mathbf{r}, \mathbf{r}'; E)$ and use the Fisher–Lee formula [20] to obtain $T(\mathbf{r}, \mathbf{r}'; E)$ [18].

Equation (5.3) is solved numerically in the same way as the general transport equation (3.24). We assume $\mu(\mathbf{r})$ to have specified values in the contacts and solve (5.3) within the device (with $\tilde{I}(\mathbf{r}) = 0$) to obtain $\mu(\mathbf{r})$. We then evaluate $\tilde{I}(\mathbf{r})$ in the contacts from (5.3) and integrate it over each contact to obtain the corresponding terminal current. Knowing $\mu(\mathbf{r})$ we can also compute the current density throughout the structure from (4.14). Using (5.2), (4.14) can be simplified to obtain the linear response current density; the

equilibrium current density $\mathbf{J}(\mathbf{r}; E)$ is not zero in general, although it can be shown that the flux crossing any of the surfaces S_i is zero at equilibrium.

$$\mathbf{J}(\mathbf{r}) = \int d\mathbf{r}' T_{j0}(\mathbf{r}, \mathbf{r}') \mu(\mathbf{r}') \tag{5.6a}$$

$$T_{j0}(\mathbf{r}, \mathbf{r}') = \int dE \left(-\frac{\partial f_0}{\partial E} \right) T_j^{(0)}(\mathbf{r}, \mathbf{r}'; E). \tag{5.6b}$$

Note, however, that the equilibrium current density

$$J_{\text{eq}} = \int d\mathbf{r}' T_j(\mathbf{r}, \mathbf{r}'; E) f_0 E$$

is not zero in a magnetic field. The change $\delta\varphi$ in the electrostatic potential under bias causes a first-order change in this equilibrium current density:

$$\delta J_{\text{eq}} = \int d\mathbf{r}' \delta T_j(\mathbf{r}, \mathbf{r}'; E) f_0(E).$$

Strictly speaking, this is also part of the linear response current density; however, we have not included it in (5.6) because it does not contribute to the terminal current.

Büttiker Formula: We will now reduce (5.3) to the same form as (1.1) and obtain explicit expressions for the transmission coefficients. As we have discussed, within the structure there are ‘contact’ regions where the electrochemical potential has a constant value; the rest of the structure is labeled the ‘device’ (figure 3). Integrating (5.3) over all \mathbf{r} included in contact i , we obtain the total current I_i coming into contact i .

$$I_i = \frac{e^2}{h} \left(\bar{T}_0(i) \mu_i - \sum_j T_0(i, j) \mu_j - \int_{\mathbf{r} \in \text{device}} d\mathbf{r} T_0(i, \mathbf{r}) \mu(\mathbf{r}) \right) \tag{5.7}$$

where

$$T_0(i, j) = \int_{\mathbf{r} \in i} d\mathbf{r} \int_{\mathbf{r}' \in j} d\mathbf{r}' T_0(\mathbf{r}, \mathbf{r}') \tag{5.8}$$

$$\bar{T}_0(i) \equiv \int_{\mathbf{r} \in i} d\mathbf{r} \bar{T}_0(\mathbf{r}) \tag{5.9}$$

$$T_0(i, \mathbf{r}) = \int_{\mathbf{r}' \in i} d\mathbf{r}' T_0(\mathbf{r}', \mathbf{r}). \tag{5.10}$$

When we neglect phase-breaking processes within the device the last term in (5.7) is zero (see equation (4.10)) so that (5.7) reduces to the same form as (1.1). We will show below that in general we can eliminate $\mu(\mathbf{r})$ from (5.7) to write it in the same form as (1.1):

$$I_i = \frac{e^2}{h} \left(\bar{T}_0(i) \mu_i - \sum_j T_{ij} \mu_j \right) \tag{5.11}$$

where

$$T_{ij} = T_0(i, j) + T_{ij}^{(1)} + T_{ij}^{(2)} + \dots \tag{5.12}$$

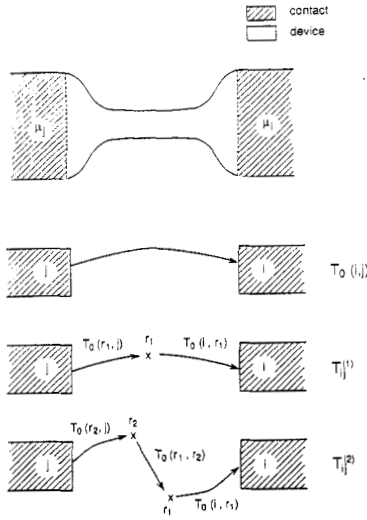


Figure 4. Interpretation of successive terms in (5.12).

$$T_{ij}^{(1)} \equiv \int_{r_1 \in \text{device}} \frac{d\mathbf{r}_1}{\bar{T}_0(\mathbf{r}_1)} T_0(i, \mathbf{r}_1) T_0(\mathbf{r}_1, j) \tag{5.13a}$$

$$T_{ij}^{(2)} = \int_{r_1, r_2 \in \text{device}} \frac{d\mathbf{r}_1}{\bar{T}_0(\mathbf{r}_2)} \int \frac{d\mathbf{r}_2}{\bar{T}_0(\mathbf{r}_2)} T_0(i, \mathbf{r}_1) T_0(\mathbf{r}_1, \mathbf{r}_2) T_0(\mathbf{r}_2, j) \tag{5.13b}$$

and so on. This result may be viewed as a generalization of the result obtained by Büttiker for a single floating probe [21]. The successive terms in (5.12) are shown schematically in figure 4. The first term $T_0(i, j)$ is the probability of coherent transmission from contact j to contact i without suffering any phase-breaking scattering within the device. The next term $T_{ij}^{(1)}$ is the probability of transmission with one phase breaking scattering event at some point \mathbf{r}_1 within the device; $T_{ij}^{(2)}$ is the probability of transmission with two scattering events at \mathbf{r}_1 and \mathbf{r}_2 within the device; and so on. It can be shown that the coefficients T_{ij} and $\bar{T}_0(i)$ indeed satisfy the relations (1.2) and (1.3).

To obtain (5.11) from (5.7) we note that within the device, the current $I(\mathbf{r}) = 0$ so that

$$0 = \bar{T}_0(\mathbf{r})\mu(\mathbf{r}) - \sum_j T_0(\mathbf{r}, j)\mu_j - \int_{r' \in \text{device}} d\mathbf{r}' T_0(\mathbf{r}, \mathbf{r}')\mu(\mathbf{r}') \quad \mathbf{r} \in \text{device} \tag{5.14}$$

or equivalently

$$\mu(\mathbf{r}) = \sum_j \frac{T_0(\mathbf{r}, j)}{\bar{T}_0(\mathbf{r})} \mu_j + \int_{r' \in \text{device}} d\mathbf{r}' \frac{T_0(\mathbf{r}, \mathbf{r}')}{\bar{T}_0(\mathbf{r})} \mu(\mathbf{r}'). \tag{5.15}$$

Equation (5.15) can be solved to obtain the electrochemical potential $\mu(\mathbf{r})$ everywhere in the device in terms of the potentials μ_j in the contacts. The solution can be written in the form of an iterative series as follows.

$$\mu(\mathbf{r}) = \mu^{(1)}(\mathbf{r}) + \mu^{(2)}(\mathbf{r}) + \dots \tag{5.16}$$

where

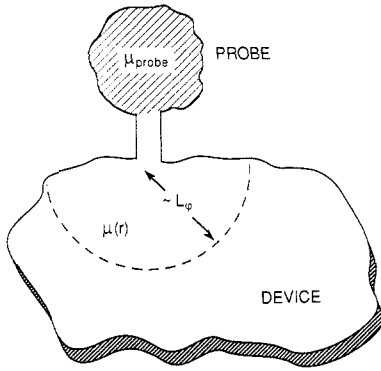


Figure 5. A weakly coupled probe connected to a device floats to a potential μ_{probe} that is a weighted average of the potential $\mu(r)$ existing within a phase-breaking length L_ϕ .

$$\mu^{(1)}(\mathbf{r}) = \sum_j \frac{T_0(\mathbf{r}, j)}{\bar{T}_0(\mathbf{r})} \mu_j \tag{5.17a}$$

$$\mu^{(n)}(\mathbf{r}) = \int_{r_1 \in \text{device}} d\mathbf{r}_1 \frac{T_0(\mathbf{r}, \mathbf{r}_1)}{\bar{T}_0(\mathbf{r})} \mu^{(n-1)}(\mathbf{r}_1) \tag{5.17b}$$

etc. Substituting $\mu(r)$ from (5.16) and (5.17a, b) into (5.7) we obtain (5.11).

Diffusion equation: We would also like to point out that in a homogeneous medium without any magnetic fields, we can reduce the linear response equation (5.3) to the familiar diffusion equation, if $\mu(r)$ is assumed to vary slowly. The integral operator on the right hand side of (5.3) then reduces to the Laplacian operator as shown in appendix D.

$$\nabla \cdot \mathbf{J} = \sigma \nabla^2 \mu(\mathbf{r}) \tag{5.18}$$

where

$$\sigma = \frac{e^2}{2h} \int d\boldsymbol{\rho} \rho_x^2 T(\boldsymbol{\rho}). \tag{5.19}$$

We have written $\boldsymbol{\rho}$ for $\mathbf{r} - \mathbf{r}'$, noting that in a homogeneous medium $T(\mathbf{r}, \mathbf{r}')$ depends only on the difference coordinate $\mathbf{r} - \mathbf{r}'$. Here $\mathbf{J}(\mathbf{r})$ is the current density in the structure, whose divergence equals $I(\mathbf{r})$.

What potential does a ‘non-invasive’ probe measure? In this paper we have defined the electrochemical potential $\mu(\mathbf{r})$ rigorously in terms of the electron density per unit energy $n(\mathbf{r}; E)$ (which is obtained from the diagonal element of the Green function $G^<(\mathbf{r}_1, \mathbf{r}_2; E)$, assuming that carriers are distributed in energy according to a Fermi distribution (equation (2.11)). An interesting question is whether this local electrochemical potential $\mu(\mathbf{r})$ can be measured using a ‘non-invasive’ probe [22]. We assume that the probe is coupled weakly enough that it does not perturb the solution to (5.3) within the device appreciably (figure 5); that is, the local electrochemical potential $\mu(\mathbf{r})$ is assumed to stay the same with and without the probe. The potential μ_{probe} to which the probe floats is obtained from (5.3) by integrating over all $\mathbf{r} \in \text{probe}$ and setting the current equal to zero.

$$0 = \mu_{\text{probe}} \int_{r \in \text{probe}} d\mathbf{r} \bar{T}_0(\mathbf{r}) - \int_{r \in \text{probe}} d\mathbf{r} \int d\mathbf{r}' T_0(\mathbf{r}, \mathbf{r}') \mu(\mathbf{r}') \tag{5.20}$$

Hence,

$$\mu_{\text{probe}} = \int d\mathbf{r}' p(\mathbf{r}') \mu(\mathbf{r}') \quad (5.21)$$

where

$$p(\mathbf{r}') = \int_{\mathbf{r} \in \text{probe}} d\mathbf{r} T_0(\mathbf{r}, \mathbf{r}') / \int_{\mathbf{r} \in \text{probe}} d\mathbf{r} \bar{T}_0(\mathbf{r}). \quad (5.22)$$

Note that (5.21) can be viewed as an extension of Büttiker's result (equation (1) of [22]) to a continuous distribution of reservoirs. Equation (5.21) shows that the potential μ_{probe} measured by the probe is a weighted average of the potentials $\mu(\mathbf{r})$ in different parts of the structure. The weighting is determined by the probe function $p(\mathbf{r})$ which represents the fraction of carriers entering the probe that suffered their *last phase-breaking scattering at \mathbf{r}* . Since $T_0(\mathbf{r}, \mathbf{r}')$ is proportional to $|G^R(\mathbf{r}, \mathbf{r}')|^2$ which decays within a phase-breaking length L_φ , μ_{probe} is affected only by the potentials within a distance L_φ . If the potential varies slowly within this distance then there is no ambiguity in the measured potential μ_{probe} . But if the potential varies significantly within a phase-breaking length then the potential μ_{probe} that a probe measures depends on the probe function $p(\mathbf{r})$ which depends on the probe-geometry and construction.

6. Summary

Starting from a model Hamiltonian we have derived a simple kinetic equation that can be solved (self-consistently with the Poisson equation) to obtain the electron density per unit energy $n(\mathbf{r}; E)$ in an arbitrary structure (equation (3.24)).

$$I(\mathbf{r}; E) = \frac{e}{\tau_\varphi(\mathbf{r}; E)} \left(n(\mathbf{r}; E) - \int d\mathbf{r}' \int dE' K(\mathbf{r}, \mathbf{r}'; E, E') n(\mathbf{r}'; E') \right). \quad (6.1)$$

We assume that the structure contains two or more contact regions where the electron density is given by a Fermi distribution with a local electrochemical potential (figure 3). We then solve (6.1) in the rest of the structure (with $I(\mathbf{r}; E) = 0$) to obtain the electron density $n(\mathbf{r}; E)$. Next we evaluate $I(\mathbf{r}; E)$ in the contact regions from (6.1); integrating it over the volume of each contact and over all energy we obtain the corresponding terminal current (see equation (3.22)). Knowing the electron density $n(\mathbf{r}; E)$ we can also compute the current density $\mathbf{J}(\mathbf{r}; E)$ throughout the structure using (3.15).

If we assume that the electrons are distributed in energy according to the Fermi distribution (see equation (4.1)), then (6.1) can be simplified to decouple quantities at different energies (equation (4.9)).

$$I(\mathbf{r}; E) = \frac{e}{h} \left(\bar{T}(\mathbf{r}; E) f(\mathbf{r}; E) - \int d\mathbf{r}' T(\mathbf{r}, \mathbf{r}'; E) f(\mathbf{r}'; E) \right). \quad (6.2)$$

Equation (6.2) can be solved in the same way as (6.1) for the distribution function $f(\mathbf{r}; E) \equiv n(\mathbf{r}, E)/N_0(\mathbf{r}; E)$, $N_0(\mathbf{r}; E)$ being the density of states. Note that (6.2) is still a non-linear transport equation; the coefficients $T(\mathbf{r}, \mathbf{r}'; E)$ are not equilibrium quantities, but are evaluated under the appropriate biasing conditions. Once (6.2) has been solved for $f(\mathbf{r}; E)$ the current density can be computed from (4.14)

Next we specialize (6.2) to linear response and obtain an equation that has the appearance of (1.1) extended to include a continuous distribution of probes (equation (5.3)).

$$\tilde{I}(\mathbf{r}) = \frac{e^2}{h} \left(\bar{T}_0(\mathbf{r})\mu(\mathbf{r}) - \int d\mathbf{r}' T_0(\mathbf{r}, \mathbf{r}')\mu(\mathbf{r}') \right). \tag{6.3}$$

This equation is solved numerically in the same way as (6.1). We assume $\mu(\mathbf{r})$ to have specified values in the contacts and solve (6.3) within the device (with $I(\mathbf{r}) = 0$) to obtain $\mu(\mathbf{r})$. We then evaluate $I(\mathbf{r})$ in the contacts from (6.3) and integrate it over each contact to obtain the corresponding terminal current. Knowing $\mu(\mathbf{r})$ the current density within the structure can be computed from (5.6).

Next we show that (6.3) can be reduced to (1.1) and obtain an explicit series solution for the coefficients T_{ij} appearing in (1.1). Also it can be shown that in a homogeneous medium with a slowly varying electrochemical potential, (6.3) reduces to the diffusion equation in the absence of magnetic fields.

The simplicity of our model leads to a clear physical picture of the transport process and establishes a bridge between the rigorous quantum kinetic approach and the intuitively appealing single-particle approach. The kinetic equation is simple enough that numerical solutions (self-consistently with the Poisson equation) seem feasible for practical structures. By comparing the predictions of our model with experiment it should be possible to establish the limitations of our model and identify new phenomena arising from spatially correlated phase-breaking processes and many-body effects that are neglected in the model. The basic approach can be applied to more sophisticated models including spatially correlated phase-breaking processes and many-body effects where the self-energy is not a delta function. The only difference is that the kinetic equation will involve not only the diagonal elements of the Green function but also the off-diagonal elements (see equation (3.1)). This makes it more difficult to obtain numerical solutions and also complicates the physical picture of the transport process.

Acknowledgments

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Appendix A. Derivation of self-energy functions

Our main objective in this appendix is to derive (2.5a, b) and (2.6a, b). We will also derive the retarded and advanced self-energy functions which are used in appendix B. We start from the relations [12]

$$\Sigma^>(X_1, X_2) = G^>(X_1, X_2)D^>(X_1, X_2) \tag{A.1a}$$

$$\Sigma^<(X_1, X_2) = G^<(X_1, X_2)D^<(X_1, X_2). \tag{A.1b}$$

Here X stands for (\mathbf{r}, t) . The electron Green functions $G^>, G^<$ are defined by

$$G^>(X_1, X_2) = (-i/\hbar)\langle\psi(X_1)\psi^\dagger(X_2)\rangle \quad (\text{A.2a})$$

$$G^<(X_1, X_2) = (i/\hbar)\langle\psi^\dagger(X_2)\psi(X_1)\rangle. \quad (\text{A.2b})$$

The functions $D^>$, $D^<$ are given by

$$D^>(X_1, X_2) = \langle H'(\mathbf{r}_1, t_1)H'(\mathbf{r}_2, t_2)\rangle \quad (\text{A.3a})$$

$$D^<(X_1, X_2) = \langle H'(\mathbf{r}_2, t_2)H'(\mathbf{r}_1, t_1)\rangle. \quad (\text{A.3b})$$

Using (2.3) for H' we obtain

$$D^>(X_1, X_2) = U^2 \sum_{m,n} \delta(\mathbf{r}_1 - \mathbf{r}_m)\delta(\mathbf{r}_2 - \mathbf{r}_n)\langle(a_m^\dagger(t_1) + a_m(t_1))(a_n^\dagger(t_2) + a_n(t_2))\rangle. \quad (\text{A.4})$$

We assume that the reservoir of oscillators is in a state of thermodynamic equilibrium, so that

$$\langle a_m^\dagger(t_1)a_n(t_2)\rangle = \delta_{mn}N(\hbar\omega_m)e^{i\omega_m(t_1-t_2)} \quad (\text{A.5a})$$

$$\langle a_m(t_1)a_n^\dagger(t_2)\rangle = \delta_{mn}(N(\hbar\omega_m) + 1)e^{-i\omega_m(t_1-t_2)} \quad (\text{A.5b})$$

$$\langle a_m(t_1)a_n(t_2)\rangle = 0 \quad (\text{A.5c})$$

$$\langle a_m^\dagger(t_1)a_n^\dagger(t_2)\rangle = 0 \quad (\text{A.5d})$$

where $N(\hbar\omega_m)$ is the average number of 'phonons' in a oscillator of frequency ω_m and is given by the Bose-Einstein factor

$$N(\hbar\omega) = 1/e^{\hbar\omega/k_B T} - 1. \quad (\text{A.6})$$

Using (A.5a-d) we obtain from equation (A.4),

$$D^>(X_1, X_2) = U^2 \delta(\mathbf{r}_1 - \mathbf{r}_2) \sum_m \delta(\mathbf{r}_1 - \mathbf{r}_m) [N(\hbar\omega_m)e^{i\omega_m(t_1-t_2)} + (N(\hbar\omega_m) + 1)e^{-i\omega_m(t_1-t_2)}]. \quad (\text{A.7})$$

Replacing the sum over m by an integral (equation (2.4)) and Fourier transforming $t_1 - t_2 \rightarrow \varepsilon$ we have,

$$D^>(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) = 2\pi\hbar U^2 J_0(\mathbf{r}_1; |\varepsilon|)\delta(\mathbf{r}_1 - \mathbf{r}_2) \times \begin{cases} N(|\varepsilon|) & \varepsilon < 0 \\ N(\varepsilon) + 1 & \varepsilon > 0. \end{cases} \quad (\text{A.8a})$$

Similarly it can be shown that

$$D^<(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) = 2\pi\hbar U^2 J_0(\mathbf{r}_1; |\varepsilon|)\delta(\mathbf{r}_1 - \mathbf{r}_2) \times \begin{cases} N(|\varepsilon|) + 1 & \varepsilon < 0 \\ N(\varepsilon) & \varepsilon > 0. \end{cases} \quad (\text{A.8b})$$

To calculate the self-energy functions we Fourier transform (A.1a, b)

$$\Sigma^>(\mathbf{r}_1, \mathbf{r}_2; E) = \int \frac{dE'}{2\pi\hbar} G^>(\mathbf{r}_1, \mathbf{r}_2; E')D^>(\mathbf{r}_1, \mathbf{r}_2; E - E') \quad (\text{A.9a})$$

$$\Sigma^<(\mathbf{r}_1, \mathbf{r}_2; E) = \int \frac{dE'}{2\pi\hbar} G^<(\mathbf{r}_1, \mathbf{r}_2; E')D^<(\mathbf{r}_1, \mathbf{r}_2; E - E'). \quad (\text{A.9b})$$

Using (A.8a, b) we obtain from (A.9a, b),

$$\Sigma^>(\mathbf{r}_1, \mathbf{r}_2; E) = (-i\hbar/\tau_n(\mathbf{r}_1; E)) \delta(\mathbf{r}_1 - \mathbf{r}_2) \tag{A.10a}$$

$$\Sigma^<(\mathbf{r}_1, \mathbf{r}_2; E) = (i\hbar/\tau_p(\mathbf{r}_1; E)) \delta(\mathbf{r}_1 - \mathbf{r}_2) \tag{A.10b}$$

where

$$\frac{1}{\tau_n(\mathbf{r}; E)} = \frac{2\pi}{\hbar} \int dE' F(\mathbf{r}; E' - E) p(\mathbf{r}; E') \tag{A.11a}$$

$$\frac{1}{\tau_p(\mathbf{r}; E)} = \frac{2\pi}{\hbar} \int dE' F(\mathbf{r}; E - E') n(\mathbf{r}; E') \tag{A.11b}$$

$$F(\mathbf{r}; \varepsilon) = U^2 J_0(\mathbf{r}; |\varepsilon|) \times \begin{cases} N(\varepsilon) & \varepsilon > 0 \\ N(|\varepsilon|) e^{|\varepsilon|/k_B T} & \varepsilon < 0. \end{cases} \tag{A.12}$$

Here we have used the relations

$$n(\mathbf{r}; E) = -iG^<(\mathbf{r}, \mathbf{r}; E)/2\pi \tag{A.13a}$$

$$p(\mathbf{r}; E) = iG^>(\mathbf{r}, \mathbf{r}; E)/2\pi. \tag{A.13b}$$

We have also used (A.6) in writing (A.12).

Finally we will evaluate the retarded and advanced self-energy functions Σ^R and Σ^A :

$$\Sigma^R(X_1, X_2) = \theta(t_1 - t_2) (\Sigma^>(X_1, X_2) - \Sigma^<(X_1, X_2)) \tag{A.14a}$$

$$\Sigma^A(X_1, X_2) = \theta(t_2 - t_1) (\Sigma^<(X_1, X_2) - \Sigma^>(X_1, X_2)) \tag{A.14b}$$

Fourier transforming with respect to $(t_1 - t_2)$ we have

$$\Sigma^R(\mathbf{r}_1, \mathbf{r}_2; E) = i \int_{-\infty}^{+\infty} \frac{dE'}{2\pi} \frac{\Sigma^>(\mathbf{r}_1, \mathbf{r}_2; E') - \Sigma^<(\mathbf{r}_1, \mathbf{r}_2; E')}{E - E' + i\varepsilon} \tag{A.15a}$$

$$\Sigma^A(\mathbf{r}_1, \mathbf{r}_2; E) = -i \int_{-\infty}^{+\infty} \frac{dE'}{2\pi} \frac{\Sigma^<(\mathbf{r}_1, \mathbf{r}_2; E') - \Sigma^>(\mathbf{r}_1, \mathbf{r}_2; E')}{E - E' - i\varepsilon}. \tag{A.15b}$$

Using (A.10a, b) we obtain from (A.15a),

$$\Sigma^R(\mathbf{r}_1, \mathbf{r}_2; E) = \frac{\hbar}{2\pi} \delta(\mathbf{r}_1 - \mathbf{r}_2) \int \frac{dE'}{E - E' + i\varepsilon} \frac{1}{\tau_\varphi(\mathbf{r}_1; E')} \tag{A.16}$$

where

$$1/\tau_\varphi(\mathbf{r}; E) = 1/\tau_n(\mathbf{r}; E) + 1/\tau_p(\mathbf{r}; E). \tag{A.17}$$

Hence, we have,

$$\text{Im}(\Sigma^R(\mathbf{r}_1, \mathbf{r}_2; E)) = (-\hbar/2\tau_\varphi(\mathbf{r}_1; E)) \delta(\mathbf{r}_1 - \mathbf{r}_2) \tag{A.18a}$$

$$\text{Re}(\Sigma^R(\mathbf{r}_1, \mathbf{r}_2; E)) = \sigma(\mathbf{r}_1; E) \delta(\mathbf{r}_1 - \mathbf{r}_2) \tag{A.18b}$$

where

$$\sigma(\mathbf{r}; E) = \frac{\hbar}{2\pi} \text{P} \int \frac{dE'}{(E - E')\tau_\varphi(\mathbf{r}; E')}. \tag{A.19}$$

P represents the principal value of the integral.

The advanced self-energy function can be obtained from the relation

$$\Sigma^A(\mathbf{r}_1, \mathbf{r}_2; E) = (\Sigma^R(\mathbf{r}_2, \mathbf{r}_1; E))^*. \quad (\text{A.20})$$

This is a general relationship between advanced and retarded functions that holds for the Green function as well:

$$G^A(\mathbf{r}_1, \mathbf{r}_2; E) = (G^R(\mathbf{r}_2, \mathbf{r}_1; E))^* \quad (\text{A.21})$$

To obtain (A.20) or (A.21) we note that from the definition of $G^<(X_1, X_2)$ in (A.2) we have

$$G^<(X_1, X_2) = (i/\hbar)\langle\psi^\dagger(X_2)\psi(X_1)\rangle = -[(i/\hbar)\langle\psi^\dagger(X_1)\psi(X_2)\rangle]^* = -[G^<(X_2, X_1)]^*. \quad (\text{A.22})$$

Since the Green functions depend only on the time differences $t = t_1 - t_2$, we can write

$$G^<(\mathbf{r}_1, \mathbf{r}_2; t) = -(G^<(\mathbf{r}_2, \mathbf{r}_1; -t))^* \quad (\text{A.23})$$

Hence, on Fourier transforming

$$G^<(\mathbf{r}_1, \mathbf{r}_2; E) = -(G^<(\mathbf{r}_2, \mathbf{r}_1; E))^* \quad (\text{A.24a})$$

The same relation holds for $G^>$ as well:

$$G^>(\mathbf{r}_1, \mathbf{r}_2; E) = -(G^>(\mathbf{r}_2, \mathbf{r}_1; E))^*. \quad (\text{A.24b})$$

Subtracting (A.24a) from (A.24b) we obtain

$$G^>(\mathbf{r}_1, \mathbf{r}_2; E) - G^<(\mathbf{r}_1, \mathbf{r}_2; E) = (G^<(\mathbf{r}_2, \mathbf{r}_1; E) - G^>(\mathbf{r}_2, \mathbf{r}_1; E))^*. \quad (\text{A.25})$$

Equation (A.21) is readily obtained using (A.25) and noting that G^R and G^A are related to $G^>$ and $G^<$ through relations analogous to (A.15a, b) for the self-energy functions. Equation (A.20) can also be obtained in a similar fashion.

Appendix B. Derivation of the kinetic equation

Our objective in this appendix is to derive (3.2) and (3.12). We start from the Dyson equation in the Keldysh formulation [12]

$$\mathbf{G}(X_1, X_2) = \mathbf{G}_0(X_1, X_2) + \int dX_3 dX_4 \mathbf{G}_0(X_1, X_3)\Sigma(X_3, X_4)\mathbf{G}(X_4, X_2) \quad (\text{B.1})$$

where X stands for (\mathbf{r}, t) . \mathbf{G} is a 2×2 matrix

$$\mathbf{G} = \begin{pmatrix} G^T & -G^< \\ G^> & -G^{\bar{T}} \end{pmatrix} \quad (\text{B.2})$$

whose elements are defined by

$$G^<(X_1, X_2) = (i/\hbar)\langle\psi^\dagger(X_2)\psi(X_1)\rangle \quad (\text{B.3a})$$

$$G^>(X_1, X_2) = -(i/\hbar)\langle\psi(X_1)\psi^\dagger(X_2)\rangle \quad (\text{B.3b})$$

$$G^T(X_1, X_2) = \theta(t_1 - t_2)G^>(X_1, X_2) + \theta(t_2 - t_1)G^<(X_1, X_2) \quad (\text{B.3c})$$

$$G^{\bar{T}}(X_1, X_2) = \theta(t_1 - t_2)G^<(X_1, X_2) + \theta(t_2 - t_1)G^>(X_1, X_2). \tag{B.3d}$$

The bracket $\langle . . . \rangle$ denotes an average over the available states of the system, that is, a trace over the reservoir states. The self-energy function Σ is also a (2×2) matrix of the same form as \mathbf{G} . \mathbf{G}_0 is the unperturbed Green function. In addition to the four functions defined in equations (B.3a–d) it is convenient to define a retarded and an advanced Green function as follows:

$$G^R(X_1, X_2) = \theta(t_1 - t_2)(G^>(X_1, X_2) - G^<(X_1, X_2)) \tag{B.4a}$$

$$G^A(X_1, X_2) = \theta(t_2 - t_1)(G^<(X_1, X_2) - G^>(X_1, X_2)) \tag{B.4b}$$

The retarded and advanced self-energy functions Σ^R, Σ^A are also defined accordingly (see appendix A).

To derive the kinetic equation we start from (B.1) noting that

$$(i\hbar \partial/\partial t_1 - H_0(r_1))\mathbf{G}_0(X_1, X_2) = \delta^4(X_1 - X_2)\mathbf{I} \tag{B.5}$$

where \mathbf{I} is the 2×2 identity matrix. Operating on (B.1) with $i\hbar \partial/\partial t_1 - H_0(r_1)$ and using (B.5) we obtain

$$\left(i\hbar \frac{\partial}{\partial t_1} - H_0(r_1)\right) \mathbf{G}(X_1, X_2) = \delta^4(X_1 - X_2)\mathbf{I} + \int dX_3 \Sigma(X_1, X_3)\mathbf{G}(X_3, X_2) \tag{B.6}$$

Each element in (B.6) is a (2×2) matrix, so that it is equivalent to four separate equations. We consider only the component involving $G^<$ on the left.

$$\begin{aligned} \left(i\hbar \frac{\partial}{\partial t_1} - H_0(r_1)\right) G^<(X_1, X_2) &= \int dX_3 (\Sigma^T(X_1, X_3)G^<(X_3, X_2) \\ &\quad - \Sigma^<(X_1, X_3)G^{\bar{T}}(X_3, X_2)). \end{aligned} \tag{B.7}$$

We note that

$$\begin{aligned} \Sigma^T(X_1, X_3) &= \theta(t_1 - t_3)\Sigma^>(X_1, X_3) + \theta(t_3 - t_1)\Sigma^<(X_1, X_3) \\ &= \Sigma^R(X_1, X_3) + \Sigma^<(X_1, X_3) \end{aligned} \tag{B.8}$$

where the retarded self-energy function Σ^R was defined earlier (equation (A.14a)). Also,

$$\begin{aligned} G^{\bar{T}}(X_3, X_2) &= \theta(t_3 - t_2)G^<(X_3, X_2) + \theta(t_2 - t_3)G^>(X_3, X_2) \\ &= -G^A(X_3, X_2) + G^<(X_3, X_2) \end{aligned} \tag{B.9}$$

where the advanced Green function G^A defined in the same way as the advanced self-energy function Σ^A (equation (A.14b)). Using equations (B.8) and (B.9) in equation (B.7) we obtain

$$\begin{aligned} \left(i\hbar \frac{\partial}{\partial t_1} - H_0(r_1)\right) G^<(X_1, X_2) &- \int dX_3 \Sigma^R(X_1, X_3)G^<(X_3, X_2) \\ &= \int dX_3 \Sigma^<(X_1, X_3)G^A(X_3, X_2). \end{aligned} \tag{B.10}$$

Fourier transforming with respect to $t_1 - t_2$ we have

$$\begin{aligned} (E - H_0(r_1))G^<(r_1, r_2; E) &- \int dr_3 \Sigma^R(r_1, r_3; E)G^<(r_3, r_2; E) \\ &= \int dr_3 \Sigma^<(r_1, r_3; E)G^A(r_3, r_2; E). \end{aligned} \tag{B.11}$$

Here we have assumed that the self-energy functions as well as the Green functions depend only on time differences like $t_1 - t_3$, and not on $t_1 + t_3$. The integrals then represent convolution products in time whose Fourier transforms are simple products in energy.

It can also be shown from (B.6) that

$$\left(i\hbar \frac{\partial}{\partial t_1} - H_0(\mathbf{r}_1)\right) G^R(X_1, X_2) - \int dX_3 \Sigma^R(X_1, X_3) G^R(X_3, X_2) = \delta^4(X_1 - X_2). \quad (\text{B.12})$$

Equation (B.13) is obtained by considering the component of (B.6) involving G^T on the left, subtracting (B.7) from it and noting that $G^R = G^T - G^<$. Fourier transforming we obtain

$$(E - H_0(\mathbf{r}_1)) G^R(\mathbf{r}_1, \mathbf{r}_2; E) - \int d\mathbf{r}_3 \Sigma^R(\mathbf{r}_1, \mathbf{r}_3; E) G^R(\mathbf{r}_3, \mathbf{r}_2; E) = \delta(\mathbf{r}_1 - \mathbf{r}_2). \quad (\text{B.13})$$

Using (B.13) we can write down the solution to (B.11) as

$$G^<(\mathbf{r}_1, \mathbf{r}_2; E) = \int d\mathbf{r}' \int d\mathbf{r}'' G^R(\mathbf{r}_1, \mathbf{r}'; E) \Sigma^<(\mathbf{r}', \mathbf{r}'', E) G^A(\mathbf{r}'', \mathbf{r}_2; E). \quad (\text{B.14})$$

Substituting for $\Sigma^<$ from (A.10b) we obtain

$$G^<(\mathbf{r}_1, \mathbf{r}_2; E) = i\hbar \int d\mathbf{r}' \frac{G^R(\mathbf{r}_1, \mathbf{r}'; E) G^A(\mathbf{r}', \mathbf{r}_2; E)}{\tau_p(\mathbf{r}', E)}. \quad (\text{B.15})$$

We now set $\mathbf{r}_1 = \mathbf{r}_2 \equiv \mathbf{r}$; using equations (A.13a) and (A.21), we have

$$n(\mathbf{r}; E) = \frac{\hbar}{2\pi} \int d\mathbf{r}' \frac{|G^R(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_p(\mathbf{r}'; E)}. \quad (\text{B.16})$$

This completes our derivation of (3.2). By considering the component of the matrix equation, (B.6), corresponding to $G^>$ instead of $G^<$ we could come up with an equation for the hole density $p(\mathbf{r}; E)$ instead of the electron density $n(\mathbf{r}; E)$. Instead of (B.16) we obtain

$$p(\mathbf{r}; E) = \frac{\hbar}{2\pi} \int d\mathbf{r}' \frac{|G^R(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_n(\mathbf{r}'; E)}. \quad (\text{B.17})$$

Adding (B.16) and (B.17) and using (A.17) we obtain an important relationship (derived again in appendix C from a different approach):

$$N_0(\mathbf{r}; E) = \frac{\hbar}{2\pi} \int d\mathbf{r}' \frac{|G^R(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_\varphi(\mathbf{r}'; E)} \quad (\text{B.18})$$

where $N_0(\mathbf{r}; E) = n(\mathbf{r}; E) + p(\mathbf{r}; E)$ is the electronic density of states. Fourier transforming $t_1 - t_2$ in (B.4a) and using (A.13) it can be shown that the density of states is also given by

$$N_0(\mathbf{r}; E) = -\text{Im}(G^R(\mathbf{r}, \mathbf{r}; E))/\pi. \quad (\text{B.19})$$

Next we will derive (3.12). The current density is obtained from the off-diagonal elements of the Green function $G^<(\mathbf{r}, \mathbf{r}'; E)$ using the relation [12]

$$\begin{aligned}
 \mathbf{J}(\mathbf{r}; E) &= \frac{-ie}{2\pi m^*} \int \frac{d\mathbf{k}}{(2\pi)^3} (\hbar\mathbf{k} - e\mathbf{A}) G^<(\mathbf{r}; \mathbf{k}; E) \\
 &= \frac{-e\hbar}{4\pi m^*} (\nabla - \nabla') G^>(\mathbf{r}, \mathbf{r}'; E) \Big|_{\mathbf{r}=\mathbf{r}'} - \frac{e^2}{m^*} \mathbf{A}(\mathbf{r}) n(\mathbf{r}; E)
 \end{aligned} \tag{B.20}$$

where ∇ and ∇' denote gradient operations with respect to \mathbf{r} and \mathbf{r}' respectively. Using (B.15), (B.16) and (A.21) we obtain from (B.20)

$$\mathbf{J}(\mathbf{r}; E) = \frac{\hbar}{2\pi} \int \frac{d\mathbf{r}'}{\tau_p(\mathbf{r}'; E)} \mathbf{J}_\delta(\mathbf{r}, \mathbf{r}'; E) \tag{B.21}$$

where

$$\mathbf{J}_\delta(\mathbf{r}, \mathbf{r}'; E) = \mathbf{j}_\delta(\mathbf{r}, \mathbf{r}'; E) - (e^2/m^*) \mathbf{A}(\mathbf{r}) n_\delta(\mathbf{r}, \mathbf{r}'; E) \tag{B.22a}$$

$$\tag{B.22b}$$

$$n_\delta(\mathbf{r}, \mathbf{r}'; E) = |G^R(\mathbf{r}, \mathbf{r}'; E)|^2$$

$$\begin{aligned}
 \mathbf{j}_\delta(\mathbf{r}, \mathbf{r}'; E) &= (-ie\hbar/2m^*) (G^R(\mathbf{r}, \mathbf{r}'; E) \nabla G^R(\mathbf{r}, \mathbf{r}'; E) \\
 &\quad - G^R(\mathbf{r}, \mathbf{r}'; E) \nabla G^R(\mathbf{r}, \mathbf{r}'; E)^*).
 \end{aligned} \tag{B.22c}$$

Writing $G^R(\mathbf{r}, \mathbf{r}'; E)$ as $|G^R(\mathbf{r}, \mathbf{r}'; E)| \exp(i\theta(\mathbf{r}, \mathbf{r}'; E))$ we can show from (B.22c) that

$$\mathbf{j}_\delta(\mathbf{r}, \mathbf{r}'; E) = n_\delta(\mathbf{r}, \mathbf{r}'; E) (e/m^*) \hbar \nabla \theta(\mathbf{r}, \mathbf{r}'; E). \tag{B.23}$$

Using (B.23) we rewrite (B.22a) as

$$\mathbf{J}_\delta(\mathbf{r}, \mathbf{r}'; E) = n_\delta(\mathbf{r}, \mathbf{r}'; E) (e/m^*) (\hbar \nabla \theta(\mathbf{r}, \mathbf{r}'; E) - e\mathbf{A}(\mathbf{r})). \tag{B.24}$$

This completes the derivation of (3.12).

Appendix C. Derivation of some useful properties of Green functions

Our objective in this appendix is to derive (3.4) and (3.19). We start from the defining equation for the retarded Green function (equation (3.3)).

$$(H_0(\mathbf{r}) + V_{\text{op}}(\mathbf{r}; E)) G^R(\mathbf{r}, \mathbf{r}'; E) = E G^R(\mathbf{r}, \mathbf{r}'; E) - \delta(\mathbf{r} - \mathbf{r}'). \tag{C.1}$$

H_0 is given by (2.1):

$$H_0 = -\frac{\hbar^2 \nabla^2}{2m^*} + \frac{ie\hbar}{m^*} \mathbf{A} \cdot \nabla + \frac{ie\hbar}{2m^*} (\nabla \cdot \mathbf{A}) + \frac{e^2 A^2}{2m^*} + eV(\mathbf{r}). \tag{C.2}$$

It can be shown that

$$(1/e) \nabla \cdot \mathbf{J}_\delta(\mathbf{r}, \mathbf{r}'; E) = (i/\hbar) ((G^R)^* H_0 G^R - G^R (H_0 G^R)^*) \tag{C.3}$$

where \mathbf{J}_δ is defined by (B.22a, b, c). Using (C.1) to substitute for $H_0 G^R$ in (C.3) we obtain

$$\begin{aligned}
 (1/e) \nabla \cdot \mathbf{J}_\delta(\mathbf{r}, \mathbf{r}'; E) &= (i/\hbar) \delta(\mathbf{r} - \mathbf{r}') (G^R(\mathbf{r}, \mathbf{r}'; E) - G^R(\mathbf{r}, \mathbf{r}'; E)^*) \\
 &\quad - (i/\hbar) |G^R(\mathbf{r}, \mathbf{r}'; E)|^2 (V_{\text{op}}(\mathbf{r}; E) - V_{\text{op}}^*(\mathbf{r}; E)).
 \end{aligned} \tag{C.4}$$

Using (2.8b) and (3.3b) we write (C.4) as

$$(1/e) \nabla \cdot \mathbf{J}_\delta(\mathbf{r}, \mathbf{r}'; E) = (2\pi/\hbar) N_0(\mathbf{r}; E) \delta(\mathbf{r} - \mathbf{r}') - |G^R(\mathbf{r}, \mathbf{r}'; E)|^2 / \tau_\phi(\mathbf{r}; E). \tag{C.5}$$

Integrating over all volume, using the divergence theorem and assuming that the surface is so far away that \mathbf{J}_δ is zero on the surface, we obtain

$$\int d\mathbf{r}' \frac{|G^R(\mathbf{r}', \mathbf{r}; E)|^2}{\tau_\phi(\mathbf{r}'; E)} = \frac{2\pi}{\hbar} N_0(\mathbf{r}; E). \quad (\text{C.6})$$

Consider (C.6) with the magnetic field \mathbf{B} (and the current density) reversed:

$$\int d\mathbf{r}' \frac{|G^R(\mathbf{r}', \mathbf{r}; E)|^2}{\tau_\phi(\mathbf{r}'; E)} \Big|_{-\mathbf{B}} = \frac{2\pi}{\hbar} N_0(\mathbf{r}; E) \Big|_{-\mathbf{B}}. \quad (\text{C.7})$$

We will show that

$$G^R(\mathbf{r}', \mathbf{r}; E) \Big|_{-\mathbf{B}} = G^R(\mathbf{r}, \mathbf{r}'; E) \Big|_{\mathbf{B}} \quad (\text{C.8a})$$

$$N_0(\mathbf{r}; E) \Big|_{-\mathbf{B}} = N_0(\mathbf{r}; E) \Big|_{\mathbf{B}} \quad (\text{C.8b})$$

$$\tau_\phi(\mathbf{r}'; E) \Big|_{-\mathbf{B}} = \tau_\phi(\mathbf{r}'; E) \Big|_{\mathbf{B}}. \quad (\text{C.8c})$$

Using (C.8a, b, c) we obtain from (C.7),

$$\int d\mathbf{r}' \frac{|G^R(\mathbf{r}', \mathbf{r}; E)|^2}{\tau_\phi(\mathbf{r}'; E)} \Big|_{\mathbf{B}} = \frac{2\pi}{\hbar} N_0(\mathbf{r}; E) \Big|_{\mathbf{B}}. \quad (\text{C.9})$$

Combining (C.6) and (C.9) we obtain (3.4).

To prove (C.8c) we note that the electron density $n(\mathbf{r}; E)$ remains the same when the magnetic field is reversed (provided the sense of current flow is also reversed). Hence the scattering times τ_n , τ_p and τ_ϕ remain unaffected (see equations (2.6a,b), (3.3d)).

To prove (C.8a) we note that the Green function $G^R(\mathbf{r}', \mathbf{r}; E)$ can be expanded in terms of the eigenfunctions $\psi_n(\mathbf{r})$ and $\phi_n(\mathbf{r})$ of the adjoint operators $H_0 + V_{\text{op}}$ and $H_p + V_{\text{op}}^*$ respectively [23].

$$(H_0 + V_{\text{op}}) \psi_n(\mathbf{r}) = \varepsilon_n \psi_n(\mathbf{r}) \quad (\text{C.10a})$$

$$(H_0 + V_{\text{op}}^*) \phi_n(\mathbf{r}) = \varepsilon_n^* \phi_n(\mathbf{r}) \quad (\text{C.10b})$$

$$G^R(\mathbf{r}, \mathbf{r}'; E) = \sum_n \frac{\psi_n(\mathbf{r}) \phi_n^*(\mathbf{r}')}{E - \varepsilon_n}. \quad (\text{C.11})$$

Taking the complex conjugate of (C.10b) we obtain (see equation (C.2))

$$(H_0(-B) + V_{\text{op}}) \phi_n^*(\mathbf{r}) = \varepsilon_n \phi_n^*(\mathbf{r}). \quad (\text{C.12})$$

Comparing (C.12) with (C.10a) it is apparent that (since $V_{\text{op}}(-B) = V_{\text{op}}(B)$)

$$\phi_n^*(\mathbf{r}) \Big|_{-\mathbf{B}} = \psi_n(\mathbf{r}) \Big|_{\mathbf{B}}. \quad (\text{C.13})$$

Equation (C.8a) follows readily from (C.11) and (C.13). Using (B.19), we obtain (C.8b) from (C.8a).

To prove (3.19), we integrate (C.5) over a volume Ω not including the source at \mathbf{r}' and use the divergence theorem to write

$$\oint \mathbf{J}_\delta(\mathbf{r}', \mathbf{r}; E) \cdot d\mathbf{S} = -e \int_{\mathbf{r} \in \Omega} d\mathbf{r} \frac{|G^R(\mathbf{r}', \mathbf{r}; E)|^2}{\tau_\phi(\mathbf{r}; E)} \quad \text{if } \mathbf{r}' \notin \Omega \quad (\text{C.14})$$

where \mathbf{S} is the closed surface surrounding the volume Ω . Now if \mathbf{r}' lies outside the contact i then we can apply (C.14) to a closed surface \mathbf{S} formed by extending \mathbf{S}_i (figure 3) to

enclose the contact at infinity. Since there is no flux through the rest of the surface (see discussion following (3.17)), we can write

$$\int \mathbf{J}_\delta(\mathbf{r}', \mathbf{r}; E) \cdot d\mathbf{S}_i = -e \int_{\mathbf{r} \in \Omega_i} d\mathbf{r} \frac{|G^R(\mathbf{r}', \mathbf{r}; E)|^2}{\tau_\phi(\mathbf{r}; E)} \quad \text{if } \mathbf{r}' \notin \Omega_i. \quad (\text{C.15a})$$

Again if \mathbf{r}' lies inside the contact i then we can extend the surface S_i so as to exclude the contact. We then obtain

$$\int \mathbf{J}_\delta(\mathbf{r}', \mathbf{r}; E) \cdot d\mathbf{S}_i = +e \int_{\mathbf{r} \in \Omega_i} d\mathbf{r} \frac{|G^R(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_\phi(\mathbf{r}; E)} \quad \text{if } \mathbf{r}' \in \Omega_i. \quad (\text{C.15b})$$

The additional negative sign arises because the outward going normal to the closed surface is now reversed with the respect to our assumed direction for S_i .

Appendix D. Derivation of the diffusion equation from the linearized kinetic equation

In this Appendix our objective is to reduce the linear response equation (5.3) to the familiar diffusion equation (5.19) assuming a homogeneous medium in which the electrochemical potential varies slowly. First we note that in the homogeneous medium we may write (5.3) in the form of a convolution (denoted by $*$)

$$I(\mathbf{r}) = \frac{e^2}{h} \int d\mathbf{r}' \tau(\mathbf{r} - \mathbf{r}') \mu(\mathbf{r}') \equiv \frac{e^2}{h} \tau(\mathbf{r}) * \mu(\mathbf{r}) \quad (\text{D.1})$$

where

$$\tau(\mathbf{r} - \mathbf{r}') \equiv \bar{T}_0 \delta(\mathbf{r} - \mathbf{r}') - T_0(\mathbf{r} - \mathbf{r}'). \quad (\text{D.2})$$

Fourier transforming (D.1) we obtain

$$I(\mathbf{q}) = (e^2/h) \tau(\mathbf{q})\mu(\mathbf{q}). \quad (\text{D.3})$$

Now we expand $\tau(\mathbf{q})$ in a Taylor series up to the quadratic term

$$\tau(\mathbf{q}) \approx \tau(0) - iq_j(\tau_1)_j - q_i q_j (\tau_2)_{ij}. \quad (\text{D.4})$$

The coefficients in this expansion are given by the moments of $\tau(\mathbf{r} - \mathbf{r}')$ in real space.

$$\tau_0 = \int d\boldsymbol{\rho} \tau(\boldsymbol{\rho}) \quad (\text{D.5})$$

$$(\tau_1)_j = \int d\boldsymbol{\rho} \rho_j \tau(\boldsymbol{\rho}) \quad j = x, y, z \quad (\text{D.6})$$

$$(\tau_2)_{ij} = \frac{1}{2} \int d\boldsymbol{\rho} \rho_i \rho_j \tau(\boldsymbol{\rho}) \quad i, j = x, y, z \quad (\text{D.7})$$

where we have written $\boldsymbol{\rho}$ for $\mathbf{r} - \mathbf{r}'$. Using (5.5a) and (D.2) it is evident from (D.5) that $\tau_0 = 0$. Also in the absence of magnetic fields $\tau(\boldsymbol{\rho}) = \tau(-\boldsymbol{\rho})$ (see equation (5.5b)) so

that $(\tau_1)_j = 0$. The only non-zero quantities are $(\tau_2)_{xx} = (\tau_2)_{yy} = (\tau_2)_{zz} \equiv \tau_2$. Equation (D.3) thus reduces to

$$I(\mathbf{q}) = -(e^2 \tau_2 / h)(q_x^2 + q_y^2 + q_z^2) \mu(\mathbf{q}). \quad (\text{D.8})$$

Fourier transforming back to real space we obtain

$$I(\mathbf{r}) = (e^2 \tau_2 / h) \nabla^2 \mu(\mathbf{r}). \quad (\text{D.9})$$

Note that $I(\mathbf{r})$ is the current entering the structure through the external probes which is equal to divergence of the current density $\mathbf{J}(\mathbf{r})$. We thus obtain the diffusion equation

$$\nabla \cdot \mathbf{J} = \sigma \nabla^2 \mu(\mathbf{r}) \quad (\text{D.10})$$

where

$$\sigma = (e^2 / h) \tau_2. \quad (\text{D.11})$$

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