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An Integral Equation for Dissipative Quantum Transport

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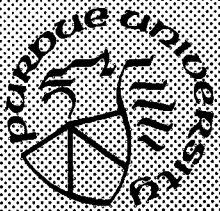
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**TR-EE 89-12
March, 1989**

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Supported by the Semiconductor Research Corporation (Contract no. 88-SJ-089)
and the National Science Foundation (Grant no. ECS-83-51-036).

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DISSIPATIVE QUANTUM TRANSPORT**

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TABLE OF CONTENTS

Abstract	1
I. Introduction.....	2
II. Overview	11
III. Inelastic Scattering Rate	16
A. Relationship Between Inelastic Scattering Rate and Self-energy.....	18
B. Self-energy in the “Golden Rule” Approximation	19
IV. The Transport Equation	23
V. Equilibrium and Linear Response.....	30
A. Effect of the Exclusion Principle	31
B. Equilibrium State.....	32
C. Linear Response	35
D. Power Dissipation and Circulating Currents.....	38
VI. Relationship to Classical Brownian Motion	41
A. Drift and Diffusion	41
B. Semiclassical Magnetoresistance	44
C. Numerical Example of Localization	47
VII. Summary.....	55
Appendix: Derivation of the Kernel from the Kubo Conductivity	58
References.....	64

ABSTRACT

We present an integral equation derived under the simplifying assumption that the inelastic scattering is caused by uncorrelated point scatterers, such as magnetic impurities or impurities with internal degrees of freedom. While this assumption is not always realistic, we believe that the model can be used to describe much of the essential physics of quantum transport in mesoscopic systems. This assumption allows us to write a transport equation that involves only the electron density and not the spatial correlations of the wavefunction. The kernel of this integral equation is calculated from the Schrödinger equation and contains all quantum interference effects. We show that at equilibrium the electron density relaxes to the expected equilibrium value with a constant chemical potential everywhere in the structure. Assuming local thermodynamic equilibrium we then derive a linear-response transport equation which resembles the Landauer-Büttiker formula extended to include a continuous distribution of probes. An alternative derivation is provided in the appendix for the kernel of the linear-response transport equation, starting from the Kubo formula for the conductivity. We discuss the conditions under which this transport equation reduces to the well-known drift-diffusion equations describing classical Brownian motion. In the present work we restrict ourselves to steady state transport and neglect many-body effects beyond the Hartree term.

I. INTRODUCTION

Much of our understanding of electron transport in solids is based on the Boltzmann transport equation (BTE).

$$\frac{\partial}{\partial t} f(\mathbf{r}; \mathbf{k}; t) + \mathbf{v} \cdot \nabla_{\mathbf{r}} f(\mathbf{r}; \mathbf{k}; t) + \frac{e\mathcal{E}}{\hbar} \cdot \nabla_{\mathbf{k}} f(\mathbf{r}; \mathbf{k}; t) = S_{\text{op}} f(\mathbf{r}; \mathbf{k}; t) \quad (1.1)$$

Here $f(\mathbf{r}; \mathbf{k}; t)$ is the distribution function in phase space that tells us the number of particles at \mathbf{r} with wavevector \mathbf{k} at time t . S_{op} is the scattering operator which is local in space.

$$S_{\text{op}} f(\mathbf{r}; \mathbf{k}; t) = \sum_{\mathbf{k}'} \left[S(\mathbf{k}, \mathbf{k}') f(\mathbf{k}') [1 - f(\mathbf{k})] - S(\mathbf{k}', \mathbf{k}) f(\mathbf{k}) [1 - f(\mathbf{k}')] \right]_{\text{at } \mathbf{r}, t} \quad (1.2)$$

The scattering function $S(\mathbf{k}, \mathbf{k}')$ is commonly obtained from Fermi's golden rule. The BTE is based on a simple semiclassical picture of transport: Electrons are particles that obey Newton's law in an external electric field (\mathcal{E}) and are scattered occasionally by phonons and impurities. Despite its impressive successes, it suffers from an important limitation; it cannot describe transport phenomena in which the wave nature of electrons plays a crucial role. A variety of such quantum effects have been discovered over the years, such as tunneling [1], resonant tunneling [2], weak and strong localization [3], the quantum Hall effect [4], etc. Since 1985, experiments on mesoscopic structures have revealed a wealth of new effects such as the Aharonov-Bohm effect, conductance fluctuations, non-local effects and the quantized conductance of point contacts [5-12]. For ultrasmall structures at low temperature, these phenomena have clearly revealed that electron transport is dominated by wave interference effects not unlike those well-known in microwave networks. It has also become clear that in mesoscopic structures, whose dimensions are comparable to the phase-breaking length, it is necessary to distinguish between sample-specific properties and ensemble-averaged properties; solid-state physics in the past had been almost exclusively concerned with the latter.

An important topic of current theoretical research is to develop a quantum transport formalism that can be used to describe the sample-specific properties of mesostructures. A satisfactory theory must not only include quantum interference effects, but also the effects of phase-

breaking processes (arising from scattering processes in which the scatterer changes its state) that are inevitably present. This is in general a very difficult problem, for it involves one of the fundamental questions of physics: How do irreversibility and dissipation creep into a system that is governed by reversible mechanics (i.e., the Schrödinger equation or Newton's law)? There have been a number of different approaches to quantum transport theory, each with its own subtle technique for introducing irreversibility.

1. In the *Kubo formalism*, linear transport coefficients such as conductivity are expressed in terms of correlation functions evaluated at equilibrium [13,14]. The conductivity tensor σ at a frequency ω is related to the current-current correlation function.

$$i\omega [\sigma_o(\mathbf{r}, \mathbf{r}'; \omega)]_{\alpha\beta} = [C_{JJ}(\mathbf{r}, \mathbf{r}'; \omega)]_{\alpha\beta} - \frac{n e^2}{m} \delta(\mathbf{r} - \mathbf{r}') \delta_{\alpha\beta} \quad (1.3)$$

where n is the electron density, m is the effective mass, $\delta_{\alpha\beta}$ is the Kronecker delta and the subscripts α, β run over x, y and z . The current-current correlation function C_{JJ} is defined as

$$C_{JJ}(\mathbf{r}, \mathbf{r}'; \omega) = \frac{i}{\hbar} \int_0^{\infty} dt e^{i\omega t} \langle \mathbf{J}(\mathbf{r}, t) \mathbf{J}(\mathbf{r}', 0) - \mathbf{J}(\mathbf{r}', 0) \mathbf{J}(\mathbf{r}, t) \rangle \quad (1.4)$$

where $\mathbf{J}(\mathbf{r}, t)$ is the current density operator in the Heisenberg picture and $\langle \dots \rangle$ denotes the expectation value. Eqs. (1.3), (1.4) and relations derived from it have been the starting point for much theoretical work on localization [15-19]. Recently Lee and co-workers and Maekawa et. al. have used this approach to study quantum transport in mesostructures [20-24]. Inelastic processes are included in this approach (also known as linear response theory) by replacing $(-i\omega)$ in the final result with $(1/\tau_i)$, where τ_i is the inelastic scattering time.

2. In the *Landauer formalism*, linear transport coefficients are expressed in terms of the scattering properties of the structure [25-28]. Usually it is assumed that inelastic scattering is negligible within the structure and occurs primarily in the contacts. Under these conditions, the current I_i at lead i is related to the chemical potential μ_j at lead j by the Landauer-Büttiker formula (Fig. 1.1) [29,30]

$$I_i = \frac{e^2}{h} \sum_j \{ (T_0)_{ji} \mu_i - (T_0)_{ij} \mu_j \} \quad (1.5)$$

where

$$(T_0)_{ij} = \int dE \left[-\frac{\partial f_0}{\partial E} \right] T_{ij}(E)$$

$$T_{ij}(E) = \text{Tr} \{ t_{ij}^\dagger(E) t_{ij}(E) \} \quad (1.6)$$

$t_{ij}(E)$ is the transmission matrix from lead j to lead i for electrons with energy E and f_0 is the Fermi-Dirac distribution function. It has been shown that the coefficients $(T_0)_{ij}$ are related to the conductivity tensor $(\sigma_o)_{\alpha\beta}$ by the following relation [31,32].

$$\frac{e^2}{h} (T_0)_{ij} = \int d(S_i)_\alpha \int d(S_j)_\beta [\sigma_o(\mathbf{r}, \mathbf{r}')]_{\alpha\beta} \quad (1.7)$$

where the vector S_i is normal to the cross-section of the lead i . Eq. (1.5) has been the starting point for much of the recent work on quantum transport in mesostructures [33-43]. Although the Landauer approach, in principle, can be applied more generally [44], eqs. (1.6) can be used to compute the coefficients $(T_0)_{ij}$ only if inelastic scattering is significant in the contacts and not within the structure. Dissipation and irreversibility in this approach arise from the coupling to the contacts which act as reservoirs, as often pointed out by Landauer [25,44]. Büttiker simulated the effects of inelastic scattering within the main structure by connecting it to a contact reservoir through a side probe and setting the current at this fictitious probe to zero [45]. The Landauer approach has so far been applied only to problems involving linear

response though, in principle, it should be applicable to non-linear response as well.

3. Finally, a variety of quantum kinetic equations have been used to describe quantum transport. The quantum Boltzmann equation (QBE) uses the Wigner distribution function $W(\mathbf{r}; \mathbf{k}; E; t)$ in place of the semiclassical Boltzmann distribution function $f(\mathbf{r}; \mathbf{k}; t)$ used in the BTE [46-53]. The Wigner distribution function is obtained from the Green function

$$G(\mathbf{r}_1, \mathbf{r}_2; t_1, t_2) = i \langle \psi^\dagger(\mathbf{r}_1, t_1) \psi(\mathbf{r}_2, t_2) \rangle \quad (1.8)$$

($\psi(\mathbf{r}, t)$ being the electron field operator) by transforming to center-of-mass

$$\mathbf{r} = \frac{1}{2} (\mathbf{r}_1 + \mathbf{r}_2), \quad t = \frac{1}{2} (t_1 + t_2)$$

and relative coordinates, and then Fourier transforming with respect to the relative coordinate.

$$\mathbf{r}_1 - \mathbf{r}_2 \rightarrow \mathbf{k}, \quad t_1 - t_2 \rightarrow E$$

The QBE is derived starting from the Dyson equation, and dissipation is introduced through the self-energy function. Alternatively, several authors have used the density matrix $\rho(\mathbf{r}_1, \mathbf{r}_2; t)$ which is proportional to the equal-time Green function $G(\mathbf{r}_1, \mathbf{r}_2; t_1, t_2) \Big|_{t_1=t_2^+}$. Dissipation has been introduced through an influence functional in the path integral technique [54], and through a boundary condition on the Wigner function corresponding to Landauer-type contact reservoirs [52]. Quantum kinetic equations provide a powerful approach to quantum transport theory, including non-linear response. The main difficulty seems to be their complexity as well as the fact that quantum distribution functions, being complex quantities, often have counter-intuitive properties, so that it is difficult to make approximations.

In this paper we present a simple quantum kinetic equation that can be solved to compute the electron density per unit energy $n(\mathbf{r}; E)$, *under steady state conditions*, neglecting many-body effects beyond the Hartree approximation. At equilibrium, $n(\mathbf{r}; E)$ is the product of the density of states $N_0(\mathbf{r}; E)$ and the Fermi-Dirac function $f_0(E)$. As the system is driven away from equilibrium by external sources, the distribution of electrons is perturbed. We assume that any external current is injected incoherently from the contacts. Our objective in this paper is to present a transport equation that can be solved to obtain this non-equilibrium distribution $n(\mathbf{r}; E)$. We emphasize that $n(\mathbf{r}; E)$ is not a semiclassical concept, but a well-defined quantum mechanical quantity, proportional to the Wigner distribution function $W(\mathbf{r}; \mathbf{k}; E; t)$ *integrated over all \mathbf{k}* (t is absent because we have restricted ourselves to steady state). The kernel of this integral transport equation is computed from the Schrödinger equation and contains all quantum interference effects due to elastic scatterers. Space-charge effects are taken into account by including in the Schrödinger equation the electrostatic Hartree potential obtained self-consistently from the Poisson equation.

In general it is not possible to write an integral equation involving only the electron density; spatial correlations of the wavefunction must also be taken into account. The transport equation presented in this paper represents a major simplification for two reasons. Firstly, the number of independent variables is reduced from $(\mathbf{r}_1; \mathbf{r}_2; E)$ (or equivalently, $(\mathbf{r}; \mathbf{k}; E)$) to $(\mathbf{r}; E)$. Secondly, the transport equation involves only positive quantities, so that it is easy to make intuitive approximations. Monte Carlo analysis based on a probabilistic interpretation should also be possible. In order to achieve this simplification, we assume that inelastic scattering is caused by a distribution of independent oscillators, each of which interacts with the electrons through a *delta potential*. We also assume that inelastic scattering processes are weak and infrequent, just as one does in deriving Fermi's golden rule; however, the elastic processes are treated exactly. This model closely approximates a laboratory sample with magnetic impurities, or impurities with internal degrees of freedom. For other types of inelastic scattering the model may not be realistic; however, we believe that it should still be possible to describe much of the

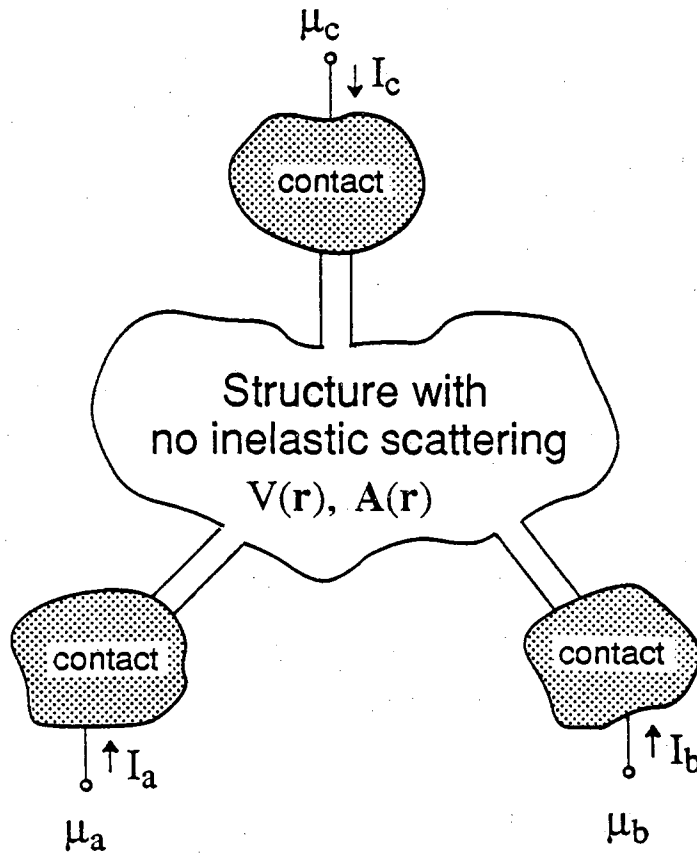


Fig. 1.1: The Landauer-Büttiker formula relates I_i to μ_j assuming that all inelastic scattering processes are confined to the contact reservoirs.

essential physics of dissipation in quantum transport.

Physically, it is easy to see why the above assumption leads to a simple transport equation that does not involve spatial correlations of the wavefunction. In the “golden rule” approximation, each scatterer acts independently. Since we have assumed a delta interaction potential, an inelastic scattering event only involves the wavefunction at a particular point and is insensitive to spatial correlations. In fact, inelastic scattering events in our model may be viewed as quantum measurements of the position and energy of the electron. Every time an electron is inelastically scattered it leaves one of these oscillators in an excited state, and energy is dissipated into the surroundings as the oscillator relaxes back to its state of thermodynamic equilibrium. An observer who monitors the states of the oscillators will see a series of flashes with different energies from different spatial locations and can, in principle, deduce the electron density $n(\mathbf{r}; E)$ from the observations. Our transport equation is thus formulated in terms of a variable that is actually measured rather than a conceptual quantity from which observable quantities can be deduced. We believe that it is for this reason that the transport equation involves only real positive quantities.

In this paper we adopt a microscopic approach starting from a model Hamiltonian for the inelastic scatterers; however, our model is closely related to the Landauer picture. Since the inelastic scattering process 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 (Fig 1.2). Indeed, when we simplify our transport equation to linear response we obtain what looks like the Landauer-Büttiker formula (eq. (1.5)) generalized to include a continuous distribution of probes. Moreover, the kernel of this linear-response transport equation can be derived directly from the Kubo formula for the conductivity (eq. (1.3)) using the Lee-Fisher formula (eq. (1.7)); this is shown in the appendix. Therefore, our transport equation reduces to well-known results in the limit of linear response. We believe that even the full (non-linear response) transport equation can also be derived from a Landauer picture if we

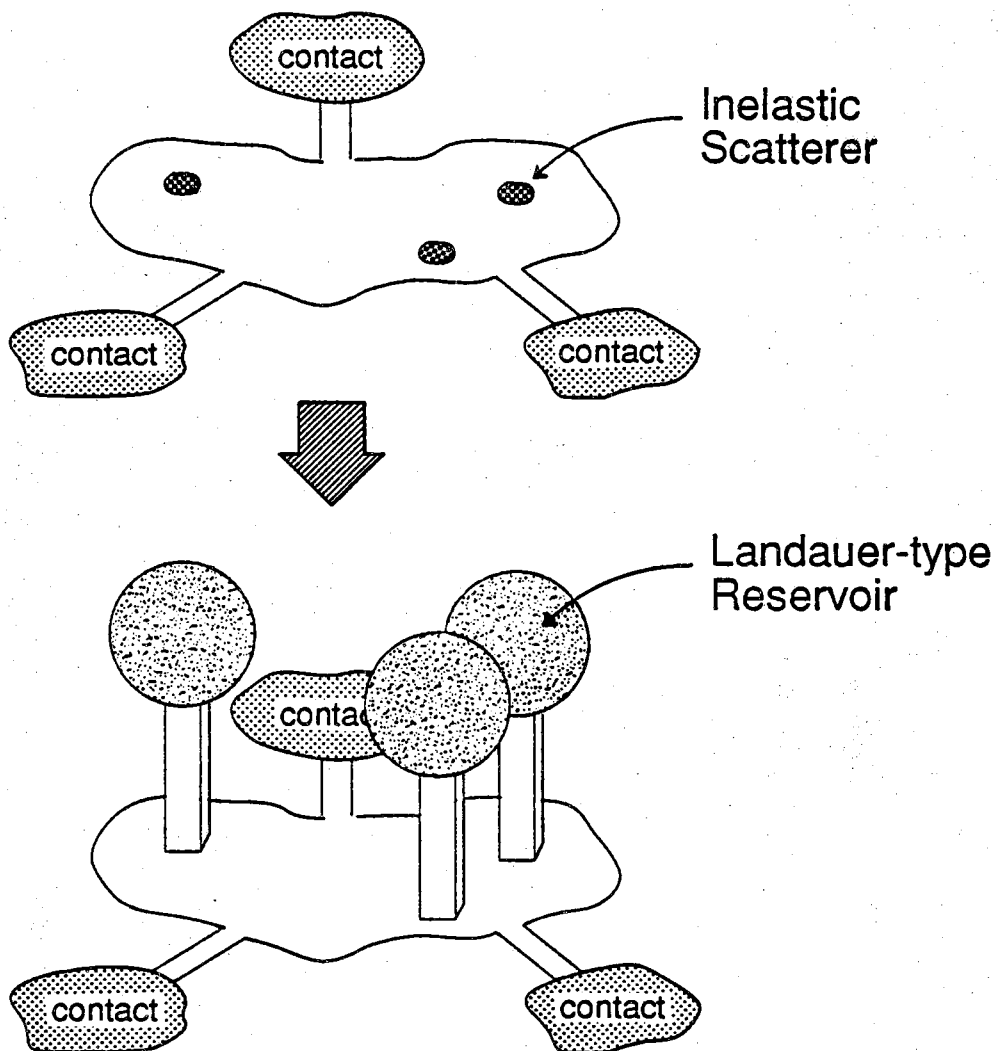


Fig. 1.2: In the limit of linear response at zero-temperature, the transport equation can be viewed as a generalization of the Landauer-Büttiker formula to a continuous distribution of reservoirs. Each reservoir simulates the action of an inelastic scatterer.

assume an appropriate relationship between the energy spectra of carriers entering and leaving the reservoirs. A direct generalization of the Landauer-Büttiker formula, however, would appear to be a phenomenological approach to simulating inelastic scattering. Our paper provides the rigorous justification for such an approach, by deriving the transport equation mentioned above directly from a model Hamiltonian making certain well-defined assumptions.

This paper also serves to clarify the meaning of the chemical potential $\mu(\mathbf{r})$ in quantum transport theory. As we mentioned earlier, the transport equation derived in this paper is formulated in terms of the electron density per unit energy $n(\mathbf{r}; E)$. We emphasize that this is a well-defined quantum mechanical quantity. The energy variable E is derived from the temporal correlations of the wavefunction at a point \mathbf{r} , and bears no relationship to \mathbf{k} ; there is thus no violation of the uncertainty principle since conjugate variables (like \mathbf{r} and \mathbf{k} or E and t) are never invoked simultaneously. In order to derive the linear-response transport equation, we assume *local thermodynamic equilibrium* so that we can write the electron density $n(\mathbf{r}; E)$ in terms of a local chemical potential $\mu(\mathbf{r})$

$$n(\mathbf{r}; E) = N_0(\mathbf{r}; E) \frac{1}{e^{(E-\mu(\mathbf{r}))/k_B T} + 1} \quad (1.9)$$

where $N_0(\mathbf{r}; E)$ is the electronic density of states. It is with this assumption that our transport equation simplifies to a form resembling the Landauer-Büttiker formula generalized to a continuous distribution of probes. On the other hand, if the driving forces are large enough (or the inelastic scattering weak enough) then local thermodynamic equilibrium may not be maintained. It is then not appropriate to talk in terms of a local chemical potential; we should solve for the actual distribution $n(\mathbf{r}; E)$ using the more general transport equation.

The outline of the paper is as follows. In Section II we describe the model that we use and provide an overview of the main results. In Section III we show that, in our model, the inelastic scattering rate at any point is proportional to the local electron density and does not involve spatial correlations of the wavefunction. The transport equation is then derived in Section IV, using a one-electron picture. An extra factor in the kernel arising from the exclusion principle

is added in Section V, using thermodynamic arguments for the equilibrium state; the linear-response transport equation is also derived in this section, assuming local thermodynamic equilibrium. In Section VI we discuss the conditions under which the linear-response transport equation reduces to the drift-diffusion equation that is widely used to describe classical Brownian motion. The diffusion coefficient is computed for a few simple examples (analytically as well as numerically). Finally in Section VII we conclude by summarizing our important results.

II. OVERVIEW

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

$$H_0 = \frac{[\mathbf{p} - e \mathbf{A}(\mathbf{r})]^2}{2m} + e V(\mathbf{r}) \quad (2.1)$$

The vector and scalar potentials $\mathbf{A}(\mathbf{r})$ and $V(\mathbf{r})$ include the Hartree potential obtained from a self-consistent solution with the Poisson equation, as well as externally imposed potentials, and all sources of *elastic* scattering such as impurities, defects, boundaries, etc. For the inelastic scattering we assume a reservoir of independent oscillators labeled by the index m ,

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

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

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

Note that we have assumed the interaction strength U to be constant. There is no loss of generality since the strength of inelastic 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.

$$\sum_m \Rightarrow \int d\mathbf{r} \int d(\hbar\omega) J_0(\mathbf{r}; \hbar\omega) \quad (2.4)$$

We will show in Section III that, with the assumption of a delta interaction potential, the self-energy function $\Sigma(\mathbf{r}_1, \mathbf{r}_2; E)$ in the simplest approximation reduces to a point function in space,

$$\Sigma(\mathbf{r}_1, \mathbf{r}_2; E) = -\frac{i\hbar}{2\tau_i(\mathbf{r}_1; E)} \delta(\mathbf{r}_1 - \mathbf{r}_2) \quad (2.5)$$

where $\tau_i(\mathbf{r}; E)$ is defined as the inelastic scattering time. Physically, this simplification arises from the fact that an individual inelastic scatterer sees only the electron wavefunction at a point. In general, the scattering rate would depend not only on the local electron density $n(\mathbf{r}) \sim \langle \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}) \rangle$ but also on the spatial correlations of the wavefunction $\sim \langle \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}') \rangle$. As a consequence of eq. (2.5), however, the inelastic scattering rate per unit volume per unit (initial) energy at a point can be written solely in terms of local quantities.

$$i_S(\mathbf{r}; E)/e \equiv \frac{n(\mathbf{r}; E)}{\tau_i(\mathbf{r}; E)} \quad (2.6)$$

where $i_S(\mathbf{r}; E)$ is defined as the inelastic scattering current per unit volume per unit energy. We will show in Section IV that in the absence of external sources, the scattering current must satisfy an integral equation of the form

$$i_S(\mathbf{r}; E) = \int d\mathbf{r}' \int dE' K(\mathbf{r}, \mathbf{r}'; E, E') i_S(\mathbf{r}'; E') \quad (2.7)$$

where the kernel $K(\mathbf{r}, \mathbf{r}'; E, E')$ is proportional to the square of the Green function of the Schrödinger equation, and thus contains all quantum interference effects due to elastic scatterers, boundaries, etc. It is interesting to note that the BTE (eq. (1.1)) without the diffusion and field terms,

$$\frac{d}{dt} f_{\mathbf{k}} = -\frac{f_{\mathbf{k}}}{\tau_{\mathbf{k}}} + \sum_{\mathbf{k}'} S_{\mathbf{k}, \mathbf{k}'} (1 - f_{\mathbf{k}}) f_{\mathbf{k}'} \quad (2.8)$$

can also be written in a form similar to eq. (2.7) above, assuming steady state ($df_{\mathbf{k}}/dt = 0$) and defining a scattering current $(i_S)_{\mathbf{k}}/e \equiv f_{\mathbf{k}}/\tau_{\mathbf{k}}$.

$$(i_s)_k = \sum_{k'} K_{k,k'} (i_s)_{k'} \quad (2.9)$$

where

$$K_{k,k'} \equiv S_{k,k'} (1 - f_k) \tau_{k'} \quad (2.10)$$

Eq. (2.8) is derived assuming that the momentum eigenstates $|k\rangle$ are energy eigenstates with definite energies E_k . For this reason, the energy variable does not appear explicitly in eq. (2.8). The fact that the position eigenstates $|r\rangle$ are not energy eigenstates makes the derivation of eq. (2.7) somewhat more complicated than that of eq. (2.8). Indeed, were it not for our assumption of point-size inelastic scatterers, it would not be possible to write down an equation such as eq. (2.7) solely in terms of the electron density; in general, such an equation would also involve spatial correlations of the wavefunction.

We assume that any external current $I(\mathbf{r}; E)$ flowing in and out of the contacts is completely incoherent and can simply be added to eq. (2.7).

$$i_s(\mathbf{r}; E) = I(\mathbf{r}; E) + \int d\mathbf{r}' \int dE' K(\mathbf{r}, \mathbf{r}'; E, E') i_s(\mathbf{r}'; E') \quad (2.11)$$

In general, the externally injected current may have spatial correlations, which we are neglecting in this treatment. This is the transport equation that must be solved to determine the inelastic scattering current $i_s(\mathbf{r}; E)$, or equivalently, the electron density $n(\mathbf{r}; E)$. Given the static potentials $V(\mathbf{r})$ and $A(\mathbf{r})$ (eq. (2.1)), and a distribution of inelastic scatterers $J_0(\mathbf{r}; \hbar\omega)$, the kernel $K(\mathbf{r}, \mathbf{r}'; E, E')$ can be computed. We can then proceed to solve eq. (2.11). At any node $(\mathbf{r}; E)$ we have two variables: the external current $I(\mathbf{r}; E)$ and the electron density $n(\mathbf{r}; E)$ (or equivalently, $i_s = en/\tau_i$). At all nodes which are not connected to some external source, $I(\mathbf{r}; E) = 0$, and we must solve for $n(\mathbf{r}; E)$. At contact nodes, we can assume $n(\mathbf{r}; E)$ to be given by a thermodynamic distribution characterized by a local chemical potential, and solve instead for $I(\mathbf{r}; E)$. It should be noted that I is the current flowing into the structure and not the current density \mathbf{J} within the structure; the two are related by $I = -\nabla \cdot \mathbf{J}$.

In Section V we will first show that in the absence of external sources ($I = 0$) eq. (2.11) does predict the expected equilibrium electron density $n_{\text{eq}}(\mathbf{r}; E)$

$$n_{\text{eq}}(\mathbf{r}; E) \equiv N_0(\mathbf{r}; E) f_0(E) \quad (2.12)$$

Here $f_0(E)$ is the Fermi-Dirac function

$$f_0(E) = \frac{1}{e^{(E - e\mu_0)/k_B T} + 1} \quad (2.13)$$

with a constant chemical potential μ_0 . $N_0(\mathbf{r}; E)$ is the electronic density of states given by

$$N_0(\mathbf{r}; E) = \sum_M |\phi_M(\mathbf{r})|^2 \delta(E - \epsilon_M) \quad (2.14)$$

where $\phi_M(\mathbf{r})$ are the eigenfunctions of H_0 (eq. (2.1)) with eigenvalues ϵ_M . In writing eq. (2.14) we assume weak inelastic scattering, so that level broadening effects may be neglected.

The remainder of Section V is devoted to simplifying the transport equation (eq. (2.11)) assuming a small perturbation from equilibrium. Below we state briefly the main results in order to show the resemblance between the simplified transport equation and the Landauer-Büttiker formula. In this linear response regime, we assume local thermodynamic equilibrium; the electron density $n(\mathbf{r}; E)$ can be described by a spatially varying chemical potential $\mu(\mathbf{r})$ (cf. eqs. (2.12), (2.13)).

$$n(\mathbf{r}; E) = N_0(\mathbf{r}; E) \frac{1}{e^{(E - e\mu(\mathbf{r}))/k_B T} + 1} \quad (2.15)$$

For linear response at low temperatures, only electrons within a narrow range of energies near the Fermi surface ($E = E_F$) contribute to the transport process. Consequently, the linear-response transport equation at zero-temperature looks much like eq. (2.11), but with the energy argument dropped:

$$i_S(\mathbf{r}) = \tilde{I}(\mathbf{r}) + \int d\mathbf{r}' P(\mathbf{r}, \mathbf{r}') i_S(\mathbf{r}') \quad (2.16)$$

where it is understood that all quantities are evaluated at $E = E_F$ and

$$P(\mathbf{r}, \mathbf{r}'; E') = \int dE K(\mathbf{r}, \mathbf{r}'; E, E') \quad (2.17)$$

We have changed nothing by writing eq. (2.16) in the form

$$\tilde{I}(\mathbf{r}) = \int d\mathbf{r}' \{P(\mathbf{r}', \mathbf{r}) i_S(\mathbf{r}) - P(\mathbf{r}, \mathbf{r}') i_S(\mathbf{r}')\} \quad (2.18)$$

because $\int d\mathbf{r}' P(\mathbf{r}', \mathbf{r}) = 1$, as we will see in Section IV. Noting that $i_S = e n / \tau_i$ and $n = N_0 \mu$, we may write eq. (2.18) in terms of the chemical potential as follows.

$$\tilde{I}(\mathbf{r}) = \frac{e^2}{h} \int d\mathbf{r}' \{T_0(\mathbf{r}', \mathbf{r}) \mu(\mathbf{r}) - T_0(\mathbf{r}, \mathbf{r}') \mu(\mathbf{r}')\} \quad (2.19)$$

where we have defined

$$T_0(\mathbf{r}, \mathbf{r}') \equiv \frac{h N_0(\mathbf{r}')}{\tau_i(\mathbf{r}')} P(\mathbf{r}, \mathbf{r}') \quad (2.20)$$

This form of the transport equation bears a striking similarity to the Landauer-Büttiker formula, repeated here for convenience

$$I_i = \frac{e^2}{h} \sum_j \{(T_0)_{ji} \mu_i - (T_0)_{ij} \mu_j\} \quad (2.21)$$

Eq. (2.19) can be viewed as an extension of the Landauer-Büttiker formula to include a continuous distribution of reservoirs, connected through perfectly conducting probes with infinitesimally small cross-sections to the main structure (Fig. 1.2). A single reservoir whose coupling can be varied has been used in the past to simulate the effect of inelastic scattering [45,55]. A better model for distributed inelastic scattering processes is a continuous distribution of reservoirs that repeatedly absorb and reinject electrons. From this point of view eq. (2.19) would seem to be an obvious extension of the Landauer-Büttiker formula. It is not obvious, however, how the kernel $T_0(\mathbf{r}, \mathbf{r}')$ is to be calculated for a given structure. Furthermore, the assumptions implicit in such an approach are not readily apparent. Indeed, critics would argue that this means of incorporating dissipation is purely phenomenological. This paper serves to rigorously justify such an approach, by deriving an integral equation starting directly from the Hamiltonian and making certain well-defined assumptions. Moreover, it extends the approach

to include non-linear response as well.

III. INELASTIC SCATTERING RATE

Our objective in this section is to show, starting from the Hamiltonian stated in Section II (eqs. (2.1)-(2.3)), that the inelastic scattering rate depends only on local properties, as expressed by eq. (2.6). To accomplish this, we first relate the inelastic scattering rate to the self-energy. It will be evident from this relationship that the inelastic scattering rate depends only on local properties if the self-energy is a delta function in space. We will then show that in our model, with point inelastic scatterers, the self-energy is indeed a delta function.

Our approach is to use a one-electron Hamiltonian H_0 , coupled to a bath of oscillators H_p through the interaction Hamiltonian H' (eqs. (2.1)-(2.3)). A correction factor due to the exclusion principle will be inserted later in Section V. The state vector Ψ for the entire many-particle system comprising the electron and the oscillators obeys the equation

$$i\hbar \frac{\partial \Psi}{\partial t} = (H_0 + H_p + H') \Psi \quad (3.1)$$

We expand the state vector Ψ using the position representation $|r\rangle$ for the electron and the eigenstates $|\alpha\rangle$ for the oscillators.

$$\Psi = \sum_{\alpha} \psi_{\alpha}(r) |\alpha\rangle |r\rangle e^{-iE_{\alpha}t/\hbar} \quad (3.2)$$

where E_{α} is the total energy of the system (electron plus oscillators). The ket $|\alpha\rangle$ represents an eigenstate of the oscillator Hamiltonian H_p (eq. (2.2)), which can be expressed as a direct product of the individual oscillator eigenstates.

$$|\alpha\rangle = \prod_m |N_m\rangle_m \quad (3.3)$$

Here, the subscript m indexes each of the oscillators, and N_m is the number of "phonons" in oscillator m . The corresponding energy eigenvalue ϵ_{α} is given by

$$\epsilon_{\alpha} = \sum_m \hbar \omega_m (N_m + \frac{1}{2}) \quad (3.4)$$

Substituting eq. (3.2) into eq. (3.1) and taking the projection onto $|\alpha\rangle$ we obtain

$$(E_T - \epsilon_{\alpha} - H_0) \psi_{\alpha}(\mathbf{r}) = \sum_{\alpha'} H'_{\alpha\alpha'}(\mathbf{r}) \psi_{\alpha'}(\mathbf{r}) \quad (3.5)$$

Eq. (3.5) is a system of spatial differential equations coupled by the matrix elements of the interaction Hamiltonian. The probability amplitude $\psi_{\alpha}(\mathbf{r})$ can be written as the product of two terms: the amplitude Φ_{α} for the oscillators to be in state $|\alpha\rangle$, and the amplitude $\psi(\mathbf{r})$ for the electron to be at $|\mathbf{r}\rangle$: $\psi_{\alpha}(\mathbf{r}) = \Phi_{\alpha} \psi(\mathbf{r})$. Irreversibility is later introduced into the model by assuming that the phonon bath is maintained in thermal equilibrium, so that the phonon density matrix is always diagonal,

$$\Phi_{\alpha}^* \Phi_{\beta} = 0 \quad \text{for } \alpha \neq \beta \quad (3.6)$$

The electron density matrix $\rho(\mathbf{r}, \mathbf{r}')$ is obtained by tracing over the oscillator eigenstates.

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_{\alpha} \psi_{\alpha}(\mathbf{r}) \psi_{\alpha}^*(\mathbf{r}') \quad (3.7a)$$

Our transport equation will only involve the diagonal element of the density matrix, which can be identified as the electron density $n(\mathbf{r})$,

$$n(\mathbf{r}) = \rho(\mathbf{r}, \mathbf{r}) = \sum_{\alpha} |\psi_{\alpha}(\mathbf{r})|^2 \quad (3.7b)$$

We define the electron density per unit energy $n(\mathbf{r}; E)$ to be

$$n(\mathbf{r}; E) = \sum_{\alpha} |\psi_{\alpha}(\mathbf{r})|^2 \delta(E - E_{\alpha}) \quad (3.8a)$$

where the electron energy E_{α} is obtained by subtracting the oscillator energy ϵ_{α} from the total energy E_T .

$$E_{\alpha} = E_T - \epsilon_{\alpha} \quad (3.8b)$$

Note that we obtain the total electron density $n(\mathbf{r})$ (eq. (3.7b)) if we integrate eq. (3.8a) over all energy.

A. RELATIONSHIP BETWEEN INELASTIC SCATTERING RATE AND SELF-ENERGY

We could rewrite eq. (3.5) in terms of the Green function, rather than the wavefunction, as follows.

$$(E_\alpha - H_0) G_{\alpha\beta}(\mathbf{r}, \mathbf{r}') - \sum_{\alpha'} H'_{\alpha\alpha'}(\mathbf{r}) G_{\alpha'\beta}(\mathbf{r}, \mathbf{r}') = \delta_{\alpha\beta} \delta(\mathbf{r} - \mathbf{r}') \quad (3.9)$$

Note that eq. (3.9), like its counterpart eq. (3.5), is a coupled system of differential equations indexed by the oscillator states α and β . $G_{\alpha\beta}(\mathbf{r}, \mathbf{r}')$ represents the wavefunction $\psi_\alpha(\mathbf{r})$ due to a delta excitation at (β, \mathbf{r}') . It is well-known that the Green function $G_{\alpha\alpha}(\mathbf{r}, \mathbf{r}')$ obeys the Dyson equation [46],

$$G_{\alpha\alpha}(\mathbf{r}, \mathbf{r}') = G_0(\mathbf{r}, \mathbf{r}'; E_\alpha) + \int d\mathbf{r}_1 \int d\mathbf{r}_2 G_0(\mathbf{r}, \mathbf{r}_2; E_\alpha) \Sigma_\alpha(\mathbf{r}_2, \mathbf{r}_1) G_{\alpha\alpha}(\mathbf{r}_1, \mathbf{r}') \quad (3.10)$$

where $\Sigma_\alpha(\mathbf{r}_1, \mathbf{r}_2)$ is the self-energy function, and $G_0(\mathbf{r}, \mathbf{r}'; E_\alpha)$ is the undamped propagator defined by

$$(E_\alpha - H_0) G_0(\mathbf{r}, \mathbf{r}'; E_\alpha) = \delta(\mathbf{r} - \mathbf{r}') \quad (3.11)$$

Operating on eq. (3.10) with $(E_\alpha - H_0)$, and using eq. (3.11) we have,

$$(E_\alpha - H_0) G_{\alpha\alpha}(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') + \int d\mathbf{r}_1 \Sigma_\alpha(\mathbf{r}, \mathbf{r}_1) G_{\alpha\alpha}(\mathbf{r}_1, \mathbf{r}') \quad (3.12)$$

This equation can alternatively be written in terms of the quasi particle wavefunction as,

$$(E_\alpha - H_0) \psi_\alpha(\mathbf{r}) - \int d\mathbf{r}_1 \Sigma_\alpha(\mathbf{r}, \mathbf{r}_1) \psi_\alpha(\mathbf{r}_1) = 0 \quad (3.13)$$

The non-local ‘‘optical potential’’ in eq. (3.13) is well-known in scattering theory [56]. It is easy to show that eq. (3.13) leads to a continuity equation of the following form for the probability current density \mathbf{J}_α ,

$$\frac{1}{e} \nabla \cdot \mathbf{J}_\alpha = -\frac{2}{\hbar} \int d\mathbf{r}' \text{Re}\{i \Sigma_\alpha(\mathbf{r}, \mathbf{r}') \psi_\alpha^*(\mathbf{r}) \psi_\alpha(\mathbf{r}')\} \quad (3.14)$$

Current is not conserved because eq. (3.13) describes damped quasi particles. It includes *out-scattering* but no *in-scattering*. The term on the right represents the rate at which electrons are

inelastically scattered out.

$$iS_{\alpha}(\mathbf{r})/e = \frac{2}{\hbar} \int d\mathbf{r}' \operatorname{Re}\{i \Sigma_{\alpha}(\mathbf{r}, \mathbf{r}') \psi_{\alpha}^{*}(\mathbf{r}) \psi_{\alpha}(\mathbf{r}')\} \quad (3.15)$$

It is apparent from eq. (3.15) that the inelastic scattering rate, in general, depends on the spatial correlations of the wavefunction. However, we will now show that in our model the self-energy is a point function in space as stated earlier (eq. (2.5)), so that the inelastic scattering rate depends on purely local factors.

B. SELF-ENERGY IN THE "GOLDEN RULE" APPROXIMATION

Our approach in this paper is to treat the elastic Hamiltonian H_0 exactly, while treating the inelastic scattering in the "golden rule" approximation. As such we consider only the simplest diagram for the self-energy shown in Fig. 3.1. This diagram yields for the self-energy [56],

$$\Sigma_{\alpha}(\mathbf{r}, \mathbf{r}') \equiv \sum_{\beta} H'_{\alpha\beta}(\mathbf{r}) G_0(\mathbf{r}, \mathbf{r}'; E_{\beta}) H'_{\beta\alpha}(\mathbf{r}') \quad (3.16)$$

Our assumption of delta interaction potentials between the electron and the oscillators now leads to a simplification: The self-energy reduces to a point function. To show this, we note that (using eq. (2.3) for the electron-oscillator interaction H')

$$H'_{\alpha\beta}(\mathbf{r}) H'_{\alpha\beta}^{*}(\mathbf{r}') = |U|^2 \sum_{m,n} \delta(\mathbf{r} - \mathbf{r}_m) \delta(\mathbf{r}' - \mathbf{r}_n) \langle \alpha | a_m^{\dagger} + a_m | \beta \rangle \langle \beta | a_n^{\dagger} + a_n | \alpha \rangle \quad (3.17)$$

The factor $\langle \alpha | a_m^{\dagger} + a_m | \beta \rangle$ is non-zero only if $|\alpha\rangle$ and $|\beta\rangle$ represent states for which all oscillators are in identical states, except for the m^{th} oscillator whose state differs by one. Clearly the product of this factor and the following factor $\langle \beta | a_n^{\dagger} + a_n | \alpha \rangle$ cannot be non-zero unless $m = n$. Hence,

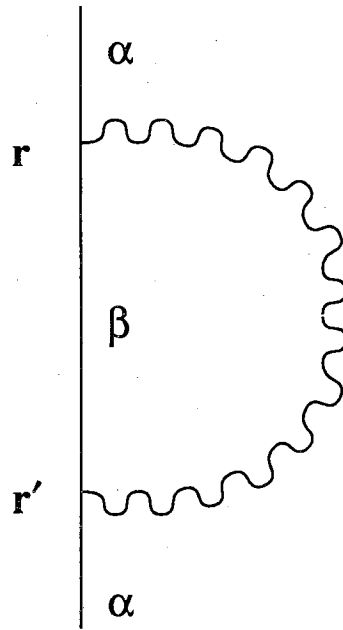


Fig. 3.1: Diagrammatic representation of $\Sigma_\alpha(r, r')$ in eq. (3.16).

$$H'_{\alpha\beta}(\mathbf{r}) H'^*_{\alpha\beta}(\mathbf{r}') = F_{\alpha\beta}(\mathbf{r}) \delta(\mathbf{r}-\mathbf{r}') \quad (3.18)$$

where

$$F_{\alpha\beta}(\mathbf{r}) \equiv \begin{cases} |U|^2 \sum_m \delta(\mathbf{r}-\mathbf{r}_m) (N_{m\alpha} + 1) , & \text{if } a_m |\beta\rangle = \sqrt{N_{m\alpha} + 1} |\alpha\rangle \\ |U|^2 \sum_m \delta(\mathbf{r}-\mathbf{r}_m) N_{m\alpha} , & \text{if } a_m^\dagger |\beta\rangle = \sqrt{N_{m\alpha}} |\alpha\rangle \\ 0 , & \text{otherwise} \end{cases} \quad (3.19)$$

Using eq. (3.18) we write the self-energy from eq. (3.16) as

$$\Sigma_\alpha(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') \sum_\beta G_0(\mathbf{r}, \mathbf{r}'; E_\beta) F_{\alpha\beta}(\mathbf{r}) \quad (3.20)$$

Using eq. (3.19) and noting that $G_0(\mathbf{r}, \mathbf{r}; E_\beta) \approx -i\pi N_0(\mathbf{r}; E_\beta)$ (neglecting the real part of the self-energy) we obtain

$$\begin{aligned} \Sigma_\alpha(\mathbf{r}, \mathbf{r}') = -i\pi \delta(\mathbf{r}-\mathbf{r}') |U|^2 \sum_m \delta(\mathbf{r}-\mathbf{r}_m) [(N_{m\alpha} + 1) N_0(\mathbf{r}; E_\alpha - \hbar\omega_m) \\ + N_{m\alpha} N_0(\mathbf{r}; E_\alpha + \hbar\omega_m)] \end{aligned} \quad (3.21)$$

Replacing the sum over m by an integral (eq. (2.4)), we obtain

$$\Sigma_\alpha(\mathbf{r}, \mathbf{r}') = \frac{-i\hbar}{2\tau_i(\mathbf{r}; E_\alpha)} \delta(\mathbf{r}-\mathbf{r}') \quad (3.22)$$

where

$$\frac{1}{\tau_i(\mathbf{r}; E)} \equiv \frac{2\pi}{\hbar} \int dE' F(\mathbf{r}; E'-E) N_0(\mathbf{r}; E') \quad (3.23)$$

$$F(\mathbf{r}; E-E') \equiv \begin{cases} |U|^2 J_0(\mathbf{r}; \hbar\omega) N(\hbar\omega) , & \text{if } \hbar\omega \equiv E-E' > 0 \\ |U|^2 J_0(\mathbf{r}; \hbar\omega) (N(\hbar\omega) + 1) , & \text{if } \hbar\omega \equiv E'-E > 0 \end{cases} \quad (3.24)$$

Assuming that the oscillators are in thermal equilibrium, the average number of "phonons" in each oscillator is related to its frequency ω by the Bose-Einstein factor.

$$N(\hbar\omega) = \frac{1}{e^{\hbar\omega/k_B T} - 1} \quad (3.25)$$

Now that we have computed the self-energy function, we substitute it into eq. (3.15) to obtain the inelastic scattering rate.

$$i_{S\alpha}(\mathbf{r})/e = |\psi_{\alpha}(\mathbf{r})|^2 / \tau_i(\mathbf{r}; E_{\alpha}) \quad (3.26)$$

The inelastic scattering current per unit energy is defined as

$$i_S(\mathbf{r}; E) = \sum_{\alpha} i_{S\alpha}(\mathbf{r}) \delta(E - E_{\alpha}) \quad (3.27)$$

Using eqs. (3.26) and (3.8a) we obtain the desired relation (eq. (2.6)).

$$i_S(\mathbf{r}; E) = \frac{e n(\mathbf{r}; E)}{\tau_i(\mathbf{r}; E)} \quad (3.28)$$

This represents the total rate at which electrons are inelastically scattered from an energy E to some other energy. The rate at which electrons are inelastically scattered into a particular energy E' is given by $e n(\mathbf{r}; E) S(\mathbf{r}; E', E)$, where $S(\mathbf{r}; E', E)$ is given by the integrand in eq. (3.23),

$$S(\mathbf{r}; E', E) = \frac{2\pi}{\hbar} F(\mathbf{r}; E' - E) N_0(\mathbf{r}; E') \quad (3.29)$$

Eq. (3.29) may be viewed as a "golden rule" describing the inelastic scattering process; however, it should be noted that unlike the usual golden rule we are using the position representation and not the energy eigenstates. This simple result is made possible by our assumption of independent point-size inelastic scatterers.

It is convenient to define a dimensionless factor $P_S(\mathbf{r}; E', E)$ as the fraction of the total inelastic scattering current $i_S(\mathbf{r}; E)$ that acquires a final energy E' after inelastically scattering from an energy E .

$$P_S(\mathbf{r}; E', E) \equiv \frac{S(\mathbf{r}; E', E)}{\int dE' S(\mathbf{r}; E', E)} = S(\mathbf{r}; E', E) \tau_i(\mathbf{r}; E) \quad (3.30)$$

Using eq. (3.29) we obtain

$$P_S(\mathbf{r}; E', E) = \frac{2\pi}{\hbar} F(\mathbf{r}; E' - E) N_0(\mathbf{r}; E') \tau_i(\mathbf{r}; E) \quad (3.31)$$

IV. THE TRANSPORT EQUATION

We have shown in Section III that the inelastic scattering process in our model is a purely local one; at any point \mathbf{r}' the rate at which electrons are inelastically scattered from an initial energy E' to a final energy E is given by $i_S(\mathbf{r}'; E') P_S(\mathbf{r}'; E, E')$, as illustrated in Fig. 4.1(a). Once the electron has been "injected" at \mathbf{r}' with an energy E (by an inelastic scattering process) it propagates *elastically* in real space. We can define a function $P(\mathbf{r}, \mathbf{r}'; E)$ as the probability that the electron will suffer its *very next* inelastic scattering event at position \mathbf{r} . Later in this section we will evaluate this function. Assuming that we know this function, it is straightforward to establish a transport equation simply by balancing the in-flow and out-flow at each "coordinate" $(\mathbf{r}; E)$, as shown in Fig. 4.1(b).

$$i_S(\mathbf{r}; E) = I(\mathbf{r}; E) + \int d\mathbf{r}' \int dE' K(\mathbf{r}, \mathbf{r}'; E, E') i_S(\mathbf{r}'; E') \quad (4.1)$$

where

$$K(\mathbf{r}, \mathbf{r}'; E, E') = P(\mathbf{r}, \mathbf{r}'; E) P_S(\mathbf{r}'; E, E') \quad (4.2)$$

The kernel $K(\mathbf{r}, \mathbf{r}'; E, E')$ is the product of two factors: The first factor $P(\mathbf{r}, \mathbf{r}'; E)$, which will be evaluated later in this section, is proportional to the square of the Green function $G(\mathbf{r}, \mathbf{r}'; E)$ and thus includes all quantum interference effects, while the second factor $P_S(\mathbf{r}'; E, E')$, which was evaluated in Section III (eq. (3.31)), contains all information regarding the spectrum of the inelastic scatterers. Our model thus provides an intuitive picture of quantum transport as a

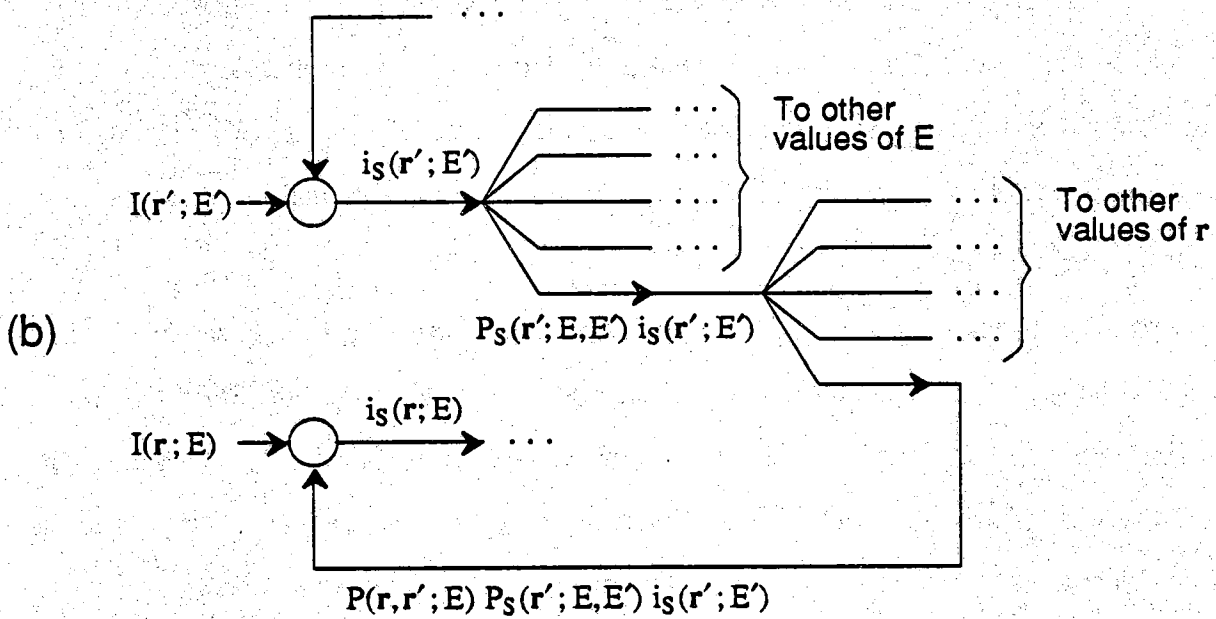
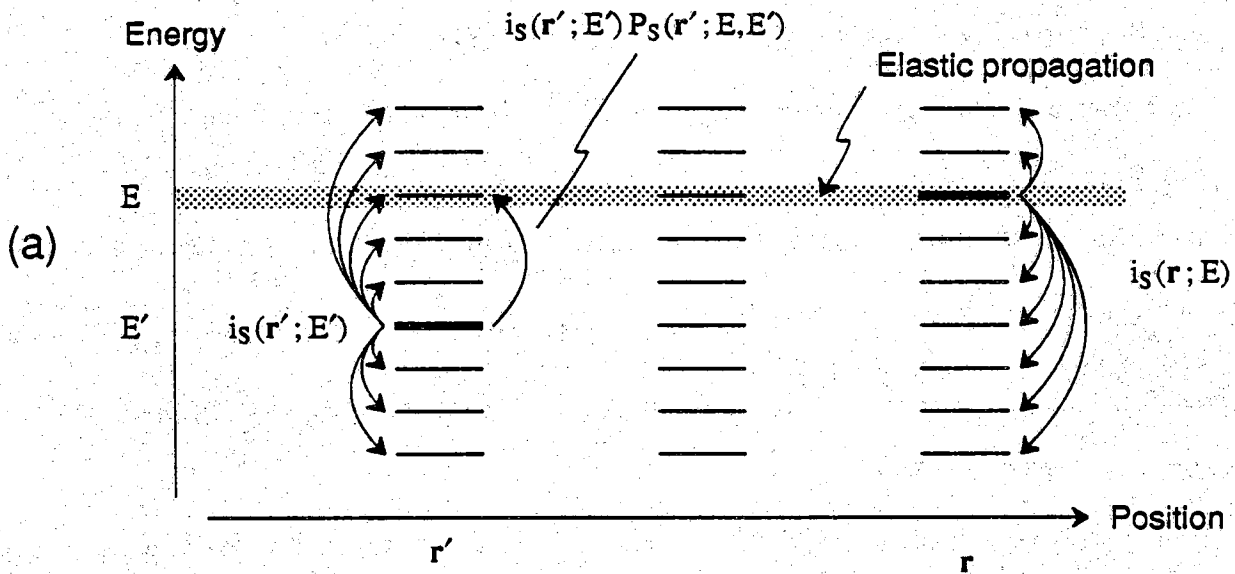


Fig. 4.1: (a) Physical picture of the transport process. (b) Schematic diagram illustrating different terms in the transport equation (4.1).

diffusion process in $(\mathbf{r}; E)$. The kernel $K(\mathbf{r}, \mathbf{r}'; E, E')$ can be viewed as a transfer function from one inelastic scattering event at $(\mathbf{r}'; E')$ to the next one at $(\mathbf{r}; E)$.

For linear response at zero-temperature, the function $P_S(\mathbf{r}'; E, E')$ does not appear since all transport occurs in a narrow range of energies around $E = E_F$. We will show in Section V that the linear-response transport equation at zero-temperature acquires a simple form as follows:

$$i_S(\mathbf{r}) = \tilde{I}(\mathbf{r}) + \int d\mathbf{r}' P(\mathbf{r}, \mathbf{r}') i_S(\mathbf{r}') \quad (4.3)$$

where all quantities are evaluated in a narrow energy slice around $E = E_F$. This linear-response equation is illustrated in Fig. 4.2.

It now remains to evaluate the factor $P(\mathbf{r}, \mathbf{r}'; E)$. As we have stated, $P(\mathbf{r}, \mathbf{r}'; E)$ represents the fraction of electrons injected at \mathbf{r}' with energy E (by inelastically scattering from some other energy) that suffer an inelastic scattering event at \mathbf{r} *without inelastically scattering in the meantime*. If this restriction (in italics) were absent, we would basically be calculating the diffusion propagator from \mathbf{r}' to \mathbf{r} , which includes the possibility that an electron inserted at \mathbf{r}' ends up at \mathbf{r} after suffering any number of inelastic scattering events. However, because of this restriction, what we are calculating is merely the piece connecting successive rungs in a ladder series diagram for the diffusion propagator.

Inelastic scattering may be viewed as a two-step process involving a decay out of an initial energy E , followed by an injection into a final energy E' . In calculating $P(\mathbf{r}, \mathbf{r}'; E)$, the second step is irrelevant. We are simply interested in the probability that an electron injected at \mathbf{r}' with energy E suffers its *very next* inelastic event at \mathbf{r} ; the reinjection at \mathbf{r} is a separate part of the problem that is already taken into account by the integral transport equation. Thus, for the purpose of calculating $P(\mathbf{r}, \mathbf{r}'; E)$ we can ignore the reinjection process and assume that we are dealing with decaying quasi particles. Such particles are described by the Schrödinger equation modified to include the optical potential (eq. (3.13)). In our model, the optical potential reduces to a purely local potential because the self-energy is a delta-function (eq. (3.22)).

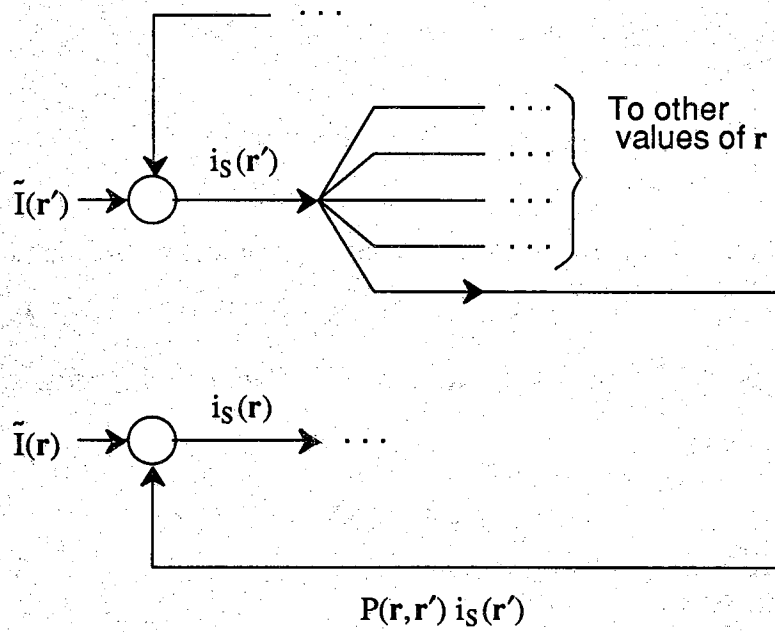


Fig. 4.2: A schematic diagram illustrating the different terms in the linearized transport equation at zero-temperature (eq. (4.3)).

$$\left[E_{\alpha} - H_0 + \frac{i\hbar}{2\tau_i(\mathbf{r}; E_{\alpha})} \right] G_{\alpha\alpha}(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \quad (4.4)$$

Since $G_{\alpha\alpha}(\mathbf{r}, \mathbf{r}')$ depends only on the energy E_{α} we can write it as

$$G_{\alpha\alpha}(\mathbf{r}, \mathbf{r}') = G(\mathbf{r}, \mathbf{r}'; E_{\alpha}) \quad (4.5)$$

where the damped propagator $G(\mathbf{r}, \mathbf{r}'; E)$ is computed from the equation

$$\left[E - H_0 + \frac{i\hbar}{2\tau_i(\mathbf{r}; E)} \right] G(\mathbf{r}, \mathbf{r}'; E) = \delta(\mathbf{r} - \mathbf{r}') \quad (4.6)$$

Since we have assumed point-size inelastic scatterers, an electron is injected as a point source by the inelastic scattering process. We can thus expect $P(\mathbf{r}, \mathbf{r}'; E)$ to be proportional to the squared magnitude of the Green function $G(\mathbf{r}, \mathbf{r}'; E)$. Consider the continuity equation obeyed by the probability density

$$n = |G(\mathbf{r}, \mathbf{r}'; E)|^2 \quad (4.7)$$

and the probability current density

$$\frac{1}{e} \mathbf{J} = \frac{i\hbar}{2m} \left[(\nabla G)^* G - G^* (\nabla G) \right] \quad (4.8)$$

that we obtain from the solution to eq. (4.6). It can be shown from eqs. (4.6), (4.7) and (4.8) that

$$\frac{1}{e} \nabla \cdot \mathbf{J} + \frac{n}{\tau_i} = \frac{i}{\hbar} \delta(\mathbf{r} - \mathbf{r}') [G - G^*] \quad (4.9)$$

Integrating over all volume, using the divergence theorem and assuming that the boundaries are far away so that no current flows out of the surface, we have

$$\int d\mathbf{r} \frac{|G(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_i(\mathbf{r}; E)} = \frac{2\pi}{\hbar} N_0(\mathbf{r}'; E) \quad (4.10)$$

since $N_0(\mathbf{r}; E) = -\text{Im}\{G(\mathbf{r}, \mathbf{r}; E)\}/\pi$ [14]. The integrand on the left in eq. (4.10) is the steady-state current n/τ_i due to electrons lost from the coherent state by inelastic scattering; the term on the right is the total steady-state current injected at \mathbf{r}' (Fig. 4.3). The ratio of these two terms

is equal to the probability function $P(\mathbf{r}, \mathbf{r}'; E)$, which is the quantity we sought.

$$P(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar}{2\pi} \frac{|G(\mathbf{r}, \mathbf{r}'; E)|^2}{N_0(\mathbf{r}'; E) \tau_i(\mathbf{r}; E)} \quad (4.11)$$

Substituting for P_S from eq. (3.31), and for P from eq. (4.11), into eq. (4.2) we obtain an expression for the kernel.

$$K(\mathbf{r}, \mathbf{r}'; E, E') = |G(\mathbf{r}, \mathbf{r}'; E)|^2 F(\mathbf{r}'; E - E') \frac{\tau_i(\mathbf{r}'; E')}{\tau_i(\mathbf{r}; E)} \quad (4.12)$$

It will be noted from eq. (3.30) that the factor P_S is normalized to unity.

$$\int dE P_S(\mathbf{r}'; E, E') = 1 \quad (4.13)$$

Again from eq. (4.10) it is evident that the factor P is also normalized to unity.

$$\int d\mathbf{r} P(\mathbf{r}, \mathbf{r}'; E) = 1 \quad (4.14)$$

Eqs. (4.13) and (4.14) together imply that the kernel K is normalized to unity.

$$\int d\mathbf{r} \int dE K(\mathbf{r}, \mathbf{r}'; E, E') = 1 \quad (4.15)$$

This normalization condition ensures that the particle current is conserved. The scattering current $i_S(\mathbf{r}'; E')$ out of a coordinate $(\mathbf{r}'; E')$ is distributed amongst the other coordinates $(\mathbf{r}; E)$ according to the kernel $K(\mathbf{r}, \mathbf{r}'; E, E')$. Eq. (4.15) ensures that no current is lost or gained in the process.

It should be noted that the assumption of point-size inelastic scatterers is crucial in arriving at such a simple description of non-linear quantum transport. Firstly, it allows us to write the function $P_S(\mathbf{r}'; E, E')$ in terms of purely local factors (eq. (3.31)). Secondly, it allows us to compute the probability function $P(\mathbf{r}, \mathbf{r}'; E)$ in a straightforward manner from the Green function. This is possible because each inelastic scattering event is assumed to reinject the electron incoherently with a new energy at a single point; the initial condition for each elastic propagation process is thus always a delta function. An extended inelastic scatterer would reinject the electron over an extended region; it would then be necessary to know the spatial correlations of

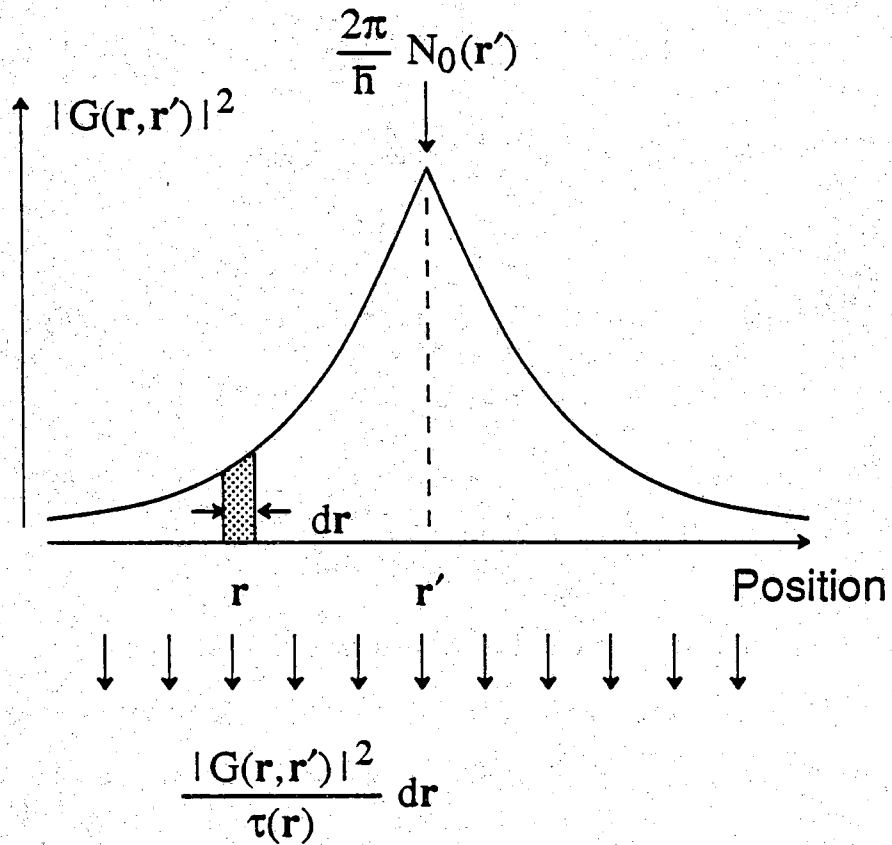


Fig. 4.3: Sketch of the probability density $|G(r, r'; E)|^2$ calculated from eq. (4.6). The index E has been dropped for convenience.

the wavefunction $\sim \langle \psi(\mathbf{r}) \psi^*(\mathbf{r}') \rangle$ in order to obtain the initial condition for the elastic propagation process.

We can rewrite the transport equation (eq. (4.1)) in terms of $n(\mathbf{r}; E)$ instead of $i_S(\mathbf{r}; E) = e n(\mathbf{r}; E) / \tau_i(\mathbf{r}; E)$.

$$n(\mathbf{r}; E) = \frac{I(\mathbf{r}; E) \tau_i(\mathbf{r}; E)}{e} + \int d\mathbf{r}' \int dE' K_n(\mathbf{r}, \mathbf{r}'; E, E') n(\mathbf{r}'; E') \quad (4.16)$$

where

$$\begin{aligned} K_n(\mathbf{r}, \mathbf{r}'; E, E') &= \frac{\tau_i(\mathbf{r}; E)}{\tau_i(\mathbf{r}'; E')} K(\mathbf{r}, \mathbf{r}'; E, E') \\ &= |G(\mathbf{r}, \mathbf{r}'; E)|^2 F(\mathbf{r}'; E - E') \end{aligned} \quad (4.17)$$

Eq. (4.16) can alternatively be derived by considering the ladder diagrams for the particle-hole propagator, and setting up a Bethe-Salpeter equation. It can then be shown that the kernel $K_n(\mathbf{r}, \mathbf{r}'; E, E')$ is simply one unit of the ladder diagram.

V. EQUILIBRIUM AND LINEAR RESPONSE

In this section, we consider solutions of the transport equation at or near equilibrium. We verify that in the absence of external sources, solution of the transport equation yields the correct distribution of electrons in energy (i.e., the Fermi-Dirac distribution). For small perturbations from equilibrium, we reformulate the equation, assuming that the distribution of electrons at any point can be characterized by a local chemical potential or quasi Fermi level. In this form, the equation bears a striking similarity to the Landauer-Büttiker formula. Each inelastic scatterer in our model acts as an independent reservoir in the Landauer model, so that our transport equation appears to be a simple extension of the Landauer-Büttiker formula to account for a continuous distribution of probes. A simple expression is derived for the two-probe conductance of any structure.

A. Effect of the Exclusion Principle

In the previous section we derived an integral transport equation (eq. (4.1)) based upon a one-electron picture. We now consider the effect of the Pauli exclusion principle and insert a correction factor into the definition of the kernel. It will be shown in Section B that this factor is necessary in order to obtain the proper equilibrium solution.

At equilibrium, the electron density should be given by the product of the density-of-states $N_0(\mathbf{r}; E)$ (eq. (2.14)) and the Fermi-Dirac factor $f_0(E)$,

$$n_{\text{eq}}(\mathbf{r}; E) = N_0(\mathbf{r}; E) f_0(E) \quad (5.1)$$

Extending this relationship to non-equilibrium situations, we define a convenient solution variable $f(\mathbf{r}; E)$ which we refer to as the distribution function:

$$n(\mathbf{r}; E) \equiv N_0(\mathbf{r}; E) f(\mathbf{r}; E) \quad (5.2)$$

Although the solution variables that we have introduced are all interchangeable,

$$i_S(\mathbf{r}; E) = \frac{e n(\mathbf{r}; E)}{\tau_i(\mathbf{r}; E)} = \frac{e N_0(\mathbf{r}; E) f(\mathbf{r}; E)}{\tau_i(\mathbf{r}; E)} \quad (5.3)$$

$f(\mathbf{r}; E)$ is particularly well-suited to discussion of the exclusion principle. Using this newly defined distribution function, the transport equation (eq. (4.11)) can be expressed as

$$\frac{e N_0(\mathbf{r}; E)}{\tau_i(\mathbf{r}; E)} f(\mathbf{r}; E) = I(\mathbf{r}; E) + \int d\mathbf{r}' \int dE' K(\mathbf{r}, \mathbf{r}'; E, E') \frac{e N_0(\mathbf{r}'; E')}{\tau_i(\mathbf{r}'; E')} f(\mathbf{r}'; E') \quad (5.4)$$

We emphasize that the distribution function $f(\mathbf{r}; E)$ as defined above is not a semiclassical concept but a well-defined quantum mechanical quantity. There is no violation of the uncertainty principle, since a knowledge of the electron's energy is conjugate to the time coordinate, not the position coordinate. This is in contrast to a semiclassical distribution such as $f(\mathbf{r}; \mathbf{k})$, used in the solution of the Boltzmann transport equation.

In Section IV we showed that the kernel $K(\mathbf{r}, \mathbf{r}'; E, E')$ is the product of two independent probabilities: $P_S(\mathbf{r}'; E, E')$ is the probability that an electron suffering an inelastic scattering event at $(\mathbf{r}'; E')$ would be scattered to an energy E ; and $P(\mathbf{r}, \mathbf{r}'; E)$ is the probability that an

electron “injected” at position \mathbf{r}' with an energy E would suffer its next inelastic scattering event at \mathbf{r} . The Pauli exclusion principle requires that an electron cannot be scattered into a state that is already filled. To account for this, we modify P_S by including a factor $[1 - f(\mathbf{r}'; E)]$ in the definition of $S(\mathbf{r}'; E, E')$.

$$S(\mathbf{r}'; E, E') = \frac{2\pi}{\hbar} F(\mathbf{r}'; E - E') N_0(\mathbf{r}'; E) [1 - f(\mathbf{r}'; E)] \quad (5.5)$$

This modifies the expressions for both P_S and τ_i as follows.

$$P_S(\mathbf{r}'; E, E') \equiv \frac{2\pi}{\hbar} F(\mathbf{r}'; E - E') N_0(\mathbf{r}'; E) [1 - f(\mathbf{r}'; E)] \tau_i(\mathbf{r}'; E') \quad (5.6)$$

$$\frac{1}{\tau_i(\mathbf{r}'; E')} \equiv \frac{2\pi}{\hbar} \int dE F(\mathbf{r}'; E - E') N_0(\mathbf{r}'; E) [1 - f(\mathbf{r}'; E)] \quad (5.7)$$

It is necessary to include this factor; without it, the distribution function $f(\mathbf{r}; E)$ would not relax to the proper equilibrium solution $f_0(E)$ in the absence of external sources. In principle, one could also modify P by using some form of exchange potential in eq. (4.6). However, we will not consider this further in our present treatment.

B. Equilibrium State

Close to equilibrium, the distribution function can be written in the form of a Fermi-Dirac function

$$f(\mathbf{r}; E) = \frac{1}{e^{(E - \epsilon\mu(\mathbf{r}))/k_B T} + 1} \quad (5.8)$$

where $\mu(\mathbf{r})$ is the local chemical potential. At equilibrium, the chemical potential is constant everywhere in the structure. In this section we will show that the distribution function in eq. (5.8) with $\mu(\mathbf{r}) = \mu_0$ (a constant) is indeed a solution to our transport equation (eq. (5.4)) with the external current $I(\mathbf{r}; E)$ set equal to zero; that is, we will show that

$$\int d\mathbf{r}' \int dE' K(\mathbf{r}, \mathbf{r}'; E, E') \frac{e N_0(\mathbf{r}'; E')}{\tau_i(\mathbf{r}'; E')} f_0(E') = \frac{e N_0(\mathbf{r}; E)}{\tau_i(\mathbf{r}; E)} f_0(E) \quad (5.9)$$

where

$$f_0(E) = \frac{1}{e^{(E - e\mu_0)/k_B T} + 1} \quad (5.10)$$

μ_0 being a constant. It is easily shown that

$$f_0(E') [1 - f_0(E)] = f_0(E) [1 - f_0(E')] e^{(E - E')/k_B T} \quad (5.11)$$

Using this fact, we can perform the energy integral in eq. (5.9) as follows. We obtain the kernel from eqs. (4.11) and (5.6),

$$\begin{aligned} K(\mathbf{r}, \mathbf{r}'; E, E') &= P_S(\mathbf{r}'; E, E') P(\mathbf{r}, \mathbf{r}'; E) \\ &= \frac{\tau_i(\mathbf{r}'; E')}{\tau_i(\mathbf{r}; E)} |G(\mathbf{r}, \mathbf{r}'; E)|^2 F(\mathbf{r}'; E - E') [1 - f(\mathbf{r}'; E)] \end{aligned} \quad (5.12)$$

This expression accounts for the exclusion principle, as described previously. Now, we substitute this definition into eq. (5.9) and apply eq. (5.11),

$$\begin{aligned} &\int dE' K(\mathbf{r}, \mathbf{r}'; E, E') \frac{e N_0(\mathbf{r}'; E')}{\tau_i(\mathbf{r}'; E')} f_0(E') \\ &= \frac{e \hbar}{2\pi} \frac{|G(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_i(\mathbf{r}, E)} \int dE' N_0(\mathbf{r}'; E') F(\mathbf{r}'; E - E') [1 - f_0(E)] f_0(E') \\ &= \frac{e \hbar}{2\pi} \frac{|G(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_i(\mathbf{r}, E)} f_0(E) \\ &\quad \int dE' N_0(\mathbf{r}'; E') F(\mathbf{r}'; E - E') [1 - f_0(E')] e^{(E - E')/k_B T} \end{aligned} \quad (5.13)$$

If our system of oscillators is in equilibrium, then the number of "phonons" with an energy $\hbar\omega$ is given by the Bose-Einstein function (eq. (3.25)). In conjunction with the definition of $F(\mathbf{r}'; E - E')$ stated in eq. (3.24), this implies that

$$F(\mathbf{r}'; E' - E) = F(\mathbf{r}'; E - E') e^{(E - E')/k_B T} \quad (5.14)$$

After substituting eq. (5.14) in eq. (5.13), the remaining integral is simply defined by eq. (5.7) to be $1/\tau_i(\mathbf{r}'; E)$. Therefore, we have simplified the integration over energy to

$$\int d\mathbf{r}' \int dE' K(\mathbf{r}, \mathbf{r}'; E, E') \frac{e N_0(\mathbf{r}'; E')}{\tau_i(\mathbf{r}'; E')} f_0(E') = \frac{e \hbar}{2\pi} \frac{f_0(E)}{\tau_i(\mathbf{r}; E)} \int d\mathbf{r}' \frac{|G(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_i(\mathbf{r}'; E)} \quad (5.15)$$

We must now evaluate the integral over the position coordinate \mathbf{r}' . It was shown in Section IV (cf. eq. (4.10)) that

$$\int d\mathbf{r}' \frac{|G(\mathbf{r}', \mathbf{r}; E)|^2}{\tau_i(\mathbf{r}'; E)} = \frac{2\pi}{\hbar} N_0(\mathbf{r}; E) \quad (5.16)$$

which is essentially the integral that we must perform, but with the coordinates interchanged in the Green function. A well-known symmetry property of the Green function is that

$$G(\mathbf{r}, \mathbf{r}'; E) \Big|_H = G(\mathbf{r}', \mathbf{r}; E) \Big|_{-H} \quad (5.17)$$

where $H \rightarrow -H$ implies a reversal of the magnetic field. From this property, we can evaluate the following integral,

$$\int d\mathbf{r}' \frac{|G(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_i(\mathbf{r}'; E)} \Big|_H = \int d\mathbf{r}' \frac{|G(\mathbf{r}', \mathbf{r}; E)|^2}{\tau_i(\mathbf{r}'; E)} \Big|_{-H} = \frac{2\pi}{\hbar} N_0(\mathbf{r}; E) \Big|_{-H} \quad (5.18)$$

We have by definition (eq. (2.14))

$$N_0(\mathbf{r}; E) = \sum_M |\phi_M(\mathbf{r})|^2 \delta(E - \epsilon_M) \quad (5.19)$$

where $\phi_M(\mathbf{r})$ are the eigenfunctions of H_0 (eq. (2.1)) with eigenvalues ϵ_M . The reversal of the magnetic field merely replaces each eigenfunction $\phi_M(\mathbf{r})$ by its complex conjugate, so that the density of states $N_0(\mathbf{r}; E)$ remains unchanged.

$$\int d\mathbf{r}' \frac{|G(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_i(\mathbf{r}'; E)} = \int d\mathbf{r}' \frac{|G(\mathbf{r}', \mathbf{r}; E)|^2}{\tau_i(\mathbf{r}'; E)} = \frac{2\pi}{\hbar} N_0(\mathbf{r}; E) \quad (5.20)$$

Substituting eq. (5.20) into eq. (5.15) we obtain eq. (5.9). This shows that in equilibrium (with source terms $I(\mathbf{r}; E)$ set to zero) the Fermi-Dirac function $f_0(E)$ is indeed the solution of our

transport equation.

It is thus fairly straightforward to calculate the equilibrium density of electrons in any structure. We first calculate the eigenfunctions $\phi_M(\mathbf{r})$ and eigenenergies ϵ_M for the elastic part of the Hamiltonian H_0 ; these are then used to obtain the density of states $N_0(\mathbf{r}; E)$ from eq. (5.19). The chemical potential μ_0 appearing in the Fermi-Dirac function $f_0(E)$ (eq. (5.10)) is adjusted to obtain the correct average density of electrons, according to eq. (5.1). In general, any uncompensated space-charge must be accounted for by performing an iterative solution for the electron density and the electrostatic potential. The electron density $n(\mathbf{r})$ should be inserted into the Poisson equation to obtain a corrected potential; the eigenfunctions $\phi_M(\mathbf{r})$ and the eigenenergies ϵ_M should then be recalculated including this potential, and iteration should continue until the solution is self-consistent.

C. Linear Response

To obtain a transport equation valid for linear response, we assume that inelastic scattering is sufficiently strong to maintain *local thermodynamic equilibrium* everywhere in the structure. If this is the case, the distribution function $f(\mathbf{r}; E)$ can be written in the form of a Fermi-Dirac function with a local chemical potential $\mu(\mathbf{r})$.

$$f(\mathbf{r}; E) = \frac{1}{e^{(E - e\mu(\mathbf{r}))/k_B T} + 1} \quad (5.21)$$

Provided that this assumption is true, the following relationship is valid:

$$f(E') [1 - f(E)] \Big|_{\text{at } \mathbf{r}} = f(E) [1 - f(E')] \Big|_{\text{at } \mathbf{r}} e^{(E - E')/k_B T} \quad (5.22)$$

Note that this is the same condition which allowed us to perform an integration over energy (eq. (5.11)) in the discussion above. Although the distribution $f(\mathbf{r}; E)$ is now a function of position, the arguments leading to eq. (5.15) are still valid. Therefore, we use this result to integrate eq. (5.4) over energy,

$$\tilde{I}(\mathbf{r}) = \frac{e}{h} \int dE \left[\frac{e N_0(\mathbf{r}; E)}{\tau_i(\mathbf{r}; E)} f(\mathbf{r}; E) - \int d\mathbf{r}' \tilde{T}(\mathbf{r}, \mathbf{r}'; E) f(\mathbf{r}'; E) \right] \quad (5.23)$$

where

$$\tilde{I}(\mathbf{r}) \equiv \int dE I(\mathbf{r}; E) \quad (5.24)$$

$$\tilde{T}(\mathbf{r}, \mathbf{r}'; E) \equiv \frac{\hbar^2 |G(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_i(\mathbf{r}; E) \tau_i(\mathbf{r}'; E)} \quad (5.25)$$

From eq. (5.20),

$$\int d\mathbf{r}' \tilde{T}(\mathbf{r}', \mathbf{r}; E) = \int d\mathbf{r}' \tilde{T}(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar N_0(\mathbf{r}; E)}{\tau_i(\mathbf{r}; E)} \quad (5.26)$$

We use this property to write eq. (5.23) in a more symmetric form.

$$\tilde{I}(\mathbf{r}) = \frac{e}{h} \int d\mathbf{r}' \int dE \{ \tilde{T}(\mathbf{r}', \mathbf{r}; E) f(\mathbf{r}; E) - \tilde{T}(\mathbf{r}, \mathbf{r}'; E) f(\mathbf{r}'; E) \} \quad (5.27)$$

In linear response theory we assume 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

$$f(\mathbf{r}; E) \simeq f_0(E) + \left[-\frac{\partial f_0}{\partial E} \right] e [\mu(\mathbf{r}) - \mu_0] \quad (5.28)$$

Substituting eq. (5.28) into eq. (5.27) and using eq. (5.26) we obtain

$$\tilde{I}(\mathbf{r}) = \frac{e^2}{h} \int d\mathbf{r}' \{ T_0(\mathbf{r}', \mathbf{r}) \mu(\mathbf{r}) - T_0(\mathbf{r}, \mathbf{r}') \mu(\mathbf{r}') \} \quad (5.29)$$

where

$$T_0(\mathbf{r}, \mathbf{r}') \equiv \int dE \left[-\frac{\partial f_0}{\partial E} \right] \tilde{T}(\mathbf{r}, \mathbf{r}'; E) \quad (5.30)$$

At low temperatures, $-\partial f_0/\partial E \simeq \delta(E - E_F)$, so that

$$T_0(\mathbf{r}, \mathbf{r}') = \tilde{T}(\mathbf{r}, \mathbf{r}'; E = E_F) = \frac{\hbar^2 |G(\mathbf{r}, \mathbf{r}')|^2}{\tau_i(\mathbf{r}) \tau_i(\mathbf{r}')} \Big|_{E = E_F} \quad (5.31)$$

Eq. (5.29) can be viewed as a generalization of the Landauer-Büttiker formula,

$$I_i = \frac{e^2}{h} \sum_j \{T_{ji} \mu_i - T_{ij} \mu_j\} \quad (5.32)$$

to a continuous distribution of probes. The coefficients $T_0(\mathbf{r}, \mathbf{r}')$ have the same symmetry properties in a magnetic field H as the coefficients T_{ij} [29,36]. Namely,

$$T_{ij} \Big|_H = T_{ji} \Big|_{-H} \quad (5.33a)$$

$$T_0(\mathbf{r}, \mathbf{r}') \Big|_H = T_0(\mathbf{r}', \mathbf{r}) \Big|_{-H} \quad (5.33b)$$

This is apparent from the definitions of $T_0(\mathbf{r}, \mathbf{r}')$ (eq. (5.30)), $\tilde{T}(\mathbf{r}, \mathbf{r}'; E)$ (eq. (5.25)) and the symmetry property of the Green function (eq. (5.17)). It has also been shown that the coefficients T_{ij} obey the following relationship [29],

$$\sum_j \{T_{ji} - T_{ij}\} = 0 \quad (5.34a)$$

Similarly, it can be shown that

$$\int d\mathbf{r}' \{T_0(\mathbf{r}', \mathbf{r}) - T_0(\mathbf{r}, \mathbf{r}')\} = 0 \quad (5.34b)$$

This property follows directly from eqs. (5.26) and (5.30).

Space-charge effects: In deriving eq. (5.29) from eq. (5.27) we have implicitly assumed that when we drive the system slightly away from equilibrium, the distribution function $f(\mathbf{r}; E)$ deviates from the equilibrium value of $f_0(E)$, but the coefficients $\tilde{T}(\mathbf{r}', \mathbf{r}; E)$ remain fixed. Actually, the coefficients $\tilde{T}(\mathbf{r}', \mathbf{r}; E)$ will change because corrections to the electrostatic potential will change the Green function $G(\mathbf{r}', \mathbf{r}; E)$, as well as the inelastic scattering times $\tau_i(\mathbf{r}; E)$. In considering the variation δI , we have accounted for one term,

$$\frac{e}{h} \int dr' \int dE \delta f_0(E) \{ \tilde{T}(r', r; E) - \tilde{T}(r, r'; E) \}$$

It would seem that we should also have a term of the form

$$\frac{e}{h} \int dr' \int dE f_0(E) \{ \delta \tilde{T}(r', r; E) - \delta \tilde{T}(r, r'; E) \}$$

where $\delta \tilde{T}$ is the change in the coefficient \tilde{T} . This term is zero, however, because of the relation (eq. (5.26)) that must be satisfied by $\tilde{T}(r', r; E)$. Consequently, in linear response theory we can use the coefficients $\tilde{T}(r', r; E)$ obtained (self-consistently) under equilibrium conditions, and ignore corrections due to the modification of the electrostatic potential under an applied bias. This, however, may not be true if there are sharp resonances in \tilde{T} ; second-order terms ($\sim \delta \tilde{T} \delta f_0$) may not be negligible in that case.

D. Power Dissipation and Circulating Currents

In general, we can solve eq. (5.29) for the potential distribution $\mu(r)$ in any structure. At equilibrium, $\mu(r)$ is equal to a constant μ_0 , and $\tilde{I}(r)$ is equal to zero. In the absence of magnetic fields ($H=0$ in eq. (5.33b)), $T_0(r', r) = T_0(r, r')$ so that at equilibrium the integrand in eq. (5.34b) is zero, and there is *detailed balance* between any two points r' and r . But in the presence of a magnetic field this is not true. There can be *circulating currents*, even at equilibrium. However, the net current out of any point is zero, as evident from eq. (5.34b). Any outflow in one direction is balanced by an inflow from another.

We can rewrite eq. (5.29) in the form

$$I(r) = \frac{e^2}{h} \int dr' \{ T_S(r', r) [\mu(r) - \mu(r')] + T_A(r', r) [\mu(r) + \mu(r')] \} \quad (5.35)$$

where

$$T_S(r', r) = \frac{1}{2} [T_0(r', r) + T_0(r, r')] \quad (5.36a)$$

$$T_A(\mathbf{r}', \mathbf{r}) = \frac{1}{2} [T_0(\mathbf{r}', \mathbf{r}) - T_0(\mathbf{r}, \mathbf{r}')] \quad (5.36b)$$

The power P_0 dissipated in the structure arises solely from the first term.

$$P_0 = \frac{e^2}{2h} \int d\mathbf{r} \int d\mathbf{r}' T_S(\mathbf{r}', \mathbf{r}) [\mu(\mathbf{r}) - \mu(\mathbf{r}')]^2 \quad (5.37)$$

The net power dissipation due to the second term is zero.

$$\frac{e^2}{2h} \int d\mathbf{r} \int d\mathbf{r}' T_A(\mathbf{r}', \mathbf{r}) [\mu^2(\mathbf{r}) - \mu^2(\mathbf{r}')] = 0 \quad (5.38)$$

Eq. (5.38) follows readily if we note that from eqs. (5.34b) and (5.36b)

$$\int d\mathbf{r}' T_A(\mathbf{r}', \mathbf{r}) = \int d\mathbf{r} T_A(\mathbf{r}', \mathbf{r}) = 0 \quad (5.39)$$

The circulating currents that are present even under equilibrium conditions thus dissipate no power. From the point of view of power dissipation we can represent any structure by a continuous network of conductors; any two volume elements $d\mathbf{r}'$ and $d\mathbf{r}$ are connected by a conductance equal to $(e^2/h) T_S(\mathbf{r}', \mathbf{r}) d\mathbf{r}' d\mathbf{r}$ (Fig. 5.1). If we have two external probes with a potential difference $\Delta\mu$ between them, the conductance g_0 seen from the terminals can be obtained by equating the total power dissipated in the network P_0 to $g_0 (\Delta\mu)^2$. From eq. (5.37) we obtain the following expression for the two-probe conductance g_0 .

$$g_0 = \frac{e^2}{2h} \int d\mathbf{r} \int d\mathbf{r}' T_S(\mathbf{r}', \mathbf{r}) \left[\frac{\mu(\mathbf{r}) - \mu(\mathbf{r}')}{\Delta\mu} \right]^2 \quad (5.40)$$

One may adopt a variational approach to calculating $\mu(\mathbf{r})$: choose a trial function and then minimize the power dissipated.

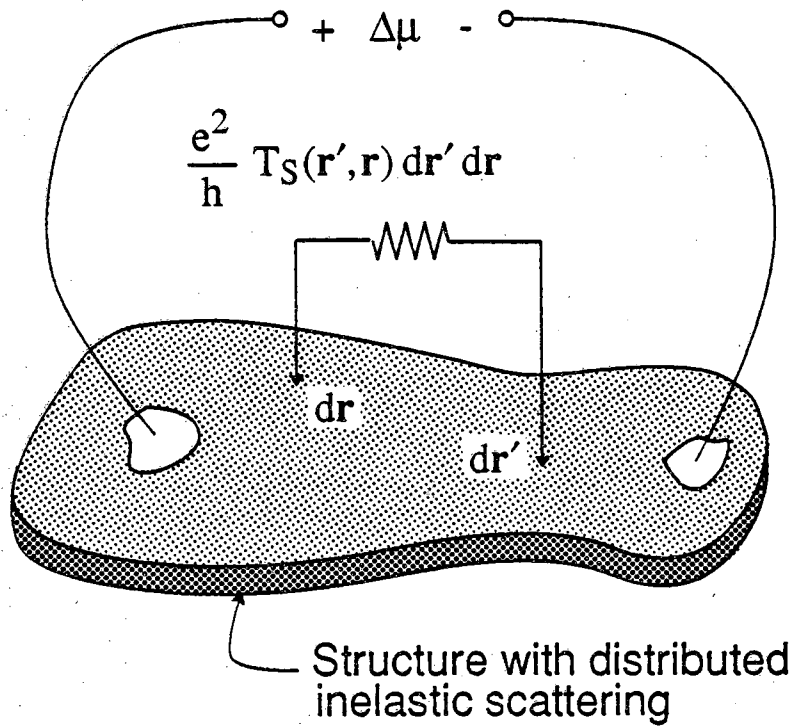


Fig. 5.1: Neglecting the circulating currents due to magnetic fields, any structure can be represented by a continuous network of conductors; any two volume elements dr' and dr are connected by a conductance equal to $(e^2/h) T_S(r', r) dr' dr$.

VI. RELATIONSHIP TO CLASSICAL BROWNIAN MOTION

The transport equation discussed in this paper (eq. (2.11)) can be viewed as describing a random diffusion process in $(\mathbf{r}; E)$, where the kernel $K(\mathbf{r}, \mathbf{r}'; E, E')$ represents the probability of “hopping” from $(\mathbf{r}'; E')$ to $(\mathbf{r}; E)$. Thus, the transport process can be viewed as classical Brownian motion; the only quantum mechanical input is in computing the kernel. In specializing to linear response (Section V), we have integrated over energy, so that we are left with a diffusion process in real space only. In this section, we will show that the linear-response transport equation (eq. (5.29)) reduces to a drift-diffusion equation, if we assume slowly varying ensemble-averaged quantities. Using this formulation, we evaluate the diffusion coefficient in a few simple cases. The purpose of these examples is not to derive any new results, but to show that our formulation reproduces well-known results. These examples involve ensemble-averaged properties of systems; this is in contrast to all previous discussion which has emphasized sample-specific solutions. The well-known expression for the semiclassical magnetoresistance is derived by determining the hopping distribution $v(\mathbf{r}, \mathbf{r}')$ from semiclassical dynamics. We then present numerical results for the ensemble-averaged diffusivity in a disordered resistor which are in agreement with the work of Thouless et. al. [18]. When the inelastic scattering time is short, the semiclassical and quantum diffusivities agree well. But as the inelastic scattering time is increased, the quantum diffusivity approaches zero due to strong localization, while the semiclassical diffusivity becomes constant.

A. Drift and Diffusion

Eq. (5.27) can be written in a slightly different form in terms of the electron density per unit energy $n(\mathbf{r}; E) = N_0(\mathbf{r}; E) f(\mathbf{r}; E)$.

$$I(\mathbf{r}; E) = e \int d\mathbf{r}' \{v(\mathbf{r}', \mathbf{r}; E) n(\mathbf{r}; E) - v(\mathbf{r}, \mathbf{r}'; E) n(\mathbf{r}'; E)\} \quad (6.1)$$

where

$$v(\mathbf{r}', \mathbf{r}; E) \equiv \frac{\tilde{T}(\mathbf{r}', \mathbf{r}; E)}{h N_0(\mathbf{r}; E)} \quad (6.2)$$

Eq. (6.1) has a simple physical interpretation. $v(\mathbf{r}', \mathbf{r}; E) d\mathbf{r}'$ tells us the fraction of electrons per unit time that "hop" from \mathbf{r} to \mathbf{r}' . The first term on the right-hand side of eq. (6.1) is the total number of electrons hopping per unit time *out* of the volume element $d\mathbf{r}$ while the second term is the number of electrons hopping per unit time *into* the volume element $d\mathbf{r}$. The net hopping frequency ν_0 is equal to the inelastic scattering rate; using eqs. (6.2) and (5.26) we have

$$\nu_0 \equiv \int d\mathbf{r}' v(\mathbf{r}', \mathbf{r}; E) = 1/\tau_i(\mathbf{r}; E) \quad (6.3)$$

Quantum transport is thus much like classical Brownian motion with a distribution of hopping lengths $v(\mathbf{r}', \mathbf{r}; E)$ that is determined quantum mechanically. In the absence of any externally injected current $I(\mathbf{r}; E)$ we can write eq. (6.1) in the following form.

$$\int d\mathbf{r}' \zeta(\mathbf{r}, \mathbf{r}'; E) n(\mathbf{r}'; E) = 0 \quad (6.4)$$

where

$$\zeta(\mathbf{r}, \mathbf{r}'; E) \equiv \frac{\delta(\mathbf{r} - \mathbf{r}')}{\tau_i(\mathbf{r}; E)} - v(\mathbf{r}, \mathbf{r}'; E) \quad (6.5)$$

The obvious question to ask is under what conditions does eq. (6.4) reduce to the drift-diffusion equation

$$-D_{ij} \nabla_i \nabla_j n + v_{dj} \nabla_j n = 0 \quad (6.6)$$

Here \mathbf{D} is the diffusion coefficient (tensor), \mathbf{v}_d is the drift velocity (vector) and summation over repeated indices is implied (x, y and z).

To get from eq. (6.4) to eq. (6.6) we first assume that we are dealing with ensemble-averaged quantities (denoted by a bar on top) so that the coefficient $\bar{\zeta}(\mathbf{r}, \mathbf{r}'; E)$ depends only on the difference coordinate.

$$\bar{\zeta}(\mathbf{r}, \mathbf{r}'; E) = \frac{1}{\tau_i} \delta(\mathbf{r} - \mathbf{r}') - \bar{v}(\mathbf{r} - \mathbf{r}'; E) \quad (6.7)$$

Next we assume that $\bar{\zeta}_n \approx \bar{\zeta} \bar{n}$ so that eq. (6.4) becomes a convolution integral.

$$\int d\mathbf{r}' \bar{\zeta}(\mathbf{r} - \mathbf{r}') \bar{n}(\mathbf{r}') = 0 \quad (6.8)$$

We have suppressed the argument E for simplicity. Fourier transforming eq. (6.8) we obtain

$$\bar{\zeta}(\mathbf{q}) \bar{n}(\mathbf{q}) = 0 \quad (6.9)$$

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

$$\bar{\zeta}(\mathbf{q}) \approx \bar{\zeta}(0) - i q_j v_{dj} - q_i q_j D_{ij} \quad (6.10)$$

The coefficients in this expansion are obtained readily from the moments of the function $\bar{\zeta}(\mathbf{r} - \mathbf{r}')$ in real space.

$$\bar{\zeta}(0) = \int d\boldsymbol{\rho} \bar{\zeta}(\boldsymbol{\rho}) \quad (6.11)$$

$$v_{dj} = \int d\boldsymbol{\rho} \rho_j \bar{v}(\boldsymbol{\rho}) \quad (6.12)$$

$$D_{ij} = \frac{1}{2} \int d\boldsymbol{\rho} \rho_i \rho_j \bar{v}(\boldsymbol{\rho}) \quad (6.13)$$

where we have written $\boldsymbol{\rho}$ for $\mathbf{r} - \mathbf{r}'$. Using eq. (6.3), (6.7) and (6.11) it is easy to show that $\bar{\zeta}(0) = 0$. Hence, inserting eq. (6.10) in eq. (6.9),

$$(i q_j v_{dj} + q_i q_j D_{ij}) \bar{n}(\mathbf{q}) = 0 \quad (6.14)$$

Fourier transforming to real space we obtain the drift-diffusion equation (eq. (6.6)).

Eqs. (6.12) and (6.13) may be used to compute the drift velocity and diffusion coefficient from the ensemble-averaged hopping function $\bar{v}(\mathbf{r} - \mathbf{r}')$. In general we also need to average over the energy E, though at low temperatures we could let E equal the Fermi energy E_F . It should be noted that a number of approximations have been made in deriving eqs. (6.12) and (6.13). We feel that in general eq. (5.29) is a better starting point for the computation of sample-specific properties that vary rapidly in space. However, for slowly varying ensemble-averaged

properties eqs. (6.12) and (6.13) are more convenient.

We will consider two simple examples where the electron density varies slowly enough that we can use these results to calculate the drift velocity and diffusion coefficient. For simplicity, the inelastic scattering time τ_i is assumed to be constant. First, we consider the semiclassical magnetoresistance of a free electron gas with isotropic scattering described by an inelastic scattering time τ_i . In this case we compute the function $v(\rho)$ directly from the classical trajectory and use it in eq. (6.12) or (6.13). The results obtained agree with the well-known semiclassical results. Next, we consider a disordered resistor with delta-function elastic scatterers distributed randomly. We compute the function $v(\rho)$ numerically, ensemble-average it and obtain the diffusion coefficient D from eq. (6.13) for different values of the inelastic scattering time τ_i (assumed constant everywhere). For small values of τ_i , we find that the semiclassical and quantum values of the diffusion coefficient D agree very well, while at large values of τ_i the two values differ significantly due to quantum localization.

B. Semiclassical Magnetoresistance

Consider an electron injected with energy E at $\mathbf{r}' = \mathbf{0}$ and following a certain classical trajectory $\mathbf{r}_0(t)$. The probability $P(\mathbf{r}, \mathbf{0}; E) d\mathbf{r}$ that it will suffer its next inelastic scattering in the volume element $d\mathbf{r}$ is given by (τ_i is the inelastic scattering time, assumed constant)

$$P(\mathbf{r}, \mathbf{0}; E) = \int_0^{\infty} \frac{dt}{\tau_i} \delta(\mathbf{r} - \mathbf{r}_0(t)) e^{-t/\tau_i} \quad (6.15)$$

This simply states that as an electron follows the classical trajectory, it decays from the coherent state with a lifetime of τ_i . The factor $1/\tau_i$ is included so that the function is properly normalized. We note from eqs. (5.26) and (6.2) that

$$\int d\mathbf{r} v(\mathbf{r}, \mathbf{0}; E) = 1/\tau_i \quad (6.16)$$

Since $v(\mathbf{r}, \mathbf{0}; E)$ is proportional to $P(\mathbf{r}, \mathbf{0}; E)$, and the latter is normalized to one, we must have

$$v(\mathbf{r}, \mathbf{0}; E) = \int_0^{\infty} \frac{dt}{\tau_i^2} \delta(\mathbf{r} - \mathbf{r}_0(t)) e^{-t/\tau_i} \quad (6.17)$$

Using eqs. (6.12) and (6.13) we obtain

$$v_{dx} = \int_0^{\infty} \frac{dt}{\tau_i^2} e^{-t/\tau_i} x_0(t) \quad (6.18)$$

$$D_{xx} = \frac{1}{2} \int_0^{\infty} \frac{dt}{\tau_i^2} e^{-t/\tau_i} x_0^2(t) \quad (6.19)$$

where $x_0(t)$ is the x-component of the trajectory $\mathbf{r}_0(t)$. The other components may be evaluated similarly.

Now we need the classical trajectory $x_0(t)$. To start with, we consider a classical electron moving without any influence from electric and magnetic fields. Assuming the particle has an initial velocity v_x in the x-direction, the x-component of the trajectory is $x_0(t) = v_x t$. Because we are interested in the collective behavior for an ensemble of electrons, we must average over all possible initial states. We assume that the initial velocity of an electron is uniformly distributed over all directions in a sample, due to the action of scattering processes. With these assumptions, we evaluate eqs. (6.18) and (6.19):

$$\langle v_{dx} \rangle = \left\langle \int_0^{\infty} \frac{dt}{\tau_i^2} v_x t e^{-t/\tau_i} \right\rangle = \langle v_x \rangle = 0 \quad (6.20)$$

$$\langle D_{xx} \rangle = \left\langle \int_0^{\infty} \frac{dt}{\tau_i^2} v_x^2 t^2 e^{-t/\tau_i} \right\rangle = \langle v_x^2 \tau_i \rangle \neq 0 \quad (6.21)$$

where we have used the angle brackets $\langle \dots \rangle$ to denote ensemble averaging. Without the influence of fields, the drift velocity of an ensemble of electrons is zero; the diffusion coefficient is not.

As a second example, we consider the effect of an electric field in the x-direction, causing an electron to accelerate: $x_0(t) = v_x t + a_x t^2 / 2$, where $a_x = e\mathcal{E} / m$ is the acceleration due to the field. We evaluate the drift velocity and obtain,

$$\langle v_{dx} \rangle = \left\langle \int_0^{\infty} \frac{dt}{\tau_i^2} \left(v_x t + \frac{a_x t^2}{2} \right) e^{-t/\tau_i} \right\rangle = \langle v_x \rangle + \langle a_x \tau_i \rangle \quad (6.22)$$

After averaging over all initial velocities, we again find that $\langle v_x \rangle = 0$. Because of the acceleration, however, the drift velocity is not zero,

$$\langle v_{dx} \rangle = \frac{e \tau_i}{m} \mathcal{E}_x \quad (6.23)$$

Next, we consider the more complicated problem of semiclassical magnetoresistance. We assume a magnetic field along the z-axis, and an electric field in the x-y plane. It can be shown [57] that the x-component of the classical trajectory is:

$$x_0(t) = \left[\frac{a_x}{\omega_c^2} - \frac{v_y}{\omega_c} \right] (1 - \cos \omega_c t) + \left[\frac{a_y}{\omega_c^2} + \frac{v_x}{\omega_c} \right] \sin \omega_c t - \frac{a_y}{\omega_c} t \quad (6.24)$$

where we have introduced the cyclotron frequency for an electron $\omega_c = |e|B/m$. Substituting eq. (6.24) into eq. (6.18) and performing the necessary integrals, we obtain the drift velocity,

$$v_{dx} = \left[\frac{a_x}{\omega_c} - v_y \right] \frac{\omega_c \tau_i}{1 + \omega_c^2 \tau_i^2} + \left[\frac{a_y}{\omega_c} + v_x \right] \frac{1}{1 + \omega_c^2 \tau_i^2} - \frac{a_y}{\omega_c} \quad (6.25)$$

If we average over all initial velocities, $\langle v_x \rangle$ and $\langle v_y \rangle$ vanish, leaving only the terms involving acceleration. By substituting in the acceleration due to the electric field,

$$\langle v_{dx} \rangle = \frac{e \tau_i}{m} \left[\frac{\mathcal{E}_x}{1 + \omega_c^2 \tau_i^2} - \frac{\mathcal{E}_y \omega_c \tau_i}{1 + \omega_c^2 \tau_i^2} \right] \quad (6.26)$$

This velocity defines the x-component of the drift current, which we can use to determine conductivity:

$$\sigma_{xx} = \left. \frac{e n v_{dx}}{\mathcal{E}_x} \right|_{\mathcal{E}_y=0} = \frac{\sigma_0}{1 + \omega_c^2 \tau_i^2} \quad (6.27a)$$

$$\sigma_{xy} = \left. \frac{e n v_{dx}}{\mathcal{E}_y} \right|_{\mathcal{E}_x=0} = -\sigma_0 \frac{\omega_c \tau_i}{1 + \omega_c^2 \tau_i^2} \quad (6.27b)$$

Following a similar derivation for the y-component of the drift velocity, we can define σ_{yx} and

σ_{yy} , and obtain the usual magnetoconductivity tensor [58],

$$\sigma = \frac{\sigma_0}{1 + \omega_c^2 \tau_i^2} \begin{bmatrix} 1 & -\omega_c \tau_i \\ \omega_c \tau_i & 1 \end{bmatrix} \quad (6.28)$$

We have shown that some familiar results can be obtained by assuming a classical motion of electrons. We now proceed to demonstrate quantum mechanical effects in a numerical example.

C. Numerical Example of Localization

In recent years, considerable attention has been given to the effects of disorder on electron transport. In particular, Anderson has shown that for a sufficiently high degree of disorder, and in the absence of inelastic scattering, conductance decreases exponentially with length [59]. Electron wavefunctions become spatially localized, having envelope functions that decay exponentially with distance. As the overlap between localized states decreases, the conductance vanishes. In the presence of inelastic scattering, however, electrons can “hop” between localized states so that inelastic scattering actually *improves* the conductance.

An illustration of this effect is well suited to our model. In principle, we can calculate the diffusion coefficient D for any chain of randomly spaced impurities. We consider the average diffusion coefficient of many such chains, as a function of the inelastic scattering time τ_i . We will show that as τ_i increases, D rapidly approaches zero. Furthermore, if we treat electrons semiclassically (i.e., work with probabilities rather than probability *amplitudes*), localization behavior is destroyed, and D is limited by impurity scattering for large τ_i . Our numerical solution has been described in detail elsewhere [37,57,60]. In the following discussion, we focus more on the physical assumptions in our model, rather than on the details of computing a numerical solution.

To this point we have worked in the position representation, using the basis $|r\rangle$. A change of basis is convenient for modeling narrow wires, in which a confining potential in the transverse direction gives rise to a set of sub-bands or modes. From this standpoint, transport is

analogous to electromagnetic waves traveling in a waveguide, and is conveniently described using the basis $|x, k_{y,m}\rangle$, where m enumerates modes in the transverse (y) direction. Using this basis, the hopping distribution $v(\mathbf{r}, \mathbf{r}'; E)$ becomes

$$v(\mathbf{r}, \mathbf{r}'; E) \rightarrow v_{mn}(x, x'; E)$$

and is interpreted as the fraction of electrons per unit time that “hop” from position x' and mode n to position x and mode m . Strictly speaking, such a change of basis is not straightforward. The transport equation takes on a simple form in the position representation because each inelastic scattering event in our model measures the position of the electron. In principle, one could conceive of an inelastic scattering potential (possibly non-local) that measures the “coordinate” in some other basis. The transport equation would then take on a simple form in that basis. Although this necessitates a change in our assumptions regarding the inelastic scatterers, we believe that the essential physics of dissipative transport is still described. In the following example, τ_i should be viewed more as a phenomenological parameter than as a well-defined microscopic quantity.

We can evaluate the ensemble-averaged diffusion coefficient by determining the second moment of the distribution $\bar{v}(\rho)$

$$D_{xx,n} = \frac{1}{2} \sum_m \left[\int d\rho_x \rho_x^2 v_{mn}(\rho_x) \right] \quad (6.29)$$

where $D_{xx,n}$ represents diffusion due to electrons injected into mode n . We average the contributions of all possible injected modes to obtain

$$D_{xx} = \frac{1}{2M} \int d\rho_x \rho_x^2 \left[\sum_{m,n} v_{mn}(\rho_x) \right] \quad (6.30)$$

where M is the total number of propagating modes. In general, the function $v_{mn}(\rho_x)$ falls off exponentially away from $\rho_x = 0$, due to the imaginary potential $i\hbar/2\tau_i(\mathbf{r}; E)$ in the Schrödinger equation (eq. (4.6)). For each configuration of impurities, however, $v_{mn}(\rho_x)$ will have a characteristic “noise” superimposed on the exponential decay. In an ensemble-averaged sense, the

“noise” components average to zero, and the remaining exponential decay can be characterized by a decay length L_D ,

$$\langle \sum_{m,n} v_{mn}(\rho_x) \rangle \equiv v_0 e^{-|\rho_x|/L_D} \quad (6.31)$$

The constant v_0 is determined so that the function is properly normalized:

$$\sum_m \int d\rho_x v_{mn}(\rho_x) = \frac{1}{\tau_{i,n}} \quad (6.32)$$

where $\tau_{i,n}$ is the inelastic scattering time for mode n . We assume for simplicity that the inelastic scattering time is a constant, independent of both position and mode number. In this case, the normalization condition for v_0 becomes

$$\int d\rho_x \langle \sum_{m,n} v_{mn}(\rho_x) \rangle = \frac{M}{\tau_i} \quad (6.33)$$

After determining v_0 , we evaluate eq. (6.30) with the functional form stated in eq. (6.31).

$$D_{xx} = \frac{1}{4\tau_i L_D} \int_{-\infty}^{+\infty} d\rho_x \rho_x^2 e^{-|\rho_x|/L_D} = \frac{L_D^2}{\tau_i} \quad (6.34)$$

Our solution hinges upon determining the ensemble-averaged decay length L_D for the hopping distribution within a long wire. We expect that, for small τ_i , the decay length should increase as $L_D \approx v_F \tau_i$ for both semiclassical and quantum mechanical analyses. This is because in this limit, inelastic scattering events are so frequent that transport between successive events is essentially ballistic. On the other hand, for long τ_i , the electron will elastically scatter many times between two inelastic scattering events. Consequently, the semiclassical $L_D = \sqrt{D_{el} \tau_i}$, where D_{el} is the diffusivity due to the elastic scatterers. The quantum mechanical L_D , however, tends to a constant equal to the localization length L_c . It is apparent from eq. (6.34), therefore, that D_{xx} will initially increase with τ_i . The semiclassical result will then level off to D_{el} , while the quantum mechanical result will decrease as L_c^2/τ_i , due to localization. This is precisely what we obtain from our numerical solution (Fig. 6.3), which is described below.

For each random configuration of impurities, we must determine the Green function of the Schrödinger equation, as shown schematically in Fig. 6.1. $G_{mn}(\rho_x)$ represents the amplitude in mode m at position ρ_x for an electron injected in mode n at position $\rho_x = 0$. Solutions for the wavefunction on either side of $\rho_x = 0$ can be determined by ordinary means--for example, with the use of scattering matrices, as described in Ref. [37]. Each impurity is represented by a scattering matrix, which specifies the coupling between various modes introduced by a particular scattering potential. Regions between scatterers are represented by diagonal matrices, which account for the phase shift (and attenuation) acquired by each mode while propagating through a given region. These individual scattering matrices can be combined to determine an overall scattering matrix, representing transmission through a given region. To connect the two solutions on either side of $\rho_x = 0$, we introduce the following boundary conditions:

$$G_{mn}(\rho_x = 0^+) = G_{mn}(\rho_x = 0^-) \quad (6.35a)$$

$$\left. \frac{dG_{mn}}{d\rho_x} \right|_{\rho_x=0^+} - \left. \frac{dG_{mn}}{d\rho_x} \right|_{\rho_x=0^-} = \frac{2m}{\hbar^2} \delta_{mn} \quad (6.35b)$$

A semiclassical result can also be obtained using this method, if the elements of all scattering matrices are replaced with their squared magnitudes. In this case, the solution vector $G_{mn}(\rho_x)$ is comprised of (real) probabilities rather than (complex) probability amplitudes. In any event, the solution of $G_{mn}(\rho_x)$ for a particular impurity configuration determines the hopping distribution, which is fit to a decaying exponential (eq. (6.31)) to determine the decay length L_D . Decay lengths for a large number of random samples are then averaged, to determine the ensemble-averaged diffusion coefficient $D \equiv L_D^2 / \tau_i$. A final concern is the averaging process used to determine L_D . In the localized regime, fluctuations in L_D from sample to sample can be quite large; however, Anderson et. al. [61] have shown that the inverse localization length L_D^{-1} has a well behaved distribution. For this reason, we determine the average of L_D^{-1} and invert it, to determine the ensemble-averaged L_D .

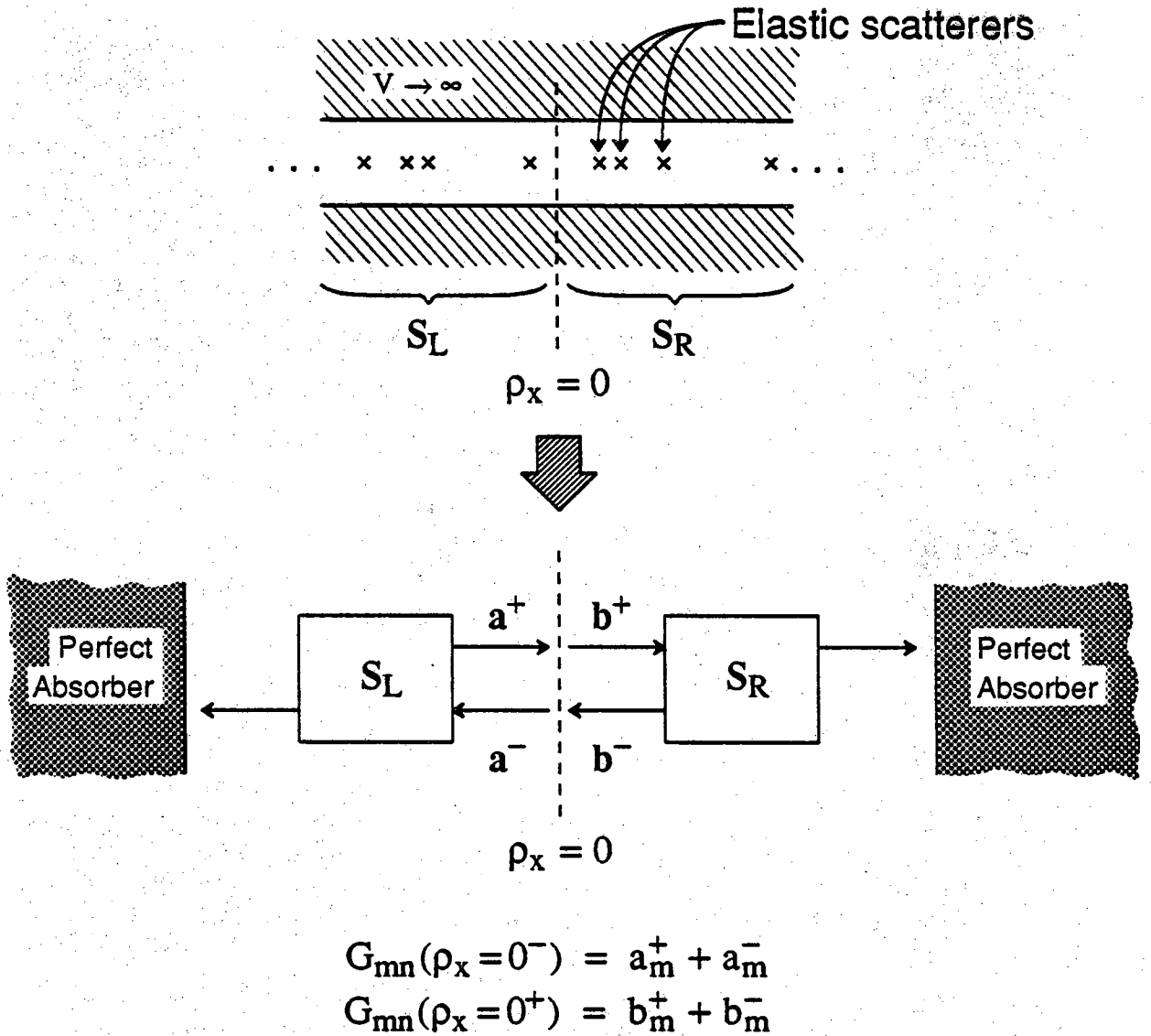


Fig. 6.1: A narrow wire with randomly spaced impurities is represented by two scattering matrices, one on either side of the injection point ($\rho_x = 0$).

We have applied this model to samples with five propagating modes and 400 impurities with an average spacing of $1.5 \mu\text{m}$; the injection point ($\rho_x = 0$) was immediately left of the 200th impurity. All impurities were characterized by the same scattering matrix, and the impurity strength was chosen so that the elastic scattering length Λ_{el} was 4 impurities, corresponding to an elastic scattering time of $\tau_0 = 2.87 \times 10^{-11}$ s [37]. An estimate of the localization length is $\Lambda_{loc} \approx M\Lambda_{el}$ [62], where M is the number of propagating modes. For the present example, samples should exhibit localization when the inelastic scattering length Λ_i exceeds 20 impurities. Inelastic scattering times were chosen between 10^{-12} s and 10^{-8} s, corresponding to Λ_i between 0.2 and 95 impurities. All results were verified against longer chains, to ensure that edge effects due to the finite length of the chain were negligible.

To provide some insight into the arguments concerning the decay length L_D , we have plotted the hopping distribution for two arbitrary samples with different scattering times τ_i . These results are presented in Fig. 6.2 on identical logarithmic scales. For $\tau_i = 10^{-10}$ s ($\Lambda_i = 9$ impurities), the sample is in the so-called weak localization regime. The distribution is predominantly characterized by its exponential decay, although small fluctuations are clearly visible. As the inelastic scattering time is increased, the fluctuations become larger. For $\tau_i = 10^{-8}$ s ($\Lambda_i = 95$ impurities), the general character of exponential decay remains, but the fluctuations have added considerable scatter to the decay length L_D .

In Fig. 6.3 we present the ensemble-averaged diffusion coefficient D for both semiclassical and quantum analyses. For small τ_i , inelastic scattering dominates, and both solutions are in close agreement. As τ_i increases, however, the quantum mechanical solution rapidly approaches zero, while the semiclassical result levels off to the value dictated by impurity scatterers. This clearly demonstrates that localization must be understood in the context of quantum mechanics. Both semiclassical and quantum solution methods are identical, except that elements of the semiclassical scattering matrices are replaced by their squared magnitudes. By neglecting interference of the electronic wavefunction between successive scatterers, the semiclassical analysis cannot account for localization.

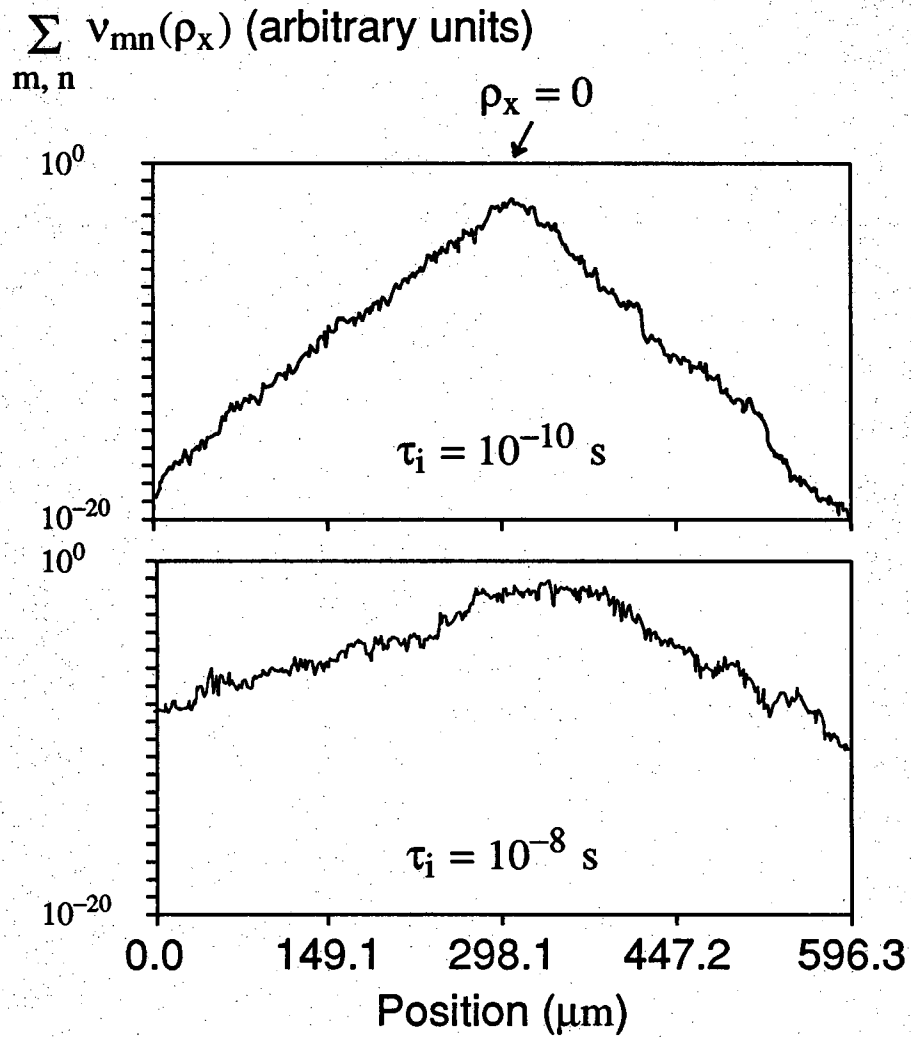


Fig. 6.2: The hopping distribution $\sum_{m,n} v_{mn}(\rho_x)$ for two arbitrary samples with different inelastic scattering times τ_i . Both functions exhibit the general character of exponential decay.

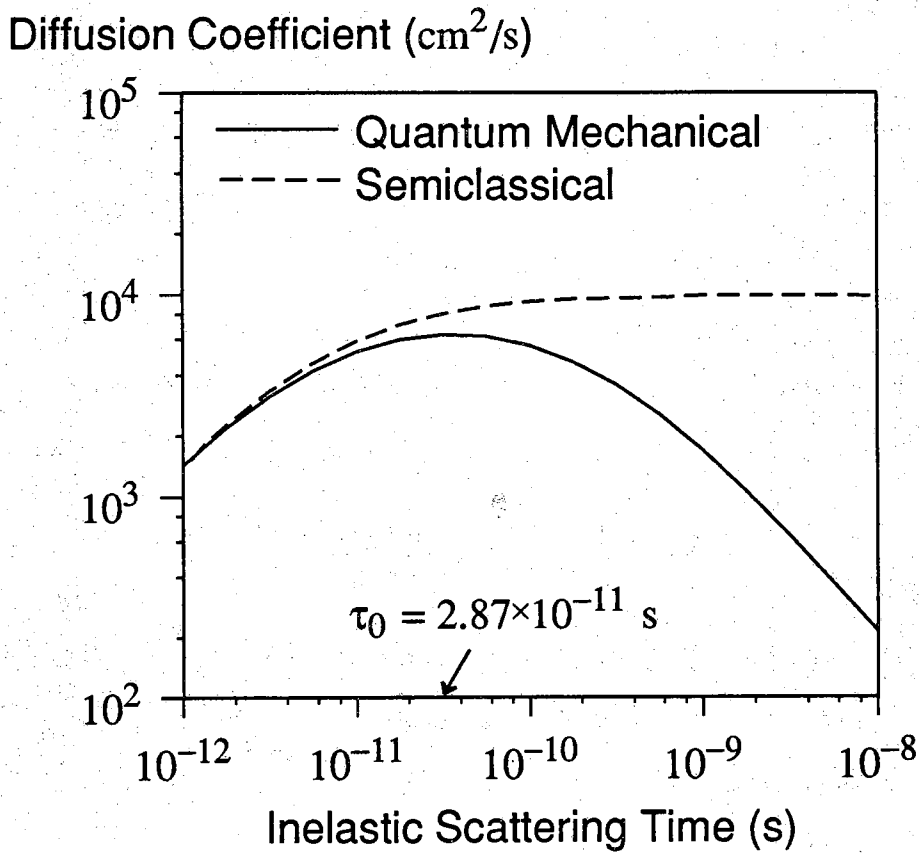


Fig. 6.3: The ensemble-averaged diffusion coefficient as a function of τ_i for both semiclassical and quantum analyses. The quantum result decreases rapidly for large τ_i , a demonstration of strong localization.

VII. SUMMARY

In the preceding sections we have developed an integral transport equation which incorporates dissipation into quantum transport theory:

$$i_S(\mathbf{r}; E) = I(\mathbf{r}; E) + \int d\mathbf{r}' \int dE' K(\mathbf{r}, \mathbf{r}'; E, E') i_S(\mathbf{r}'; E') \quad (7.1)$$

where $i_S(\mathbf{r}; E)$ is the current per unit volume of electrons inelastically scattered at position \mathbf{r} from an energy E to all other energies. In deriving this equation we have assumed that inelastic scattering processes can be modeled by a continuous distribution of independent point-size oscillators. This assumption allowed us to simplify the one-electron self-energy to a point function. From this we showed that the inelastic scattering current could be expressed in terms of local properties at \mathbf{r} .

$$i_S(\mathbf{r}; E) = \frac{e n(\mathbf{r}; E)}{\tau_i(\mathbf{r}; E)} = \frac{e N_0(\mathbf{r}; E) f(\mathbf{r}; E)}{\tau_i(\mathbf{r}; E)} \quad (7.2)$$

where $n(\mathbf{r}; E)$ is the electron density per unit volume per unit energy, $N_0(\mathbf{r}; E)$ is the electronic density of states, and $f(\mathbf{r}; E)$ is the probability of occupation for the coordinate $(\mathbf{r}; E)$. The inelastic scattering time $\tau_i(\mathbf{r}; E)$ is defined by

$$\frac{1}{\tau_i(\mathbf{r}; E)} \equiv \frac{2\pi}{\hbar} \int dE' F(\mathbf{r}; E' - E) N_0(\mathbf{r}; E') [1 - f(\mathbf{r}; E')] \quad (7.3)$$

where $F(\mathbf{r}; E' - E)$ is a property of the inelastic scatterers, defined by eq. (3.24). It is apparent from eq. (7.2) that three solution variables (i_S , n and f) can be used interchangeably in the solution of eq. (7.1).

The kernel of the integral equation was shown to be a product of two independent probabilities:

$$K(\mathbf{r}, \mathbf{r}'; E, E') = P_S(\mathbf{r}'; E, E') P(\mathbf{r}, \mathbf{r}'; E) \quad (7.4)$$

where $P_S(\mathbf{r}'; E, E')$ is the probability that an electron at position \mathbf{r}' having an energy E' will be inelastically scattered to an energy E ,

$$P_S(\mathbf{r}'; E, E') \equiv \frac{2\pi}{\hbar} F(\mathbf{r}'; E - E') N_0(\mathbf{r}'; E) [1 - f(\mathbf{r}'; E)] \tau_i(\mathbf{r}'; E') \quad (7.5)$$

and $P(\mathbf{r}, \mathbf{r}'; E)$ is the probability that an electron "injected" at a position \mathbf{r}' with an energy E (by inelastically scattering from some other energy) will suffer its next inelastic scattering event at \mathbf{r} .

$$P(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar}{2\pi} \frac{|G(\mathbf{r}, \mathbf{r}'; E)|^2}{N_0(\mathbf{r}'; E) \tau_i(\mathbf{r}; E)} \quad (7.6)$$

$G(\mathbf{r}, \mathbf{r}'; E)$ is the Green function of the Schrödinger equation modified to include the optical potential

$$\left[E - H_0 + \frac{i\hbar}{2\tau_i(\mathbf{r}; E)} \right] G(\mathbf{r}, \mathbf{r}'; E) = \delta(\mathbf{r} - \mathbf{r}') \quad (7.7)$$

where H_0 is the exact elastic Hamiltonian (eq. (2.1)).

For any arbitrary structure, a solution of eq. (7.1) can be obtained as follows. Some initial guess is used to establish the distribution function $f(\mathbf{r}; E)$ everywhere within the structure. An example of this is to assume that each point is in local equilibrium, so that $f(\mathbf{r}; E)$ is characterized by a local chemical potential, as shown in eq. (5.21). One then assumes some distribution of the chemical potential, thereby establishing $f(\mathbf{r}; E)$. The inelastic scattering time τ_i is then calculated using eq. (7.3). The kernel $K(\mathbf{r}, \mathbf{r}'; E, E')$ is calculated from eqs. (7.4), (7.5) and (7.6) once the Green function $G(\mathbf{r}, \mathbf{r}'; E)$ has been determined from eq. (7.7). Given the kernel, eq. (7.1) can be solved to determine a new guess for $i_S(\mathbf{r}; E)$ (or equivalently, $f(\mathbf{r}; E)$). Because τ_i is dependent on $f(\mathbf{r}; E)$, this solution process must be repeated until the solution for $f(\mathbf{r}; E)$ has converged.

In this work, we have restricted ourselves to steady-state transport and neglected many-body effects beyond the Hartree term. We believe that it should be possible in the future to extend the work, to remove these restrictions. However, our assumption of delta interaction potentials is essential in obtaining a simple transport equation in the position representation that involves only the electron density, and not the spatial correlations of the wavefunction. For a

different type of inelastic scattering potential it may be possible to conceive of another representation which would again simplify the transport equation, though it is not obvious how such a representation would be determined. We believe that the simplicity of this transport equation will make it feasible to obtain numerical solutions for specific mesostructures, and thereby quantitatively answer some of the fundamental questions of quantum transport [44]. Also, by comparing the predictions of our model with experiment, it should be possible to identify new phenomena arising from correlations between inelastic scatterers, and to shed light on the microscopic origin of irreversibility.

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Appendix: Derivation of the Kernel from the Kubo Conductivity

In Section V we assumed that, for small perturbations from equilibrium, inelastic scattering was strong enough to maintain local equilibrium everywhere in a sample. In this linear response regime, the transport equation was reduced to a simple form (eq. (5.29)) which resembles the Landauer-Büttiker formula (eq. (5.32)) generalized to include a continuous distribution of reservoirs. The purpose of this appendix is to reproduce our expression for the kernel $\tilde{T}(\mathbf{r}, \mathbf{r}'; E)$ of this integral equation. We start from the Kubo formula for the conductivity (eq. (1.3)), and apply the Lee-Fisher formula (eq. (1.7)) to determine the “transmission” between reservoirs at \mathbf{r} and \mathbf{r}' .

In the Kubo formalism, the conductivity tensor σ at a frequency ω is related to the current-current correlation function [13,14],

$$i\omega[\sigma_0(\mathbf{r}, \mathbf{r}'; \omega)]_{\alpha\beta} = [C_{JJ}(\mathbf{r}, \mathbf{r}'; \omega)]_{\alpha\beta} - \frac{ne^2}{m} \delta(\mathbf{r} - \mathbf{r}') \delta_{\alpha\beta} \quad (\text{A.1})$$

where n is the electron density, m is the effective mass, $\delta_{\alpha\beta}$ is the Kronecker delta and the subscripts α, β run over x, y and z . The current-current correlation function C_{JJ} is defined as

$$C_{JJ}(\mathbf{r}, \mathbf{r}'; \omega) = \frac{i}{\hbar} \int_0^{\infty} dt e^{i\omega t} \langle \mathbf{J}(\mathbf{r}, t) \mathbf{J}(\mathbf{r}', 0) - \mathbf{J}(\mathbf{r}', 0) \mathbf{J}(\mathbf{r}, t) \rangle \quad (\text{A.2})$$

where $\mathbf{J}(\mathbf{r}, t)$ is the current density operator in the Heisenberg picture, and $\langle \dots \rangle$ denotes the ensemble-averaged expectation value. For convenience, we define each of the terms composing

C_{JJ} :

$$C_1(\mathbf{r}, \mathbf{r}'; \omega) = \frac{i}{\hbar} \int_0^{\infty} dt e^{i\omega t} \langle \mathbf{J}(\mathbf{r}, t) \mathbf{J}(\mathbf{r}', 0) \rangle \quad (\text{A.3a})$$

$$C_2(\mathbf{r}, \mathbf{r}'; \omega) = \frac{i}{\hbar} \int_0^{\infty} dt e^{i\omega t} \langle \mathbf{J}(\mathbf{r}', 0) \mathbf{J}(\mathbf{r}, t) \rangle \quad (\text{A.3b})$$

The current density operator can be written as

$$\mathbf{J}(\mathbf{r}, t) = \sum_{N, M} \mathbf{J}_{NM}(\mathbf{r}) a_N^\dagger(t) a_M(t) \quad (\text{A.4})$$

where $\mathbf{J}_{NM}(\mathbf{r})$ is defined in terms of the eigenfunctions $\phi_N(\mathbf{r})$ of H_0 (eq. (2.1)),

$$\mathbf{J}_{NM}(\mathbf{r}) \equiv \frac{i e \hbar}{2m} [(\nabla \phi_N)^* \phi_M - \phi_N^* (\nabla \phi_M)] \quad (\text{A.5})$$

and a_N^\dagger, a_N are the creation and annihilation operators for the eigenstate N . Substituting eq. (A.4) into eq. (A.3a),

$$\begin{aligned} C_1(\mathbf{r}, \mathbf{r}'; \omega) &= \sum_{N, M} \sum_{N', M'} \mathbf{J}_{NM}(\mathbf{r}) \mathbf{J}_{N'M'}(\mathbf{r}') \\ &\quad \frac{i}{\hbar} \int_0^\infty dt e^{i\omega t} \langle a_N^\dagger(t) a_M(t) a_{N'}^\dagger(0) a_{M'}(0) \rangle \end{aligned} \quad (\text{A.6})$$

Since N, M, N', M' are eigenstates, the expectation value on the right hand side is zero unless $N' = M$ and $M' = N$. Hence

$$C_1(\mathbf{r}, \mathbf{r}'; \omega) = \sum_{N, M} \mathbf{J}_{NM}(\mathbf{r}) \mathbf{J}_{MN}(\mathbf{r}') F_1(\omega) \quad (\text{A.7a})$$

where

$$\begin{aligned} F_1(\omega) &= \frac{i}{\hbar} \int_0^\infty dt e^{i\omega t} \langle a_N^\dagger(t) a_N(0) \rangle \langle a_M(t) a_M^\dagger(0) \rangle \\ &= - \frac{f_0(\epsilon_N) [1 - f_0(\epsilon_M)]}{\hbar\omega + \epsilon_N - \epsilon_M + i\eta} \end{aligned} \quad (\text{A.7b})$$

η is an infinitesimal positive quantity ($\eta = 0^+$). Similarly it can be shown that

$$C_2(\mathbf{r}, \mathbf{r}'; \omega) = \sum_{N, M} \mathbf{J}_{NM}(\mathbf{r}) \mathbf{J}_{MN}(\mathbf{r}') F_2(\omega) \quad (\text{A.8a})$$

$$\text{where } F_2(\omega) = - \frac{f_0(\epsilon_M) [1 - f_0(\epsilon_N)]}{\hbar\omega + \epsilon_N - \epsilon_M + i\eta} \quad (\text{A.8b})$$

Substituting eqs. (A.7a,b) and (A.8a,b) into eq. (A.2) we have

$$C_{JJ}(\mathbf{r}, \mathbf{r}'; \omega) = \sum_{N, M} J_{NM}(\mathbf{r}) J_{MN}(\mathbf{r}') F_{NM}(\omega) \quad (\text{A.9a})$$

$$\text{where } F_{NM}(\omega) = F_1 - F_2 = \frac{f_o(\epsilon_M) - f_o(\epsilon_N)}{\hbar\omega + \epsilon_N - \epsilon_M + i\eta} \quad (\text{A.9b})$$

We will now rewrite $F_{NM}(\omega)$ in a somewhat different form by proceeding as follows.

$$F_{NM}(\omega) = \int d\epsilon \left[-\frac{f_o(\epsilon + \hbar\omega) \delta(\epsilon - \epsilon_M + \hbar\omega)}{\epsilon - \epsilon_N - i\eta} - \frac{f_o(\epsilon) \delta(\epsilon - \epsilon_N)}{\epsilon - \epsilon_M + \hbar\omega + i\eta} \right] \quad (\text{A.10})$$

Using the relation

$$\delta(x) = \frac{1}{2\pi i} \left[\frac{1}{x - i\eta} - \frac{1}{x + i\eta} \right]$$

we obtain from eq. (A.10),

$$F_{NM}(\omega) = \int \frac{d\epsilon}{2\pi i} \left[-f_o(\epsilon + \hbar\omega) G_N^A(\epsilon) [G_M^A(\epsilon + \hbar\omega) - G_M^R(\epsilon + \hbar\omega)] \right. \\ \left. - f_o(\epsilon) G_M^R(\epsilon + \hbar\omega) [G_N^A(\epsilon) - G_N^R(\epsilon)] \right] \quad (\text{A.11})$$

where

$$G_M^R(\epsilon) \equiv \frac{1}{\epsilon - \epsilon_M + i\eta} \quad (\text{A.12a})$$

$$G_M^A(\epsilon) \equiv \frac{1}{\epsilon - \epsilon_M - i\eta} \quad (\text{A.12b})$$

For small ω , we can write eq. (A.11) as

$$F_{NM}(\omega) \approx i\omega a_{NM} + b_{NM} \quad (\text{A.13a})$$

where

$$a_{NM} = \frac{\hbar}{2\pi} \int d\epsilon \left[-\frac{\partial f_0}{\partial \epsilon} \right] G_M^R(\epsilon) G_N^A(\epsilon) \quad (\text{A.13b})$$

$$b_{NM} = \frac{1}{2\pi i} \int d\epsilon f_0(\epsilon) [G_N^R(\epsilon) G_M^R(\epsilon) - G_N^A(\epsilon) G_M^A(\epsilon)] \quad (\text{A.13c})$$

Using eqs. (A.9a) and (A.13a), we obtain from eq. (A.1)

$$[\sigma_0(\mathbf{r}, \mathbf{r}')]_{\alpha\beta} = A + \frac{1}{i\omega} \left(B - \frac{ne^2}{m} \delta(\mathbf{r}-\mathbf{r}') \delta_{\alpha\beta} \right) \quad (\text{A.14a})$$

$$\text{where} \quad A = \sum_{N,M} [J_{NM}(\mathbf{r}) \otimes J_{MN}(\mathbf{r}')]_{\alpha\beta} a_{NM} \quad (\text{A.14b})$$

$$B = \sum_{N,M} [J_{NM}(\mathbf{r}) \otimes J_{MN}(\mathbf{r}')]_{\alpha\beta} b_{NM} \quad (\text{A.14c})$$

It can be shown that A and B are both real quantities so that the real part of the conductivity is simply equal to A. From eqs. (A.13b) and (A.14b) we obtain a familiar expression for the Kubo conductivity [32],

$$\sigma_0(\mathbf{r}, \mathbf{r}') = \int dE \left[-\frac{\partial f_0}{\partial E} \right] \sigma(\mathbf{r}, \mathbf{r}'; E) \quad (\text{A.15a})$$

$$\sigma(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar}{2\pi} \sum_{N,M} [J_{NM}(\mathbf{r}) \otimes J_{MN}(\mathbf{r}')] G_M^R(E) G_N^A(E) \quad (\text{A.15b})$$

So far in this appendix, we have neglected inelastic scattering; the energy η in eqs. (A.12) is then a true infinitesimal. As we have seen in Section III, inelastic scattering causes damping of the quasi particle propagator, which is described by including the optical potential $i\hbar/2\tau_i(\mathbf{r}; E)$ in the defining equation for the Green function (eq. (4.7)); consequently, we modify eqs. (A.12) to

$$G_M^R(\epsilon) \equiv \frac{1}{\epsilon - \epsilon_M + i\hbar/2\tau_M} \quad (\text{A.16a})$$

$$G_M^A(\epsilon) \equiv \frac{1}{\epsilon - \epsilon_M - i\hbar/2\tau_M} \quad (\text{A.16b})$$

Since the inelastic scattering time $\tau_i(\mathbf{r}; E)$ is not a constant but can vary spatially, we have used different lifetimes τ_M for the different eigenstates; in principle, these may be obtained from the imaginary parts of the eigenenergies ϵ_M calculated using the Hamiltonian $(H_0 - i\hbar/2\tau_i(\mathbf{r}; E))$. However, we assume that the imaginary potential is small enough that we can neglect any complication due to the non-orthogonality of the corresponding eigenfunctions $\phi_M(\mathbf{r})$.

We obtain the conductivity which accounts for inelastic scattering by inserting eqs. (A.16a,b) into eq. (A.15b),

$$\sigma_{\alpha\beta}(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar}{2\pi} \sum_{N,M} \frac{[\mathbf{J}_{NM}(\mathbf{r}) \otimes \mathbf{J}_{MN}(\mathbf{r}')]_{\alpha\beta}}{(E - \epsilon_M + i\hbar/2\tau_M)(E - \epsilon_N - i\hbar/2\tau_N)} \quad (\text{A.17})$$

We can relate this expression to the kernel $\tilde{T}(\mathbf{r}, \mathbf{r}'; E)$ by recalling the Landauer interpretation of the linear-response transport equation: The kernel $\tilde{T}(\mathbf{r}, \mathbf{r}'; E)$ corresponds to the transmission coefficient between reservoirs connected to the infinitesimal volume elements at \mathbf{r} and \mathbf{r}' . With this physical picture, we invoke the Lee-Fisher formula (eq. (1.7)) which links transmission to conductivity. In the limit of a continuous distribution of probes, each probe has an infinitesimal cross-section, so that eq. (1.7) is extended to

$$\frac{e^2}{h} \tilde{T}(\mathbf{r}, \mathbf{r}'; E) d\mathbf{r} d\mathbf{r}' = \frac{\hbar}{2\pi} \sum_{N,M} \frac{(\mathbf{J}_{NM}(\mathbf{r}) \cdot \hat{\mathbf{n}}(\mathbf{r}) d\mathbf{r})(\mathbf{J}_{MN}(\mathbf{r}') \cdot \hat{\mathbf{n}}(\mathbf{r}') d\mathbf{r}')}{(E - \epsilon_M + i\hbar/2\tau_M)(E - \epsilon_N - i\hbar/2\tau_N)} \quad (\text{A.18})$$

where $\hat{\mathbf{n}}(\mathbf{r})$ is the unit vector normal to the probe at \mathbf{r} . But $\mathbf{J} \cdot \hat{\mathbf{n}}$ is the current entering the probe at \mathbf{r} due to inelastic scattering; as shown in Section III, this current is $i_s = e n / \tau_i$.

$$\tilde{T}(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar^2}{e^2} \sum_{N,M} \frac{\rho_{NM}(\mathbf{r}) \rho_{MN}(\mathbf{r}') / \tau_i(\mathbf{r}; E) \tau_i(\mathbf{r}'; E)}{(E - \epsilon_M + i\hbar/2\tau_M)(E - \epsilon_N - i\hbar/2\tau_N)} \quad (\text{A.19})$$

where $\rho_{NM}(\mathbf{r}) \equiv e \phi_N^*(\mathbf{r}) \phi_M(\mathbf{r})$, so that

$$\tilde{T}(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar^2}{\tau_i(\mathbf{r}; E) \tau_i(\mathbf{r}'; E)} \sum_N \frac{\phi_N^*(\mathbf{r}) \phi_N(\mathbf{r}')}{(E - \epsilon_N - i\hbar/2\tau_N)} \sum_M \frac{\phi_M(\mathbf{r}) \phi_M^*(\mathbf{r}')}{(E - \epsilon_M + i\hbar/2\tau_M)} \quad (\text{A.20})$$

We note that the Green function can be expanded in terms of the eigenstates $\phi_M(\mathbf{r})$ as

$$G(\mathbf{r}, \mathbf{r}'; E) = \sum_M \frac{\phi_M(\mathbf{r}) \phi_M^*(\mathbf{r}')}{(E - \epsilon_M + i\hbar/2\tau_M)} \quad (\text{A.21})$$

Therefore, we have obtained our previous expression for the kernel (cf. eq. (5.25)):

$$\tilde{T}(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar^2 |G(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_i(\mathbf{r}; E) \tau_i(\mathbf{r}'; E)} \quad (\text{A.22})$$

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