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Supriyo Datta  
*Purdue University*

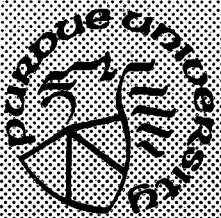
Michael J. McLennan  
*Purdue University*

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Supriyo Datta  
Michael J. McLennan

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School of Electrical Engineering  
Purdue University  
West Lafayette, Indiana 47907

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LINEAR AND NON-LINEAR RESPONSE**

Supriyo Datta  
Michael J. McLennan

School of Electrical Engineering  
Purdue University  
West Lafayette, Indiana 47907

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## ABSTRACT

We present a quantum transport equation derived under the simplifying assumption that the inelastic scattering is caused by uncorrelated point scatterers, such as magnetic impurities. 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 quantum transport equation that involves only the diagonal elements of the density matrix which we use to define a distribution function  $f(\mathbf{r}; E)$ . The kernel of this integral equation is calculated from the Schrödinger equation and contains all quantum interference effects. We show that at equilibrium the distribution function relaxes to the Fermi-Dirac function with a constant chemical potential everywhere in the structure. Assuming local thermodynamic equilibrium we then derive a linearized transport equation which has the appearance of a continuous version of the multiprobe Landauer formula. An alternative derivation is provided for the linearized transport equation starting from the multiprobe Landauer formula. Numerical results are presented for the conductivity of a disordered resistor with distributed inelastic scattering. A clear transition is observed from weak to strong localization as the inelastic scattering time is increased. In the present work we restrict ourselves to steady state transport and neglect many-body effects.

## FOREWORD

The purpose of this report is to present a quantum transport equation derived under the simplifying assumption that the inelastic scattering is caused by uncorrelated point scatterers. We believe that this equation will be useful in describing both linear and non-linear quantum transport in mesoscopic systems. The outline of the report is as follows. Section 1.2 provides an overview of the main results, which are then derived systematically in Chapters 2, 3 and 4. Sections 1.3 and 1.4 provide alternative derivations for the linearized transport equation which we call the “Continuous-Probe Landauer Formula.” In Chapter 2 we describe the model that we use for the inelastic scatters and compute the inelastic scattering rate from a model Hamiltonian using Fermi’s golden rule. The general non-linear quantum transport equation is derived in Chapter 3, which is then linearized in Chapter 4 assuming local thermodynamic equilibrium. A few examples are also discussed in Chapter 4 illustrating the relationship between semiclassical and quantum transport.

## CHAPTER 1: INTRODUCTION

### 1.1. Background

Much of our understanding of electron transport in solids is based on the Boltzmann Transport Equation (BTE). At steady state (which will be our primary concern in this paper),

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

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

$$S_{\text{op}} f(\mathbf{r}; \mathbf{k}) = \sum_{\mathbf{k}'} \left[ S(\mathbf{k}, \mathbf{k}') f(\mathbf{k}') [1 - f(\mathbf{k})] - S(\mathbf{k}', \mathbf{k}) f(\mathbf{k}) [1 - f(\mathbf{k}')] \right]_{\text{at } \mathbf{r}} \quad (1.2)$$

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 three separate 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]. The conductivity tensor  $\sigma$  at a frequency  $\omega$  is related to the current-current correlation function.

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

where  $n$  is the electron density,  $m$  is the effective mass,  $\delta_{\alpha\beta}$  is the Kronecker delta and the subscripts  $\alpha, \beta$  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 ensemble-averaged expectation value. Eqs. (1.3), (1.4) and relations derived from it have been the starting point for much theoretical work on localization [14-17]. Recently Lee and co-workers and Maekawa et. al. have used this approach



to study quantum transport in mesostructures [18-23]. Inelastic processes are included in this approach (also known as linear response theory) by replacing  $(-i\omega)$  with  $(1/\tau_i)$  where  $\tau_i$  is the inelastic scattering time.

2. In the *Landauer formalism*, linear transport coefficients are expressed in terms of the scattering properties of the structure [24-28]. 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  $\mu_j$  at lead  $j$  by the multiprobe Landauer formula (Fig. 1.1) [29]

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

where

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

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

$\mathbf{t}_{ij}(E)$  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 [30,31].

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

where the vector  $\mathbf{S}_i$  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 [32-34]. Although the Landauer approach, in principle, can be applied more generally [35], 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 [24,25,35]. 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 [36]. 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. The third approach to quantum transport theory has been to develop transport equations similar to the BTE [37]. Instead of the semiclassical distribution function  $f(\mathbf{r}; \mathbf{k})$ , such a *Quantum Boltzmann Equation* (QBE) uses a quantum distribution function which is derived from the density matrix  $\rho(\mathbf{r}, \mathbf{r}')$ . For example, the Wigner distribution function  $f(\mathbf{R}, \mathbf{k})$  is obtained from the density matrix  $\rho(\mathbf{r}, \mathbf{r}')$  by transforming to center-of-mass ( $\mathbf{R} = (\mathbf{r} + \mathbf{r}')/2$ ) and relative ( $\mathbf{r} - \mathbf{r}'$ ) coordinates and then Fourier transforming with respect to the relative coordinate. Dissipation is usually introduced using a relaxation time approximation [38] or through an influence functional in the Feynman path integral technique [39]. Although the QBE may provide a powerful and general approach to quantum transport theory (including non-linear response), it has not been used as widely as the Kubo or the Landauer formula. Moreover, quantum distribution functions have counter-intuitive properties (such as not being positive definite) and it is more difficult to make intuitive approximations.

In the present work we assume that the inelastic scattering is caused by a continuous distribution of point oscillators. 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. Since the oscillators are assumed to be points in space, each inelastic scattering event can be viewed as a *quantum measurement of the position of the electron*. An observer who monitors the states of the oscillators will see a

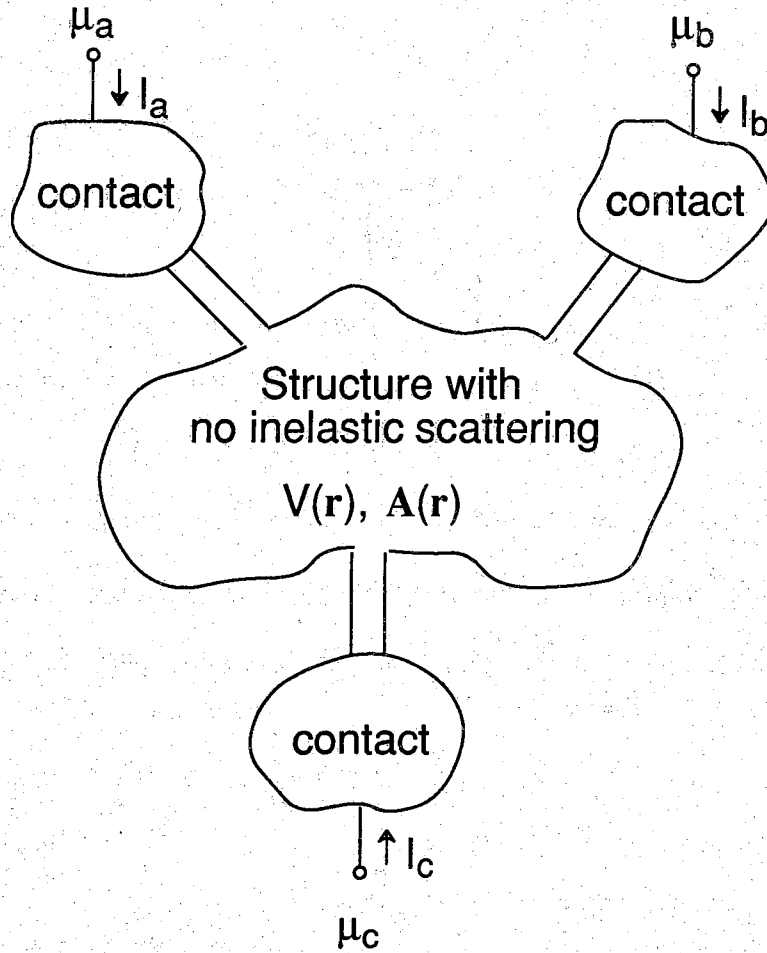


Fig. 1.1: The multiprobe Landauer formula relates  $I_i$  to  $\mu_j$  assuming that all inelastic scattering processes are confined to the contact reservoirs.

series of flashes from different spatial locations. Transport can thus be viewed as a series of “hops” (Fig. 1.2). Each “hop” starts with one inelastic scattering event at some location  $\mathbf{r}'$  and ends with another at some location  $\mathbf{r}$ ; in between, the electron propagates without inelastic scattering. We use the Schrödinger equation to obtain the probability  $P(\mathbf{r}, \mathbf{r}'; E)$  that an electron, having an energy  $E$  after suffering an inelastic scattering event at  $\mathbf{r}'$ , will suffer its next inelastic scattering event at  $\mathbf{r}$ . This probability function  $P(\mathbf{r}, \mathbf{r}'; E)$  contains all interference effects. Since all phase information is lost at the beginning and at the end of each “hop,” successive “hops” do not interfere. This allows us to write an integral transport equation describing the overall transport of carriers. The kernel of this integral equation depends on the probability function  $P(\mathbf{r}, \mathbf{r}'; E)$  and thus contains all the effects of quantum interference.

There is a similarity between this description and the Landauer description. An inelastic scattering event can be viewed as an exit into a reservoir followed by emission from the reservoir. It is as if there is a continuous distribution of reservoirs connected to the main structure by side probes through which electrons are absorbed and reinjected. In fact when we linearize our general transport equation assuming local thermodynamic equilibrium, we arrive at what looks like a continuous version of the multiprobe formula (eq. (1.5)). For this reason we have named the linearized transport equation the “*Continuous-Probe Landauer Formula*” [40]. In this section we will provide two alternative derivations of this formula (a) using a simple physical argument (Section 1.3) and (b) starting from the multiprobe Landauer formula and using linear response theory (Section 1.4). But first let us present a brief overview of the main results of this paper (Section 1.2).

## 1.2. Overview of Main Results

In this report we present a quantum transport equation derived under the simplifying assumption that the inelastic scattering is caused by *uncorrelated point scatterers*, like magnetic impurities. While this assumption may not always be realistic, we believe that this model can be used to describe much of the essential physics of quantum transport in mesostructures. This

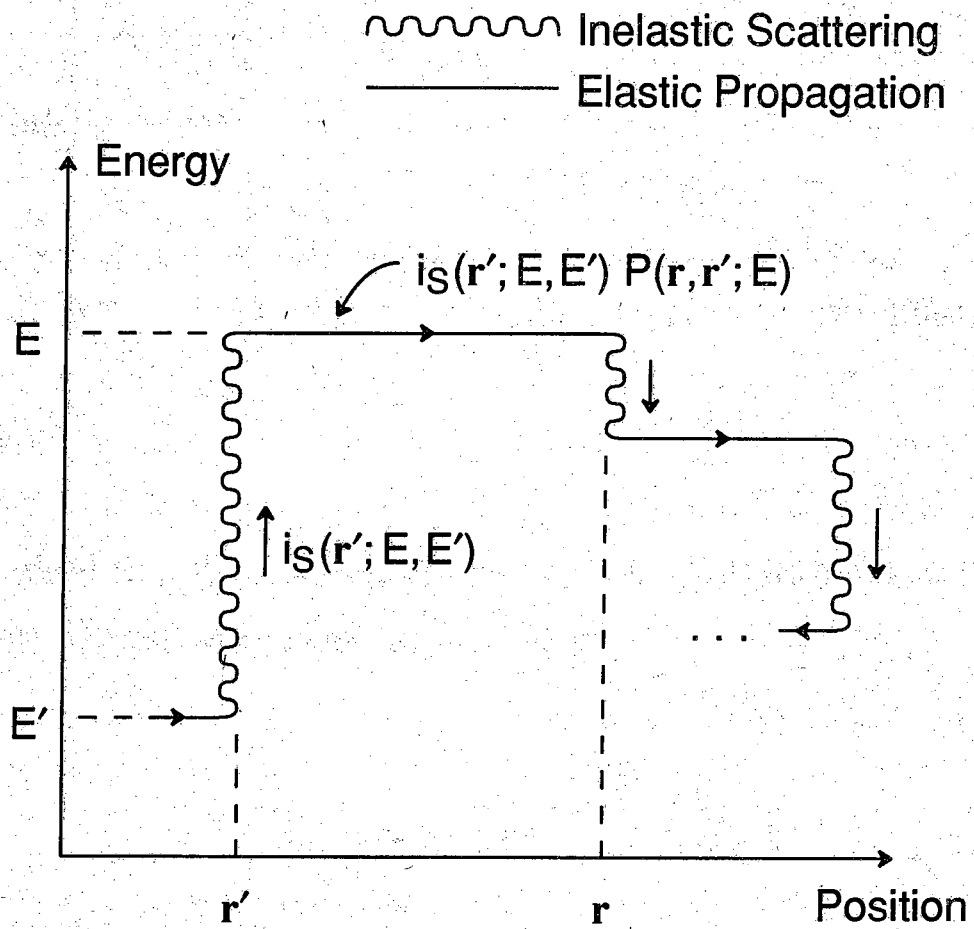


Fig. 1.2: Transport is viewed as a series of "hops." Each "hop" starts with an inelastic scattering event and ends with one.

assumption allows us to write a quantum transport equation entirely in terms of the *diagonal elements* of the density matrix which we use to define a distribution function  $f(\mathbf{r}; E)$ . We then linearize the transport equation assuming local thermodynamic equilibrium. The resulting linear transport equation (eq. (1.27)) has the appearance of a continuous version of the multiprobe Landauer formula (eq. (1.5)), as if the main structure were linked to a continuous distribution of reservoirs through side probes (Fig. 1.4). Either the full quantum transport equation or its linearized version can be used to describe linear and non-linear quantum transport in mesostructures. We make several assumptions in the present work that can possibly be removed in future extensions of the theory: (1) we restrict ourselves to steady state transport and many-body effects are neglected, (2) the inelastic scattering events are assumed instantaneous so that the wiggly lines in Fig. 1.2 are vertical and (3) we assume that the inelastic scattering is weak enough that the broadening of energy levels can be neglected.

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

$$H_0 = \frac{(\mathbf{p} - e\mathbf{A}(\mathbf{r}))^2}{2m} + eV(\mathbf{r}) \quad (1.8)$$

The vector and scalar potentials  $\mathbf{A}(\mathbf{r})$  and  $V(\mathbf{r})$  include external fields and self-consistent fields, as well as all sources of *elastic* scattering such as impurities, defects, boundaries etc. Assuming that the eigenfunctions  $\phi_M(\mathbf{r})$  of  $H_0$  (eq. (1.8)) have eigenvalues  $\epsilon_M$ , the density of states  $N_0(\mathbf{r}; E)$  per unit volume per unit energy is given by (we assume weak inelastic scattering)

$$N_0(\mathbf{r}; E) = \sum_M |\phi_M(\mathbf{r})|^2 \delta(E - \epsilon_M) \quad (1.9)$$

At equilibrium the electron density (which is the diagonal element of the density matrix  $\rho(\mathbf{r}, \mathbf{r}')$ ) is given by

$$\begin{aligned} n_{\text{eq}}(\mathbf{r}) &= \int dE N_0(\mathbf{r}; E) f_0(E) \\ &\equiv \int dE n_{\text{eq}}(\mathbf{r}; E) \end{aligned} \quad (1.10)$$

where  $f_0(E)$  is the usual Fermi-Dirac function. We extend eq. (1.10) to non-equilibrium problems to define a distribution function  $f(\mathbf{r}; E)$ .

$$n(\mathbf{r}; E) = N_0(\mathbf{r}; E) f(\mathbf{r}; E) \quad (1.11)$$

$$n(\mathbf{r}) = \int dE n(\mathbf{r}; E) \quad (1.12)$$

Note that the distribution function  $f(\mathbf{r}; E)$  as defined above is not a semiclassical concept but a well-defined quantum mechanical quantity. The electron density per unit energy  $n(\mathbf{r}; E)$  can be written in terms of field operators as

$$n(\mathbf{r}; E) = \frac{1}{2\pi} \int dE' e^{iE't/\hbar} \langle \psi^\dagger(\mathbf{r}; t) \psi(\mathbf{r}; 0) \rangle \quad (1.13a)$$

so that the total electron density  $n(\mathbf{r})$  is given by

$$n(\mathbf{r}) = \int dE n(\mathbf{r}; E) = \langle \psi^\dagger(\mathbf{r}; t) \psi(\mathbf{r}; 0) \rangle_{t=0^+} \quad (1.13b)$$

Our objective is to derive a transport equation that can be solved to obtain the distribution function  $f(\mathbf{r}; E)$ , or equivalently, the electron density per unit energy  $n(\mathbf{r}; E)$ . At equilibrium, with source terms set equal to zero, the distribution function relaxes to the Fermi Dirac function  $f_0(E)$  with a constant chemical potential, as we might expect.

The inelastic scattering is modeled as a continuous distribution of independent oscillators, each of whom interacts with the electron through a delta-function potential. We show in Chapter 2 that the inelastic scattering rate per unit volume per unit energy is equal to  $n(\mathbf{r}; E)/\tau_i(\mathbf{r}; E)$  where the *inelastic scattering time*  $\tau_i(\mathbf{r}; E)$  is given by

$$\frac{1}{\tau_i(\mathbf{r}; E)} = \int dE' [1 - f(\mathbf{r}; E')] N_0(\mathbf{r}; E') J(\mathbf{r}; E-E') \quad (1.14)$$

$J(\mathbf{r}; \hbar\omega)$  is a function that describes the spectral density of the oscillators responsible for the inelastic scattering (eq. (2.6)). The net inelastic scattering current per unit volume per unit energy

is given by  $e n(\mathbf{r}; E) / \tau_i(\mathbf{r}; E)$ ; using eqs. (1.11) and (1.14) we could write this quantity as

$$\frac{e n(\mathbf{r}; E)}{\tau_i(\mathbf{r}; E)} = \int dE' i_S(\mathbf{r}; E', E) \quad (1.15)$$

where

$$i_S(\mathbf{r}; E', E) = e \left[ J(E' - E) N_0(E) N_0(E') f(E) [1 - f(E')] \right]_{\text{at } \mathbf{r}} \quad (1.16)$$

$i_S(\mathbf{r}; E', E) dE' dE$  is the inelastic scattering current per unit volume from an initial energy interval  $dE$  to a final energy interval  $dE'$ ; as we might expect, it is proportional to the electron density at  $E$  ( $N_0(E) f(E)$ ) and to the "hole" density at  $E'$  ( $N_0(E') [1 - f(E')]$ ). Note that the inelastic scattering rate at any point depends on purely local factors at the same point.

Now we can write down a master equation quite straightforwardly as follows.

$$\frac{e n(\mathbf{r}; E)}{\tau_i(\mathbf{r}; E)} = \tilde{I}(\mathbf{r}; E) + \int d\mathbf{r}' \int dE' i_S(\mathbf{r}'; E, E') P(\mathbf{r}, \mathbf{r}'; E) \quad (1.17a)$$

This equation is illustrated in Fig. 1.3. Let us for the moment ignore the first term of the right-hand side and consider the second term.  $i_S(\mathbf{r}'; E, E')$  tells us the rate at which electrons are scattered at  $\mathbf{r}'$  from an initial energy  $E'$  to a final energy  $E$ ;  $P(\mathbf{r}, \mathbf{r}'; E)$  gives us the fraction of the electrons injected at  $\mathbf{r}'$  with energy  $E$  that suffer their next inelastic scattering event at  $\mathbf{r}$ . Integrating  $i_S(\mathbf{r}'; E, E') P(\mathbf{r}, \mathbf{r}'; E)$  over all  $\mathbf{r}'$  and  $E'$ , we should obtain the net rate at which electrons with energy  $E$  are inelastically scattered at  $\mathbf{r}$ , which is the quantity on the left-hand side  $e n(\mathbf{r}; E) / \tau_i(\mathbf{r}; E)$ . The first term on the right-hand side  $\tilde{I}(\mathbf{r}; E)$  is the current per unit volume per unit energy injected from external sources. Eq. (1.17a) can equivalently be written as

$$\tilde{I}(\mathbf{r}; E) = \int d\mathbf{r}' \int dE' \{ i_S(\mathbf{r}; E', E) P(\mathbf{r}', \mathbf{r}; E') - i_S(\mathbf{r}'; E, E') P(\mathbf{r}, \mathbf{r}'; E) \} \quad (1.17b)$$

Eq. (1.17b) follows readily from eq. (1.17a) using eq. (1.15) and noting that by definition, for a probability function we must have  $\int d\mathbf{r}' P(\mathbf{r}', \mathbf{r}; E) = 1$ .

Using eqs. (1.11) and (1.16) we can write eq. (1.17a) in terms of the distribution function  $f(\mathbf{r}; E)$ .



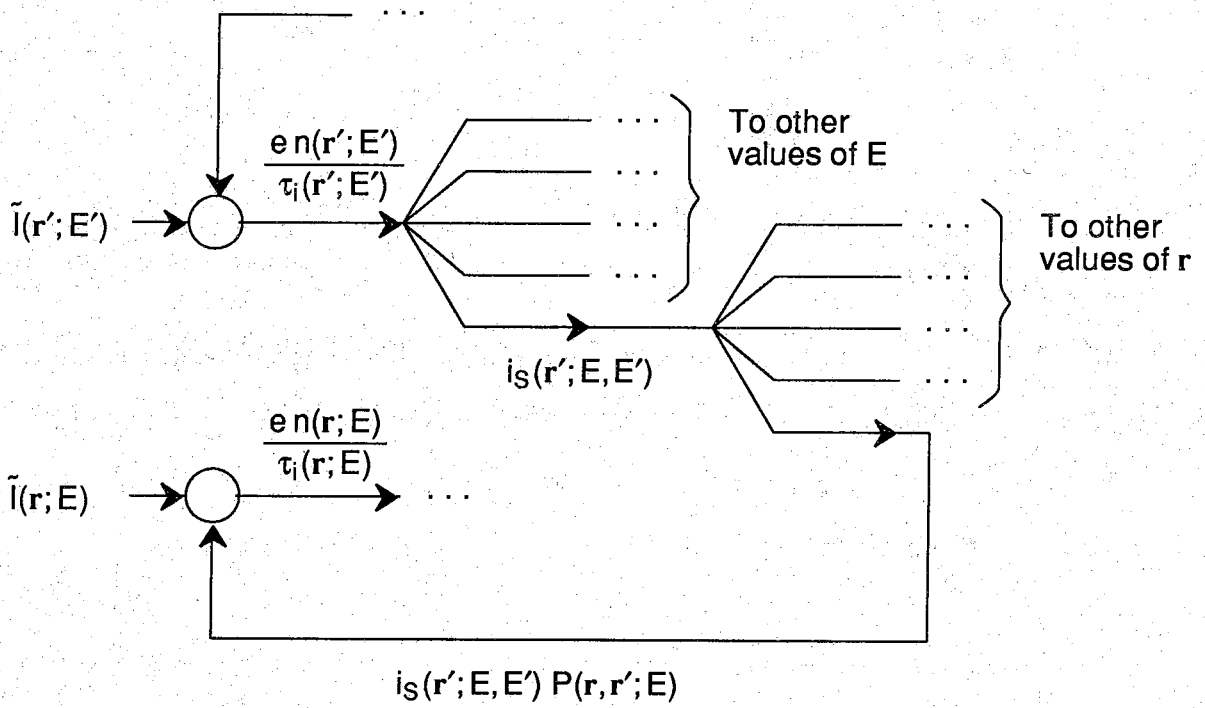


Fig. 1.3: A schematic diagram illustrating the different terms in eq. (1.17a).

$$\frac{e N_0(\mathbf{r}; E) f(\mathbf{r}; E)}{\tau_i(\mathbf{r}; E)} = \tilde{I}(\mathbf{r}; E) + \frac{e}{\hbar} \int d\mathbf{r}' \int dE' \tilde{T}(\mathbf{r}, \mathbf{r}'; E, E') f(\mathbf{r}'; E') [1 - f(\mathbf{r}'; E)] \quad (1.18)$$

Equivalently from eq. (1.17b) we obtain

$$\begin{aligned} \tilde{I}(\mathbf{r}; E) = & \frac{e}{\hbar} \int d\mathbf{r}' \int dE' \{ \tilde{T}(\mathbf{r}', \mathbf{r}; E', E) f(\mathbf{r}; E) [1 - f(\mathbf{r}; E')] \\ & - \tilde{T}(\mathbf{r}, \mathbf{r}'; E, E') f(\mathbf{r}'; E') [1 - f(\mathbf{r}'; E)] \} \end{aligned} \quad (1.19)$$

It will be noted that there is a close similarity between the right-hand side of eq. (1.19) and the scattering operator in the Boltzmann equation (eq. (1.2)). One describes hopping processes in real space, while the other describes hopping processes in  $\mathbf{k}$ -space. The energy variable does not appear explicitly in eq. (1.2) because the momentum states are assumed to be energy eigenstates; a given  $\mathbf{k}$  has a unique energy  $E_{\mathbf{k}}$ .

The kernel  $\tilde{T}$  of this integral equation is given by

$$\tilde{T}(\mathbf{r}, \mathbf{r}'; E, E') = \hbar P(\mathbf{r}, \mathbf{r}'; E) v_S(\mathbf{r}'; E, E') \quad (1.20)$$

where

$$v_S(\mathbf{r}'; E, E') = \left[ J(E - E') N_0(E) N_0(E') \right]_{\text{at } \mathbf{r}} \quad (1.21)$$

We show in Chapter 3 that the probability function  $P(\mathbf{r}, \mathbf{r}'; E)$  can be obtained from the Green function  $G(\mathbf{r}, \mathbf{r}'; E)$  of the time-independent Schrödinger equation modified to include an additional imaginary potential  $i\hbar/2\tau_i(\mathbf{r}; E)$ .

$$P(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar}{2\pi} \frac{|G(\mathbf{r}, \mathbf{r}'; E)|^2}{N_0(\mathbf{r}'; E) \tau_i(\mathbf{r}; E)} \quad (1.22)$$

$$\left[ E - H_0 + \frac{i\hbar}{2\tau_i(\mathbf{r}; E)} \right] G(\mathbf{r}, \mathbf{r}'; E) = \delta(\mathbf{r} - \mathbf{r}') \quad (1.23)$$

where  $H_0$  is the Hamiltonian defined in eq. (1.8).

The kernel  $\tilde{T}(\mathbf{r}, \mathbf{r}'; E, E')$  of the integral equation (1.18) thus contains all quantum interference effects through the Green function  $G(\mathbf{r}, \mathbf{r}'; E)$ . Once the kernel has been computed we can solve eq. (1.18) to obtain the distribution function  $f(\mathbf{r}; E)$  for a given external source function  $\tilde{I}(\mathbf{r}; E)$ ; alternatively, we could specify  $f(\mathbf{r}; E)$  in certain parts of the structure (like the contacts) and compute the resulting  $\tilde{I}(\mathbf{r}; E)$ .

It should be noted that the assumption of point inelastic scatterers is crucial in arriving at such a simple description of non-linear quantum transport. Firstly, it allows us to write the scattering rate  $i_S(\mathbf{r}; E', E)$  in terms of purely local factors (eq. (1.16)). 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 (Fig. 1.2) is thus always a delta function. We believe that the assumption of point inelastic scatterers can only be relaxed at the expense of considerable added complexity.

We show in Chapter 3 that at equilibrium with  $\tilde{I}(\mathbf{r}; E) = 0$ , the distribution function  $f(\mathbf{r}; E)$  relaxes to the Fermi-Dirac function  $f_0(E)$  with a constant chemical potential everywhere in the structure. To obtain the linearized transport equation (Chapter 4) we first simplify eq. (1.19) to the following form, under the assumption that the distribution function  $f(\mathbf{r}; E)$  can be written as a Fermi-Dirac function with a *local chemical potential*  $\mu(\mathbf{r})$  (see eq. (4.7)).

$$I(\mathbf{r}) = \frac{e}{h} \int d\mathbf{r}' \int dE [T(\mathbf{r}', \mathbf{r}; E) f(\mathbf{r}; E) - T(\mathbf{r}, \mathbf{r}'; E) f(\mathbf{r}'; E)] \quad (1.24)$$

where

$$T(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar^2 |G(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_i(\mathbf{r}; E) \tau_i(\mathbf{r}'; E)} \quad (1.25)$$

$I(\mathbf{r})$  is the total current (over all energies) that is injected per unit volume at  $\mathbf{r}$  from external sources. We also show that (eq. (3.15))

$$\int d\mathbf{r}' [T(\mathbf{r}', \mathbf{r}; E) - T(\mathbf{r}, \mathbf{r}'; E)] = 0 \quad (1.26)$$

Eq. (1.26) ensures that at equilibrium with  $I(\mathbf{r}) = 0$ , the distribution function  $f(\mathbf{r}; E)$  relaxes to a constant  $f_0(E)$  with a constant chemical potential  $\mu_0$  throughout the structure. In linear response theory we assume that the local chemical potential  $\mu(\mathbf{r})$  deviates only slightly from the equilibrium chemical potential  $\mu_0$ . Using a Taylor series expansion for  $f(\mathbf{r}; E)$  we obtain the linearized transport equation (see eq. (4.11)).

$$I(\mathbf{r}) = \frac{e^2}{h} \int d\mathbf{r}' \{T_0(\mathbf{r}', \mathbf{r}) \mu(\mathbf{r}) - T_0(\mathbf{r}, \mathbf{r}') \mu(\mathbf{r}')\} \quad (1.27)$$

where

$$T_0(\mathbf{r}, \mathbf{r}') = \int dE \left[ -\frac{\partial f_0}{\partial E} \right] T(\mathbf{r}, \mathbf{r}'; E) \quad (1.28)$$

Once again the kernel  $T_0(\mathbf{r}, \mathbf{r}')$  contains all quantum interference effects through the Green function  $G(\mathbf{r}, \mathbf{r}'; E)$ . We believe that either the non-linear transport equation (eq. (1.19)) or its linearized version (eq. (1.27)) can be used to describe quantum transport in mesostructures of arbitrary size and shape.

In principle, eqs. (1.19) or (1.27) should be solved self-consistently with the Poisson equation; the self-consistent potential which enters the one-electron Schrödinger equation affects the kernels ( $\tilde{T}(\mathbf{r}, \mathbf{r}'; E, E')$  or  $T_0(\mathbf{r}, \mathbf{r}')$ ) appearing in these equations. However, in linear response theory we can use the coefficients  $T(\mathbf{r}, \mathbf{r}'; E)$  obtained (self-consistently) under equilibrium conditions. This is because the first-order change in the right-hand side of eq. (1.24) due to a small change  $\delta T$  in the coefficient  $T$

$$\frac{e}{h} \int d\mathbf{r}' \int dE f_0(E) [\delta T(\mathbf{r}', \mathbf{r}; E) - \delta T(\mathbf{r}, \mathbf{r}'; E)]$$

is zero on account of the relation (eq. (1.26)) that must be satisfied by  $T$ . This means that for small applied bias the current is not affected by the self-consistent readjustment of charges within the structure. This, however, may not be true if there are sharp resonances in  $T$ ; second-

order terms ( $\sim \delta T \delta f_0$ ) may not be negligible in that case.

Eq. (1.27) can be viewed as a continuous version of the multiprobe Landauer formula stated earlier (eq. (1.5)) and we call it the “*Continuous-Probe Landauer Formula.*” It is as if we have added a continuous distribution of reservoirs connected through probes to the main structure (Fig. 1.4). A single reservoir whose coupling can be varied has been used in the past to simulate the effect of inelastic scattering [36,41]. 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. (1.27) would seem to be an obvious extension of the multiprobe Landauer formula to include inelastic scattering within the structure. What is not obvious, however, is how the kernel  $T_0(\mathbf{r}, \mathbf{r}')$  is to be calculated in a given structure. In view of the importance of eq. (1.27) we will now provide two alternative derivations for it -- one using a simple physical argument (Section 1.3) and the other starting from linear response theory (Section 1.4).

### 1.3. Simple Derivation of the Linearized Transport Equation

We can obtain the linearized transport equation at zero-temperature directly by starting from a simplified version of eq. (1.17a).

$$\frac{e n(\mathbf{r})}{\tau_i(\mathbf{r})} = I(\mathbf{r}) + \int d\mathbf{r}' \frac{e n(\mathbf{r}')}{\tau_i(\mathbf{r}')} P(\mathbf{r}, \mathbf{r}') \quad (1.29)$$

The physical basis for this equation is very similar to that for eq. (1.17a), and is illustrated in Fig. 1.5. Here we are assuming that all the transport occurs within a narrow range of energies right around the Fermi level, and  $n(\mathbf{r})$  is the total electron density in this energy range. We have suppressed the energy  $E$  is the probability function  $P(\mathbf{r}, \mathbf{r}'; E)$ , which is assumed to equal the Fermi energy. The net rate at which electrons are inelastically scattered at  $\mathbf{r}'$  is given by  $n(\mathbf{r}')/\tau_i(\mathbf{r}')$ ; of these, a fraction equal to  $P(\mathbf{r}, \mathbf{r}')$  suffer their next inelastic scattering event at  $\mathbf{r}$ . Integrating over all  $\mathbf{r}'$  and adding the externally injected current ( $I(\mathbf{r})/e$ ) we obtain the net rate at which electrons are inelastically scattered at  $\mathbf{r}$ , which is the term on the left-hand side,

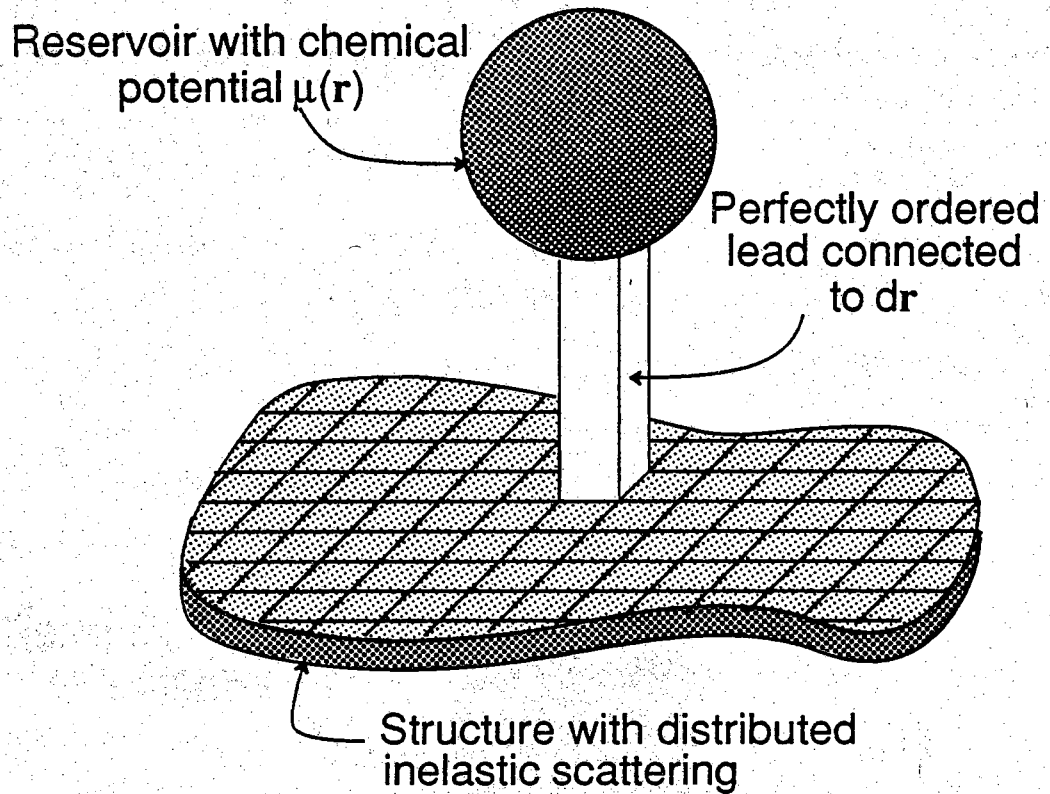


Fig. 1.4: Eq. (1.27) can be viewed as a generalization of the multiprobe Landauer formula to a structure with a continuous distribution of probes linking each volume element  $dr$  to a conceptual reservoir of carriers.

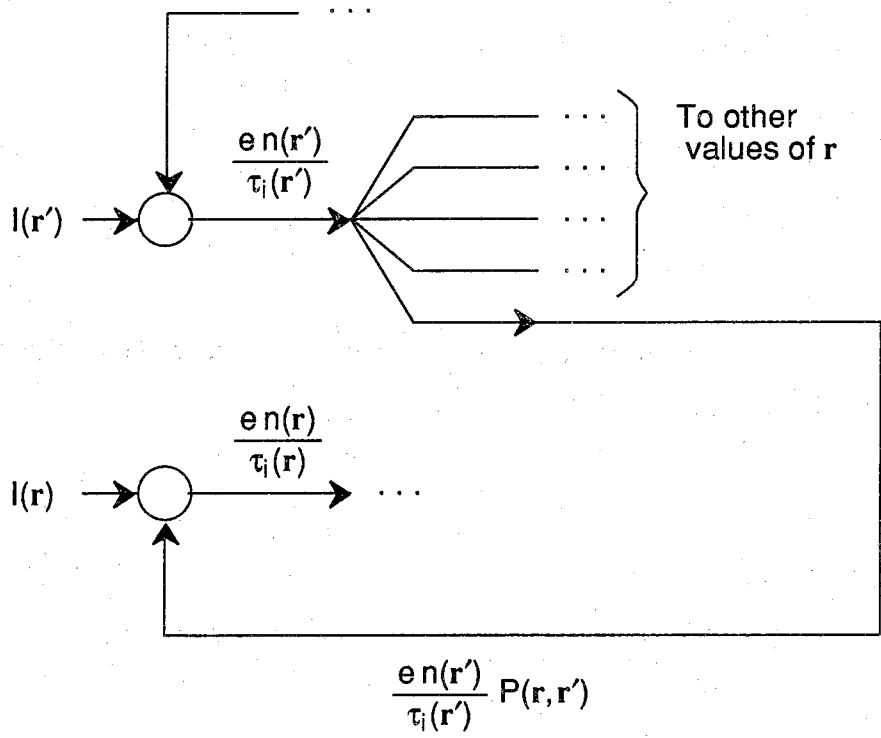


Fig. 1.5: Schematic diagram illustrating the different terms in eq. (1.29).

$n(\mathbf{r})/\tau_i(\mathbf{r})$ . Once again using the property of probability functions  $\int d\mathbf{r}' P(\mathbf{r}',\mathbf{r}) = 1$ , we can write eq. (1.29) as

$$I(\mathbf{r}) = \int d\mathbf{r}' \left[ \frac{e n(\mathbf{r})}{\tau_i(\mathbf{r})} P(\mathbf{r}',\mathbf{r}) - \frac{e n(\mathbf{r}')}{\tau_i(\mathbf{r}')} P(\mathbf{r},\mathbf{r}') \right] \quad (1.30)$$

Writing  $n(\mathbf{r}) = e N_0(\mathbf{r}) \mu(\mathbf{r})$ , where  $e \mu(\mathbf{r})$  is the chemical potential measured from some reference energy near the Fermi energy, we obtain from eq. (1.29),

$$\frac{e N_0(\mathbf{r})}{\tau_i(\mathbf{r})} \mu(\mathbf{r}) = I(\mathbf{r}) + \frac{e^2}{h} \int d\mathbf{r}' T(\mathbf{r},\mathbf{r}') \mu(\mathbf{r}') \quad (1.31)$$

where

$$T(\mathbf{r},\mathbf{r}') = \frac{h N_0(\mathbf{r}') P(\mathbf{r},\mathbf{r}')}{\tau_i(\mathbf{r}')} \quad (1.32)$$

Using eq. (1.22) for  $P(\mathbf{r},\mathbf{r}')$  it is easy to check that  $T(\mathbf{r},\mathbf{r}')$  is given by the same expression as stated earlier (eq. (1.25)). Note that in this section we have suppressed the energy  $E$  which is assumed to equal the Fermi energy; this is because we are restricting our attention to linear transport at zero-temperature.

Again, starting from the alternative form given in eq. (1.30) we obtain the alternative version of eq. (1.31),

$$I(\mathbf{r}) = \frac{e^2}{h} \int d\mathbf{r}' \{ T(\mathbf{r}',\mathbf{r}) \mu(\mathbf{r}) - T(\mathbf{r},\mathbf{r}') \mu(\mathbf{r}') \} \quad (1.32)$$

#### 1.4. Linearized Transport Equation from the Multiprobe Landauer Formula

As we discussed in Section 1.2, the linearized transport equation (eq. (1.27)) is an obvious extension of the multiprobe Landauer formula (eq. (1.5)). What is not obvious is how we obtain the kernel  $T_0(\mathbf{r},\mathbf{r}')$ . In this section we derive  $T(\mathbf{r},\mathbf{r}';E)$  starting from the Kubo formula for the conductivity  $\sigma(\mathbf{r},\mathbf{r}';E)$  (eq. (1.3)) and using the Lee-Fisher formula (eq. (1.7)) to obtain  $T$  from  $\sigma$ . As shown in the Appendix, eq. (1.3) can be simplified to yield



$$\sigma_0(\mathbf{r}, \mathbf{r}') = \int dE \left[ -\frac{\partial f_0}{\partial E} \right] \sigma(\mathbf{r}, \mathbf{r}'; E) \quad (1.34a)$$

$$\sigma_{\alpha\beta}(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar}{2\pi} \sum_{N,M} [\mathbf{J}_{NM}(\mathbf{r}) \otimes \mathbf{J}_{MN}(\mathbf{r}')]_{\alpha\beta} G_M^R(E) G_N^A(E) \quad (1.34b)$$

where

$$\mathbf{J}_{NM}(\mathbf{r}) = \frac{ie\hbar}{2m} [(\nabla\phi_N)^* \phi_M - \phi_N^* (\nabla\phi_M)] \quad (1.35)$$

$$G_M^R(E) = \frac{1}{(E - \epsilon_M + i\eta)} \quad (1.36a)$$

$$G_M^A(E) = \frac{1}{(E - \epsilon_M - i\eta)} \quad (1.36b)$$

$\phi_M(\mathbf{r})$  are the eigenfunctions of  $H_0$  (eq. (1.8)); the corresponding eigenenergies  $\epsilon_M$  of  $H_0$  are purely real.  $\eta$  is an infinitesimal positive quantity. The problem now is to include the effect of inelastic scattering in the Green functions  $G_M^{R,A}(E)$ . One approach that has often been used to incorporate inelastic scattering processes is to let

$$\eta = \hbar/2\tau_i \quad (1.37)$$

where  $\tau_i$  is the inelastic scattering time, assumed to be constant everywhere. This is equivalent to adding an imaginary potential  $i\hbar/2\tau_i$  to the Hamiltonian  $H_0$  so that the eigenenergies  $\epsilon_M$  acquire an imaginary part. It is easy to show that the ‘‘Schrodinger’’ equation

$$E \Psi = \left[ H_0 - \frac{i\hbar}{2\tau_i} \right] \Psi \quad (1.38)$$

leads to a continuity equation of the following form for the probability density ( $\rho/e$ ) and the probability current density ( $\mathbf{J}/e$ ).

$$\nabla \cdot \mathbf{J} = -\frac{\rho}{\tau_i} \quad (1.39)$$

Thus by identifying  $\eta$  with  $\hbar/2\tau_i$  we are effectively describing particles that *decay* with a

lifetime  $\tau_i$ . This is clearly not an accurate representation of the scattering process which involves not only the decay from an initial state but also the subsequent reinsertion into another state. Now, it is well-known that if we assume the eigenstates to be plane wave states,  $\mathbf{k}$ , and identify  $\eta$  with  $\hbar/2\tau$  where  $\tau$  is the total (elastic as well as inelastic) scattering time

$$G_{\mathbf{k}}^{R,A}(E) = \frac{1}{E - \epsilon_{\mathbf{k}} \pm i\hbar/2\tau} \quad (1.40)$$

then we obtain the correct Boltzmann conductivity from eq. (1.34b) *only if the scattering is isotropic*; any scattering event then causes a complete decay of the momentum and the subsequent reinsertion into another state (which we neglect) has no effect on the current-current correlation. But for anisotropic scattering processes it is well-known that this simple procedure is inadequate [13]. What we are trying to do here is to include inelastic scattering processes in a Boltzmann-like manner while treating the elastic processes quantum mechanically by using the exact eigenstates  $\phi_{\mathbf{M}}(\mathbf{r})$  (rather than the plane wave states  $e^{i\mathbf{k}\cdot\mathbf{r}}$ ). Since the inelastic scattering processes have been assumed to be isotropic we can include them simply by identifying  $\eta$  with  $\hbar/2\tau_i$  in eqs. (1.25a,b) as noted by Thouless and Kirkpatrick [17].

$$G_{\mathbf{M}}^R(E) = \frac{1}{E - \epsilon_{\mathbf{M}} + i\hbar/2\tau_{\mathbf{M}}} \quad (1.41a)$$

$$G_{\mathbf{M}}^A(E) = \frac{1}{E - \epsilon_{\mathbf{M}} - i\hbar/2\tau_{\mathbf{M}}} \quad (1.41b)$$

Since the inelastic scattering time  $\tau_i(\mathbf{r}; E)$  is not a constant  $\tau_i$  but can vary spatially (eq. (1.14)), we have used different lifetimes  $\tau_{\mathbf{M}}$  for the different eigenstates; in principle, these may be obtained from the imaginary parts of the eigenenergies  $\epsilon_{\mathbf{M}}$  obtained from eq. (1.38). However, we assume that the imaginary potential  $i\hbar/2\tau_i(\mathbf{r}; E)$  is small enough that we can neglect any complication due to the non-orthogonality of the eigenfunctions  $\phi_{\mathbf{M}}(\mathbf{r})$  obtained from eq. (1.38).

We obtain from eq. (1.34b) using eqs. (1.41a,b),

$$\sigma_{\alpha\beta}(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar}{2\pi} \sum_{N,M} \frac{[\mathbf{J}_{NM}(\mathbf{r}) \otimes \mathbf{J}_{MN}(\mathbf{r}')]_{\alpha\beta}}{(E - \epsilon_M + i\hbar/2\tau_M)(E - \epsilon_N - i\hbar/2\tau_N)} \quad (1.42)$$

Next, we use the Lee-Fisher formula linking  $T$  to  $\sigma$  (eq. (1.7)). Since each probe has an infinitesimal cross-section we can write

$$\frac{e^2}{h} T(\mathbf{r}, \mathbf{r}'; E) d\mathbf{r} d\mathbf{r}' = \frac{\hbar}{2\pi} \sum_{N,M} \frac{(\mathbf{J}_{NM}(\mathbf{r}) \cdot \hat{\mathbf{n}}(\mathbf{r}) d\mathbf{r})(\mathbf{J}_{MN}(\mathbf{r}') \cdot \hat{\mathbf{n}}(\mathbf{r}') d\mathbf{r}')}{(E - \epsilon_M + i\hbar/2\tau_M)(E - \epsilon_N - i\hbar/2\tau_N)} \quad (1.43)$$

where  $\hat{\mathbf{n}}(\mathbf{r})$  is the unit vector normal to the probe at  $\mathbf{r}$  (Fig. 1.2). But  $\mathbf{J} \cdot \hat{\mathbf{n}}$  is the current entering the probe at  $\mathbf{r}$  due to inelastic scattering; by definition, it must equal  $\rho/\tau_i$ .

$$T(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar^2}{e^2} \sum_{N,M} \frac{\rho_{NM}(\mathbf{r}) \rho_{MN}(\mathbf{r}') / \tau_i(\mathbf{r}; E) \tau_i(\mathbf{r}'; E)}{(E - \epsilon_M + i\hbar/2\tau_M)(E - \epsilon_N - i\hbar/2\tau_N)} \quad (1.44)$$

Since  $\rho_{NM}(\mathbf{r}) = e \phi_N^*(\mathbf{r}) \phi_M(\mathbf{r})$ , we have

$$T(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar^2}{\tau_i(\mathbf{r}; E) \tau_i(\mathbf{r}'; E)} \sum_N \frac{\phi_N^*(\mathbf{r}) \phi_N(\mathbf{r}')}{E - \epsilon_N - i\hbar/2\tau_N} \sum_M \frac{\phi_M(\mathbf{r}) \phi_M^*(\mathbf{r}')}{E - \epsilon_M + i\hbar/2\tau_M} \quad (1.45)$$

Eq. (1.25) follows from eq. (1.45) if we note that,

$$G(\mathbf{r}, \mathbf{r}'; E) = \sum_M \frac{\phi_M(\mathbf{r}) \phi_M^*(\mathbf{r}')}{E - \epsilon_M + i\hbar/2\tau_M} \quad (1.46)$$

## CHAPTER 2: THE MODEL FOR INELASTIC SCATTERERS

In Section 1.2 we outlined the derivation of the non-linear quantum transport equation. Two “details” were not discussed in Chapter 1, namely, (1) how the expression for  $i_s$  (eq. (1.16)) is obtained and (2) how the expression for  $P$  (eq. (1.22)) is obtained. We will discuss the second point in Chapter 3. Our objective in this chapter is to describe the model that we use for the inelastic scatterers and to derive expressions for the inelastic scattering rate starting from a model Hamiltonian.

### 2.1. Model Hamiltonian

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

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

The vector and scalar potentials  $\mathbf{A}(\mathbf{r})$  and  $V(\mathbf{r})$  include external fields and self-consistent fields, as well as all sources of *elastic scattering* such as impurities, defects, boundaries etc. For the *inelastic scattering* we adopt the following model: we assume a continuous distribution of oscillators whose interaction with the electrons is described by the Hamiltonian

$$H_i = \sum_m \sum_{\alpha} U_{m,\alpha} \delta(\mathbf{r} - \mathbf{r}_m) (a_{m,\alpha}^{\dagger} + a_{m,\alpha}) \quad (2.2)$$

Here  $U_{m,\alpha}$  (dimensions  $-eV-\text{\AA}^3$ ) is the interaction potential between the electron and the oscillator  $\alpha$  at the location  $\mathbf{r}_m$ , whose creation and annihilation operators are  $a_{m,\alpha}^{\dagger}$  and  $a_{m,\alpha}$  respectively (Fig. 2.1). We will assume that the number of oscillators per unit volume with frequencies lying between  $\omega$  and  $\omega + d\omega$  is given by some function  $J_0(\mathbf{r}; \hbar\omega) d(\hbar\omega)$ .

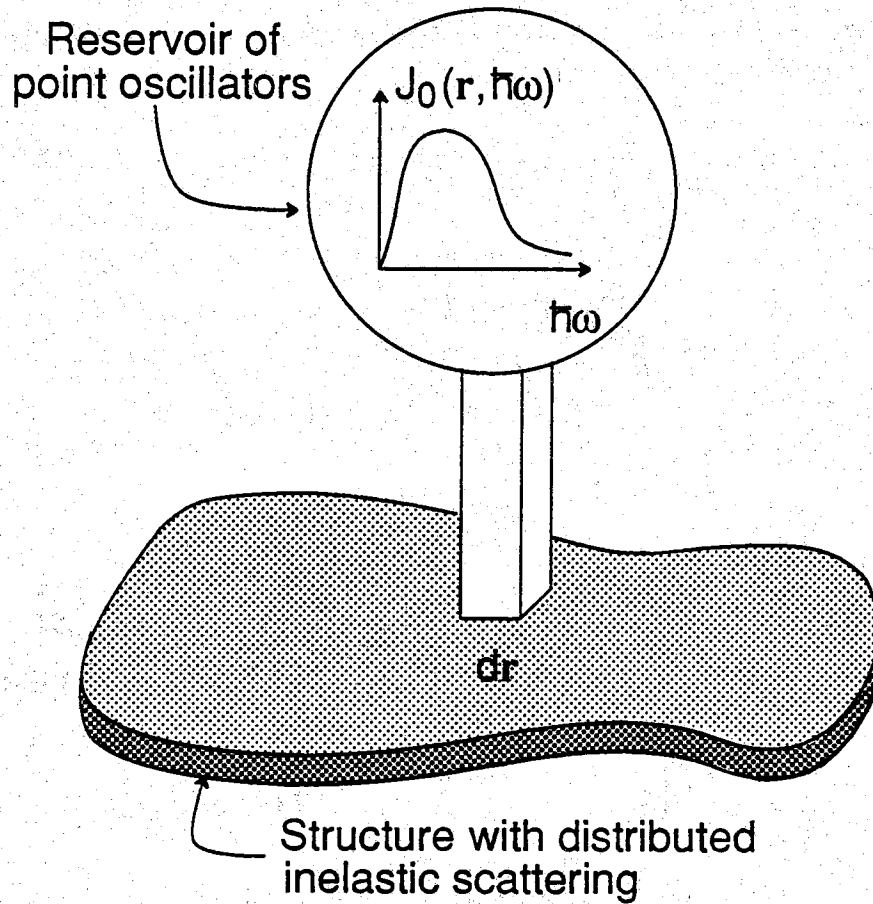


Fig. 2.1: Inelastic scattering is modeled with a continuous distribution of point scatterers. The number of oscillators per unit volume with frequencies lying between  $\omega$  and  $\omega+d\omega$  is equal to  $J_0(\mathbf{r}; \hbar\omega) d(\hbar\omega)$ .

## 2.2. Scattering Rate from Fermi's Golden Rule

Consider an electron with energy  $E$  having the wave function

$$\Psi(\mathbf{r}, t) = \Phi(\mathbf{r}) e^{-iEt/\hbar} \quad (2.3)$$

Assuming that the eigenfunctions  $\phi_M(\mathbf{r})$  of  $H_0$  (eq. (2.1)) have eigenvalues  $\epsilon_M$ , we can write the inelastic scattering rate  $v_i$  from Fermi's golden rule as follows.

$$v_i = \frac{2\pi}{\hbar} \sum_m \sum_\alpha |U_{m,\alpha}|^2 \sum_M \left| \langle \phi_M(\mathbf{r}) | \delta(\mathbf{r}-\mathbf{r}_m) | \Phi(\mathbf{r}) \rangle \right|^2 \{ N_{m,\alpha} \delta(E - \epsilon_M + \hbar\omega_{m,\alpha}) + (N_{m,\alpha} + 1) \delta(E - \epsilon_M - \hbar\omega_{m,\alpha}) \} \quad (2.4)$$

Here  $N_{m,\alpha}$  is the number of "phonons" occupying the oscillator  $m, \alpha$ . We now convert the summations over  $m, \alpha$  into integrals, assuming that the number of oscillators in a volume  $d\mathbf{r}$  with energies lying between  $\hbar\omega$  and  $\hbar(\omega+d\omega)$  is given by  $J_0(\mathbf{r}; \hbar\omega) d\mathbf{r} d(\hbar\omega)$ .

$$v_i = \frac{2\pi}{\hbar} \int d\mathbf{r} |\Phi(\mathbf{r})|^2 \int_0^\infty d(\hbar\omega) J_0(\mathbf{r}; \hbar\omega) |U(\mathbf{r}; \hbar\omega)|^2 \sum_M |\phi_M(\mathbf{r})|^2 \{ N(\mathbf{r}; \hbar\omega) \delta(E - \epsilon_M + \hbar\omega) + (N(\mathbf{r}; \hbar\omega)+1) \delta(E - \epsilon_M - \hbar\omega) \} \quad (2.5)$$

We can write eq. (2.5) in a more compact form by defining

$$J(\mathbf{r}; \hbar\omega) = \begin{cases} \frac{2\pi}{\hbar} |U(\mathbf{r}; \hbar\omega)|^2 J_0(\mathbf{r}; \hbar\omega) (N(\mathbf{r}; \hbar\omega)+1) , & \hbar\omega > 0 \\ \frac{2\pi}{\hbar} |U(\mathbf{r}; -\hbar\omega)|^2 J_0(\mathbf{r}; -\hbar\omega) N(\mathbf{r}; -\hbar\omega) , & \hbar\omega < 0 \end{cases} \quad (2.6)$$

Note that  $J(\mathbf{r}; \hbar\omega)$  has the dimensions of  $\text{\AA}^3/\text{sec}$ .

$$v_i = \int d\mathbf{r} |\Phi(\mathbf{r})|^2 \int_{-\infty}^{+\infty} d(\hbar\omega) J(\mathbf{r}; \hbar\omega) N_0(\mathbf{r}; E-\hbar\omega) \quad (2.7)$$

where  $N_0(\mathbf{r}; E)$  is the *electronic density of states* which is written in terms of the eigenfunctions  $\phi_M(\mathbf{r})$  as follows.

$$N_0(\mathbf{r}; E) = \sum_M |\phi_M(\mathbf{r})|^2 \delta(E - \epsilon_M) \quad (2.8)$$

It will be noted from eq. (2.7) that the inelastic scattering rate at a point  $\mathbf{r}$  is proportional to the *local electron density*  $n(\mathbf{r}) = |\Phi(\mathbf{r})|^2$  and involves only local factors such as  $J(\mathbf{r}; \hbar\omega)$  and  $N_0(\mathbf{r}; \hbar\omega)$ . It is this property of point inelastic scatterers that we exploit in this paper to develop a simplified description of quantum transport. In deriving eq. (2.7) we assumed that all electrons have the same energy  $E$ . In general, we can integrate over the distribution of electrons  $n(\mathbf{r}; E)$  per unit energy per unit volume.

$$v_i = \int d\mathbf{r} \int dE n(\mathbf{r}; E) \int_{-\infty}^{+\infty} dE' N_0(\mathbf{r}; E') J(\mathbf{r}; E-E') \quad (2.9)$$

### 2.3. Distribution Function

We now define a distribution function  $f(\mathbf{r}; E)$ , so that the density of  $n(\mathbf{r})$  can be determined by summing the contributions at all energies.

$$n(\mathbf{r}) = \int dE n(\mathbf{r}; E) = \int dE N_0(\mathbf{r}; E) f(\mathbf{r}; E) \quad (2.10)$$

The distribution function  $f(\mathbf{r}; E)$  relaxes to the Fermi-Dirac function at equilibrium. In the next chapter we will derive a transport equation that can be solved to obtain  $f(\mathbf{r}; E)$  when the structure is driven away from equilibrium; however, for our present purpose, eq. (2.10) can be used to simplify eq. (2.9) to the form

$$\begin{aligned} v_i &= \int d\mathbf{r} \int dE \int dE' v_s(\mathbf{r}; E', E) f(\mathbf{r}; E) [1 - f(\mathbf{r}; E')] \\ &= \int d\mathbf{r} \int dE \int dE' \left[ v_s(E', E) f(E) [1 - f(E')] \right]_{\text{at } \mathbf{r}} \end{aligned} \quad (2.11)$$

where

$$v_s(\mathbf{r}; E', E) = J(E-E') N_0(E') N_0(E) \Big|_{\text{at } \mathbf{r}} \quad (2.12a)$$

We have added the factor  $[1 - f(E')]$  in eq. (2.11) to account for the exclusion principle, which was not considered earlier. The inelastic scattering current  $i_s(\mathbf{r}; E', E)$  used in Section 1.2 is given by the integrand in eq. (2.11) multiplied by the electronic charge.

$$i_s(\mathbf{r}; E', E) = e v_s(\mathbf{r}; E', E) f(E) [1 - f(E')] \quad (2.12b)$$

Note that in eq. (2.11) the integrand  $v_s(E', E) f(E) [1 - f(E')] \Big|_{\text{at } \mathbf{r}}$  is a local function and can be interpreted as the inelastic scattering rate per unit volume, per unit energy range of initial states (E), per unit energy range of final states (E'). The function  $v_s(E', E)$  is the product of three terms (eq. (2.12a)): the density of initial states  $N_0(E)$ , the density of final states  $N_0(E')$  and the coupling  $J(\hbar\omega)$  between the electrons and the oscillators that comprise the inelastic scatterers (eq. (2.6)). It can be seen from eqs. (2.6) and (2.12a) that if the system of oscillators is in equilibrium so that the number of "phonons"  $N(\hbar\omega)$  is given by the Bose-Einstein function then we have the following relationship

$$v_s(\mathbf{r}; E', E) = v_s(\mathbf{r}; E, E') e^{(E-E')/k_B T} \quad (2.13)$$

since

$$J(E-E') = J(E'-E) e^{(E-E')/k_B T} \quad (2.14)$$

#### 2.4. Inelastic Scattering Time

Finally we will derive an expression for the inelastic scattering time  $\tau_i(\mathbf{r}; E)$ . As discussed in Section 1.1, the inelastic scattering rate per unit volume per unit energy depends only on the local properties of the system, and can be expressed as  $n(\mathbf{r}; E)/\tau_i(\mathbf{r}; E)$ . Equating this to the result from eq. (2.11),



$$\frac{n(\mathbf{r}; E)}{\tau_i(\mathbf{r}; E)} = \int dE' \left[ v_s(E', E) f(E) [1 - f(E')] \right]_{\text{at } \mathbf{r}} \quad (2.15)$$

Using eqs. (2.10) and (2.12a) we obtain

$$\frac{1}{\tau_i(\mathbf{r}; E)} = \int dE' \left[ [1 - f(E')] N_0(E') J(E-E') \right]_{\text{at } \mathbf{r}} \quad (2.16)$$

## CHAPTER 3: NON-LINEAR QUANTUM TRANSPORT EQUATION

The derivation of the non-linear quantum transport equation has already been outlined in Section 1.2 (eqs. (1.18) - (1.22)).

$$\frac{e N_0(\mathbf{r}; E) f(\mathbf{r}; E)}{\tau(\mathbf{r}; E)} = \tilde{I}(\mathbf{r}; E) + \frac{e}{h} \int d\mathbf{r}' \int dE' \tilde{T}(\mathbf{r}, \mathbf{r}'; E, E') f(\mathbf{r}'; E') [1 - f(\mathbf{r}'; E)] \quad (3.1)$$

or equivalently,

$$\begin{aligned} \tilde{I}(\mathbf{r}; E) = & \frac{e}{h} \int d\mathbf{r}' \int dE' \{ \tilde{T}(\mathbf{r}', \mathbf{r}; E', E) f(\mathbf{r}; E) [1 - f(\mathbf{r}; E')] \\ & - \tilde{T}(\mathbf{r}, \mathbf{r}'; E, E') f(\mathbf{r}'; E') [1 - f(\mathbf{r}'; E)] \} \end{aligned} \quad (3.2)$$

where

$$\tilde{T}(\mathbf{r}, \mathbf{r}'; E, E') \equiv h P(\mathbf{r}, \mathbf{r}'; E) v_S(\mathbf{r}'; E, E') \quad (3.3)$$

Two “details” that were not discussed in Chapter 1, namely, (1) how the expression for  $v_S$  (eq. (1.21)) is obtained, and (2) how the expression for  $P$  (eq. (1.22)) is obtained. The first item has already been discussed in Chapter 2. In this chapter we will address the question of how the probability function is obtained (Section 3.1). This function is also used in the simplified derivation of the linearized transport equation presented in Section 1.3. In Section 3.2 we will show that at equilibrium the distribution function  $f(\mathbf{r}; E)$  relaxes to the Fermi-Dirac function with a constant chemical potential.

### 3.1. Derivation of the Probability Function

The probability function  $P(\mathbf{r}, \mathbf{r}'; E)$  tells us the fraction of electrons injected at  $\mathbf{r}'$  with energy  $E$  (by inelastic scattering from some other energy) that suffer an inelastic scattering event at  $\mathbf{r}$  *without suffering any inelastic scattering event 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 like one rung in a ladder series 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 a reinjection into a final energy  $E'$ . However, in calculating  $P(\mathbf{r}, \mathbf{r}'; E)$ , the second step is irrelevant. We just want the probability that an electron injected at  $\mathbf{r}'$  suffers its *very next* scattering event at  $\mathbf{r}$ ; the subsequent reinjection 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 particles having a decay rate of  $n/\tau_i$  per unit volume. The simplest way to describe decaying particles is to include an imaginary potential  $i\hbar/2\tau_i(\mathbf{r}; E)$  in the Schrödinger equation. More generally one could use an optical potential derived from the one-particle self-energy. Since we have assumed point 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  $G(\mathbf{r}, \mathbf{r}'; E)$  of the Schrödinger equation modified to include an imaginary potential  $i\hbar/2\tau_i(\mathbf{r}; E)$ , where  $\tau_i(\mathbf{r}; E)$  is the inelastic scattering time defined by eq. (2.16).

$$\left[ E - H_0 + \frac{i\hbar}{2\tau_i(\mathbf{r}; E)} \right] G(\mathbf{r}, \mathbf{r}'; E) = \delta(\mathbf{r} - \mathbf{r}') \quad (3.4)$$

Consider the continuity equation obeyed by the probability density

$$n = |G(\mathbf{r}, \mathbf{r}'; E)|^2 \quad (3.5a)$$

and the probability current density

$$\mathbf{J} = \frac{i\hbar}{2m} \left[ (\nabla G)^* G - G^* (\nabla G) \right] \quad (3.5b)$$

that we obtain from the solution to eq. (3.4). It can be shown from eqs. (3.4) and (3.5a,b) that

$$\nabla \cdot \mathbf{J} + \frac{n}{\tau_i} = \frac{i}{\hbar} \delta(\mathbf{r}-\mathbf{r}') [G-G^*] \quad (3.6)$$

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

$$\int d\mathbf{r} \frac{|G(\mathbf{r},\mathbf{r}';E)|^2}{\tau_i(\mathbf{r};E)} = \frac{2\pi}{\hbar} N_0(\mathbf{r}';E) \quad (3.7)$$

since  $N_0(\mathbf{r};E) = -\text{Im}\{G(\mathbf{r},\mathbf{r};E)\}/\pi$  [13]. The integrand on the left in eq. (3.4) is the steady-state current due to electrons lost from the coherent state by inelastic scattering (eq. (2.15)); the term on the right is the total steady-state current injected at  $\mathbf{r}'$  (Fig. 3.1). The ratio of these two terms is equal to the probability function  $P(\mathbf{r},\mathbf{r}';E)$ .

$$P(\mathbf{r},\mathbf{r}';E) = \frac{\hbar}{2\pi} \frac{|G(\mathbf{r},\mathbf{r}';E)|^2}{N_0(\mathbf{r}';E) \tau_i(\mathbf{r};E)} \quad (3.8)$$

### 3.2. Equilibrium State

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

$$f(\mathbf{r};E) = \frac{1}{1 + e^{(E - e\mu(\mathbf{r}))/k_B T}} \quad (3.9)$$

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. (3.9) with  $\mu(\mathbf{r}) = \mu_0$  (a constant) is indeed a solution to our transport equation (eq. (3.1)) with the external current  $\tilde{I}(\mathbf{r};E)$  set equal to zero; that is, we will show that

$$\frac{e}{\hbar} \int d\mathbf{r}' \int dE' \tilde{T}(\mathbf{r},\mathbf{r}';E,E') f_0(E') [1 - f_0(E)] = \frac{e N_0(\mathbf{r};E) f_0(E)}{\tau_i(\mathbf{r};E)} \quad (3.10)$$

where

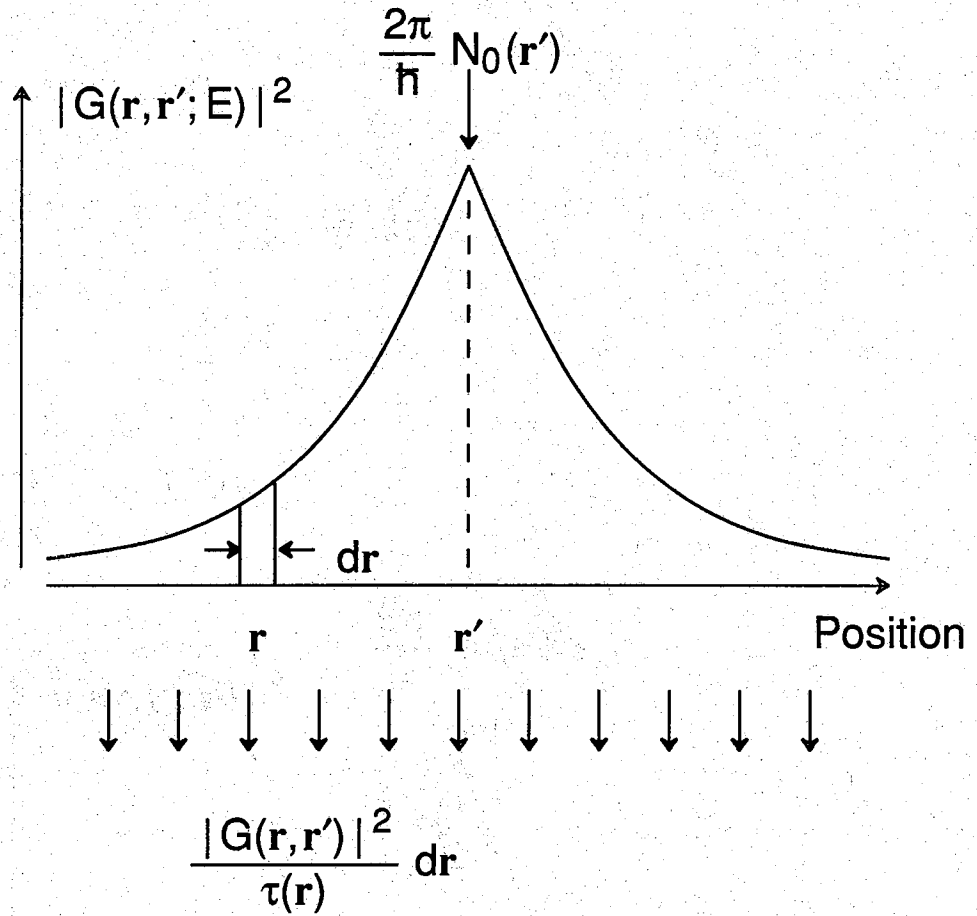


Fig. 3.1: Sketch of the probability density  $|G(\mathbf{r}, \mathbf{r}'; E)|^2$  calculated from eq. (3.4).

$$f_0(E) = \frac{1}{1 + e^{(E - e\mu_0)/k_B T}} \quad (3.11)$$

$\mu_0$  being a constant. It is easily shown that

$$f_0(E') [1 - f_0(E)] = f_0(E) [1 - f_0(E')] e^{(E - E')/k_B T} \quad (3.12)$$

It can be shown that (see Appendix)

$$\begin{aligned} \int dE' \tilde{T}(\mathbf{r}, \mathbf{r}'; E, E') [1 - f(\mathbf{r}'; E')] e^{(E - E')/k_B T} \\ = \hbar^2 \frac{|G(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_i(\mathbf{r}; E) \tau_i(\mathbf{r}'; E)} \equiv T(\mathbf{r}, \mathbf{r}'; E) \end{aligned} \quad (3.13)$$

Using eqs. (3.12) and (3.13) we can simplify the left-hand side of eq. (3.10) as follows.

$$\begin{aligned} \frac{e}{h} \int d\mathbf{r}' \int dE' \tilde{T}(\mathbf{r}, \mathbf{r}'; E, E') f_0(E') [1 - f_0(E)] \\ = \frac{e}{h} f_0(E) \int d\mathbf{r}' \int dE' \tilde{T}(\mathbf{r}, \mathbf{r}'; E, E') [1 - f_0(E')] e^{(E - E')/k_B T} \\ = \frac{e}{h} f_0(E) \int d\mathbf{r}' T(\mathbf{r}, \mathbf{r}'; E) \end{aligned} \quad (3.14)$$

It is further shown in the Appendix that

$$\int d\mathbf{r}' T(\mathbf{r}, \mathbf{r}'; E) = \int d\mathbf{r}' T(\mathbf{r}', \mathbf{r}; E) = \frac{\hbar N_0(\mathbf{r}; E)}{\tau_i(\mathbf{r}; E)} \quad (3.15)$$

Using eq. (3.15) in eq. (3.14) we obtain eq. (3.10), which is what we set out to prove.

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  $\epsilon_M$ ; these are then used to obtain the density of states  $N_0(\mathbf{r}; E)$  from eq. (2.8). The electron density  $n(\mathbf{r})$  can then be calculated from

$$n(\mathbf{r}) = \int dE f_0(E) N_0(\mathbf{r}; E) \quad (3.16)$$

The chemical potential  $\mu_0$  appearing in the Fermi-Dirac function  $f_0(E)$  (eq. (3.11)) is adjusted to obtain the correct average density of electrons in the structure. In general, the electron density  $n(\mathbf{r})$  obtained from eq. (3.16) should be inserted into the Poisson equation to obtain a corrected potential; the eigenfunctions  $\phi_M(\mathbf{r})$  and the eigenenergies  $\epsilon_M$  should then be recalculated including this potential, and iteration should continue until the solution is self-consistent.

## CHAPTER 4: LINEAR RESPONSE

In Section 4.1 we linearize the transport equation (eq. (3.2)) assuming local thermodynamic equilibrium, to obtain the ‘‘Continuous-Probe Landauer Formula.’’ We then obtain an expression for the dissipated power in Section 4.2. In Section 4.3 we discuss the conditions under which the ‘‘Continuous-Probe Landauer Formula’’ reduces to the drift-diffusion equations that are used to describe classical Brownian motion. Finally in Section 4.4 we compute the diffusion coefficient in a few simple cases using the present approach. Numerical results are presented for the conductivity of a disordered resistor. When the inelastic scattering time is short, the semiclassical and quantum conductivities agree well. But as the inelastic scattering is reduced, the quantum conductivity approaches zero due to strong localization while the semiclassical conductivity becomes constant.

### 4.1. Continuous-Probe Landauer Formula

To obtain the linear transport equation we assume that the structure is in *local thermodynamic equilibrium* so that the distribution function  $f(\mathbf{r}; E)$  can be written in the form of a Fermi-Dirac function with a local chemical potential  $\mu(\mathbf{r})$ .

$$f(\mathbf{r}; E) = \frac{1}{1 + e^{(E - e\mu(\mathbf{r}))/k_B T}} \quad (4.1)$$

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

$$f(E') [1 - f(E)] \Big|_{\text{at } \mathbf{r}} = f(E) [1 - f(E')] \Big|_{\text{at } \mathbf{r}} e^{(E - E')/k_B T} \quad (4.2)$$

Using eq. (4.2) we can simplify the non-linear transport equation (eq. (3.2)) as follows. First we integrate eq. (3.2) over  $E$  to obtain

$$I(\mathbf{r}) = \frac{e}{h} \int d\mathbf{r}' \{i(\mathbf{r}', \mathbf{r}) - i(\mathbf{r}, \mathbf{r}')\} \quad (4.3)$$

where



$$I(\mathbf{r}) = \int dE \tilde{I}(\mathbf{r}; E) \quad (4.4)$$

$$\begin{aligned} i(\mathbf{r}, \mathbf{r}') &\equiv \int dE \int dE' i(\mathbf{r}, \mathbf{r}'; E, E') \\ &= \int dE \int dE' \tilde{T}(\mathbf{r}, \mathbf{r}'; E, E') f(\mathbf{r}'; E') [1 - f(\mathbf{r}'; E)] \end{aligned} \quad (4.5)$$

Next we use eq. (4.2) to write

$$i(\mathbf{r}, \mathbf{r}') = \int dE f(\mathbf{r}'; E) \int dE' \tilde{T}(\mathbf{r}, \mathbf{r}'; E, E') [1 - f(\mathbf{r}'; E')] e^{(E-E')/k_B T} \quad (4.6)$$

Using eqs. (4.6) and (3.13) we can write eq. (4.3) as

$$I(\mathbf{r}) = \frac{e}{h} \int d\mathbf{r}' \int dE \{T(\mathbf{r}', \mathbf{r}; E) f(\mathbf{r}; E) - T(\mathbf{r}, \mathbf{r}'; E) f(\mathbf{r}'; E)\} \quad (4.7)$$

where

$$T(\mathbf{r}, \mathbf{r}'; E) = \hbar^2 \frac{|G(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_1(\mathbf{r}; E) \tau_1(\mathbf{r}'; E)} \quad (4.8)$$

$I(\mathbf{r})$  is the total current (over all energies) that is injected per unit volume at  $\mathbf{r}$ . At equilibrium,  $I(\mathbf{r}) = 0$  and the distribution function  $f(\mathbf{r}; E)$  is equal to a constant  $f_0(E)$  (eq. (3.11)) throughout the structure. It is easy to see that eq. (4.7) is satisfied under these conditions noting that (see eq. (3.15))

$$\int d\mathbf{r}' \{T(\mathbf{r}', \mathbf{r}; E) - T(\mathbf{r}, \mathbf{r}'; E)\} = 0 \quad (4.9)$$

Now 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

$$f(\mathbf{r}; E) \approx f_0(E) + \left[ \frac{-\partial f_0}{\partial E} \right] e (\mu(\mathbf{r}) - \mu_0) \quad (4.10)$$

Substituting eq. (4.10) into eq. (4.7) and using eq. (4.9) we obtain

$$I(\mathbf{r}) = \frac{e^2}{h} \int d\mathbf{r}' \{T_0(\mathbf{r}', \mathbf{r}) \mu(\mathbf{r}) - T_0(\mathbf{r}, \mathbf{r}') \mu(\mathbf{r}')\} \quad (4.11)$$

where

$$T_0(\mathbf{r}, \mathbf{r}') = \int dE \left[ \frac{-\partial f_0}{\partial E} \right] T(\mathbf{r}, \mathbf{r}'; E) \quad (4.12)$$

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

$$T_0(\mathbf{r}, \mathbf{r}') \approx T(\mathbf{r}, \mathbf{r}'; E = E_F) = \hbar^2 \frac{|G(\mathbf{r}, \mathbf{r}')|^2}{\tau_i(\mathbf{r}) \tau_i(\mathbf{r}')} \Big|_{E=E_F} \quad (4.13)$$

Eq. (4.11) can be viewed as a generalization of Büttiker's multiprobe Landauer formula,

$$I_i = \frac{e^2}{h} \sum_j \{T_{ji} \mu_i - T_{ij} \mu_j\} \quad (4.14)$$

to a continuous distribution of probes. For this reason we call it the "*Continuous-Probe Landauer Formula*." The coefficients  $T(\mathbf{r}, \mathbf{r}'; E)$  have the same symmetry properties in a magnetic field,  $H$  as the coefficients  $T_{ij}$ . Namely,

$$T(\mathbf{r}, \mathbf{r}'; E) \Big|_H = T(\mathbf{r}', \mathbf{r}; E) \Big|_{-H} \quad (4.15)$$

This is shown in the Appendix.

*Self-consistency:* In deriving eq. (4.11) from eq. (4.7) 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  $T(\mathbf{r}', \mathbf{r}; E)$  remain fixed. Actually the coefficients  $T(\mathbf{r}', \mathbf{r}; E)$  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 variations  $\delta I$ , we have accounted for one term,

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

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

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

where  $\delta T$  is the change in the coefficient  $T$ . This term is zero, however, because of the relation (eq. (4.9)) that must be satisfied by  $T(\mathbf{r}', \mathbf{r}; E)$ . Consequently, in linear response theory we can use the coefficients  $T(\mathbf{r}', \mathbf{r}; E)$  obtained (self-consistently) under equilibrium conditions, and ignore corrections due to the modification of the electrostatic potential by the applied bias.

#### 4.2. Power Dissipation and Circulating Currents

In general, we can solve eq. (4.11) for the potential distribution  $\mu(\mathbf{r})$  in any structure. At equilibrium,  $\mu(\mathbf{r})$  is equal to a constant  $\mu_0$ , and  $I(\mathbf{r})$  is equal to zero. Under these conditions it can be seen that eq. (4.11) is satisfied since (from eqs. (4.9) and (4.12))

$$\int d\mathbf{r}' \{T_0(\mathbf{r}', \mathbf{r}) - T_0(\mathbf{r}, \mathbf{r}')\} = 0 \quad (4.16)$$

Also, we note that (from eqs. (4.15) and (4.12)),

$$T_0(\mathbf{r}', \mathbf{r}) \Big|_H = T_0(\mathbf{r}, \mathbf{r}') \Big|_{-H} \quad (4.17)$$

In the absence of magnetic fields ( $H=0$ ),  $T_0(\mathbf{r}', \mathbf{r}) = T_0(\mathbf{r}, \mathbf{r}')$  so that at equilibrium the integrand in eq. (4.16) is zero, and there is *detailed balance* between any two points  $\mathbf{r}'$  and  $\mathbf{r}$ . 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. (4.16). Any outflow in one direction is balanced by an inflow from another.

We can rewrite eq. (4.11) in the form

$$I(\mathbf{r}) = \frac{e^2}{h} \int d\mathbf{r}' \{T_S(\mathbf{r}', \mathbf{r}) [\mu(\mathbf{r}) - \mu(\mathbf{r}')] + T_A(\mathbf{r}', \mathbf{r}) [\mu(\mathbf{r}) + \mu(\mathbf{r}')] \} \quad (4.18)$$

where

$$T_S(\mathbf{r}', \mathbf{r}) = \frac{1}{2} [T_0(\mathbf{r}', \mathbf{r}) + T_0(\mathbf{r}, \mathbf{r}')] \quad (4.19a)$$

$$T_A(\mathbf{r}', \mathbf{r}) = \frac{1}{2} [T_0(\mathbf{r}', \mathbf{r}) - T_0(\mathbf{r}, \mathbf{r}')] \quad (4.19b)$$

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

$$P_0 = \frac{e^2}{2h} \int d\mathbf{r} \int d\mathbf{r}' T_S(\mathbf{r}', \mathbf{r}) [\mu(\mathbf{r}) - \mu(\mathbf{r}')]^2 \quad (4.20)$$

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

$$\frac{e^2}{2h} \int d\mathbf{r} \int d\mathbf{r}' T_A(\mathbf{r}', \mathbf{r}) [\mu^2(\mathbf{r}) - \mu^2(\mathbf{r}')] = 0 \quad (4.21)$$

Eq. (4.21) follows readily if we note that from eqs. (4.9) and (4.12)

$$\int d\mathbf{r}' T_A(\mathbf{r}', \mathbf{r}) = \int d\mathbf{r} T_A(\mathbf{r}', \mathbf{r}) = 0 \quad (4.22)$$

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. 4.1). 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. (4.20) we obtain the following expression for the two-probe conductance  $g_0$ .

$$g_0 = \frac{e^2}{2h} \int d\mathbf{r} \int d\mathbf{r}' T_S(\mathbf{r}', \mathbf{r}) \left[ \frac{\mu(\mathbf{r}) - \mu(\mathbf{r}')}{\Delta\mu} \right]^2 \quad (4.23)$$

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

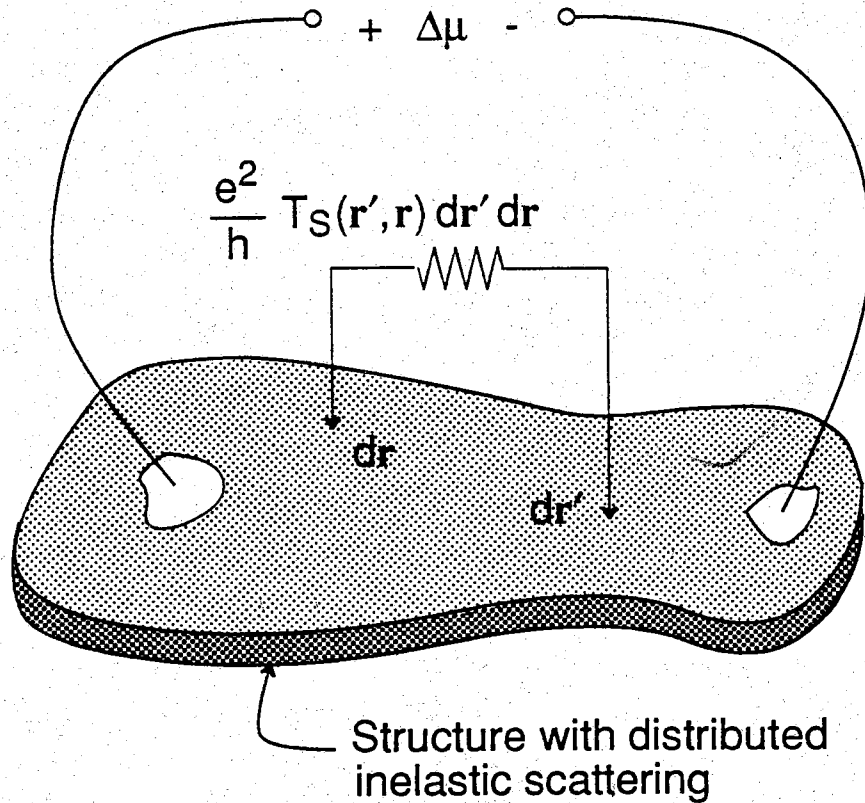


Fig. 4.1: Neglecting the circulating currents due to magnetic fields, any structure can be represented by a continuous network of conductors; any two volume elements  $d\mathbf{r}'$  and  $d\mathbf{r}$  are connected by a conductance equal to  $(e^2/h) T_S(\mathbf{r}', \mathbf{r}) d\mathbf{r}' d\mathbf{r}$ .

### 4.3. Relation to Classical Brownian Motion

Eq. (4.7) can be written in a slightly different form in terms of the electron density per unit energy  $n(\mathbf{r}; E) = N_0(\mathbf{r}; E) f(\mathbf{r}; E)$ .

$$\tilde{I}(\mathbf{r}; E) = e \int d\mathbf{r}' [\mathbf{v}(\mathbf{r}', \mathbf{r}; E) n(\mathbf{r}; E) - \mathbf{v}(\mathbf{r}, \mathbf{r}'; E) n(\mathbf{r}'; E)] \quad (4.24)$$

where

$$\mathbf{v}(\mathbf{r}', \mathbf{r}; E) = \frac{T(\mathbf{r}', \mathbf{r}; E)}{h N_0(\mathbf{r}; E)} \quad (4.25)$$

Eq. (4.24) has a simple physical interpretation.  $\mathbf{v}(\mathbf{r}', \mathbf{r}; E) d\mathbf{r}'$  tells us the fraction of electrons per unit time that “hop” from  $\mathbf{r}$  to  $\mathbf{r}'$ . The first term on the right of eq. (4.24) 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  $\nu_0$  is equal to the inelastic scattering rate; using eqs. (4.25) and (3.15) we have

$$\nu_0 \equiv \int d\mathbf{r}' \nu(\mathbf{r}', \mathbf{r}; E) = 1/\tau_i(\mathbf{r}; E) \quad (4.26)$$

Quantum transport is thus much like classical Brownian motion with a distribution of hopping lengths  $\mathbf{v}(\mathbf{r}', \mathbf{r}; E)$  that is determined quantum mechanically. In the absence of any externally injected current  $\tilde{I}(\mathbf{r}; E)$  we can write eq. (4.24) in the following form.

$$\int d\mathbf{r}' \zeta(\mathbf{r}, \mathbf{r}'; E) n(\mathbf{r}'; E) = 0 \quad (4.27)$$

where

$$\zeta(\mathbf{r}, \mathbf{r}'; E) = \frac{\delta(\mathbf{r} - \mathbf{r}')}{\tau_i(\mathbf{r}; E)} - \mathbf{v}(\mathbf{r}, \mathbf{r}'; E) \quad (4.28)$$

The obvious question to ask is under what conditions does eq. (4.27) reduce to the drift-diffusion equation

$$-D_{ij} \nabla_i \nabla_j n + v_{dj} \nabla_j n = 0 \quad (4.29)$$

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. (4.27) to eq. (4.29) 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.

$$\bar{\zeta}(\mathbf{r}, \mathbf{r}'; E) = \frac{1}{\tau_i} \delta(\mathbf{r} - \mathbf{r}') - \bar{\mathbf{v}}(\mathbf{r} - \mathbf{r}'; E) \quad (4.30)$$

Next we assume that  $\bar{\zeta} \bar{\mathbf{n}} \approx \bar{\zeta} \bar{\mathbf{n}}$  so that eq. (4.27) becomes a convolution integral.

$$\int d\mathbf{r}' \bar{\zeta}(\mathbf{r} - \mathbf{r}') \bar{\mathbf{n}}(\mathbf{r}') = 0 \quad (4.31)$$

We have suppressed the argument E for simplicity. Fourier transforming eq. (4.31) we obtain

$$\bar{\zeta}(\mathbf{q}) \bar{\mathbf{n}}(\mathbf{q}) = 0 \quad (4.32)$$

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

$$\bar{\zeta}(\mathbf{q}) \approx \bar{\zeta}(0) - i q_j v_{dj} - q_i q_j D_{ij} \quad (4.33)$$

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

$$\bar{\zeta}(0) = \int d\boldsymbol{\rho} \bar{\zeta}(\boldsymbol{\rho}) \quad (4.34)$$

$$v_{dj} = \int d\boldsymbol{\rho} \rho_j \bar{\mathbf{v}}(\boldsymbol{\rho}) \quad (4.35)$$

$$D_{ij} = \frac{1}{2} \int d\boldsymbol{\rho} \rho_i \rho_j \bar{\mathbf{v}}(\boldsymbol{\rho}) \quad (4.36)$$

where we have written  $\boldsymbol{\rho}$  for  $\mathbf{r} - \mathbf{r}'$ . Using eq. (4.26), (4.30) and (4.34) it is easy to show that  $\bar{\zeta}(0) = 0$ . Hence, inserting eq. (4.33) in eq. (4.32),

$$(i q_j v_{dj} + q_i q_j D_{ij}) \bar{\mathbf{n}}(\mathbf{q}) = 0 \quad (4.37)$$

Fourier transforming to real space we obtain the drift-diffusion equation (eq. (4.29)).

Eqs. (4.35) and (4.36) may be used to compute the drift velocity and diffusion coefficient from the ensemble-averaged hopping function  $\bar{\mathbf{v}}(\mathbf{r} - \mathbf{r}')$ . 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. (4.35) and (4.36). We feel that in general eq. (4.11) 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. (4.35) and (4.36) are more convenient (see Section 4.4 for a few examples).

#### 4.4. Simple Examples

In this section we will consider two simple examples where the electron density varies slowly enough that we can use eqs. (4.35) and (4.36) to calculate the drift velocity and diffusion coefficient respectively. First we consider the semiclassical magnetoresistance of a free electron gas with isotropic scattering described by an inelastic scattering time  $\tau_i$ . In this case we compute the function  $v(\mathbf{p})$  directly from the classical trajectory and use it in eq. (4.35) or (4.36). 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  $v(\mathbf{p})$  numerically, ensemble-average it and obtain the diffusion coefficient  $D$  from eq. (4.36) for different values of the inelastic scattering time  $\tau_i$  (assumed constant everywhere). For small values of  $\tau_i$ , we find that the semiclassical and quantum values of the diffusion coefficient  $D$  agree very well while at large values of  $\tau_i$  the two values differ significantly due to quantum localization.

##### 4.4.1. 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 ( $\tau_i$  is the inelastic scattering time, assumed constant)

$$P(\mathbf{r}, \mathbf{0}; E) = \int_0^{\infty} \frac{dt}{\tau_i} \delta(\mathbf{r} - \mathbf{r}_0(t)) e^{-t/\tau_i} \quad (4.38)$$

We note from eqs. (3.15) and (4.25) that



$$\int d\mathbf{r} v(\mathbf{r}, \mathbf{0}; E) = 1/\tau_i \quad (4.39)$$

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

$$v(\mathbf{r}, \mathbf{0}; E) = \int_0^\infty \frac{dt}{\tau_i^2} \delta(\mathbf{r} - \mathbf{r}_0(t)) e^{-t/\tau_i} \quad (4.40)$$

Using eqs. (4.35) and (4.36) we obtain

$$v_{dx} = \int_0^\infty \frac{dt}{\tau_i^2} e^{-t/\tau_i} x_0(t) \quad (4.41)$$

$$D_{xx} = \frac{1}{2} \int_0^\infty \frac{dt}{\tau_i^2} e^{-t/\tau_i} x_0^2(t) \quad (4.42)$$

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

Next 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. (4.41) and (4.42):

$$\langle v_{dx} \rangle = \left\langle \int_0^\infty \frac{dt}{\tau_i^2} v_x t e^{-t/\tau_i} \right\rangle = \langle v_x \rangle = 0 \quad (4.43)$$

$$\langle D_{xx} \rangle = \left\langle \int_0^\infty \frac{dt}{\tau_i^2} v_x^2 t^2 e^{-t/\tau_i} \right\rangle = \langle v_x^2 \tau_i \rangle \neq 0 \quad (4.44)$$

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,

$$\langle v_{dx} \rangle = \left\langle \int_0^{\infty} \frac{dt}{\tau_i^2} \left( v_x t + \frac{a_x t^2}{2} \right) e^{-t/\tau_i} \right\rangle = \langle v_x \rangle + \langle a_x \tau_i \rangle \quad (4.45)$$

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,

$$\langle v_{dx} \rangle = \frac{e \tau_i}{m} \mathcal{E}_x \quad (4.46)$$

Finally, we assume a magnetic field along the z-axis, and an electric field in the x-y plane. It can be shown [43] that the x-component of the classical trajectory is:

$$x_0(t) = \left[ \frac{a_x}{\omega_c^2} - \frac{v_y}{\omega_c} \right] (1 - \cos \omega_c t) + \left[ \frac{a_y}{\omega_c^2} + \frac{v_x}{\omega_c} \right] \sin \omega_c t - \frac{a_y}{\omega_c} t \quad (4.47)$$

where we have introduced the cyclotron frequency for an electron  $\omega_c = |e|B/m$ . Substituting eq. (4.47) into eq. (4.41) and performing the necessary integrals, we obtain the drift velocity,

$$v_{dx} = \left[ \frac{a_x}{\omega_c} - v_y \right] \frac{\omega_c \tau_i}{1 + \omega_c^2 \tau_i^2} + \left[ \frac{a_y}{\omega_c} + v_x \right] \frac{1}{1 + \omega_c^2 \tau_i^2} - \frac{a_y}{\omega_c} \quad (4.48)$$

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,

$$\langle v_{dx} \rangle = \frac{e \tau_i}{m} \left[ \frac{\mathcal{E}_x}{1 + \omega_c^2 \tau_i^2} - \frac{\mathcal{E}_y \omega_c \tau_i}{1 + \omega_c^2 \tau_i^2} \right] \quad (4.49)$$

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

$$\sigma_{xx} = \left. \frac{e n v_{dx}}{\mathcal{E}_x} \right|_{\mathcal{E}_y=0} = \frac{\sigma_0}{1 + \omega_c^2 \tau_i^2} \quad (4.50a)$$

$$\sigma_{xy} = \left. \frac{e n v_{dx}}{\mathcal{E}_y} \right|_{\mathcal{E}_x=0} = -\sigma_0 \frac{\omega_c \tau_i}{1 + \omega_c^2 \tau_i^2} \quad (4.50b)$$

Following a similar derivation for the y-component of the drift velocity, we can define  $\sigma_{yx}$  and  $\sigma_{yy}$ , and obtain the usual magnetoconductivity tensor [42],

$$\sigma = \frac{\sigma_0}{1 + \omega_c^2 \tau_i^2} \begin{bmatrix} 1 & -\omega_c \tau_i \\ \omega_c \tau_i & 1 \end{bmatrix} \quad (4.51)$$

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.

#### 4.4.2. 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, the conductance decreases exponentially with length. Electron wave functions 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.

A 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  $\tau_i$ . We will show that as  $\tau_i$  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  $\tau_i$ . Our numerical solution has been described in detail elsewhere [33,42]. In the following discussion, we focus more

on the physical assumptions in our model, rather than the details of computing a numerical solution.

To this point we have worked in the position representation, using a basis  $|r\rangle$ ; we could, however, rephrase all previous discussion to correspond to another basis, say  $|k\rangle$ . In this case, inelastic scatterers would be independent point-sources not in position, but in momentum. Such 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. Borrowing from the solution techniques used in microwave engineering, we will describe transport using the basis  $|x, k_{y,m}\rangle$ , where  $m$  enumerates modes in the transverse ( $y$ ) direction. In 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  $m$ . We can evaluate the ensemble-averaged diffusion coefficient as described in Section 4.3 by determining the second moment of the distribution  $\bar{v}(\rho)$

$$D_{xx,n} = \frac{1}{2} \sum_m \left[ \int d\rho_x \rho_x^2 v_{mn}(\rho_x) \right] \quad (4.52)$$

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

$$D_{xx} = \frac{1}{2M} \int d\rho_x \rho_x^2 \left[ \sum_{m,n} v_{mn}(\rho_x) \right] \quad (4.53)$$

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. (3.4)). 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  $L_D$ ,

$$\left\langle \sum_{m,n} v_{mn}(\rho_x) \right\rangle \equiv v_0 e^{-|\rho_x|/L_D} \quad (4.54)$$

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

$$\sum_m \int d\rho_x v_{mn}(\rho_x) = \frac{1}{\tau_{i,n}} \quad (4.55)$$

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

$$\int d\rho_x \left\langle \sum_{m,n} v_{mn}(\rho_x) \right\rangle = \frac{M}{\tau_i} \quad (4.56)$$

After determining  $v_0$ , we evaluate eq. (4.53) with the functional form stated in eq. (4.54).

$$D_{xx} = \frac{1}{4\tau_i L_D} \int_{-\infty}^{+\infty} d\rho_x \rho_x^2 e^{-|\rho_x|/L_D} = \frac{L_D^2}{\tau_i} \quad (4.57)$$

Our solution hinges upon determining the ensemble-averaged decay length  $L_D$  for the transmission function within a long wire. The numerical solution proceeds as follows.

For each random configuration of impurities, we must determine the Green function of the Schrödinger equation:

$$\left[ \frac{d^2}{dx^2} + k_m^2 \right] G_{mn}(x) = \delta(x) \delta_{mn} \quad (4.58)$$

where  $G_{mn}(x)$  represents the amplitude in mode  $m$  at position  $x$  for an electron injected in mode  $n$  at position  $x=0$ . Solutions for the wavefunction on either side of  $x=0$  can be determined by ordinary means--for example, with the use of scattering matrices, as described in Ref. [33]. Each impurity is represented by a scattering matrix, which specifies coupling between the 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  $x=0$ , we introduce the following boundary conditions:

$$G_{mn}(x=0^+) = G_{mn}(x=0^-) \quad (4.59a)$$

$$\left. \frac{dG_{mn}}{dx} \right|_{x=0^+} - \left. \frac{dG_{mn}}{dx} \right|_{x=0^-} = \delta_{mn} \quad (4.59b)$$

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  $G_{mn}(x)$  is comprised of (real) probabilities rather than (complex) probability amplitudes. In any event, the solution of  $G_{mn}(x)$  for a particular impurity configuration determines the hopping distribution, which is fit to a decaying exponential (eq. (4.54)) 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. [44] 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  $L_D$ .

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 was immediately left of the 200<sup>th</sup> impurity. All impurities were characterized by the same scattering matrix, and the impurity strength was chosen so that the elastic scattering length  $\Lambda_{el}$  was 4 impurities, corresponding to an elastic scattering time of  $\tau_0 = 2.87 \times 10^{-11}$  s [33]. An estimate of the localization length is  $\Lambda_{loc} \approx M\Lambda_{el}$  [45], where  $M$  is the number of propagating modes. For the present example, samples should exhibit localization when the inelastic scattering length  $\Lambda_i$  exceeds 20 impurities. Inelastic scattering times were chosen between  $10^{-12}$  s and  $10^{-8}$  s, corresponding to  $\Lambda_i$  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  $\tau_i$ . These results are presented in Fig. 4.2 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. 4.3 we present the ensemble-averaged diffusion coefficient  $D$  for both semiclassical and quantum analyses. For small  $\tau_i$ , inelastic scattering dominates, and both solutions are in close agreement. As  $\tau_i$  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 wave function between successive scatterers, the semiclassical analysis cannot account for localization.

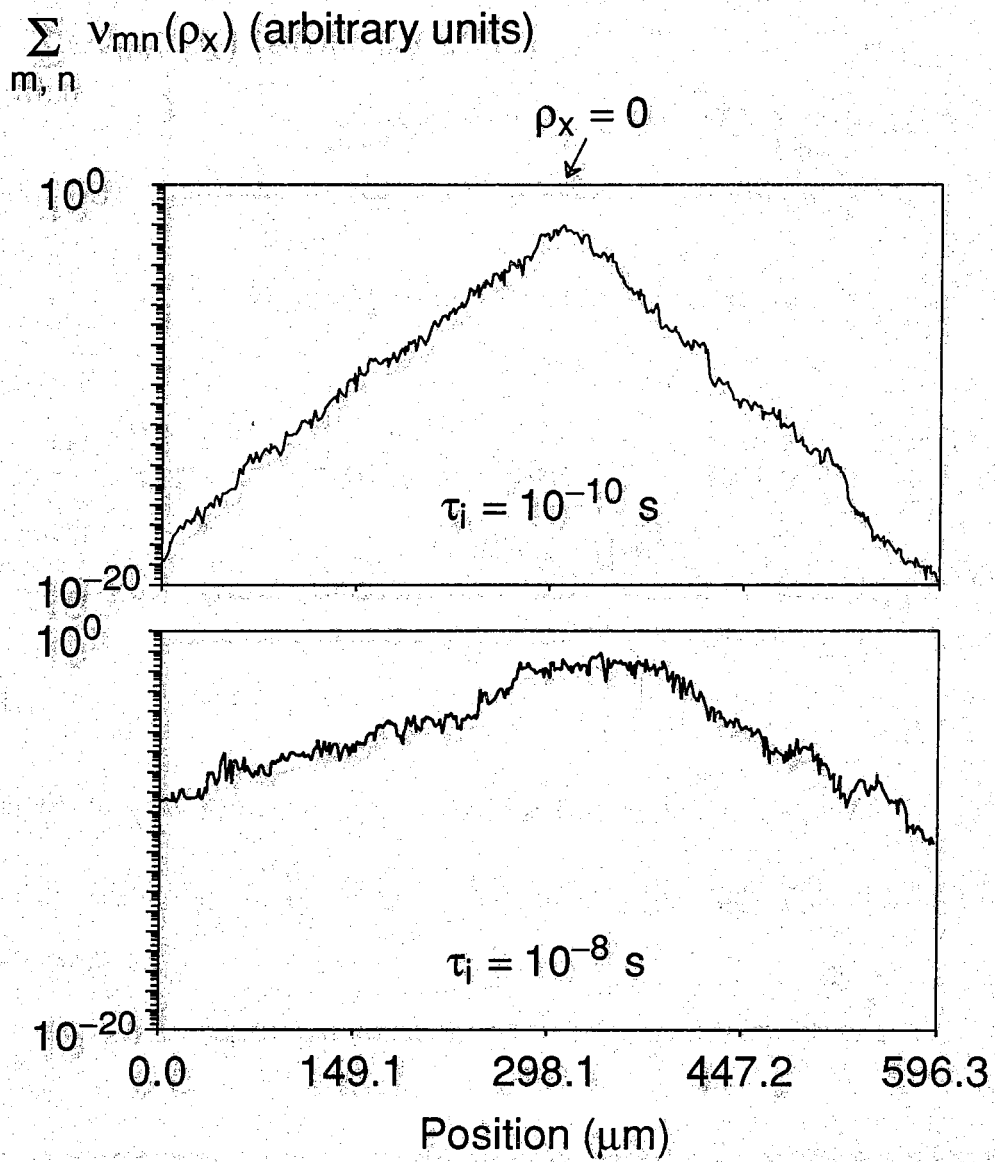


Fig. 4.2: The hopping distribution  $\sum_{m,n} v_{mn}(\rho_x)$  for two arbitrary samples with different inelastic scattering times  $\tau_i$ . Both functions exhibit the general character of exponential decay.



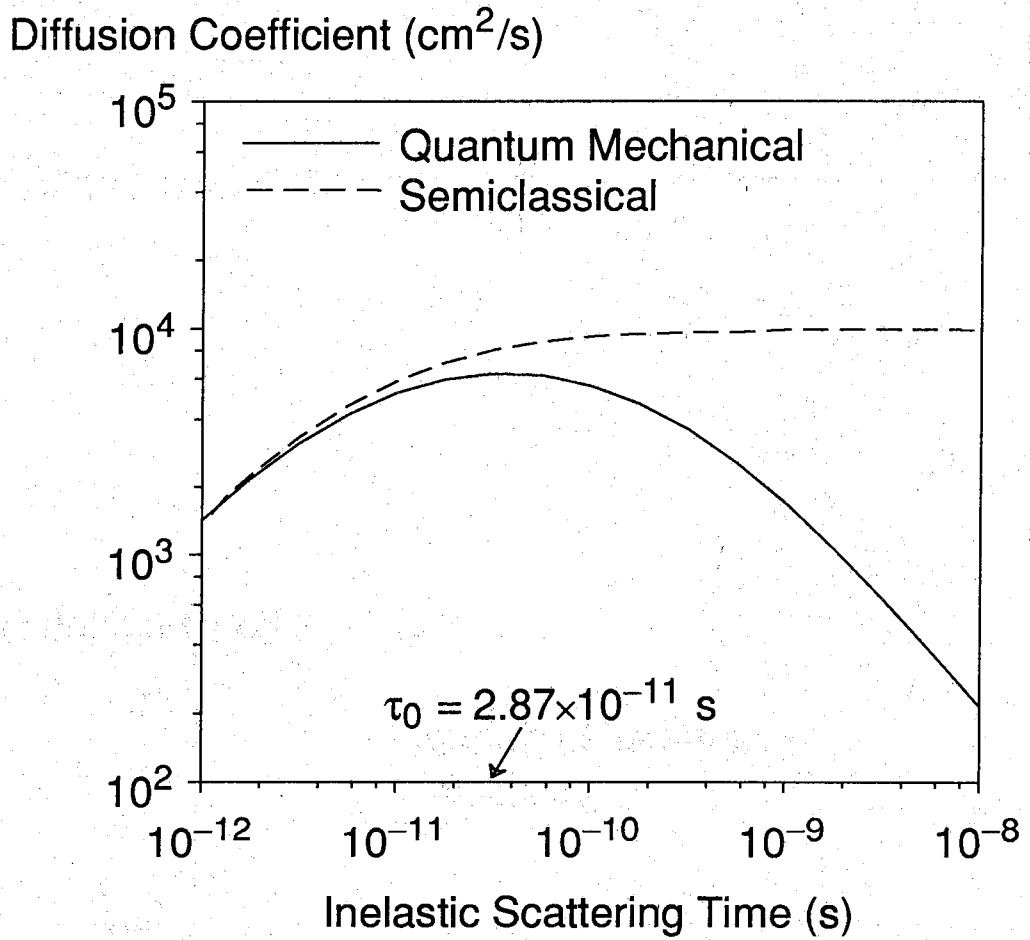


Fig. 4.3: The ensemble-averaged diffusion coefficient as a function of  $\tau_i$  for both semiclassical and quantum analyses. The quantum result decreases rapidly for large  $\tau_i$ , a demonstration of strong localization.

## SUMMARY OF IMPORTANT RESULTS

### *The Model*

Electron propagation is assumed to be described by the one electron Hamiltonian

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

having eigenfunctions  $\Phi_M(\mathbf{r})$  with eigenvalues  $\epsilon_M$ . Inelastic scattering is assumed to arise from a continuous distribution of point oscillators whose distribution per unit volume per unit energy is given by  $J_0(\mathbf{r}; \hbar\omega)$ .

$$J(\mathbf{r}, \hbar\omega) = \begin{cases} \frac{2\pi}{\hbar} |U(\mathbf{r}; \hbar\omega)|^2 J_0(\mathbf{r}; \hbar\omega) (N(\mathbf{r}; \hbar\omega) + 1) , & \hbar\omega > 0 \\ \frac{2\pi}{\hbar} |U(\mathbf{r}; -\hbar\omega)|^2 J_0(\mathbf{r}; -\hbar\omega) N(\mathbf{r}; -\hbar\omega) , & \hbar\omega < 0 \end{cases} \quad (2.6)$$

where  $N(\mathbf{r}; \hbar\omega)$  is the number of phonons occupying an oscillator with frequency  $\omega$  at  $\mathbf{r}$  and  $U(\mathbf{r}; \hbar\omega)$  is the interaction potential between the electron and the oscillators.

### *Density of states, $N_0(\mathbf{r}; E)$*

$$N_0(\mathbf{r}; E) = \sum_M |\Phi_M(\mathbf{r})|^2 \delta(E - \epsilon_M) \quad (2.8)$$

### *Distribution function, $f(\mathbf{r}; E)$*

$$n(\mathbf{r}) = \int dE n(\mathbf{r}; E) = \int dE N_0(\mathbf{r}; E) f(\mathbf{r}; E) \quad (2.10)$$

*Inelastic Lifetime,  $\tau_i(\mathbf{r}; E)$*

$$\frac{1}{\tau_i(\mathbf{r}; E)} = \int dE' \left[ [1 - f(E')] N_0(E') J(E-E') \right]_{\text{at } \mathbf{r}} \quad (2.16)$$

*Transport Equation*

$$\frac{e N_0(\mathbf{r}; E) f(\mathbf{r}; E)}{\tau(\mathbf{r}; E)} = \tilde{I}(\mathbf{r}; E) + \frac{e}{h} \int d\mathbf{r}' \int dE' \tilde{T}(\mathbf{r}, \mathbf{r}'; E, E') f(\mathbf{r}'; E') [1 - f(\mathbf{r}'; E)] \quad (3.1)$$

$$\begin{aligned} \tilde{I}(\mathbf{r}; E) = & \frac{e}{h} \int d\mathbf{r}' \int dE' \{ \tilde{T}(\mathbf{r}', \mathbf{r}; E', E) f(\mathbf{r}; E) [1 - f(\mathbf{r}; E')] \\ & - \tilde{T}(\mathbf{r}, \mathbf{r}'; E, E') f(\mathbf{r}'; E') [1 - f(\mathbf{r}'; E)] \} \end{aligned} \quad (3.2)$$

*Kernel,  $\tilde{T}(\mathbf{r}, \mathbf{r}'; E, E')$*

$$\tilde{T}(\mathbf{r}, \mathbf{r}'; E, E') \equiv h P(\mathbf{r}, \mathbf{r}'; E) v_s(\mathbf{r}'; E, E') \quad (3.3)$$

$$P(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar}{2\pi} \frac{|G(\mathbf{r}, \mathbf{r}'; E)|^2}{N_0(\mathbf{r}'; E) \tau_i(\mathbf{r}; E)} \quad (3.8)$$

$$v_s(\mathbf{r}; E', E) = J(E-E') N_0(E') N_0(E) \Big|_{\text{at } \mathbf{r}} \quad (2.12a)$$

*Green Function,  $G(\mathbf{r}, \mathbf{r}'; E)$*

$$\left[ E - H_0 + \frac{i\hbar}{2\tau_i(\mathbf{r}; E)} \right] G(\mathbf{r}, \mathbf{r}'; E) = \delta(\mathbf{r} - \mathbf{r}') \quad (3.4)$$

*Linearized Transport Equation*

$$I(r) = \frac{e^2}{h} \int dr' \{ T_0(r', r) \mu(r) - T_0(r, r') \mu(r') \} \quad (4.11)$$

where

$$f(r; E) = \frac{1 + e^{(E - e\mu(r))/k_B T}}{1} \quad (4.1)$$

*Kernel,  $T_0(r, r')$*

$$T_0(r, r') = \int dE \left[ -\frac{\partial f_0}{\partial E} \right] T(r, r'; E) \quad (4.12)$$

$$T(r, r'; E) = \hbar^2 \frac{t_1(r; E) t_1(r'; E)}{|G(r, r'; E)|^2} \quad (4.8)$$

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**Appendix: Derivations of Important Relations Used in the Text**

**1. Eqs. (1.34a,b):**

$$\sigma_o(\mathbf{r}, \mathbf{r}') = \int dE \left[ -\frac{\partial f_o}{\partial E} \right] \sigma(\mathbf{r}, \mathbf{r}'; E)$$

$$\sigma(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar}{2\pi} \sum_{N,M} \left[ \mathbf{J}_{NM}(\mathbf{r}) \otimes \mathbf{J}_{MN}(\mathbf{r}') \right] G_M^R(E) G_N^A(E)$$

We start from eq. (1.4) in the text and write it as

$$C_{JJ} = C_1 - C_2 \quad (A.1)$$

where 
$$C_1(\mathbf{r}, \mathbf{r}'; \omega) = \frac{i}{\hbar} \int_0^{\infty} dt e^{i\omega t} \langle \mathbf{J}(\mathbf{r}, t) \mathbf{J}(\mathbf{r}, 0) \rangle \quad (A.2a)$$

$$C_2(\mathbf{r}, \mathbf{r}'; \omega) = \frac{i}{\hbar} \int_0^{\infty} dt e^{i\omega t} \langle \mathbf{J}(\mathbf{r}, 0) \mathbf{J}(\mathbf{r}, t) \rangle \quad (A.2b)$$

The current density operator can be written as

$$\mathbf{J}(\mathbf{r}, t) = \sum_{N,M} \mathbf{J}_{NM}(\mathbf{r}) a_N^\dagger(t) a_M(t) \quad (A.3)$$

where  $\mathbf{J}_{NM}(\mathbf{r})$  is defined in eq. (1.35) and  $a_N^\dagger, a_N$  are the creation and annihilation operators for the eigenstate N. Substituting eq. (A.3) into eq. (A.2a),

$$C_1(\mathbf{r}, \mathbf{r}'; \omega) = \sum_{N,M,N',M'} \mathbf{J}_{NM}(\mathbf{r}) \mathbf{J}_{N'M'}(\mathbf{r}') \frac{i}{\hbar} \int_0^{\infty} dt e^{i\omega t} \langle a_N^\dagger(t) a_M(t) a_{N'}^\dagger(0) a_{M'}(0) \rangle \quad (A.4)$$

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



$$C_1(\mathbf{r}, \mathbf{r}'; \omega) = \sum_{N,M} \mathbf{J}_{NM}(\mathbf{r}) \mathbf{J}_{MN}(\mathbf{r}') F_1(\omega) \quad (\text{A.5a})$$

where

$$\begin{aligned} F_1(\omega) &= \frac{i}{\hbar} \int_0^{\infty} dt e^{i\omega t} \langle a_N^\dagger(t) a_N(0) \rangle \langle a_M(t) a_M^\dagger(0) \rangle \\ &= - \frac{f_o(\epsilon_N) [1 - f_o(\epsilon_M)]}{\hbar\omega + \epsilon_N - \epsilon_M + i\eta} \end{aligned} \quad (\text{A.5b})$$

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

$$C_2(\mathbf{r}, \mathbf{r}'; \omega) = \sum_{N,M} \mathbf{J}_{NM}(\mathbf{r}) \mathbf{J}_{MN}(\mathbf{r}') F_2(\omega) \quad (\text{A.6a})$$

$$\text{where } F_2(\omega) = - \frac{f_o(\epsilon_M) [1 - f_o(\epsilon_N)]}{\hbar\omega + \epsilon_N - \epsilon_M + i\eta} \quad (\text{A.6b})$$

Substituting eqs. (A.5a,b) and (A.6a,b) into eq. (A.1) we have

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

$$\text{where } F_{NM}(\omega) = F_1 - F_2 = \frac{f_o(\epsilon_M) - f_o(\epsilon_N)}{\hbar\omega + \epsilon_N - \epsilon_M + i\eta} \quad (\text{A.7b})$$

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

$$F_{NM}(\omega) = \int d\epsilon \left[ - \frac{f_o(\epsilon + \hbar\omega) \delta(\epsilon - \epsilon_M + \hbar\omega)}{\epsilon - \epsilon_N - i\eta} - \frac{f_o(\epsilon) \delta(\epsilon - \epsilon_N)}{\epsilon - \epsilon_M + \hbar\omega + i\eta} \right] \quad (\text{A.8})$$

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.8),

$$F_{NM}(\omega) = \int \frac{d\epsilon}{2\pi i} \left[ -f_0(\epsilon + \hbar\omega) G_N^A(\epsilon) [G_M^A(\epsilon + \hbar\omega) - G_M^R(\epsilon + \hbar\omega)] \right. \\ \left. - f_0(\epsilon) G_M^R(\epsilon + \hbar\omega) [G_N^A(\epsilon) - G_N^R(\epsilon)] \right] \quad (\text{A.9})$$

where

$$G_M^R(\epsilon) \equiv \frac{1}{\epsilon - \epsilon_M + i\eta} \quad (\text{A.10a})$$

$$G_M^A(\epsilon) \equiv \frac{1}{\epsilon - \epsilon_M - i\eta} \quad (\text{A.10b})$$

For small  $\omega$ , we can write eq. (A.9) as

$$F_{NM}(\omega) \approx i\omega a_{NM} + b_{NM} \quad (\text{A.11a})$$

where

$$a_{NM} = \frac{\hbar}{2\pi} \int d\epsilon \left[ -\frac{\partial f_0}{\partial \epsilon} \right] G_M^R(\epsilon) G_N^A(\epsilon) \quad (\text{A.11b})$$

$$b_{NM} = \frac{1}{2\pi i} \int d\epsilon f_0(\epsilon) [G_N^R(\epsilon) G_M^R(\epsilon) - G_N^A(\epsilon) G_M^A(\epsilon)] \quad (\text{A.11c})$$

Using eqs. (A.7a), (A.11) and (A.12a,b) we obtain from eq. (1.3)

$$[\sigma_0(\mathbf{r}, \mathbf{r}')]_{\alpha\beta} = A + \frac{1}{i\omega} \left( B - \frac{ne^2}{m} \delta(\mathbf{r} - \mathbf{r}') \delta_{\alpha\beta} \right) \quad (\text{A.12a})$$

$$\text{where} \quad A = \sum_{N,M} [\mathbf{J}_{NM}(\mathbf{r}) \otimes \mathbf{J}_{MN}(\mathbf{r}')]_{\alpha\beta} a_{NM} \quad (\text{A.12b})$$

$$B = \sum_{N,M} [\mathbf{J}_{NM}(\mathbf{r}) \otimes \mathbf{J}_{MN}(\mathbf{r}')]_{\alpha\beta} b_{NM} \quad (\text{A.12c})$$

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.11b) and (A.12b) we obtain eqs. (1.34a,b):

$$\sigma_o(\mathbf{r}, \mathbf{r}') = \frac{\hbar}{2\pi} \int d\epsilon \left[ -\frac{\partial f_o}{\partial \epsilon} \right] \sum_{N,M} [\mathbf{J}_{NM}(\mathbf{r}) \otimes \mathbf{J}_{MN}(\mathbf{r}')] G_M^R(\epsilon) G_N^A(\epsilon) \quad (\text{A.13})$$

2. Eq. (3.13):

$$\begin{aligned} & \int dE' \tilde{T}(\mathbf{r}, \mathbf{r}'; E, E') [1 - f(\mathbf{r}'; E')] e^{(E-E')/k_B T} \\ &= \hbar^2 \frac{|G(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_i(\mathbf{r}; E) \tau_i(\mathbf{r}'; E)} \equiv T(\mathbf{r}, \mathbf{r}'; E) \end{aligned}$$

To prove the above relation we start with the left hand side and use eqs. (3.3), (3.8) and (2.12a) to substitute for  $\tilde{T}$ .

$$\begin{aligned} & \int dE' \tilde{T}(\mathbf{r}, \mathbf{r}'; E, E') [1 - f(\mathbf{r}'; E')] e^{(E-E')/k_B T} \\ &= \frac{\hbar^2 |G(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_i(\mathbf{r}; E)} \int dE' e^{(E-E')/k_B T} \left[ [1 - f(E')] N_0(E') J(E'-E) \right]_{\text{at } \mathbf{r}'} \quad (\text{A.14}) \end{aligned}$$

Using eqs. (2.14) and (2.16),

$$\begin{aligned} & \int dE' e^{(E-E')/k_B T} \left[ [1 - f(E')] N_0(E') J(E'-E) \right]_{\text{at } \mathbf{r}'} \\ &= \int dE' \left[ [1 - f(E')] N_0(E') J(E-E') \right]_{\text{at } \mathbf{r}'} \\ &= 1/\tau_i(\mathbf{r}'; E) \quad (\text{A.15}) \end{aligned}$$

Using eq. (A.15) in eq. (A.14) we obtain the desired relationship.

3. Eq. (4.15):

$$T(\mathbf{r}, \mathbf{r}'; E) \Big|_H = T(\mathbf{r}', \mathbf{r}; E) \Big|_{-H}$$

We know from eq. (3.13) that

$$T(\mathbf{r}, \mathbf{r}'; E) = \hbar^2 \frac{|G(\mathbf{r}, \mathbf{r}'; E)|^2}{\tau_i(\mathbf{r}, E) \tau_i(\mathbf{r}'; E)} \quad (\text{A.16})$$

The above relationship (eq. (4.15)) follows from the well-known symmetry property of the Green function:

$$G(\mathbf{r}, \mathbf{r}'; E) \Big|_H = G(\mathbf{r}', \mathbf{r}; E) \Big|_{-H} \quad (\text{A.17})$$

4. Eq. (3.15):

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

We showed in Chapter 3 that (see eq. (3.7))

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

Using eqs. (A.16) and (A.18) we obtain

$$\int d\mathbf{r} T(\mathbf{r}, \mathbf{r}'; E) = \frac{\hbar N_0(\mathbf{r}'; E)}{\tau_i(\mathbf{r}'; E)} \quad (\text{A.19})$$

This proves half the desired result. To prove the other half we note that, using eq. (4.15) derived earlier,

$$\begin{aligned} \int d\mathbf{r} T(\mathbf{r}', \mathbf{r}; E) \Big|_H &= \int d\mathbf{r} T(\mathbf{r}, \mathbf{r}'; E) \Big|_{-H} \\ &= \frac{\hbar N_0(\mathbf{r}'; E)}{\tau_i(\mathbf{r}'; E)} \Big|_{-H} \quad (\text{using eq. (A.18)}) \end{aligned} \quad (\text{A.20})$$

But we have by definition (eq. (2.8)),

$$N_0(\mathbf{r}; E) = \sum_M |\phi_M(\mathbf{r})|^2 \delta(E - \epsilon_M) \quad (\text{A.21})$$

where  $\phi_M(\mathbf{r})$  are the eigenfunctions of  $H_0$  (eq. (2.1)) with eigenvalues  $\epsilon_M$ . The reversal of the magnetic field  $H$  merely replaces each eigenfunction  $\phi_M(\mathbf{r})$  by its complex conjugate leaving the density of states  $N_0(\mathbf{r}; E)$  intact. Hence

$$N_0(\mathbf{r}; E) \Big|_H = N_0(\mathbf{r}; E) \Big|_{-H} \quad (\text{A.22})$$

Another way to prove eq. (A.22) is to note that  $N_0(\mathbf{r}; E) = -\text{Im}\{G(\mathbf{r}, \mathbf{r}; E)\}/\pi$  and to use eq. (A.18). Also from eqs. (2.16) and (A.22) we have

$$\tau_i(\mathbf{r}; E) \Big|_H = \tau_i(\mathbf{r}; E) \Big|_{-H} \quad (\text{A.23})$$

Using eqs. (A.22) and (A.23) in eq. (A.20) we obtain

$$\int d\mathbf{r} T(\mathbf{r}', \mathbf{r}; E) \Big|_H = \frac{\hbar N_0(\mathbf{r}'; E)}{\tau_i(\mathbf{r}'; E)} \Big|_{-H} \quad (\text{A.24})$$

This completes our proof.