

What is measured when you measure a resistance?— The Landauer formula revisited

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We re-examine the question of what constitutes the physically relevant quantum-mechanical expression for the resistance of a disordered conductor in light of recent experimental and theoretical advances in our understanding of the conducting properties of mesoscopic systems. It is shown that in the absence of a magnetic field, the formula proposed by Büttiker, which expresses the current response of a multi-port conductor in terms of transmission matrices, is derivable straightforwardly from linear response theory. We also present a general formalism for solving these equations for the resistance given the scattering matrix. This Landauer-type formula reduces to $g = (e^2/h) \text{Tr}(tt^\dagger)$, where g is the conductance and t is the transmission matrix, for the two-probe case. It is suggested

that this formula provides the best description of the present class of experiments performed in two-probe or multi-probe measuring configurations, and that the subtleties leading to various different Landauer formulae are not relevant to these experiments. This is not because of the large number of channels in real conductors, but is due to the fact that apparently no present experiment probes a “local chemical potential” in the conductor. Certain standard objections to deriving a Landauer-type formula from linear response theory are answered. Applications of this formula to fluctuations in disordered multi-probe conductors are discussed.

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1. Introduction

It is entirely appropriate that a volume on the physics of mesoscopic systems contain an updated discussion of the Landauer formula. The new discoveries concerning the novel conducting properties of small systems have certainly clarified and sharpened many of the issues that have been raised by a variety of authors who have attempted to

understand the relationship between the conductance of a quantum-mechanical system and an associated scattering problem. Furthermore, Landauer's great insight, that conduction in solids can be thought of as a scattering problem, has certainly been of great practical importance in guiding our intuition to an understanding of quantum transport in mesoscopic systems. This paper has somewhat the character of a review article, and is divided into four main sections. First, we summarize the major developments in modern thinking about the Landauer formula since 1980, leading up to the very recent developments relating to the physics of multi-probe mesoscopic devices. Second, we present a complete and rigorous derivation of a multi-probe generalization of the Landauer formula from linear response theory. This formula was first written down explicitly and justified on phenomenological grounds by Büttiker [1]. An alternative representation of the current response of a multi-probe conductor in terms of Green functions, starting from the Kubo formula, has been widely employed recently to calculate voltage fluctuations in mesoscopic multi-probe devices [2-7]; these calculations give excellent qualitative, and reasonable quantitative, agreement with experiment. Our calculations prove the explicit equivalence of the Green function approach to that of Büttiker (in the absence of a magnetic field). The proof requires a nontrivial application of scattering theory, and we find that the previous literature on this subject contains a number of technical errors, which we correct. The equivalence of the two approaches, and the success of the Green function calculations, suggest that this newly proposed multi-probe Landauer formula captures most of the relevant physics of these mesoscopic devices. Third, we discuss the plausibility of the formula on physical grounds, and its relationship to other Landauer formulae which have been proposed in the literature. Most of the points we make have been made by other authors (to whom we shall refer at appropriate points); however, the new collective wisdom of the field concerning these issues has not been assembled in one article. Fourth, we discuss very briefly the applications of this formula to conductance and voltage fluctuations in small devices.

The basic purpose of this exercise is twofold. On one hand, due to previous controversies concerning the "correct" Landauer formula, many researchers in the wider community have been cautious about employing this approach in quantitative calculations of transport phenomena. By showing that this most recent multi-channel generalization is equivalent to a well-defined linear response calculation (and indeed equivalent to precisely the calculation that one standardly performs for these systems), we hope to show that there *is* no more rigorous formalism. Calculations explicitly appealing to this Landauer formula are no more or less convincing than they would be in the Green function approach (unless of course the actual calculational technique employed for evaluating the formula

is less accurate or involves more unverified assumptions). Conversely, some authors have suggested that there are subtle physical assumptions implicit in the Landauer approach which cannot be included naturally in standard linear response theory. We show that this is not the case, at least for the particular formula we derive, and explicitly discuss several of the frequently raised objections to a linear response calculation of the conductance. In the spirit of Landauer, we occasionally give our somewhat subjective characterizations of the prevailing sentiment about certain issues at certain times. Let us emphasize that our intention is not to assign priority or credit to certain individuals, but rather to allow an interested bystander to read this paper and sort out the rather confusing developments concerning this topic over the past eight years.

2. Historical background

As is now well known, Landauer proposed the novel point of view that transport should be viewed as a consequence of incident carrier flux [8] in this very journal in 1957 [9], and later gave a more complete discussion in 1970 [9], when he proposed that the conductance of a one-dimensional conductor sandwiched between two phase-randomizing reservoirs (where all the dissipation occurs) is given by

$$g = \frac{e^2}{h} \frac{T}{R}, \quad (1)$$

where T and R are the transmission and reflection coefficients of the conductor treated as a single complex scattering center, and only one spin direction is included. The formula (1) was rediscovered in 1980 by Anderson et al. [10], who brought it to the attention of the wider transport community by proposing a generalization of the formula to the many-channel case and employing it in a rigorous formulation of the scaling theory of localization. However, this approach was a complete success only in the strictly one-dimensional case, which, though quite interesting theoretically, had little impact on experimental work on quantum transport phenomena.

The rekindled theoretical interest in Equation (1) at this time led to several attempts to reexamine it in the 1D case, and also to generalize it to higher dimensions (many transverse scattering channels), so that it could be used in quantitative calculations of the conducting properties of real physical systems. Landauer's original derivation of Equation (1) was not based on standard linear response theory, but on a sort of "counting argument," and an appeal to the Einstein relation between the mobility and the diffusion constant [9]. A slightly higher electrochemical potential in, e.g., the left reservoir creates a current due to the presence of filled "right-going" states in the left reservoir and unfilled "left-going" states in the right reservoir; the magnitude of the current is just proportional to T , the transmission coefficient of the resistor connecting them. In steady state, the particle

densities in the leads are also unequal, differing by factors of $(1 + R)$ and $(1 - R)$, due to the reflected and transmitted particles. This creates a density gradient proportional to $2R$ over the length of the sample. Relating the current and the density gradient by means of a diffusion equation, one obtains the diffusion coefficient of the sample, and, by using the Einstein relation, its conductance, given by Equation (1). The argument contained several steps that were apparently difficult to formalize in the language of standard linear response theory; this motivated a number of authors to attempt to derive Equation (1) using that approach.

The initial result was obtained by Economou and Soukoulis [11], who derived the result $g = (e^2/h)T$, in the strictly 1D quantum limit, instead of (1). Shortly thereafter, in a calculation most relevant to our work below, Fisher and Lee [12] generalized this result to N channels, obtaining the result

$$g = \frac{e^2}{h} \text{Tr}(tt^\dagger) \quad (2)$$

where t is the $N \times N$ transmission matrix connecting the incident flux in the various channels on one side of the disordered region to the outgoing flux in the channels on the other side. (The Hermitian conjugate is represented by a dagger, and Tr is the trace of the matrix.) It is important to note that they obtained this result exactly, for the linear response of the system to an applied field with spatial variation only in the disordered region (the precise description of their calculation and assumptions is given below, when we present our generalization). Several authors [10, 13, 14], both before and after the work of Fisher and Lee appeared, proposed multi-channel generalizations of (1) which reduced to (2) in certain limits.

Equation (2) of course contradicts Equation (1) (in the one-channel case), and has the counterintuitive feature that, as the scattering caused by the disordered region goes to zero (the transmission matrix goes to the identity), the conductance of the system goes to $N(e^2/h)$, not to infinity; i.e., the resistance of a "perfect" conductor is not zero according to (2). This feature of Equation (2) was considered very puzzling and suspicious by many researchers (at least one of the present authors included), and initially this led to critical scrutiny of the derivations leading to (2). Independently, Thouless [15] and Langreth and Abrahams [16] produced alternative derivations that yielded Equation (1) in the one-channel case. Neither of these derivations actually revealed a straightforward calculational error in the derivations leading to (2); rather, they argued on physical grounds that one had to perform a *self-consistent* linear response calculation in order to get a physically meaningful result, and upon performing slightly different versions of such a calculation, both were able to obtain Equation (1) in the one-channel case. We argue below that it is now not at all clear that the self-consistency conditions that these

authors impose correspond better to the physical conditions relevant to real conductance measurements than those imposed in the derivations leading to Equation (2). However, it is probably accurate to say that at that time the general sentiment was relief that some kind of linear response derivation could be made to yield the result that was "obviously" correct on physical grounds. In addition, at that time Langreth and Abrahams generalized their approach to many channels and obtained an implicit formula for the conductance in terms of the transmission and reflection coefficients, which in general could not be re-expressed as a simple explicit function of these quantities; this suggested that for the many-channel case a generalized Landauer formula might be of little practical value in calculations. Indeed, the only significant quantitative application of a Landauer formula to many-channel quantum transport at that time was by Lee and Fisher [17], who used the "incorrect" formula (2) to test the scaling theory of localization in 2D and 3D, and obtained reasonably good agreement with the expected behavior of the scaling function $\beta(g)$.

At about the same time, Engquist and Anderson [18] also reexamined the derivation of Equation (1), but not from the point of view of finding a rigorous derivation from linear response theory. Instead, they introduced a fundamentally new point of view by stressing the need to consider the actual physical conditions corresponding to a measurement. In particular, they argued that if there is a current flowing out of one reservoir and into the other, strictly speaking the chemical potential of the reservoirs is not well-defined, and instead one should consider a system with (at least) four reservoirs, two to act as current source and sink, and two which define reference chemical potentials for the voltage measurement. It was also pointed out that this theoretical definition corresponded closely to a common measuring configuration, in which the current through the entire circuit is controlled by some large resistance in series with the sample of interest, so that a fixed current can be fed in through one set of leads, and the resulting voltage drop across regions of the sample can be measured by attaching different sets of voltage leads [this is known as a *four-probe* (or, if there are many voltage leads, *multi-probe*) measurement]. The basic physical idea underlying the new derivation by Engquist and Anderson was that once the current was imposed, one would "turn on" the voltmeter, i.e., let current flow back and forth between the current leads and the measuring reservoirs until the net current into each reservoir was zero (on average); then the measuring reservoirs would possess well-defined chemical potentials. The current in the current leads divided by the induced chemical potential difference gave the conductance in this four-probe configuration. Engquist and Anderson then introduced a scattering matrix to describe the scattering of particles between the current leads and the measuring

reservoirs. The crucial assumption that they made was that *the measuring reservoirs were weakly coupled to the current leads*; then, with several auxiliary assumptions which had much the same flavor as those in Landauer's original argument, they were able to derive the formula (1) (to lowest order in the small coupling to the measuring reservoir). The authors also made clearly a point of tremendous importance for recent work on mesoscopic conductors: "The measured resistances for sections of the chain add linearly. Because of long-range coherence for each energy, however, they are determined by all scatterers in the sample, *not just those between the measurement points* (italics added) . . . Only when the inelastic scattering is strong enough to destroy phase coherence between the measurement points can local resistances be defined."

The implications of this insight for conductance measurements in mesoscopic systems were not appreciated at the time; however, the derivation of Equation (1) was welcome. Not only could it be derived explicitly from linear response theory, but it was apparently correct on physical grounds since it was the result corresponding to a four-probe measurement. Such a conclusion was somewhat hasty; it was by no means clear that the assumption of weak coupling to the measuring reservoir corresponded to a typical experimental four-probe measurement. It has been argued [1, 19], and we argue below, that such an assumption does not correspond well to the measuring configuration of typical multi-probe mesoscopic conductors.

Little further progress was made in understanding the questions raised by the Landauer formula and its generalizations until 1985, when Büttiker et al. [13] extended the approach of Engquist and Anderson to the many-channel case. They were (at least in part) motivated by a calculation due to Gefen et al. [20], which computed the conductance of a one-channel ring in a magnetic field using Equation (1) and proposed that the usual (h/e period) Aharonov-Bohm effect might be observable in small normal-metal rings. Büttiker et al. again considered current fed in from two reservoirs acting as source and sink, but stressed that the "local chemical potential" difference between the two ends of the sample was not equal to the difference between the chemical potentials of the current reservoirs; instead, it was smaller due to the nonequilibrium distribution of carriers in the leads. They defined the "local chemical potential" as the chemical potential that would correspond to that density of carriers *if they were in equilibrium*, and suggested, in the spirit of Engquist and Anderson, that this is the chemical potential that a weakly coupled voltage probe would measure. This approach of course gave Equation (1) in the one-channel case, and a generalization of it to many channels:

$$g = \left(\frac{e^2}{h} \sum_{ij} T_{ij} \right) \frac{2 \sum_i v_i^{-1}}{\sum_i (1 + \sum_j R_{ij} - \sum_j T_{ij}) v_i^{-1}}, \quad (3)$$

where T_{ij} and R_{ij} are the transmission and reflection probabilities from channels i to j and v_i is the longitudinal velocity associated with channel i (these quantities are defined more precisely in Section 4). This result had been obtained earlier by Azbel [14], but the discussion by Büttiker et al. greatly clarified the physical assumptions upon which (3) is based. Thus, unlike those of Langreth and Abrahams, this set of assumptions leads to an explicit formula for g in terms of the scattering matrix of the sample, even in the multi-channel case. Note, however, that this is still a two-probe formula; the properties of the voltage leads do not enter into the measured conductance, and the scattering matrix elements involved only refer to scattering between the current reservoirs. The origin of the difference between the result obtained by Büttiker et al. and that obtained by Langreth and Abrahams was pointed out by the former, and is quite important in the context of our present concerns. It arose from the different assumptions each made about the "local chemical potential" in the leads. Büttiker et al. defined it in the manner described above, which has the consequence that the carrier densities in the different channels of the leads must be out of equilibrium. Langreth and Abrahams defined the density difference between the two leads by insisting that there be a single chemical potential for all the channels in each lead. Büttiker et al. have a brief discussion of the plausibility of the different hypotheses. The important point for us, however, is that it had become clear that any derivation which required defining a "local chemical potential" in the leads, which was different from that of the current reservoirs, would require a set of physical assumptions about the quasi-equilibrium in the leads. Therefore, there might be no "correct" multi-channel Landauer formula; the result obtained appeared to be sensitive to rather abstract and difficult-to-verify assumptions about the nature of the leads.

In summary, by 1985, just prior to the point at which mesoscopic systems became fashionable, the original 1D Landauer formula [Equation (1)] was prospering. It had been derived five or six different ways, including "rigorously" from linear response theory. However, the multi-channel generalizations of Equation (1) were not doing so well. There appeared to be no unique generalization, and since almost any calculation which proposed to make quantitative contact with experiment required considering a large number of channels, it was unclear whether calculations using the Landauer approach would be of great value. The general community was aware that there were subtle and substantial issues relating to the validity of any particular formula, and therefore regarded the approach with suspicion. On the other hand, most researchers were perfectly happy to perform quantitative calculations on small systems using the Kubo linear response formalism and diagrammatic techniques, apparently believing that somehow one did not have to confront these issues in that approach. We show below that

using the Kubo formalism does amount to making a choice of the appropriate multi-channel Landauer formula; it is equivalent to choosing Equation (2) in the two-probe case, and the natural generalization of those assumptions to the many-probe case. In other words, it is equivalent to assuming that a conductance measurement at fixed current measures the chemical potential at a set of reservoirs, and not the "local chemical potential" in the sample. On the basis of the agreement of recent experimental and theoretical results, and some new physical arguments, this is apparently a rather good assumption, as is discussed below.

3. The Bronze Age of mesoscopics

About this time the cogitations of theorists on these topics were beginning to be disturbed by the sometimes unsettling confrontation with reality, in the form of a series of landmark experiments on the conductance of ultra-small metallic devices measured primarily in multi-probe configurations [21–34]. These experiments revealed for the first time the presence of both the normal-metal Aharonov–Bohm effect and the sample-specific time-independent magnetoresistance fluctuations, which later became known as "universal conductance fluctuations" [35–40]. Two recent review articles [22, 23] describe in detail the experiments, their motivation, and some of the related theoretical work, focusing primarily on the Aharonov–Bohm effect. These experimental advances made the question of the appropriate approach for calculating quantum conductance substantially more interesting and important than it had appeared to be prior to the new discoveries; however, it is impossible to do them complete justice here, and readers are referred to [22, 23]. We focus on several points of relevance to the issue of the appropriate multi-probe multi-channel generalization of the Landauer formula.

The earliest published experimental data on aperiodic "reproducible noise" in the magnetoresistance of conventional normal metals is due to the IBM group [21, 24]. However, as intriguing as their results were, they were treated with some suspicion for two reasons: First, although many authors had discussed the possibility of observing periodic magnetoresistance oscillations in multiply connected conductors [13, 20, 41], no one had anticipated finding *aperiodic* behavior. Second, the magnetoresistance noise was observed to be *asymmetric* around $B = 0$; i.e., $g(B) \neq g(-B)$, which at least some authors took to be a violation of one of Onsager's relations [42]. The Fisher–Lee formula [Equation (2)] must yield an exactly symmetric conductance under field reversal, due to an exact symmetry of the S -matrix; however, the formula [Equation (3)] of Azbel and Büttiker et al. does not possess this property. The symmetries of the S -matrix in the presence of a field are insufficient to imply $g(B) = g(-B)$ in Equation (3), and Büttiker and Imry [42] suggested at that time that the asymmetry allowed by Equation (3) might

provide the explanation for the experimental observation.

Numerical simulations of small metallic conductors by Stone [36] clearly established that aperiodic conductance fluctuations as a function of magnetic field or Fermi energy with many of the features observed in the experiments were obtainable simply from the multi-channel Landauer formula. Stone initially used Equation (3); however, he found that results obtained using Equation (2) were quantitatively very close to those obtained from Equation (3) [43]. Although it is easy to show that Equation (3) approaches Equation (2) when all the T_{ij} are much less than one, in fact Imry argued that the convergence is much more rapid [39]; all that is needed is $\langle g \rangle \ll N(e^2/h)$ (where N is the number of channels, or equivalently, $l/L \ll 1$, where l is the elastic mean free path and L is the sample length). This condition is essentially what distinguishes the metallic or diffusive regime from the ballistic regime, and was satisfied by all samples measured except in the most recent experiments [44]. Thus, the approximate agreement of Equations (2) and (3) found by Stone in the simulations was not too surprising. The only feature distinguishing the two formulae in the simulations was that Equation (3) did yield an asymmetry in the magnetoconductance, while Equation (2) did not. However, the magnitude of the asymmetry found in the simulations was much smaller than that observed in the experiment, suggesting that Equation (3) could not fully explain the observed effect.

Shortly after the numerical simulations, there were a series of experimental breakthroughs in this area, beginning with the dramatic observation by Webb et al. [25] of the h/e Aharonov–Bohm effect in a normal metal. This stimulated further theoretical efforts to understand quantitatively these quantum fluctuation phenomena. It was rapidly shown that both the aperiodic magnetoresistance fluctuations and the h/e Aharonov–Bohm effect were manifestations of the same random interference effect. Calculations [35, 37–40] were performed both analytically (using diagrammatic perturbation theory) and numerically, predicting that the rms amplitude of such conductance fluctuations should always be of order (e^2/h) independent of the average conductance, hence the term "universal conductance fluctuations" (UCF). Lee and Stone considered a two-probe model, and explicitly appealed to the Landauer formula of Equation (2) to establish these results; Al'tshuler and coworkers made no such explicit appeal, but, as we discuss below, the formalism they used (including the boundary conditions imposed) was equivalent to Equation (2). The universality of $\text{rms}(g)$ was only established for this two-probe case, and only when the inelastic mean free path, L_{in} , was greater than or equal to the sample length L (a quantitative extension to the case $L_{\text{in}} \ll L$ was also made [35]). It is the opinion of one of the authors that the limitations of the two-probe theory were not fully appreciated in the earliest papers on the UCF, leading to

some confusion about the sense in which the measured fluctuations were expected to be universal. Most of the experiments to be explained were done in a multi-probe measuring configuration, and the sample length in the two-probe theory was somewhat naively assumed to correspond to the spacing of the voltage probes in the multi-probe measurements. In fact, this correspondence worked extremely well in explaining the magnitude and correlation length of the conductance fluctuations in all the early experiments [35], and therefore its general validity was not examined too closely.

The only qualitative feature of the experiments that remained unexplained was the magnetic field asymmetry in the conductance fluctuations, which, as noted above, was completely ruled out by any approach equivalent to Equation (2) above. In hindsight it seems obvious that the failure of theories based on Equation (2) to predict the observed asymmetry was a reflection of the limitations of the two-probe theories; however, this was not so clear at the time [45]. The inadequacy of the two-probe theory to describe the complete range of multi-probe experiments became more apparent, however, as the experimentalists began to study samples with many measuring probes attached at points along the current leads separated by a distance much less than L_{in} [27–29]. Here the naive application of the two-probe theory to a multi-probe measurement ran up against a paradox. Suppose the measurement is performed in a Hall geometry, with the voltage probes opposite one another and perpendicular to the current flow; then the average voltage developed between the two leads will be zero (in the absence of a magnetic field), and as one changes, e.g., the impurity configuration of the sample at fixed current, the ratio of the current to the voltage will fluctuate around an infinite value. If one insists on calling this a measurement of the conductance of the current channel between the leads, these “conductance” fluctuations will certainly be much greater than e^2/h , and such a measuring configuration is not even roughly in correspondence with the two-probe measurement assumed in Equation (2). The point is that in the two-probe theory the sample length provides a coherence cutoff very similar to that due to true inelastic scattering [35]; therefore it corresponds well to a multi-probe measurement (excluding consideration of the asymmetry) when L_{in} is approximately equal to the probe spacing. It corresponds very poorly when L_{in} is much greater than the probe spacing. However, in this case, as noted by Engquist and Anderson, the phase-coherent sample is not just the part of the current leads between the voltage probes; it includes upstream and downstream portions of the current leads, and also, crucially, the voltage leads as well. What is needed, then, is a formalism and a theory for describing the voltage fluctuations of multi-probe devices at fixed current.

The realization that such an extension of the theory was needed was due to many authors [1–6, 28, 29, 46]; certainly,

however, one should mention Benoit et al. [27, 28] and Skocpol et al. [29] on the experimental side, and Isawa, Ebisawa, and Maekawa [3] and Büttiker [1] on the theoretical side. Maekawa et al. [3] were the first to attempt to calculate voltage fluctuations using the Kubo formula, explicitly including the effects of the voltage leads in the calculation. Although there were minor technical errors in their initial approach, many of their results turned out to be correct, and certainly the physical motivation of their work was correct. However, they did not connect their approach to the Landauer formalism. Büttiker, on the other hand, proposed an extension of the multi-channel Landauer formula to multi-probe devices. The argument was extremely simple, but differed from the arguments described above in one crucial feature. Büttiker considered a four-probe device leading to four reservoirs with different chemical potentials, and assumed that all the leads were macroscopically the same; i.e., there was no qualitative distinction between current and voltage leads. Then he evaluated the current flowing into or out of each reservoir by the standard Landauer counting argument: The current flowing between two reservoirs with a chemical potential difference $\Delta\mu = \mu_1 - \mu_2$ is just $(e^2/h)T_{12}\Delta\mu$, where T_{12} is the transmission coefficient from one to two in the one-channel case, and the trace of the transmission matrix times its Hermitian conjugate in the many-channel case. Then he departed from the previous arguments discussed above by arguing, in effect, that the density or voltage difference corresponding to this current is really the difference of the chemical potentials of the reservoirs (and not some local chemical potential difference in the leads), at least in the case where the current flows only between two of the reservoirs and the chemical potential differences are measured between the other two. This simple argument leads to the straightforward generalization of Equation (2) to the case of N_L leads:

$$I_m = \sum_{n=1}^{N_L} g_{mn} V_n \quad \left\{ \begin{array}{l} g_{mn} = \frac{e^2}{h} \text{Tr}\{t_{mn}t_{mn}^\dagger\}, \quad m \neq n, \\ g_{nn} = \frac{e^2}{h} \text{Tr}\{r_{nn}r_{nn}^\dagger - 1\}, \end{array} \right. \quad (4)$$

where the conductance coefficients $\{g_{mn}\}$ are given in terms of the transmission and reflection matrices between leads m and n . Büttiker made the crucial assumption that this formulation was valid in the presence of a magnetic field, the only effect of which was to reduce the symmetry of the S -matrix due to the breaking of time-reversal symmetry.

The usefulness of this formulation was that it was now easy to define an Onsager-like conductance tensor by imposing the appropriate boundary conditions on the incoming and outgoing currents, which could easily be shown to have the familiar symmetries, simply due to the symmetries of the S -matrix. It could also easily be shown that the resistance, defined as the ratio of the voltage drop

between reservoirs 1 and 2 (with no current flowing) to the current between reservoirs 3 and 4, need not be symmetric when the field was reversed, since it was expressed as a combination of elements of this Onsager tensor with differing symmetry under field reversal. He also showed in this formulation that by interchanging current and voltage leads, it was possible to obtain composite resistances which are symmetric or antisymmetric under field reversal. This was a fact well known to experimentalists [47], but this procedure usually was not necessary when measuring a long wire in a four-probe configuration. The importance of employing this more correct procedure was convincingly demonstrated at the same time by Benoit et al. [27], confirming that the mysterious asymmetry was really due to mistakenly studying a transport coefficient which does not have any simple symmetry under field reversal. Of course, under normal circumstances, in macroscopic wires with voltage probes well-separated along the leads, this quantity will have such a symmetry to a very good approximation [22], and therefore it was not immediately obvious that one should look for such an explanation.

For the reasons just discussed, the multi-probe Landauer formula of Equation (4) is quite appealing. On the basis of this formula, and some simple assumptions about the statistical behavior of the S -matrix in the diffusive regime, Büttiker [46] went on to propose a theory of the voltage fluctuations in a three-port device that would explain qualitatively the observed experimental behavior. Fairly recent Kane et al. [2], Baranger et al. [6], Hershfeld and Ambegaokar [4], and DiVincenzo and Kane [7] have all performed quantitative calculations of voltage fluctuations in multi-probe conductors based either directly on Equation (4) or on applications of the Kubo formula which can be put in an apparently equivalent form, with the transmission matrices replaced by various matrix elements of the relevant Green function. These calculations (discussed briefly below) are in quite good qualitative and semiquantitative agreement with experiment, although they showed that the statistical assumptions made by Büttiker were, in general, not correct [2, 6]. However, what has still not been done anywhere in the literature is to show that Equation (4) can be explicitly derived from linear response theory, and if so, in what model, with what assumptions. We provide such a derivation, for the case of zero magnetic field, in the following section.

4. Derivation of Büttiker's formula from linear response theory

In this section we compute the $T \cong 0$, dc current response of a multi-probe disordered system in the absence of a magnetic field. The result, when expressed in terms of the quantum-mechanical reflection and transmission coefficients of the system, is precisely Equation (4) above.

• Definition of the model

We define below a precise quantum-mechanical model of a multi-probe conductor, and then solve it rigorously in the

linear response approximation. We do not assume the Kubo formula; instead, we calculate the formula from first principles using the density-matrix formulation of the many-particle Schrödinger equation. Our purpose is to exhibit explicitly the careful treatment of all boundary conditions, and the physical motivation for the order of limits taken. We find that an appropriate intermediate stage of the derivation yields expressions identical to those obtained by recent approaches starting from the Kubo formula [2, 5], so the initial section of our derivation is included primarily for pedagogical reasons.

The quantum-mechanical model we use is intended to correspond roughly to an experiment in which the leads of the multi-probe system are connected to oscillating voltage sources of dominant frequency Ω , and the in-phase ac current response (i.e., the dissipative component of the current) at each lead is measured. In order to have the frequency well-defined, the experiment is run for a long enough time, $1/\delta$, to allow many oscillations. This requires that the two experimentally controllable parameters Ω and δ be chosen to satisfy

$$\Omega \gg \delta. \quad (5)$$

In principle, the dc current response of the system is then obtained by extrapolating the result to $\Omega \rightarrow 0$, always maintaining the condition (5). It is worth noting that in fact almost all experiments measuring the "dc" current response of mesoscopic multi-probe devices are performed at small but finite ac driving frequency [and, of course, they are run for a long enough time to satisfy condition (5)]. Therefore, any model calculation where the results depend on Ω and δ being literally zero is suspect. Our calculation is valid for small but finite Ω and δ (where "small" is measured with respect to other relevant physical time scales, such as scattering times). Further discussion of the accuracy and validity of our model in describing experiments of the type considered above is deferred to the following sections. The main goal of this section is to solve carefully a well-defined quantum-mechanical problem.

We consider a system consisting of N_L infinite, perfectly conducting, straight "leads" of arbitrary widths, attached to a disordered region of arbitrary shape (see Figure 1). The absence of a magnetic field makes the distinction between simply and multiply connected systems irrelevant. Time-reversal symmetry is assumed, and the carriers are taken to be noninteracting fermions at $T \cong 0$. We restrict our discussion to two dimensions and to spinless particles (under the assumption that all quantities are spin-diagonal), for the purpose of avoiding the excessive proliferation of indices in a notation that is already quite complicated. The derivation in the more general case runs completely parallel to that given here and most of the equations (though not all) are formally identical; one only needs to bear in mind that in the general case there are two transverse directions instead of one, that

some symbols represent spin matrices instead of c-numbers, and the time-reversal operator T has a different meaning.

The Hamiltonian for each particle, before we turn on the driving field, is

$$H_0 = \frac{1}{2M} \mathbf{p}^2 + U(\mathbf{x}), \quad (6)$$

where $U(\mathbf{x})$ vanishes outside the disordered region. The eigenstates $\{\psi_\alpha\}$ of the unperturbed Hamiltonian are zero at all the boundaries except at infinity, and they can be chosen to form a delta-function normalized orthogonal basis of the Hilbert space. Because these states will be labeled by both discrete channel indices and continuous energy indices, their proper normalization is somewhat subtle. This technical point is important because it relates directly to the correct definition of a unitary S -matrix for this problem, a point which we address in detail in Appendix A. Time-reversal invariance implies that $\{T\psi_\alpha\}$ is also an orthonormal basis of eigenstates of H_0 (where T is the time-reversal operator). In each lead, the hard-wall boundary conditions impose a quantization of the transverse momentum, leading to a finite number of propagating solutions for any fixed energy ϵ , referred to as channels. All channels with transverse energies larger than ϵ will have amplitudes that decay exponentially along the lead in the outgoing direction from the disordered region. The regions of the leads that are far enough from the disordered region to ensure that all the decaying channels at energy ϵ_F have vanishing amplitudes will be called the *asymptotic region*.

Our derivation proceeds in three steps: First we use the linear response approximation to obtain an expression for the generalized conductance coefficients in terms of the eigenstates of the unperturbed system. Then we translate the result into the language of Green functions. Finally, we use scattering theory to relate the Green functions to the quantum-mechanical reflection and transmission amplitudes of the system, in order to express the linear response coefficients in terms of those quantities and compare the result with Equation (4). The final two stages in the derivation are very similar in spirit to the approach used by Fisher and Lee [12] to derive Equation (2).

• Conductance coefficients in terms of exact eigenstates

Following the usual linear response approach, we initially assume that a fixed external electric field $\mathbf{E}(\mathbf{x}, t)$ is imposed on our system, and find the current response of the system to first order in $\mathbf{E}(\mathbf{x}, t)$. However, the crucial point emerges shortly that only the electrical potential in the asymptotic region need be specified to determine fully the current response [2].

Driving field

We take $\mathbf{E}(\mathbf{x}, t)$ to be given by

$$\mathbf{E}(\mathbf{x}, t) = \mathbf{E}(\mathbf{x}) \cos \Omega t \cdot e^{-\delta|t|}, \quad (7)$$

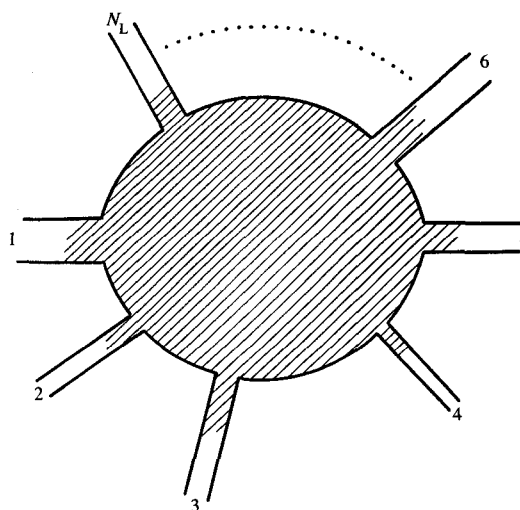


Figure 1

The system consists of a disordered region (shaded area) and N_L infinite perfectly conducting "leads" attached to it. The "leads" are straight, but have arbitrary widths.

where $\mathbf{E}(\mathbf{x})$ is assumed to be zero in the asymptotic region but is otherwise unconstrained. Ω and δ are going to be taken to zero at the end of the calculation, in a way consistent with (5), for the reasons discussed above. Choosing a gauge in which the scalar potential is identically zero,

$$\mathbf{E}(\mathbf{x}, t) = -\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t}(\mathbf{x}, t), \quad (8)$$

and the Hamiltonian for each particle (of charge e and mass M) becomes

$$H = \frac{1}{2M} \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + U(\mathbf{x}). \quad (9)$$

Since we want to use (6) as the unperturbed Hamiltonian, the choice of $\mathbf{A}(\mathbf{x}, t)$ is restricted, in addition to Equation (8), by the further condition

$$\mathbf{A}(\mathbf{x}, t \rightarrow -\infty) = 0. \quad (10)$$

Let $\tilde{E}(\omega)$ be the Fourier transform of the time-dependent part of $\mathbf{E}(\mathbf{x}, t)$,

$$\begin{aligned} \tilde{E}(\omega) &= \int_{-\infty}^{\infty} \frac{dt}{2\pi} \cos \Omega t \cdot e^{-\delta|t|} e^{i\omega t} \\ &= \frac{i}{4\pi} \left[\frac{-1}{\omega + \Omega - i\delta} + \frac{-1}{\omega - \Omega - i\delta} \right. \\ &\quad \left. + \frac{1}{\omega + \Omega + i\delta} + \frac{1}{\omega - \Omega + i\delta} \right]. \end{aligned} \quad (11)$$

Then,

$$\mathbf{E}(\mathbf{x}, t) = \mathbf{E}(\mathbf{x}) \int_{-\infty}^{\infty} d\omega \tilde{E}(\omega) e^{-i\omega t}, \quad (12)$$

and

$$\begin{aligned} \mathbf{A}(\mathbf{x}, t) &= -c \int_{-\infty}^t \mathbf{E}(\mathbf{x}, t') dt' \\ &= c \mathbf{E}(\mathbf{x}) \int_{-\infty}^{\infty} d\omega \tilde{E}(\omega) \frac{-i}{\omega + i\eta} e^{-i\omega t}. \end{aligned} \quad (13)$$

The positive infinitesimal parameter η has been introduced in the denominator to define the integral at $\omega = 0$ while at the same time preserving (10). Unlike the parameters Ω and δ , which have physical significance for nonzero values, η is a true infinitesimal, introduced simply to define the Fourier transform of $\mathbf{A}$ in terms of the Fourier transform of $\mathbf{E}$. Before embarking on the calculation, we point out that the Maxwell equation

$$|\nabla \times \mathbf{E}(\mathbf{x}, t)| = \left| \frac{1}{c} \frac{\partial \mathbf{B}}{\partial t}(\mathbf{x}, t) \right| \sim \Omega |\mathbf{B}|, \quad (14)$$

together with the condition $|\mathbf{B}| \sim |\mathbf{E}|$ (which is a consequence of the $\nabla \times \mathbf{B}$ Maxwell equation), implies that $\nabla \times \mathbf{E} = 0$ to first order in the small quantities Ω and $|\mathbf{E}|$. Therefore, at the level of approximation at which we are working, the line integral between any two points is path-independent; i.e., we could have chosen to work in a gauge where there is only a time-dependent scalar potential and no $\mathbf{A}$ field at all. Later in the calculation we use the fact that there exists a scalar function $V(\mathbf{x})$ such that

$$\mathbf{E}(\mathbf{x}) = -\nabla V(\mathbf{x}), \quad (15)$$

even though at this point we have made a different gauge choice.

Equations of motion in linear response

To begin the derivation, we identify in (9) the part of H that is linear in $\mathbf{E}$, and neglect the quadratic one:

$$\begin{aligned} H &\simeq H_0 + \left(-\frac{e}{2Mc} \right) (\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}) \\ &\equiv H_0 + H_1. \end{aligned} \quad (16)$$

Using (13), we get for the Fourier transform of H_1

$$\begin{aligned} \tilde{H}_1(\mathbf{x}, \omega) &= \frac{ie\hbar}{2M} (\nabla \cdot \mathbf{E}(\mathbf{x}) + \mathbf{E}(\mathbf{x}) \cdot \nabla) \tilde{E}(\omega) \frac{-i}{\omega + i\eta}. \end{aligned} \quad (17)$$

Since we are treating our system as approximately noninteracting, the exact many-body eigenstates can always be expressed as Slater determinants of single-particle wavefunctions. For such a system, the expectation value of any single-body operator O_1 , evolving according to the time-

dependent Schrödinger equation, can be expressed as $\langle O_1 \rangle = \text{Tr} \{ \rho(t) O_1 \}$, where $\rho(t)$ is the single-particle density matrix satisfying the equation of motion $i\hbar(d/dt)\rho(t) = [H, \rho]$. The unperturbed system in equilibrium at $T \cong 0$ is then described by the density matrix

$$\rho_0 = \sum_{\alpha} f(\epsilon_{\alpha}) |\psi_{\alpha}\rangle \langle \psi_{\alpha}|, \quad (18)$$

with $f(\epsilon_{\alpha}) \cong \theta(\epsilon_F - \epsilon_{\alpha})$, while the perturbed system is described, up to linear order in $\mathbf{E}(\mathbf{x})$, by the density operator

$$\rho(t) = \rho_0 + \rho_1(t). \quad (19)$$

The Fourier transform of the equation of motion for $\rho(t)$, also up to linear order in $\mathbf{E}(\mathbf{x})$, gives

$$\hbar\omega \tilde{\rho}_1 = [H_0, \tilde{\rho}_1] + [\tilde{H}_1, \rho_0]. \quad (20)$$

Evaluating (20) between states $\langle \alpha |$ and $|\beta \rangle$ and solving for $(\tilde{\rho}_1)_{\alpha\beta}$, we get

$$(\tilde{\rho}_1)_{\alpha\beta} = \frac{f(\epsilon_{\beta}) - f(\epsilon_{\alpha})}{\epsilon_{\beta\alpha} + \hbar\omega + i\eta} (\tilde{H}_1)_{\alpha\beta}, \quad (21)$$

where the positive infinitesimal quantity η in the denominator has been introduced again to define the Fourier integral when $\epsilon_{\beta\alpha} + \hbar\omega \equiv \epsilon_{\beta} - \epsilon_{\alpha} + \hbar\omega = 0$ and ensure that $\rho_1(t \rightarrow -\infty) = 0$.

Expectation value of the current density operator

The current response is given by the expectation value of the current density operator

$$\begin{aligned} \mathbf{j}(\mathbf{x}, t) &= \frac{e}{2} [n(\mathbf{x})\mathbf{v} + \mathbf{v}n(\mathbf{x})] \\ &= \frac{e}{2M} \left\{ n(\mathbf{x}) \left[\mathbf{p} - \frac{e}{c} \mathbf{A}(\mathbf{x}, t) \right] \right. \\ &\quad \left. + \left[\mathbf{p} - \frac{e}{c} \mathbf{A}(\mathbf{x}, t) \right] n(\mathbf{x}) \right\}, \end{aligned} \quad (22)$$

where $n(\mathbf{x})$ is the particle density operator. The coordinate representation of $\mathbf{j}(\mathbf{x}, t) = \mathbf{j}_0(\mathbf{x}) + \mathbf{j}_1(\mathbf{x}, t)$ is obtained from

$$\begin{aligned} \langle \mathbf{x}' | \mathbf{j}_0(\mathbf{x}) | \psi \rangle &= \frac{-ie\hbar}{2M} [\delta(\mathbf{x}' - \mathbf{x}) \nabla' + \nabla' \delta(\mathbf{x}' - \mathbf{x})] \psi(\mathbf{x}') \end{aligned} \quad (23)$$

and

$$\langle \mathbf{x}' | \mathbf{j}_1(\mathbf{x}, t) | \psi \rangle = \frac{-e^2}{Mc} \mathbf{A}(\mathbf{x}, t) \delta(\mathbf{x}' - \mathbf{x}) \psi(\mathbf{x}'). \quad (24)$$

The expectation value of $\mathbf{j}(\mathbf{x}, t)$ is obtained, as usual, by multiplying it by the density operator and taking the trace. Keeping terms up to first order in $\mathbf{E}$,

$$\langle \mathbf{j}(\mathbf{x}, t) \rangle = \text{Tr} \{ \rho_0 \mathbf{j}_0 \} + \text{Tr} \{ \rho_0 \mathbf{j}_1 \} + \text{Tr} \{ \rho_1 \mathbf{j}_0 \}. \quad (25)$$

Next, we use the orthonormal basis $\{ \psi_{\alpha} \}$ of eigenstates of H_0 to compute the traces. The matrix elements of the density

operators ρ_0 and $\rho_1(t)$ can be read from (18) and (21). Those of $\mathbf{j}_0(\mathbf{x})$, at finite $\mathbf{x}$, are found from (23) to be

$$\begin{aligned} [\mathbf{j}_0(\mathbf{x})]_{\beta\alpha} &= \int d\mathbf{x}' \langle \psi_\beta | \mathbf{x}' \rangle \langle \mathbf{x}' | \mathbf{j}_0(\mathbf{x}) | \psi_\alpha \rangle \\ &= \frac{-ie\hbar}{2M} W_{\beta\alpha}(\mathbf{x}), \end{aligned} \quad (26)$$

where an integration by parts has been performed, and the integral over the part of the boundary that is not at infinity vanishes because the wavefunctions are zero there. The symbol $W_{\beta\alpha}(\mathbf{x})$ in (26) is defined following Economou and Soukoulis [11] by

$$\begin{aligned} W_{\beta\alpha}(\mathbf{x}) &\equiv \psi_\beta^*(\mathbf{x}) \vec{\nabla} \psi_\alpha(\mathbf{x}) \\ &= \psi_\beta^*(\mathbf{x}) [\nabla \psi_\alpha(\mathbf{x})] - [\nabla \psi_\beta^*(\mathbf{x})] \psi_\alpha(\mathbf{x}). \end{aligned} \quad (27)$$

For later use, we point out here two properties of $W_{\beta\alpha}$:

$$W_{\beta\alpha}(\mathbf{x}) = -W_{\alpha\beta}^*(\mathbf{x}) \quad (28)$$

and

$$W_{(T\beta)(T\alpha)}(\mathbf{x}) = W_{\beta\alpha}^*(\mathbf{x}), \quad (29)$$

where $T\alpha$, $T\beta$ are the time-reversed states corresponding to ψ_α and ψ_β . Note also that as a consequence of (28) and (29),

$$W_{(T\alpha)(T\alpha)}(\mathbf{x}) = -W_{\alpha\alpha}(\mathbf{x}). \quad (30)$$

Using (24), we find the matrix elements of $\mathbf{j}_1(\mathbf{x}, t)$ to be

$$\begin{aligned} [\mathbf{j}_1(\mathbf{x}, t)]_{\beta\alpha} &= \int d\mathbf{x}' \langle \psi_\beta | \mathbf{x}' \rangle \langle \mathbf{x}' | \mathbf{j}_1(\mathbf{x}, t) | \psi_\alpha \rangle \\ &= -\frac{e^2}{Mc} \mathbf{A}(\mathbf{x}, t) \psi_\beta^*(\mathbf{x}) \psi_\alpha(\mathbf{x}). \end{aligned} \quad (31)$$

Going back to (25), we see that the equilibrium term $Tr\{\rho_0 \mathbf{j}_0\}$ vanishes as a consequence of time-reversal invariance [Equation (30)]:

$$\begin{aligned} Tr\{\rho_0 \mathbf{j}_0(\mathbf{x})\} &= \frac{1}{2} \left[\sum_\alpha \langle \alpha | \rho_0 \mathbf{j}_0(\mathbf{x}) | \alpha \rangle + \sum_{T\alpha} \langle T\alpha | \rho_0 \mathbf{j}_0(\mathbf{x}) | T\alpha \rangle \right] \\ &= \frac{-ie\hbar}{4M} \left[\sum_\alpha f(\epsilon_\alpha) W_{\alpha\alpha}(\mathbf{x}) + \sum_\alpha f(\epsilon_\alpha) W_{(T\alpha)(T\alpha)}(\mathbf{x}) \right] = 0. \end{aligned} \quad (32)$$

The second term in (25) gives rise to the diamagnetic term

$$Tr\{\rho_0 \mathbf{j}_1(\mathbf{x}, t)\} = -\frac{e^2}{Mc} \mathbf{A}(\mathbf{x}, t) \sum_\alpha f(\epsilon_\alpha) |\psi_\alpha(\mathbf{x})|^2, \quad (33)$$

and the third term is

$$\begin{aligned} Tr\{\rho_1(t) \mathbf{j}_0(\mathbf{x})\} &= \frac{-ie\hbar}{2M} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \sum_{\alpha, \beta} \frac{f(\epsilon_\beta) - f(\epsilon_\alpha)}{\epsilon_{\beta\alpha} + \hbar\omega + i\hbar\eta} (\hat{H}_1)_{\alpha\beta} W_{\beta\alpha}(\mathbf{x}). \end{aligned} \quad (34)$$

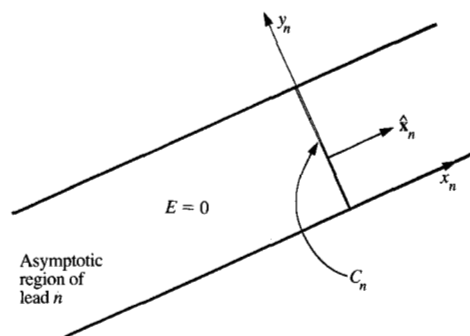


Figure 2

C_n is a transverse line in lead n located in the asymptotic region where the electric field is zero. At each lead we define local coordinates (x_n, y_n) and we indicate by $\hat{x}_n$ the normal to C_n . The part of the total system bounded by the lines $\{C_n\}$ is called $\mathcal{A}$.

$(\hat{H}_1)_{\alpha\beta}$ can be calculated from (17), and after an integration by parts in which the integral over the boundary is found to vanish because either ψ is zero or $\mathbf{E} = 0$ at infinity, we get

$$(\hat{H}_1)_{\alpha\beta} = \frac{ie\hbar}{2M} \left[\int d\mathbf{x}' \mathbf{E}(\mathbf{x}') \cdot W_{\alpha\beta}(\mathbf{x}') \right] \tilde{E}(\omega) \frac{-i}{\omega + i\eta}. \quad (35)$$

Cancellation of the diamagnetic term

At this point we have to introduce some further notation: In the asymptotic region of each lead n , where there is no electric field, we consider a transverse line C_n , and define local coordinates (x_n, y_n) as indicated in Figure 2. We call $\mathcal{A}$, the portion of the system that is bounded by the "surfaces" $\{C_1, \dots, C_N\}$. Roughly speaking, these "surfaces" correspond to the interfaces between the disordered region and the perfect leads; however, to be completely rigorous we choose them to be far enough away from the disordered region so that the propagating channels have assumed their asymptotic forms in terms of reflection and transmission matrices, and the evanescent waves have decayed to a negligible amplitude.

The integral in (35) can be restricted to the domain $\mathcal{A}$, since $\mathbf{E} = 0$ outside of it. After using (15) and integrating by parts, we are left, in addition to a line integral over the curves C_n , with an integral over $\mathcal{A}$. That integral can be further transformed by means of the following relation, which is a consequence of the single-particle Schrödinger equation:

$$\nabla \cdot W_{\alpha\beta}(\mathbf{x}) = -\frac{2M}{\hbar^2} \epsilon_{\beta\alpha} \psi_\alpha^*(\mathbf{x}) \psi_\beta(\mathbf{x}). \quad (36)$$

The result we obtain is

$$\int dx' \mathbf{E}(\mathbf{x}') \cdot \mathbf{W}_{\alpha\beta}(\mathbf{x}') = - \sum_{n=1}^{N_L} V_n \int_{C_n} \mathbf{W}_{\alpha\beta} \cdot \hat{\mathbf{x}}_n dy_n - \frac{2M}{\hbar^2} \epsilon_{\beta\alpha} \int_A dx' V(\mathbf{x}') \psi_{\alpha}^*(\mathbf{x}') \psi_{\beta}(\mathbf{x}'), \quad (37)$$

where the constants V_n multiplying the line integrals are the constant values of the voltage $V(\mathbf{x})$ on the leads external to the curves $\{C_n\}$. We are now going to transform (34) using the equality

$$\frac{1}{\epsilon_{\beta\alpha} + \hbar\omega + i\eta} = \frac{1}{\epsilon_{\beta\alpha}} - \frac{\hbar(\omega + i\eta)}{(\epsilon_{\beta\alpha} + \hbar\omega + i\eta)\epsilon_{\beta\alpha}}. \quad (38)$$

The first part in (38) gives rise to

$$\begin{aligned} & \frac{-ie\hbar}{2M} \sum_{\alpha\beta} \frac{f(\epsilon_{\beta}) - f(\epsilon_{\alpha})}{\epsilon_{\beta\alpha}} (\tilde{H}_1)_{\alpha\beta} \mathbf{W}_{\beta\alpha}(\mathbf{x}) \\ &= \left(\frac{e\hbar}{2M} \right)^2 (-i) \frac{\tilde{E}(\omega)}{\omega + i\eta} \left\{ - \sum_{n=1}^{N_L} V_n \mathbf{K}_n - \frac{2M}{\hbar^2} \sum_{\alpha\beta} [f(\epsilon_{\beta}) - f(\epsilon_{\alpha})] \mathbf{W}_{\beta\alpha}(\mathbf{x}) \int_A dx' V(\mathbf{x}') \psi_{\alpha}^*(\mathbf{x}') \psi_{\beta}(\mathbf{x}') \right\} \end{aligned} \quad (39)$$

where we have used (37) and we have defined

$$\mathbf{K}_n \mathbf{x} \equiv \sum_{\alpha\beta} \frac{f(\epsilon_{\beta}) - f(\epsilon_{\alpha})}{\epsilon_{\beta\alpha}} \mathbf{W}_{\beta\alpha}(\mathbf{x}) \int_{C_n} \mathbf{W}_{\alpha\beta} \cdot \hat{\mathbf{x}}_n dy_n. \quad (40)$$

After splitting the square bracket, writing explicitly $\mathbf{W}_{\beta\alpha}(\mathbf{x})$, using the closure relation $\sum_{\alpha} \psi_{\alpha}(\mathbf{x}) \psi_{\alpha}^*(\mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}')$ and then (15), the second term in braces in (39) gives

$$\frac{4M}{\hbar^2} \mathbf{E}(\mathbf{x}) \sum_{\alpha} f(\epsilon_{\alpha}) \psi_{\alpha}^*(\mathbf{x}) \psi_{\alpha}(\mathbf{x}), \quad (41)$$

and therefore the contribution of (39) to $\text{Tr}\{\rho_1(t) \mathbf{j}_0(\mathbf{x})\}$ is

$$\int_{-\infty}^{\infty} d\omega e^{-i\omega t} \left(\frac{e\hbar}{2M} \right)^2 \tilde{E}(\omega) \frac{-i}{\omega + i\eta} \left\{ - \sum_{n=1}^{N_L} V_n \mathbf{K}_n + \frac{4M}{\hbar^2} \mathbf{E}(\mathbf{x}) \sum_{\alpha} f(\epsilon_{\alpha}) |\psi_{\alpha}(\mathbf{x})|^2 \right\}. \quad (42)$$

Looking at (13), we see that the second term in (42) cancels the diamagnetic term (33). Adding up the contributions of the first term in (42) and the second term in (38), we obtain

$$\langle \mathbf{j}(\mathbf{x}, t) \rangle = \left(\frac{e\hbar}{2M} \right)^2 \int_{-\infty}^{\infty} d\omega \left\{ \sum_{n=1}^{N_L} V_n \mathbf{K}_n \frac{i}{\omega + i\eta} + i\hbar \sum_{\alpha\beta} \frac{f(\epsilon_{\beta}) - f(\epsilon_{\alpha})}{\epsilon_{\beta\alpha}} \mathbf{W}_{\beta\alpha}(\mathbf{x}) \left(\int dx' \mathbf{E} \cdot \mathbf{W}_{\alpha\beta} \right) \frac{1}{\epsilon_{\beta\alpha} + \hbar\omega + i\hbar\eta} \right\} \tilde{E}(\omega) e^{-i\omega t}. \quad (43)$$

Identification of reactive and dissipative terms

We now consider $t < 0$, and perform the integration $d\omega$ by closing the contour in the upper complex ω -plane [48]. After setting $\eta = 0$, we are left with

$$\begin{aligned} \langle \mathbf{j}(\mathbf{x}, t) \rangle &= \left(\frac{e\hbar}{2M} \right)^2 \frac{e^{\delta t}}{2} \left\{ i \sum_{n=1}^{N_L} V_n \mathbf{K}_n \left[\frac{e^{-i\Omega t}}{\Omega + i\delta} + \frac{e^{i\Omega t}}{-\Omega + i\delta} \right] \right. \\ &\quad \left. + i\hbar \sum_{\alpha\beta} \frac{f(\epsilon_{\beta}) - f(\epsilon_{\alpha})}{\epsilon_{\beta\alpha}} \mathbf{W}_{\beta\alpha}(\mathbf{x}) \left(\int dx' \mathbf{E} \cdot \mathbf{W}_{\alpha\beta} \right) \left[\frac{e^{-i\Omega t}}{\epsilon_{\beta\alpha} + \hbar\Omega + i\hbar\delta} + \frac{e^{i\Omega t}}{\epsilon_{\beta\alpha} - \hbar\Omega + i\hbar\delta} \right] \right\}. \end{aligned} \quad (44)$$

Now we take $\delta \rightarrow 0$ and make use of Dirac's formula $\lim_{\epsilon \rightarrow 0} 1/(x \pm i\epsilon) = P(1/x) \mp i\pi\delta(x)$ inside the "integral" $\sum_{\alpha\beta}$ to get

$$\langle \mathbf{j}(\mathbf{x}, t) \rangle = \left(\frac{e\hbar}{2M} \right)^2 \left\{ \sum_{n=1}^{N_L} V_n \mathbf{K}_n \frac{\sin \Omega t}{\Omega} + \frac{i\hbar}{2} \sum_{\alpha\beta} \frac{f(\epsilon_\beta) - f(\epsilon_\alpha)}{\epsilon_{\beta\alpha}} \mathbf{W}_{\beta\alpha}(\mathbf{x}) \left(\int d\mathbf{x}' \mathbf{E} \cdot \mathbf{W}_{\alpha\beta} \right) \cdot \left[e^{-i\Omega t} \left(P\left(\frac{1}{\epsilon_{\beta\alpha} + \hbar\Omega}\right) - i\pi\delta(\epsilon_{\beta\alpha} + \hbar\Omega) \right) + e^{i\Omega t} \left(P\left(\frac{1}{\epsilon_{\beta\alpha} - \hbar\Omega}\right) - i\pi\delta(\epsilon_{\beta\alpha} - \hbar\Omega) \right) \right] \right\}. \quad (45)$$

Then, we write $e^{\pm i\Omega t} = \cos \Omega t \pm i \sin \Omega t$ and we group the terms that multiply $\cos \Omega t$ and $\sin \Omega t$, respectively.

By exchanging dummy labels $\alpha \leftrightarrow \beta$ and making use of (28), we get the equality

$$\begin{aligned} & \sum_{\alpha,\beta} \frac{f(\epsilon_\beta) - f(\epsilon_\alpha)}{\epsilon_{\beta\alpha}} \mathbf{W}_{\beta\alpha}(\mathbf{x}) \int d\mathbf{x}' \mathbf{E} \cdot \mathbf{W}_{\alpha\beta} \left[P\left(\frac{1}{\epsilon_{\beta\alpha} - \hbar\Omega}\right) \pm P\left(\frac{1}{\epsilon_{\beta\alpha} + \hbar\Omega}\right) \right] \\ &= \sum_{\alpha,\beta} \frac{f(\epsilon_\beta) - f(\epsilon_\alpha)}{\epsilon_{\beta\alpha}} P\left(\frac{1}{\epsilon_{\beta\alpha} - \hbar\Omega}\right) \left[\mathbf{W}_{\beta\alpha}(\mathbf{x}) \int d\mathbf{x}' \mathbf{E} \cdot \mathbf{W}_{\alpha\beta} \mp \mathbf{W}_{\beta\alpha}^*(\mathbf{x}) \int d\mathbf{x}' \mathbf{E} \cdot \mathbf{W}_{\alpha\beta}^* \right]. \end{aligned} \quad (46)$$

After the square brackets are split, the second term arising from (46) can be shown to equal the first by using (29) and by noticing that the sum can be carried out using the basis $\{T\psi_\alpha\}$ instead of $\{\psi_\alpha\}$. Consequently, the expression with the minus sign in (46) vanishes, while that with the plus sign can be written as

$$\sum_{\alpha,\beta} \frac{f(\epsilon_\beta) - f(\epsilon_\alpha)}{\epsilon_{\beta\alpha}} P\left(\frac{1}{\epsilon_{\beta\alpha} - \hbar\Omega}\right) \left[\mathbf{W}_{\beta\alpha}(\mathbf{x}) \int d\mathbf{x}' \mathbf{E} \cdot \mathbf{W}_{\alpha\beta} + \mathbf{W}_{\alpha\beta}(\mathbf{x}) \int d\mathbf{x}' \mathbf{E} \cdot \mathbf{W}_{\beta\alpha} \right] \quad (47)$$

with the help of (28). The same trick used in obtaining (46) shows that

$$\begin{aligned} & \sum_{\alpha,\beta} \frac{f(\epsilon_\beta) - f(\epsilon_\alpha)}{\epsilon_{\beta\alpha}} \mathbf{W}_{\beta\alpha}(\mathbf{x}) \int d\mathbf{x}' \mathbf{E} \cdot \mathbf{W}_{\alpha\beta} [\delta(\epsilon_{\beta\alpha} - \hbar\Omega) \pm \delta(\epsilon_{\beta\alpha} + \hbar\Omega)] \\ &= \sum_{\alpha,\beta} \frac{f(\epsilon_\beta) - f(\epsilon_\alpha)}{\epsilon_{\beta\alpha}} \delta(\epsilon_{\beta\alpha} - \hbar\Omega) \left[\mathbf{W}_{\beta\alpha}(\mathbf{x}) \int d\mathbf{x}' \mathbf{E} \cdot \mathbf{W}_{\alpha\beta} \pm \mathbf{W}_{\beta\alpha}^*(\mathbf{x}) \int d\mathbf{x}' \mathbf{E} \cdot \mathbf{W}_{\alpha\beta}^* \right], \end{aligned} \quad (48)$$

and also, as before, the expression with the minus sign vanishes.

The results obtained leave us with a current density $\langle \mathbf{j}(\mathbf{x}, t) \rangle$ that is composed of a dissipative term that oscillates as $\cos \Omega t$,

$$\langle \mathbf{j}_D(\mathbf{x}, t) \rangle = \frac{e^2 \hbar^3 \pi}{8M^2} \left\{ \sum_{\alpha,\beta} \frac{f(\epsilon_\beta) - f(\epsilon_\alpha)}{\epsilon_{\beta\alpha}} \mathbf{W}_{\beta\alpha}(\mathbf{x}) \int d\mathbf{x}' \mathbf{E} \cdot \mathbf{W}_{\alpha\beta} [\delta(\epsilon_{\beta\alpha} - \hbar\Omega) + \delta(\epsilon_{\beta\alpha} + \hbar\Omega)] \right\} \cos \Omega t, \quad (49)$$

and a reactive term that oscillates as $\sin \Omega t$,

$$\begin{aligned} \langle \mathbf{j}_R(\mathbf{x}, t) \rangle &= \frac{e^2 \hbar^2}{4M^2} \left\{ \frac{1}{\Omega} \sum_{n=1}^{N_L} V_n \mathbf{K}_n - \frac{\hbar}{2} \sum_{\alpha,\beta} \frac{f(\epsilon_\beta) - f(\epsilon_\alpha)}{\epsilon_{\beta\alpha}} P\left(\frac{1}{\epsilon_{\beta\alpha} - \hbar\Omega}\right) \right. \\ &\quad \cdot \left. \left[\mathbf{W}_{\beta\alpha}(\mathbf{x}) \int d\mathbf{x}' \mathbf{E} \cdot \mathbf{W}_{\alpha\beta} + \mathbf{W}_{\alpha\beta}(\mathbf{x}) \int d\mathbf{x}' \mathbf{E} \cdot \mathbf{W}_{\beta\alpha} \right] \right\} \sin \Omega t. \end{aligned} \quad (50)$$

dc limit

Since we are interested in the behavior of $\langle \mathbf{j}(\mathbf{x}, t) \rangle$ when $\Omega \rightarrow 0$, we now proceed to consider that limit in (49) and (50). The relevant experiments are usually performed at temperatures T and frequencies Ω such that $\hbar\Omega \ll k_B T$, so we consider the limit $\Omega \rightarrow 0$ before taking $T \rightarrow 0$. We first write

$$\sum_{\alpha, \beta} \frac{f(\epsilon_\beta) - f(\epsilon_\alpha)}{\epsilon_{\beta\alpha}} \mathbf{W}_{\beta\alpha}(\mathbf{x}) \int d\mathbf{x}' \mathbf{E} \cdot \mathbf{W}_{\alpha\beta} \delta(\epsilon_{\beta\alpha} \pm \hbar\Omega) = \sum_{\substack{\alpha, \beta \\ \epsilon_\beta = \epsilon_\alpha \mp \hbar\Omega}} \frac{f(\epsilon_\alpha \mp \hbar\Omega) - f(\epsilon_\alpha)}{\mp \hbar\Omega} \mathbf{W}_{\beta\alpha}(\mathbf{x}) \int d\mathbf{x}' \mathbf{E} \cdot \mathbf{W}_{\alpha\beta}, \quad (51)$$

and observe that in the limit $\Omega \rightarrow 0$ and $T \rightarrow 0$

$$\frac{f(\epsilon_\alpha \mp \hbar\Omega) - f(\epsilon_\alpha)}{\mp \hbar\Omega} = \left. \frac{\partial f}{\partial \epsilon} \right|_{\epsilon = \epsilon_\alpha} = -\delta(\epsilon_\alpha - \epsilon_\alpha). \quad (52)$$

Consequently, (51) leads to the simple expression

$$-\sum'_{\alpha, \beta} \mathbf{W}_{\beta\alpha}(\mathbf{x}) \int d\mathbf{x}' \mathbf{E}(\mathbf{x}') \cdot \mathbf{W}_{\alpha\beta}(\mathbf{x}'), \quad (53)$$

in which we have used $\sum'_{\alpha, \beta}$ to represent a sum extended over all states α and β with energies $\epsilon_\alpha = \epsilon_\beta = \epsilon_F$.

We can further transform (49) by taking advantage of (37) to obtain

$$\sum_{n=1}^{N_L} V_n \left[\sum'_{\alpha, \beta} \mathbf{W}_{\beta\alpha}(\mathbf{x}) \int_{C_n} \mathbf{W}_{\alpha\beta} \cdot \hat{\mathbf{x}}_n dy_n \right], \quad (54)$$

with which the dissipative current density becomes

$$\langle \mathbf{j}_D(\mathbf{x}, t) \rangle = \sum_{n=1}^{N_L} \left[\frac{e^2 \hbar^3 \pi}{4M^2} \sum'_{\alpha, \beta} \mathbf{W}_{\beta\alpha}(\mathbf{x}) \int_{C_n} \mathbf{W}_{\alpha\beta} \cdot \hat{\mathbf{x}}_n dy_n \right] V_n \cos \Omega t. \quad (55)$$

We now look at the reactive piece of the current density. In the limit $\Omega \rightarrow 0$, the "integrand" in the second sum in (50) becomes odd under the exchange of dummy indices $\alpha \leftrightarrow \beta$, and therefore the sum vanishes. The resulting low-frequency expression,

$$\langle \mathbf{j}_R(\mathbf{x}, t) \rangle = \frac{e^2 \hbar^2}{4M^2} \sum_{n=1}^{N_L} \frac{1}{\Omega} \mathbf{K}_n V_n \sin \Omega t, \quad (56)$$

has the property that unless all $\{\mathbf{K}_n\}$ are zero, the reactive current grows monotonically with decreasing Ω , and can become arbitrarily large as the driving field is turned on more and more slowly. One expects this behavior for a pure noninteracting electron gas, but not in the presence of scattering; and somehow the transition between the two cases must show up in a correct calculation of these coefficients. Since the dissipative current is our main focus in this paper, we shall not pursue this question further at this time.

We note here the fact that the current density at every position is found to depend only on the constant values the electric potential $V(\mathbf{x})$ has in the asymptotic region. We can then regard $\langle \mathbf{j}(\mathbf{x}, t) \rangle$ as the response of the system to voltages applied at the leads (an easily realized experimental

condition), rather than to a specific externally imposed $\mathbf{E}(\mathbf{x})$ (something which is rather hard to realize experimentally). This point was first made (to the best of our knowledge) by Kane et al. [2], who make a physical argument concerning the natural electric field to consider if one is content to examine the system on length scales much larger than the screening length. We return to this point below.

By integrating (55) over the curve C_m , we find the total outgoing dissipative current I_m at lead m to be

$$I_m = \sum_{n=1}^{N_L} g_{mn} V_n, \quad (57)$$

where the generalized conductance coefficients are given by

$$g_{mn} = \frac{e^2 \hbar^3 \pi}{4M^2} \sum'_{\alpha, \beta} \left(\int_{C_m} \mathbf{W}_{\beta\alpha} \cdot \hat{\mathbf{x}}_m dy_m \right) \left(\int_{C_n} \mathbf{W}_{\alpha\beta} \cdot \hat{\mathbf{x}}_n dy_n \right). \quad (58)$$

Before we go on, let us cast (58) in a form that shows explicitly the units of g_{mn} . Our choice of dimensionless wavefunctions and the normalization condition $\sum_\alpha \psi_\alpha^*(\mathbf{x}) \psi_\alpha(\mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}')$ show that $\sum_\alpha$ has dimensions of inverse length square, whereas the integrals in (58) are dimensionless. Therefore, recalling that $\sum'_{\alpha, \beta}$ involves two energy delta-functions,

$$g_{mn} = \frac{e^2 \pi^2}{\hbar^2} \left[\frac{\hbar^4}{M^2} \sum'_{\alpha, \beta} \left(\int_{\text{lead } m} \mathbf{W}_{\beta\alpha} \cdot \hat{\mathbf{x}}_m dy_m \right) \cdot \left(\int_{\text{lead } n} \mathbf{W}_{\alpha\beta} \cdot \hat{\mathbf{x}}_n dy_n \right) \right] \quad (59)$$

has units of $e^2/\hbar$ as expected. We remark that (58) is a basis-independent formula, in the sense that it can be computed using any *orthonormal* basis to the subspace of eigenvectors of H_0 with eigenvalue ϵ_F .

• Conductance coefficients in terms of Green functions

Since our ultimate goal is to express the coefficients g_{mn} in terms of the quantum-mechanical reflection and transmission coefficients of the system, one would then be

tempted to use scattering states $\{\psi_\alpha^{(+)}\}$ to evaluate (58). Scattering states are the standard eigenbasis for scattering problems [50]; they correspond to a single incoming wave and outgoing waves whose amplitudes are essentially the reflection and transmission amplitudes (we define these states with great care below). This is in fact the way Langreth and Abrahams [16] proceed in their derivation of a multichannel Landauer formula. However, as was first pointed out by Fisher and Lee [12], in the multichannel case the scattering states do not form an orthonormal basis, so their use in (58) is *prima facie* unjustified. The basic reason for the nonorthogonality of the scattering states in this problem is that in a waveguide type of geometry the propagating states carry different amounts of flux per unit probability density; thus, unitarity of the S -matrix, which guarantees conservation of flux, does not imply that the states $\{\psi_\alpha^{(+)}\}$ are orthogonal. Since in one dimension the states of a given energy carry the same flux, this problem does not arise in the one-dimensional case; similarly, in the spherical scattering geometry all the states carry the same flux at infinity, so again the problem does not arise. A proof of the nonorthogonality of the scattering states is given in Appendix A, along with a careful discussion of the appropriate definition of the S -matrix for this problem. Nonetheless, despite the fact that the exact eigenstates in Equation (58) are assumed to be orthonormal in its derivation, it turns out that the evaluation of (58) using the nonorthogonal states $\{\psi_\alpha^{(+)}\}$ yields the correct result. Thus, in this particular context the extra contributions to the expectation value of the current due to the nonorthogonality of the states must cancel; however, the reason for this, and how general a result it is, remains unclear to the authors [49].

In [12], Fisher and Lee noted this problem; they then introduced the clever idea of avoiding it by relating the conductance to the Green functions of scattering theory and then relating the S -matrix directly to the Green functions and not the $\{\psi_\alpha^{(+)}\}$. Our method follows that general approach, but our derivation differs from theirs not only in that it extends the result to the case of a multiprobe system, but also in that it is computationally more straightforward. Some further notation is required at this point: We represent by $\mathbf{x}_m$ a point in the asymptotic region of lead m whose local coordinates, as defined in Figure 2, are (x_m, y_m) . We start by using Dirac's formula to express the difference between $G^{(+)}$ and $G^{(-)}$, the full Green functions of the problem, in terms of the exact eigenstates of H_0 :

$$\begin{aligned}\Delta G(\mathbf{x}, \mathbf{x}') &= (G^{(+)} - G^{(-)})(\mathbf{x}, \mathbf{x}') \\ &= \sum_{\alpha} \psi_{\alpha}(\mathbf{x}) \psi_{\alpha}^{*}(\mathbf{x}') \left[\frac{1}{\epsilon - \epsilon_{\alpha} + i\eta} - \frac{1}{\epsilon - \epsilon_{\alpha} - i\eta} \right] \\ &= -2\pi i \sum_{\alpha} \psi_{\alpha}(\mathbf{x}) \psi_{\alpha}^{*}(\mathbf{x}') \delta(\epsilon - \epsilon_{\alpha}).\end{aligned}\quad (60)$$

Using definition (27), we can expand the expression appearing in (58) as follows:

$$\begin{aligned}\mathbf{W}_{\beta\alpha}(\mathbf{x}_m) \cdot \hat{\mathbf{x}}_m \mathbf{W}_{\alpha\beta}(\mathbf{x}'_n) \cdot \hat{\mathbf{x}}_n \\ = \frac{\partial}{\partial x_m} [\psi_{\alpha}(\mathbf{x}_m) \psi_{\alpha}^{*}(\mathbf{x}'_n)] \frac{\partial}{\partial x'_n} [\psi_{\beta}(\mathbf{x}'_n) \psi_{\beta}^{*}(\mathbf{x}_m)] \\ + \frac{\partial}{\partial x'_n} [\psi_{\alpha}(\mathbf{x}_m) \psi_{\alpha}^{*}(\mathbf{x}'_n)] \frac{\partial}{\partial x_m} [\psi_{\beta}(\mathbf{x}'_n) \psi_{\beta}^{*}(\mathbf{x}_m)] \\ - [\psi_{\alpha}(\mathbf{x}_m) \psi_{\alpha}^{*}(\mathbf{x}'_n)] \frac{\partial^2}{\partial x_m \partial x'_n} [\psi_{\beta}(\mathbf{x}'_n) \psi_{\beta}^{*}(\mathbf{x}_m)] \\ - \frac{\partial^2}{\partial x_m \partial x'_n} [\psi_{\alpha}(\mathbf{x}_m) \psi_{\alpha}^{*}(\mathbf{x}'_n)] [\psi_{\beta}(\mathbf{x}'_n) \psi_{\beta}^{*}(\mathbf{x}_m)].\end{aligned}\quad (61)$$

It is here that our derivation makes contact with the usual Kubo formula. Using (51)–(53) in (49), one can immediately find that the conductivity tensor is given by

$$\sigma_{\text{Kubo}}(\mathbf{x}, \mathbf{x}') = \frac{e^2 \hbar^3 \pi}{4M^2} \sum_{\alpha, \beta} \mathbf{W}_{\beta\alpha}(\mathbf{x}) \otimes \mathbf{W}_{\alpha\beta}(\mathbf{x}'), \quad (62)$$

which can be seen to be precisely the Kubo conductivity tensor by using (61) and (60) to express it in terms of the Green functions. Combining Equations (58), (60), and (61) yields the Green function expressions for the g_{mn} obtained and evaluated in perturbation theory, e.g., by Kane et al. [2, 5].

We now call $\chi_a^{(m)}(y_m)$ the normalized transverse sine waves corresponding to channel a in the asymptotic region of lead m , and define the Fourier transforms of the Green functions by

$$G^{(\pm)}(\mathbf{x}_m, \mathbf{x}'_n) = \sum_{a, a'} G_{a, a'}^{(\pm)}(x_m, x'_n) \chi_a^{(m)}(y_m) \chi_{a'}^{(n)}(y'_n). \quad (63)$$

Combining (58), (60), (61), and (63) and taking advantage of the orthonormality of the χ 's, we obtain

$$\begin{aligned}g_{mn} &= \frac{e^2 \hbar^3}{16\pi M^2} \sum_{a, a'} \left[\Delta G_{aa'} \frac{\partial^2}{\partial x_m \partial x'_n} \overline{\Delta G_{a'a}} \right. \\ &\quad + \frac{\partial^2}{\partial x_m \partial x'_n} \Delta G_{aa'} \overline{\Delta G_{a'a}} \\ &\quad - \frac{\partial}{\partial x_m} \Delta G_{aa'} \frac{\partial}{\partial x'_n} \overline{\Delta G_{a'a}} \\ &\quad \left. - \frac{\partial}{\partial x'_n} \Delta G_{aa'} \frac{\partial}{\partial x_m} \overline{\Delta G_{a'a}} \right],\end{aligned}\quad (64)$$

where $\Delta G_{aa'}$ and $\overline{\Delta G_{a'a}}$ stand for $\Delta G_{aa'}(x_m, x'_n)$ and $\Delta G_{a'a}(x'_n, x_m)$, respectively, and $\mathbf{x}_m, \mathbf{x}'_n$ are points on the curves C_m and C_n .

Conductance coefficients in terms of S -matrix elements

We now intend to express the Green functions in (64) in terms of the reflection and transmission coefficients of the

system, and then substitute the result in (64) to obtain g_{mn} in terms of those coefficients. It is important to note that the operators $G^{(\pm)}$ involved are singular and are not ordinary operators on the Hilbert space [50], so standard operator manipulations can lead to incorrect results [51]. The properties of these operators are well-described in Messiah's classic book on quantum mechanics, where he introduced them with the warning: "... their manipulation requires caution and a certain flair." We shall certainly use caution and hopefully exhibit some flair in our proof below.

Relation of Green functions to elements of the S-matrix

Let us denote by $\psi_{(n,a)}^{(+)}$ and $\phi_{(n,a)}$ the eigenstates of the Hamiltonians with and without disorder, respectively, that have only one incident wave from infinity, coming through lead n , in channel a . As usual, the two states are related by the equation

$$\psi_{(n,a)}^{(+)}(\mathbf{x}) = \phi_{(n,a)}(\mathbf{x}) + \int_{\mathcal{A}} d\mathbf{x}' G^{(+)}(\mathbf{x}, \mathbf{x}') U(\mathbf{x}') \phi_{(n,a)}(\mathbf{x}'). \quad (65)$$

The forms of $\psi_{(n,a)}^{(+)}$ and $\phi_{(n,a)}$ in the asymptotic region of the system are given by

$$\phi_{(n,a)}(\mathbf{x}) = \begin{cases} \frac{\exp\{-ik_a^{(n)}x_n\}}{\sqrt{k_a^{(n)}}} \chi_a^{(n)}(y_n) + \sum_{a'} r_{nn,a'a}^B \frac{\exp\{ik_{a'}^{(l)}x_l\}}{\sqrt{k_{a'}^{(l)}}} \chi_{a'}^{(n)}(y_l) & \text{for } \mathbf{x} \text{ in lead } n, \\ \sum_{a'} t_{ln,a'a}^B \frac{\exp\{ik_{a'}^{(n)}x_n\}}{\sqrt{k_{a'}^{(n)}}} \chi_{a'}^{(n)}(y_n) & \text{for } \mathbf{x} \text{ in lead } l \neq n, \end{cases} \quad (66)$$

and

$$\psi_{(n,a)}^{(+)}(\mathbf{x}) = \begin{cases} \frac{\exp\{-ik_a^{(n)}x_n\}}{\sqrt{k_a^{(n)}}} \chi_a^{(n)}(y_n) + \sum_{a'} r_{nn,a'a} \frac{\exp\{ik_{a'}^{(n)}x_n\}}{\sqrt{k_{a'}^{(n)}}} \chi_{a'}^{(n)}(y_n) & \text{for } \mathbf{x} \text{ in lead } n, \\ \sum_{a'} t_{ln,a'a} \frac{\exp\{ik_{a'}^{(l)}x_l\}}{\sqrt{k_{a'}^{(l)}}} \chi_{a'}^{(l)}(y_l) & \text{for } \mathbf{x} \text{ in lead } l \neq n, \end{cases} \quad (67)$$

where the B in (66) stands for "ballistic," and all the k 's are defined to be positive. This emphasizes an important new feature of the multi-probe problem with a disordered region of arbitrary shape: Even in the absence of bulk disorder, the "free" scattering states involve transmitted and reflected waves, due to the geometry of the system. They are not simply quantized plane waves, and this complicates the derivation as compared to that of Fisher and Lee or Langreth and Abrahams. However, this feature is also of physical importance, since it reflects the fact that in very clean devices, the dominant scattering mechanism may be surface scattering due to the device geometry; one would like then to ensure that this formula is valid in that "ballistic" limit as well. We also call the attention of the reader to the

nonstandard definition of the reflection and transmission coefficients in (66) and (67). As discussed in Appendix A, these definitions are needed in order to ensure that these quantities are the matrix elements of a unitary S-matrix.

We begin by considering $\mathbf{x}$ to be a point on lead m , closer to the disordered region than C_m (i.e., $\mathbf{x}$ is inside $\mathcal{A}$). Due to the equation satisfied by $G^{(+)}(\mathbf{x}, \mathbf{x}')$, we can make the substitution

$$G^{(+)}(\mathbf{x}, \mathbf{x}') U(\mathbf{x}') = \left(\epsilon + \frac{\hbar^2 \nabla'^2}{2M} \right) G^{(+)}(\mathbf{x}, \mathbf{x}') - \delta(\mathbf{x} - \mathbf{x}') \quad (68)$$

in the integral in (65), and after a couple of integrations by parts, we obtain for that term

$$\frac{\hbar^2}{2M} \sum_{l=1}^{N_L} \int_{C_l} dy'_l \phi_{(n,a)}(\mathbf{x}'_l) \frac{\partial}{\partial x'_l} G^{(+)}(\mathbf{x}_m, \mathbf{x}'_l) - \phi_{(n,a)}(\mathbf{x}_m). \quad (69)$$

Using the asymptotic forms (66), we get

$$\int_{C_l} dy'_l \phi_{(n,a)}(\mathbf{x}'_l) \frac{\partial}{\partial x'_l} G^{(+)}(\mathbf{x}_m, \mathbf{x}'_l) = \sum_{a'} t_{ln,a'a}^B \frac{\exp\{ik_{a'}^{(l)}x_l\}}{\sqrt{k_{a'}^{(l)}}} \frac{\partial}{\partial x'_l} G_{a'}^{(+)}(\mathbf{x}_m, \mathbf{x}'_l) \quad l \neq n \quad (70)$$

and

$$\begin{aligned} \int_{C_n} dy'_n \phi_{(n,a)}(\mathbf{x}'_n) \frac{\partial}{\partial x'_n} G^{(+)}(\mathbf{x}_m, \mathbf{x}'_n) &= \frac{\exp\{-ik_a^{(n)}x'_n\}}{\sqrt{k_a^{(n)}}} \frac{\partial}{\partial x'_n} G_{a'}^{(+)}(\mathbf{x}_m, \mathbf{x}'_n) \\ &+ \sum_{a'} r_{nn,a'a}^B \frac{\exp\{ik_{a'}^{(n)}x'_n\}}{\sqrt{k_{a'}^{(n)}}} \frac{\partial}{\partial x'_n} G_{a'}^{(+)}(\mathbf{x}_m, \mathbf{x}'_n), \end{aligned} \quad (71)$$

where $G_{a'}^{(+)}(\mathbf{x}, \mathbf{x}')$ is the Fourier transform of $G^{(+)}(\mathbf{x}, \mathbf{x}')$ with respect to y' only. Substituting (70) and (71) into (65), and carrying out the differentiations, we obtain

$$\psi_{(n,a)}^{(+)}(\mathbf{x}_m) = \frac{\hbar^2}{2M} \left\{ \left(\frac{\partial}{\partial x'_n} + ik_a^{(n)} \right) G_{.a}^{(+)}(\mathbf{x}_m, x'_n) \frac{\exp\{-ik_a^{(n)}x'_n\}}{\sqrt{k_a^{(n)}}} + \sum_{a'} r_{nn,a'a}^B \left(\frac{\partial}{\partial x'_n} - ik_{a'}^{(n)} \right) G_{.a'}^{(+)}(\mathbf{x}_m, x'_n) \frac{\exp\{-ik_{a'}^{(n)}x'_n\}}{\sqrt{k_{a'}^{(n)}}} \right. \\ \left. + \sum_{l \neq n} \sum_{a'} t_{ln,a'a}^B \left(\frac{\partial}{\partial x'_l} - ik_{a'}^{(l)} \right) G_{.a'}^{(+)}(\mathbf{x}_m, x'_l) \frac{\exp\{ik_{a'}^{(l)}x'_l\}}{\sqrt{k_{a'}^{(l)}}} \right\}. \quad (72)$$

$G_{.a}^{(+)}(\mathbf{x}, x')$ contains only outgoing waves [50] in the sense that if we consider a fixed $\mathbf{x}$, and look at the dependence of $G_{.a}^{(+)}(\mathbf{x}, x')$ on x' at a point $\mathbf{x}'$ in the asymptotic region, *farther than $\mathbf{x}$ from the scattering sources*, then

$$G_{.a}^{(+)}(\mathbf{x}, x') \sim \exp\{ik_a x'\}. \quad (73)$$

The condition in italics is irrelevant when $\mathbf{x}$ and $\mathbf{x}'$ belong to different leads, but is important when both points lie on the same lead. Writing

$$G_{.a}^{(+)}(\mathbf{x}, x') = \sum_b G_{ba}^{(+)}(x, x') \chi_b(y'), \quad (74)$$

and taking advantage of (73) to evaluate the derivatives in (72), we arrive at

$$\psi_{(n,a)}^{(+)}(\mathbf{x}_m) = \frac{\hbar^2}{2M} \sum_b 2ik_a^{(n)} G_{ba}^{(+)}(x_m, x'_n) \frac{\exp\{-ik_a^{(n)}x'_n\}}{\sqrt{k_a^{(n)}}} \chi_b^{(m)}(y_m). \quad (75)$$

Comparing with (67) and identifying the coefficients of the χ 's, we obtain

$$G_{ba}^{(+)}(x_n, x'_n) = \frac{-i}{\hbar v_a^{(n)}} \left[\delta_{ba} \exp\{ik_a^{(n)}(x'_n - x_n)\} + r_{nn,ba} \sqrt{\frac{k_a^{(n)}}{k_b^{(n)}}} \exp\{ik_b^{(n)}x_n + ik_a^{(n)}x'_n\} \right] \quad x_n \leq x'_n, \quad (76)$$

$$G_{ba}^{(+)}(x_m, x'_n) = \frac{-i}{\hbar v_a^{(n)}} t_{mn,ba} \sqrt{\frac{k_a^{(n)}}{k_b^{(m)}}} \exp\{ik_b^{(m)}x_m + ik_a^{(n)}x'_n\} \quad m \neq n. \quad (77)$$

We call the attention of the reader to the fact that the Green function in (76), which corresponds to the case in which both points $\mathbf{x}$ and $\mathbf{x}'$ are on the same lead, does not only contain outgoing waves at $\mathbf{x}$ (the point standing closer to the disordered region) [52]. Similar expressions can be obtained for $G_{ba}^{(-)}$ by using the general relationship

$$G_{ba}^{(-)}(x, x') = [G_{ab}^{(+)}(x', x)]^*. \quad (78)$$

Final result for g_{mn}

To obtain g_{mn} , all that remains to be done is to substitute (76) and (77) into (64). When $m \neq n$,

$$\frac{\partial}{\partial x_m} G_{ba}^{(\pm)}(x_m, x'_n) = \pm ik_b^{(m)} G_{ba}^{(\pm)}(x_m, x'_n), \quad (79)$$

$$\frac{\partial}{\partial x'_n} G_{ba}^{(\pm)}(x_m, x'_n) = \pm ik_a^{(n)} G_{ba}^{(\pm)}(x_m, x'_n). \quad (80)$$

To obtain the analogous formulas for $G_{ab}^{(\pm)}(x'_n, x_m)$, we simply exchange labels $a \leftrightarrow b$, $m \leftrightarrow n$, and $x \leftrightarrow x'$ in (79) and (80). Computing ΔG and $\overline{\Delta G}$, using (78) and substituting into (64), we obtain

$$g_{mn} = \frac{e^2 \hbar^3}{4\pi M^2} \sum_{a,a'} k_a^{(m)} k_{a'}^{(n)} \{ |G_{aa'}^{(+)}(x_m, x'_n)|^2 + |G_{a'a}^{(+)}(x'_n, x_m)|^2 \} \quad m \neq n, \quad (81)$$

which can be immediately transformed by means of (77) to yield

$$g_{mn} = \frac{e^2}{4\pi \hbar} \sum_{a,a'} \{ |t_{mn,aa'}|^2 + |t_{nm,a'a}|^2 \} \quad m \neq n, \quad (82)$$

where the sums on a and a' run over the channels of leads m and n , respectively. We can cast (82) into a nicer form by defining the matrices t_{mn} whose elements are

$$(t_{mn})_{aa'} \equiv t_{mn,aa'}. \quad (83)$$

When we represent Hermitian conjugation by a dagger and the trace in the space of the matrices just defined by Tr , (82)

acquires the more compact form

$$g_{mn} = \frac{e^2}{4\pi \hbar} Tr \{ t_{mn} t_{mn}^\dagger + t_{nm} t_{nm}^\dagger \} \quad m \neq n. \quad (84)$$

This formula can be further simplified by appealing to time-reversal invariance, to yield the familiar-looking

$$g_{mn} = \frac{e^2}{2\pi \hbar} Tr \{ t_{mn} t_{mn}^\dagger \} \quad m \neq n. \quad (85)$$

In the special case of a two-lead system, (85) can be obtained from (84) by using only the unitarity conditions satisfied by r and t , as noted in [12]. This can easily be seen by taking the trace of Equations (115) and (118) and comparing them. Had we considered two coupled spin polarizations, we would have arrived at Equation (82) too, except that now the channel label would need to be interpreted as an index for

channel and spin, and the trace in (85) would be over those "composed indices."

In order to obtain g_{nn} , we can avoid a somewhat lengthy calculation by noticing that as a consequence of (36) and (58) [see Equations (98)–(100) in Appendix A],

$$\sum_{n=1}^{N_L} g_{nn} = \sum_{m=1}^{N_L} g_{mm} = 0. \quad (86)$$

Using (84) in (86), we arrive at

$$g_{nn} = -\frac{e^2}{4\pi\hbar} \text{Tr} \left\{ \sum_{m \neq n} (t_{mn} t_{mn}^\dagger + t_{nm} t_{nm}^\dagger) \right\}, \quad (87)$$

which can be transformed into

$$g_{nn} = \frac{e^2}{2\pi\hbar} \text{Tr} \{ r_{nn} r_{nn}^\dagger - 1 \} \quad (88)$$

by means of the cyclic property of the trace, and the unitarity conditions (115) and (118). Equations (57), (85), and (88) complete the rigorous derivation of Equation (4).

Equation (4) expresses the current response of the multi-probe conductor in terms of applied external voltages on the leads. Often in experiments the measurements are done under conditions where the injected current is effectively fixed, and the induced voltages are measured. This requires inverting Equation (4) for a given set of injected currents. This is not entirely straightforward, since the matrix g_{mn} is not invertible. Explicit solutions for the voltage response to an applied current for the three- and four-probe cases have been given by Büttiker [1, 46]; a general procedure for solving Equation (4) for arbitrary injected currents and an arbitrary number of probes is given in Appendix B.

5. Can a perfect conductor have a resistance after all?

We have now seen that the multi-probe Landauer formula proposed by Büttiker [Equation (4)] can be explicitly derived from linear response theory for a particular model system. In the limit of only two probes, this formula reduces to the one derived previously by Fisher and Lee [Equation (2)], which eight years ago caused such consternation because it predicted that a "perfect conductor" would still have a finite resistance, $R_0 = (Ne^2/h)^{-1}$. In particular, the work of Thouless [15] and Langreth and Abrahams [16] suggested that although Equation (2) was derivable from standard linear response theory, it was physically implausible because it failed to take into account important self-consistency conditions. If this is correct in the two-probe case, it is by no means clear that a similar criticism should not be leveled at Equation (4). In addition, there was the physical argument originally due to Engquist and Anderson [18] and generalized by Büttiker et al. [13], which suggested that Equations (1) and (3) were appropriate for describing a four-probe measurement. However, the correctness of these

original criticisms of Equation (2) is now much more doubtful than it appeared initially; particularly insofar as they were given plausibility by the intuitive expectation that a "perfect conductor" should exhibit zero resistance. Imry [53] and more recently Landauer [54] have emphasized that the minimum resistance obtained from Equation (2) can be thought of as a true contact resistance, which would influence a real two-probe measurement. Therefore, it is by no means clear that a *finite* perfect conductor, connected to reservoirs, should be expected to exhibit zero resistance. We summarize these arguments with slight modifications; readers are referred to [53] and [54] for more details.

The argument can be stated as follows. Consider in free space two macroscopic closed containers each containing degenerate neutral Fermi gases in equilibrium at $T = 0$, with different chemical potentials μ_1 and μ_2 . Imagine now poking a small hole in the side of each container, connecting them with a perfect tube, and observing the time-dependent current that flows between them. On very long time scales it is possible for the current to oscillate as the excess density sloshes back and forth between the two containers, since this is essentially a many-body analogue of a double-well quantum system. But on a shorter time scale one expects an approximately steady-state current to flow from the gas of higher density to that of lower density (this quasi-steady state will occur for times such that the density change in the reservoirs induced by the current flow is much less than the initial density difference). The actual value of the steady-state current will in principle depend on the shape of the apertures leading out of the two containers and on the absolute value of the chemical potentials, since this determines the particle wavelengths, and there will be diffraction effects at the opening. However, one can imagine impedance-matching the tube to the apertures, or averaging over different shapes and sizes of apertures. Then, estimating the current that will flow as μ_1 approaches μ_2 is simply a matter of counting the density of momentum states at the Fermi level in each container which will correspond to propagating states in the tube of width W , and then weighting each state by the current it carries along the tube. This is really equivalent (up to numerical factors of the order of unity) to the standard Landauer counting argument for the current, and Imry shows that a simple calculation yields $I = \alpha(Ne^2/h)(\mu_1 - \mu_2)$, where α is a constant of the order of unity.

Thus, in this case it is clear that although the tube itself is a "perfect conductor" in the sense that it contains no scattering centers, there is a contact or "spreading resistance" necessarily present when connecting the two reservoirs that on average is of the order of the resistance $R_0 = (Ne^2/h)^{-1}$ predicted by Equation (2) for a perfect conductor. Note that in this example, it is clear that the resistance involved really is a contact resistance, since it does not depend at all on the length of the tube connecting the containers, and this could

be determined experimentally. If one now introduces scatterers into the tube, an obvious extension of the argument predicts a current proportional to $Tr(tt^\dagger)$. Thus, if one measures the conductance by dividing the current by the chemical potentials μ_1 and μ_2 , measured by probing the density of the gas in the containers far away from the opening to the tube connecting them, one will obtain a value of the order of that predicted by Equation (2). If one could instead probe the average density of carriers at the ends of the tube, without significantly affecting the density, one would measure a smaller difference in the effective chemical potentials, since not all the available momentum states are filled (there is a net current flowing); presumably one would infer a larger conductance, given approximately by Equations (1) and (3).

In other words, the point made by Büttiker et al. [13] is certainly correct; there will be a true density gradient extending from the ends of the tube some distance into the reservoirs. If it is possible to measure the local nonequilibrium density in the leads, by a four-probe measurement, *without substantially changing that density when introducing further probes*, then it seems reasonable that the conductance could be well approximated by an effective two-probe formula, such as Equation (3), which does not depend on the scattering properties of the leads. This is what the assumption of weak coupling to the measuring reservoirs achieves in the models of Engquist and Anderson and Büttiker et al. However, in the context of multi-probe measurements on mesoscopic conductors, it appears difficult to realize such an ideal weakly coupled measurement. Typically the voltage leads are about the same size and conductivity as the "current leads." More importantly, if much of the sample is phase-coherent (in the sense that the inelastic scattering length is of the order of or greater than the sample size), the transmission properties of the main channel are substantially affected by excursions into the leads. In such a situation, a formula such as Equation (4) that treats current and voltage probes on equal footing appears essential for a proper description of the conducting properties of the system. It may be possible to find an experimental realization of a weakly coupled voltage measurement, e.g., by using a scanning tunneling microscope [19]. However, whether such a probe would really correspond to the ideal weak coupling needed for Equations (1) and (3) remains an open question, as we discuss in the final section.

Returning to the "two-probe measurement" discussed above, we have argued for the inevitable presence of a contact or spreading resistance in the context of this idealized model for simplicity. However, we emphasize that this is an important and well-known physical effect that must be taken into account in understanding point contacts between real conductors [55]. More than twenty years ago Sharvin [56] estimated the spreading resistance due to a

point contact, and in the limit when the aperture width is much less than the mean free path in the conductors, Imry [53] has shown that his formula yields a contact resistance of the order of R_0 .

Very recently Van Wees et al. [57] have seen dramatic evidence for this quantum contact resistance, by observing steps in the conductance of ballistic point contacts at values of the Fermi energy corresponding to the onset of successive 1D sub-bands. The experiments observe quantized conductance values very close to Ne^2/h , whereas the present theoretical arguments would only predict a contact resistance of this order of magnitude. This suggests that the impedance-matching and diffraction effects at the junction to the constriction do not substantially alter the simple arguments cited above, a finding which requires further theoretical study to be fully understood.

The crucial point of this discussion is to emphasize that not only Equation (4), but also Equation (2) corresponds rather well to one common kind of resistance measurement. In the ideal system it corresponds to connecting the reservoirs, measuring the current that flows between them, and then measuring the density difference far away from the points of connection between the two reservoirs. In a more realistic system, Equation (2) provides a good approximate description of a real "two-probe" measurement, in which the voltage induced by a given current is measured between points on two bulk electrodes. Therefore we conclude that Equation (4), including the two-probe and one-channel limits, is the physically relevant Landauer formula for all the present experiments. The fact that Equation (2) predicts a maximum achievable conductance is not unphysical, but reflects the inevitable presence of a contact resistance whenever current flows between two reservoirs. Those who cannot accept the notion that a perfect conductor can be said to have a finite resistivity (as opposed to resistance) will perhaps be consoled by the thought that because R_0 is a contact resistance (i.e., it scales inversely with area, but is independent of length), the resistivity, $\rho = (A/L)R$, corresponding to R_0 does indeed go to zero as the sample size goes to infinity (at fixed shape).

6. What about self-consistency?

In the preceding section we have argued that the approaches that obtain Equation (1) instead of Equation (2) by invoking an ideal weakly coupled four-probe measurement are not in general convincing because such a measurement does not correspond well to a real experimental resistance measurement. Our argument does not clearly address the alternative approaches for obtaining Equation (1) based on self-consistent linear response theory due to Thouless [15] and Langreth and Abrahams [16]. The approaches of these authors are similar in spirit but differ in detail.

Thouless, in an influential comment entitled "Why Landauer's Formula for Resistance Is Right" [15],

considered a finite one-dimensional system with periodic boundary conditions, i.e., a ring, consisting of a small disordered segment imbedded in an otherwise perfect conductor. He does not consider attaching leads anywhere on the ring, and does not discuss any coupling between the electrons in the ring and, e.g., the lattice. Therefore the object he considers is an isolated quantum-mechanical system with discrete energy levels. Then, it seems that this model corresponds more closely either to a microwave absorption experiment or to an experiment where the current is generated by a time-varying flux through the loop, than to a two-probe measurement. Both of these situations have been discussed in detail in the literature [41]. Thouless calculates in the usual way the linear response to a uniform ac field applied only across the disordered region, imposing the further condition that the frequency Ω of the field cannot be taken smaller than the level spacing of the ring [58]. He shows that under this condition the uniform field generates a spatially nonuniform current in the ordered section of the ring. He then argues that this result shows that such a linear response calculation is unphysical because it allows these macroscopic charge density waves, which would be forbidden if one had properly accounted for the electron-electron interactions. Therefore, linear response theory is only sensible if one assumes that the electrons generate a self-consistent field to cancel out these charge density waves. Thouless shows that the correction to Equation (2) due to the internal field is *precisely* what is needed for the response to the total field to be given by Equation (1).

The simplicity of the result obtained by this self-consistent argument is impressive and suggests that Equation (1) does have something to do with the response of a *closed* conducting system to an applied ac field. However, it is not obvious that this self-consistency requirement should apply to an *open* system, where the disordered sample is connected directly to bulk electrodes. As we emphasized above, the total current flowing in and out of various leads in the conductor is not dependent on the detailed electric field distribution within the conductor, but only depends on the voltage applied at the end of the disordered portion of the leads. The infinite perfect leads in our model calculation are intended (in the absence of a more complete description) to simulate the effect of macroscopic electrodes which introduce substantial inelastic scattering and irreversibility. Therefore, it is not clear that a self-consistency requirement imposed to avoid charge density waves far away from the disordered region, which are supposed to correspond to points well inside the reservoir, is meaningful for the open systems we are attempting to model.

Langreth and Abrahams do consider an infinite system, in fact, exactly the same system as Fisher and Lee, i.e., a finite multi-channel two-probe disordered conductor imbedded in an infinite perfect conductor. They also note that a spatially uniform finite frequency field imposed over the disordered

region alone will lead to charge density waves in the ordered leads. Like Thouless, they argue that therefore the field cannot be assumed to be zero in the ordered region, but must be determined self-consistently by the condition that the current density remain uniform for finite frequency and that far away from the disordered region the conductivity is given by that of a homogeneous 1D electron gas. They seem to imply that these conditions are necessary even for a system of neutral particles responding to a density gradient, of the type considered in the discussion above. They state that these conditions are the correct ones to impose in order to represent an experiment in which a fixed current is driven through the sample, and the induced voltage is measured. Their linear response calculation then differs from our own and that of Fisher and Lee because there appear additional contributions to the current in the disordered region due to the field in the perfect leads. This approach, like that of Thouless, yields Equation (1) in the one-channel case.

Langreth and Abrahams went on to generalize their results to many channels. In order to accomplish this, just like Büttiker et al., they had to make some assumptions about how to define the chemical potential in the leads (since they were not allowing it to be treated as an externally imposed quantity). They assumed that all channels, whether left-going or right-going, were in perfect equilibrium with one another on both sides of the sample (this differs from the assumptions of Büttiker et al., as discussed in [13]). Thus, for Langreth and Abrahams the leads do behave like reservoirs in the sense that there is assumed to be enough inelastic scattering there to equilibrate all the channels. This reflects a very sensible desire to put the "reservoirs" more explicitly into the linear response calculation (a development which we believe is important for future progress in this area). However, the "reservoirs" responsible for the hypothesized equilibration of the channels in the leads have the property that their chemical potentials depend on the scattering properties of the conductor connecting them. This assumption leads to a different and more complex generalization of Equation (1) than that of Büttiker et al., but its properties have not been studied fully enough to determine how significantly it differs from Equation (2) or Equation (4) in various limits.

It seems very likely that a calculation of the type performed by Langreth and Abrahams can be done for a multi-probe system and would yield a result different from that of Equation (4). To be more specific, our calculation appears to predict the same long-wavelength variation in the current density in the ordered leads found by these authors for the two-probe case, although we have not studied this question carefully. However, the wavelength of these variations will go to zero as Ω goes to zero, so it is only in the limit of truly infinite leads that this effect is important. Insofar as the infinite leads are supposed to mimic the effects of inelastic scattering and phase randomization in a bulk

electrode feeding current into the system, it is not clear that these charge density waves reflect a true physical effect, as opposed to an artifact of the model.

In summary, the results of Langreth and Abrahams and of Thouless depend crucially on effects in the perfect leads, and essentially deny that it is possible to imagine the boundary condition of a fixed *external* voltage. This is troubling, because even in an interacting system, the notion of measuring the current flowing between two reservoirs with an electrochemical potential difference which is independent (to arbitrarily good approximation) of the properties of the conductor connecting them seems perfectly reasonable. (How can this fail to be true as the size of the reservoirs goes to infinity?) In the case of Langreth and Abrahams, they are essentially arguing that the boundary condition of a fixed external current would generate a different linear response than that of a fixed external voltage. As we discuss below, what is needed to really clarify this issue further is a model calculation which actually includes a representation of the reservoirs or bulk electrodes in quasi-equilibrium. We cannot dismiss entirely the concerns of these authors in the absence of such a calculation. However, as matters stand, given the agreement between calculations based on Equation (4) and experiment, and our physical understanding of the origin of the contact resistance it predicts in the two-probe case, it is not clear that the self-consistency conditions imposed in these calculations are relevant to the present class of experiments.

7. Where are the reservoirs?

Having discussed the physical plausibility of Equations (2) and (4) as compared to other Landauer formulae, we now turn briefly to several common objections to deriving a Landauer-type formula rigorously from linear response theory.

First, it is often suggested, particularly in the writings of Landauer [8, 54], that the presence of those mysterious but useful "phase-randomizing reservoirs" is essential for a correct derivation of a dissipative resistance. There are several reasons for this suggestion. It is often pointed out that in the standard Landauer argument for Equation (1), it is essential to use the scattering states $\{\psi^{(+)}\}$ and not the states $\{\psi^{(-)}\}$ related to them by time-reversal, since time-reversal reverses the current carried by the state without interchanging the densities on either side of the scattering region. Hence Landauer argued that since the states $\{\psi^{(+)}\}$ give a positive conductance, use of the states $\{\psi^{(-)}\}$ would give a negative conductance. The presence of the phase-randomizing reservoir is invoked to rule out on physical grounds the use of the time-reversed states, which require precise phase coherence between waves incident from opposite sides of the disordered region. In our calculation the results from linear response theory are obviously basis-independent because the induced current density is

expressed as a trace over states. Moreover, although in general we have not performed the calculation using either $\{\psi^{(+)}\}$ or $\{\psi^{(-)}\}$ since neither are an orthonormal basis, in the one-dimensional case, when they are orthonormal, we have checked explicitly that the same result is obtained, when either the $\{\psi^{(+)}\}$ or $\{\psi^{(-)}\}$ are substituted into Equation (58).

The second objection is that there cannot be dissipation in a system in which there is only elastic scattering, and the reservoirs are needed to dissipate the energy arising from the resistance of the conductor. This is of course correct in the following sense: The resistance we calculate in linear response is really a measure of the energy fed into the system by the external field. If there is no source of dissipation in the system, it will heat up under the influence of the field, and the linear response approximation will rapidly become invalid. The construct of reservoirs reminds us that some degree of inelastic scattering is necessary for linear response theory to make sense. Of course, if a calculation is able to include inelastic scattering explicitly, as can be done by including interaction effects in the Green function calculations performed using Equation (4), then it is clearly a matter of taste whether or not one speaks of a reservoir which causes phase-randomization and dissipation.

A related argument is that, strictly speaking, no finite closed system can exhibit irreversibility and dissipation; this raises the interesting question of the conditions under which energy fed in can be fully recovered [54]. It appears that this is an objection to calculations that attribute a resistance to a *finite* quantum system, and this is why we explicitly consider an infinite system, with continuous states, in our calculations. It is evident that in some respects the infinite perfect leads of this model do simulate the phase-randomizing effect of inelastic scattering at least in the diffusive regime. This point is explicitly demonstrated in recent numerical simulations by Baranger et al. [6]. There it is shown that subdividing a conductor by attaching perfect leads at uniform intervals along its length causes the voltage fluctuations to increase as a function of that length as if the voltage fluctuations in each segment were uncorrelated, just the same effect as occurs when the inelastic mean free path is made shorter than the sample length (without introducing additional perfect leads) [33, 35].

Much of the physical motivation for a Landauer formula approach to quantum resistance has been a desire to represent the current (i.e., the incident carrier flux) as the source of the voltages induced in the sample, whereas the linear response formalism naturally regards the fields as the source of the currents. The somewhat obvious point should be made about Equation (4) that once derived, it can be used either to find the currents induced by fixed voltages or the voltage differences induced by fixed currents. Since the matrix g_{mn} is noninvertible, there are some minor technical problems when starting with imposed currents and calculating voltage response from Equation (4). A general

procedure for solving this problem is discussed in Appendix B. Of course, this does not address the much more complicated problem of how to calculate the final steady-state charge distribution, taking into account self-consistent screening [54], but one apparently need not solve this problem to understand voltage fluctuations in mesoscopic metal conductors.

In summary, although it may be important and useful to stress the distinction between open and closed systems by invoking the concept of a phase-randomizing reservoir in deriving a resistance, it is not essential to introduce such a concept to derive Equation (4). The *infinite* perfect leads apparently simulate the phase-randomization of electrons which escape into the leads invoked in the intuitive derivation of Equation (4). Some of the limitations of this model for truly representing the bulk electrodes of an experiment are discussed below.

8. Theories of voltage fluctuations

In this section we discuss briefly the quantitative calculations of voltage fluctuations in mesoscopic conductors which have been performed recently in order to explain the observed behavior in the relevant experiments.

Briefly, the experiments [27–29] had shown voltage fluctuations $\langle (\delta V)^2 \rangle$ which varied linearly with the probe spacing L for $L_{\text{in}} \ll L$ and then changed over to an apparently constant value for $L_{\text{in}} \geq L$. The value of the corresponding conductance fluctuations for $L_{\text{in}} \sim L$ was always observed to be $\langle (\delta G)^2 \rangle^{1/2} \sim (e^2/h)$. By appropriate lead-switching operations, it was possible in some cases to examine separately the behavior of the field-symmetric and antisymmetric fluctuations [27, 28]; the former were observed to have the behavior just described, whereas the latter were found to be approximately independent of probe-spacing even for $L_{\text{in}} \ll L$. Several experiments showed a nonlocal behavior in which voltage leads remote from the current paths nonetheless exhibited voltage fluctuations [28, 29], and even a remote Aharonov–Bohm effect [31]. Several quantitative analytic and numerical calculations of voltage fluctuations have recently been undertaken to account for these effects [2–6].

The diagrammatic calculations [2, 4, 7] start from the expression for the conductance coefficients g_{mn} in terms of Green functions, and employ the impurity-averaging technique to calculate quantities like $\langle (g_{mn})^2 \rangle$ to lowest order in the small parameter $(k_F l)^{-1}$, where l is the elastic mean free path. The only point at which the geometry of the device enters the calculation is in choosing the boundary conditions on the differential equation which determines the “diffusion propagator” $\langle G^{(+)}(\mathbf{x}, \mathbf{x}') G^{(-)}(\mathbf{x}', \mathbf{x}) \rangle$. The standard boundary conditions [38] set this quantity equal to zero on the boundary with the leads, and set its normal derivative to zero on the “insulating” boundaries. Imposing these boundary conditions on a finite surface cuts off the

well-known small momentum divergence of the diffusion propagator at momenta of the order of the inverse of the size of the disordered region. In the case of a two-probe wire, this finite-size cutoff enters the calculations in much the same way as the cutoff due to inelastic scattering; thus, as noted above, the two-probe theory of universal conductance fluctuations in a finite-size conductor at $T = 0$ gives good agreement with observations on wires with probes separated by approximately the inelastic diffusion length. The crucial point in this context is that these standard boundary conditions on the diffusion propagator can be shown to be a coarse-grained version of the boundary conditions appropriate for our model of a finite disordered region with hard walls, connected to infinite perfect leads at appropriate points [59]. *Therefore our results show that $T = 0$ diagrammatic calculations based on the impurity-averaging technique are precisely equivalent to calculating voltage fluctuations using the multi-probe Landauer formula, Equation (4).* One of the major goals of this review is to emphasize the equivalence of this version of the Landauer approach and the Kubo formula approach at $T = 0$.

It is nonetheless worth noting that the two approaches are only strictly equivalent in the absence of inelastic scattering (the effects of finite temperature in causing “energy-averaging” [35, 36] can be included easily in either approach). The S -matrix appearing in Equation (4) is for elastic scattering between the various channels at the Fermi surface. It may be possible to generalize this approach to include inelastic scattering channels as well, but this has not been done, and would require a very different derivation from the one we have provided above. However, as noted above, adding perfect leads at various points along the conductor can simulate to some extent the dephasing effects of inelastic scattering. In the two-probe case this is particularly simple, because there is only one length scale associated with the distance between the two ends of the disordered leads, and one can roughly identify this with the inelastic scattering length. In the multi-probe case, Baranger et al. [6] have shown by careful numerical studies that by choosing appropriate geometries it is possible to reproduce almost all of the observed experimental effects (not relating to the asymmetry). It is worth noting that these calculations use precisely Equation (4) and not any equivalent formulation. Initially the diagrammatic calculations also employed the artifice of perfect leads to simulate inelastic scattering, with some success [3].

Nonetheless, in the multi-probe case there is no longer one length scale associated with the finite-size cutoff, and therefore there is at best a rough equivalence between the spatially localized “inelastic scattering” introduced by the leads and true spatially homogeneous inelastic scattering. In particular, the voltage fluctuations calculated from Equation (4) depend on the fictitious boundary conditions of “perfect” leads, i.e., results depend in general on the distance along the

voltage leads from the main channel to the beginning of the perfect leads, a length which has no real analogue in the experiments. Later versions of the diagrammatic Green function calculations eliminated this unphysical length simply by introducing an inelastic scattering term into the differential equation for the diffusion propagator mentioned above [2, 4]. Then it can be shown that if L_{in} is much less than the distances from the main channel to the beginning of the perfect leads, the boundary condition imposed there drops out of the problem, and one obtains results which only depend on physically meaningful lengths. An important further refinement was that recently Kane et al. [2] have developed a Kubo formula approach which is valid in the limit of weak magnetic field and weak disorder, and this has allowed them to calculate the field-symmetric and antisymmetric voltage fluctuations in this approximation; this justifies results independently obtained by Isawa et al. [3]).

These calculations are able to reproduce the following features of the experimental data on voltage fluctuations in multi-probe devices:

1. The linear dependence on probe-spacing for $L_{in} \ll L$ changing over to a weaker size-dependence when $L_{in} \geq L$, at a value consistent with the universal conductance fluctuations.
2. The difference in the L -dependence of the symmetric and antisymmetric parts of the voltage fluctuations.
3. The nonlocal behavior of the voltage fluctuations.
4. The asymmetric phase behavior of the normal-metal Aharonov-Bohm effect.

Further, the recent calculations of Kane et al. [2] predict that the voltage fluctuations are not strictly constant for $L_{in} \gg L$ but should still have a linear L -dependence with a smaller slope than for $L_{in} \ll L$. They suggest that such a behavior is actually consistent with the experimental data which were interpreted to indicate no L -dependence. The quantitative values for the fluctuations predicted by the theory agree with experiment up to factors of two. There is no obvious reason that the agreement should not be even better than that, so the residual discrepancy may indicate that there is some further physics to be understood in these systems. On the whole, however, it is fair to say that the theory based on Equation (4) has done a quite creditable job of describing the experiments.

9. Open questions about open systems

There are at least four issues left open by the derivation and discussion of Equation (4) above. These relate to 1) the validity of Equation (4) in the presence of a magnetic field; 2) the feasibility of performing a true "weakly coupled" measurement; 3) the possibility of including a model of the "reservoir" or bulk measuring electrode in a rigorous

quantum-mechanical calculation; and 4) the neglect of true fluctuations in the local electric field in the conductor.

First we consider the issue of the validity of Equation (4) in the presence of a magnetic field. The derivation we have presented depends explicitly on time-reversal symmetry in the absence of a magnetic field. Büttiker's derivation is claimed to be valid even in the presence of a field, except that the elements of the S -matrix appearing in Equation (4) have a reduced symmetry. It is quite possible that this claim is correct, at least in some approximation; but the conditions necessary for its correctness need to be determined. In particular, Kane et al. have shown that the generalized Kubo formula due to Streda [60] can be employed to calculate voltage fluctuations in the limit of weak field and weak disorder [2], because in this limit the conductivity tensor is still approximately divergenceless. They did not show that the formula they use is equivalent to Büttiker's in this approximation. What is needed is to derive, in the presence of a field, a relationship between the Green function and the S -matrix similar to the one we have derived, and then insert this relationship into the generalized linear response expression. We point out that such a generalization will not be completely trivial, because the formula we have derived for g_{mn} in terms of the transmission matrices, Equation (84), if it were valid in the presence of a field, would have the property that even when the symmetry of the transmission matrices is reduced by a magnetic field, B [$T_{mn}(B) = T_{nm}(-B)$], we would still find $g_{mn}(B) = g_{mn}(-B)$. The conductance coefficients proposed by Büttiker do not have this symmetry. However, there is no expectation that such a symmetry would hold in the presence of a field, and indeed such a symmetry would invalidate the natural explanation for the observed asymmetry in the magnetoresistance. Therefore, such a derivation will not consist of simply justifying the one we have presented above in the presence of a field.

There is also apparently a more fundamental question concerning the validity of Equation (4) in the presence of a field, first noted by Lee.* Equation (4) involves only Fermi surface properties of the electronic system, whereas the Streda [60] generalization of the Kubo formula mentioned above consists of two terms: the so-called classical term expressed in terms of Green functions at the Fermi surface, treated by Kane et al., and the "nonclassical term" which depends on all the states below the Fermi surface. The latter is related to the derivative of the density of states with respect to magnetic field, and can be assumed small for a typical metal. Nonetheless, such a term exists and apparently cannot be reproduced by Equation (4), suggesting that Equation (4) is never strictly valid in the presence of a field. The qualifier "apparently" is important, since it has been suggested that edge states at the Fermi level may fill the role

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of this nonclassical term for a finite system [61]. Recently a different multi-channel Landauer formula has been proposed for the case of high magnetic field in order to discuss the quantum Hall effect [61]. Although this formula is really based on Equation (3) and not on Equation (4), it does express the Hall resistance in terms only of quantities at the Fermi level by appealing to the existence of extended edge states.

Another question clearly raised by our discussion, but not yet answered, is whether it is possible to perform an ideal weakly coupled voltage measurement of the sort envisioned by Engquist and Anderson and by Büttiker et al. It has been suggested that one might attempt such a measurement by putting a tunnel barrier between the voltage leads and current leads, or by using a scanning tunneling microscope as a voltage probe [19]. This will certainly achieve a weak coupling between the probes and the sample. But will it achieve an ideal measurement in the sense that the voltage measured is a property of the sample, independent of the nature of the voltage probes? It seems quite possible that such a measurement will be even more sensitive to the properties of the probes, for the same reason that the resistance of a finite system in the localized regime fluctuates exponentially with changes in its configuration of disorder [10]. This question certainly requires further study; but at the moment it appears quite possible that in the mesoscopic regime there is no way to experimentally measure the four-probe resistance of a microstructure and obtain a result independent of the microscopic nature of the voltage probes used.

The third major issue relates not only to Equation (4) but to the Landauer approach generally. There is, of course, no reason to expect the resistance of a quantum-mechanical system to be independent of the manner in which it is measured. That is to say, there is no reason to expect to be able to make an arbitrary distinction between the "resistor" and the measuring "reservoirs," and then find that the measured resistance depends only on the properties of the resistor. This can be seen most explicitly in our discussion of the contact resistance predicted by Equation (2). The true contact resistance associated with any particular two-probe device will depend on the details of the junction between the channel and the bulk electrodes; it is only equal to $(Ne^2/h)^{-1}$ in some average sense. This may be relatively unimportant when the channel is much longer than the inelastic scattering length, but it may be quite important in the new generation of ballistic devices, where it really may be necessary to impedance-match the channel to the bulk electrodes to minimize reflection at the junction. Similarly, the voltage induced by an imposed current in a multi-probe configuration will depend on the shape of the voltage probes. More generally, we have the physical picture of the bulk electrodes acting as an equilibrating reservoir, and there is no reason in principle why a theoretical model for such a

reservoir cannot be included in a quantum-mechanical calculation. As pointed out by Landauer [54], such a calculation would be rather similar in spirit to the now well-developed techniques for calculating tunneling in the presence of dissipation [62]. Such a model would perhaps be conceptually more attractive than simply introducing an inelastic cutoff into the relevant Green functions, as is now done.

Finally, we are back to the question that started Landauer along this road many years ago. What is the true electric field distribution in a conductor when a steady-state current is flowing? The theory based on Equation (4) does not answer this question at all, for we have seen that it is only sensitive to the values of the potential imposed at the edges of the disordered region. This is understandable, since throughout our discussions we have treated the carriers as noninteracting quasi-particles. In real conductors self-consistent screening must be taken into account, and for a good metal the total electric field resulting from an externally applied voltage in steady state would presumably fluctuate only on microscopic length scales. Therefore, in linear response it is possible to treat only the electric field corresponding to zero net charge density within the conductor. Nonetheless, as Landauer has pointed out [9], the true local fields can be important for such processes as electromigration. A complete quantum-mechanical description of these local field effects remains an open problem.

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Appendix A

In this appendix we study the consequences of flux conservation when dealing with a multi-channel problem (as opposed to a single-channel one), and show that the requirement of flux conservation is incompatible with the orthogonality of the scattering states $\{\psi_\alpha^{(+)}\}$.

• Consequences of flux conservation

The scattering state $\psi_{(n,a)}^{(+)}$ is, by definition, the eigenstate of the Hamiltonian, with a given energy, chosen to have only one incident wave from infinity, coming through channel a of lead n . The prescribed asymptotic behavior determines the functional form of $\psi_{(n,a)}^{(+)}(\mathbf{x})$ in the asymptotic region, and it is customary in scattering theory to define reflection and transmission amplitudes by

$$\psi_{(n,a)}^{(+)}(\mathbf{x}) = \begin{cases} \eta [\exp\{-ik_a^{(n)}x_n\}\chi_a^{(n)}(y_n) + \sum_{a'} \bar{r}_{nn,a'a} \exp\{ik_{a'}^{(n)}x_n\}\chi_{a'}^{(n)}(y_n)] & \text{for } \mathbf{x} \text{ in lead } n, \\ \eta \sum_{a'} \bar{t}_{ln,a'a} \exp\{ik_{a'}^{(l)}x_l\}\chi_{a'}^{(l)}(y_l) & \text{for } \mathbf{x} \text{ in lead } l \neq n. \end{cases} \quad (89)$$

η is an overall real normalization factor that does not affect the ratios of the amplitudes of the scattered waves to the incoming wave, namely, the $\bar{r}$'s and $\bar{t}$'s. For a fixed energy, the set $\{\psi_{(n,a)}^{(+)}\}$ containing all possible (n, a) is a linearly independent and complete set in the energy subspace (i.e., a basis to that subspace). For a time-reversal invariant Hamiltonian, the time-reversal transformed states of $\{\psi_{(n,a)}^{(+)}\}$ are also a basis to the same subspace. Those states are called $\{\psi_{(n,a)}^{(-)}\}$, and their behavior in the asymptotic region can be obtained by time-reversing (89). This yields

$$\psi_{(n,a)}^{(-)}(\mathbf{x}) = \begin{cases} \eta [\exp\{ik_a^{(n)}x_n\}\chi_a^{(n)}(y_n) + \sum_{a'} \bar{r}_{nn,a'a}^* \exp\{-ik_{a'}^{(n)}x_n\}\chi_{a'}^{(n)}(y_n)] & \text{for } \mathbf{x} \text{ in lead } n, \\ \eta \sum_{a'} \bar{t}_{ln,a'a}^* \exp\{-ik_{a'}^{(l)}x_l\}\chi_{a'}^{(l)}(y_l) & \text{for } \mathbf{x} \text{ in lead } l \neq n. \end{cases} \quad (90)$$

The usual procedure for defining the scattering matrix is to define a matrix $\bar{S}$ by

$$\psi_{(n,a)}^{(+)}(\mathbf{x}) = \sum_{(l,b)} \bar{S}_{(l,b)(n,a)} \psi_{(l,b)}^{(-)}(\mathbf{x}). \quad (91)$$

The matrix elements of $\bar{S}$ can be determined by the following argument. Let us consider a point $\mathbf{x}_m$ in lead $m \neq n$. After (90) is substituted into (91), the only terms in the right-hand side of (91) that have outgoing waves at $\mathbf{x}_m$ are

$$\sum_b \bar{S}_{(m,b)(n,a)} \eta \exp\{ik_b^{(m)}x_m\}\chi_b^{(m)}(y_m). \quad (92)$$

On the other hand, looking at (89), we see that the terms with outgoing waves at $\mathbf{x}_m$ in the left-hand side of Equation (91) are

$$\sum_b \bar{t}_{mn,ba} \eta \exp\{ik_b^{(m)}x_m\}\chi_b^{(m)}(y_m). \quad (93)$$

Comparing (92) and (93), we obtain

$$\bar{S}_{(m,b)(n,a)} = \bar{t}_{mn,ba} \quad m \neq n. \quad (94)$$

In a similar fashion, when we consider a point $\mathbf{x}_n$ at lead n , we obtain

$$\bar{S}_{(n,b)(n,a)} = \bar{r}_{nn,ba}. \quad (95)$$

Equations (94) and (95) can be written compactly as

$$\bar{S} = \begin{bmatrix} \bar{r}_{11} & \bar{t}_{12} & \cdots & \bar{t}_{1N_L} \\ \bar{t}_{21} & \bar{r}_{22} & \cdots & \bar{t}_{2N_L} \\ \vdots & \vdots & \ddots & \vdots \\ \bar{t}_{N_L 1} & \bar{t}_{N_L 2} & \cdots & \bar{r}_{N_L N_L} \end{bmatrix}, \quad (96)$$

where $\bar{r}_{nn}$ and $\bar{t}_{mn}$ are the matrices defined by

$$(\bar{r}_{nn})_{ba} \equiv \bar{r}_{nn,ba}, \quad (\bar{t}_{mn})_{ba} \equiv \bar{t}_{mn,ba}. \quad (97)$$

In the usual scattering problem, the condition of flux conservation requires the matrix $\bar{S}$ to be unitary. We now show that this is not so for a multi-channel problem.

In the asymptotic region, where there are no electric fields, the elements of the current density operator between any eigenstates ψ_α and ψ_β of the Hamiltonian, whether or not they are orthonormal, are given by (26). In our context flux

conservation is stated by Equation (36). If we take there ψ_α and ψ_β such that $\epsilon_\alpha = \epsilon_\beta$, then

$$\nabla \cdot \mathbf{W}_{\alpha\beta}(\mathbf{x}) = 0, \quad (98)$$

and an integration of (98) over the domain $\mathcal{A}$ defined in Section 4 (in the subsection on cancellation of the diamagnetic term) gives

$$\sum_{l=1}^{N_L} Y_{\alpha\beta}^{(l)} = 0, \quad (99)$$

where we have defined

$$Y_{\alpha\beta}^{(l)} \equiv \int_{C_l} \mathbf{W}_{\alpha\beta} \cdot \hat{\mathbf{x}}_l dy_l = \int \psi_\alpha^*(\mathbf{x}_l) \frac{\vec{\partial}}{\partial x_l} \psi_\beta(\mathbf{x}_l) dy_l. \quad (100)$$

This is the expression for flux conservation. To see what it implies for the $\bar{r}$ and $\bar{t}$ coefficients, we take α and β to be scattering states. Taking $\psi_\alpha = \psi_{(n,a)}^{(+)}$ and $\psi_\beta = \psi_{(n,b)}^{(+)}$ in (100), we obtain

$$Y_{\alpha\beta}^{(n)} = \eta^2 2i [-\delta_{ab} k_a^{(n)} + \sum_{a'} \bar{r}_{nn,a'a}^* \bar{r}_{nn,a'b} k_{a'}^{(n)}] \quad (101)$$

$$Y_{\alpha\beta}^{(l)} = \eta^2 2i \sum_{a'} \bar{t}_{ln,a'a}^* \bar{t}_{ln,a'b} k_{a'}^{(l)} \quad l \neq n, \quad (102)$$

and so, after a little rearrangement, (99) gives

$$\sum_{a'} \bar{r}_{nn,a'a}^* \bar{r}_{nn,a'b} \frac{k_{a'}^{(n)}}{\sqrt{k_a^{(n)} k_b^{(n)}}} + \sum_{l \neq n} \left[\sum_{a'} \bar{t}_{ln,a'a}^* \bar{t}_{ln,a'b} \frac{k_{a'}^{(l)}}{\sqrt{k_a^{(n)} k_b^{(n)}}} \right] = \delta_{ab}. \quad (103)$$

When we take in (100) $\psi_\alpha = \psi_{(n,a)}^{(+)}$ and $\psi_\beta = \psi_{(m,b)}^{(+)}$ with $m \neq n$, we get

$$Y_{\alpha\beta}^{(n)} = \eta^2 2i \sum_{a'} \bar{r}_{nn,a'a}^* \bar{t}_{nm,a'b} k_{a'}^{(n)}, \quad (104)$$

$$Y_{\alpha\beta}^{(m)} = \eta^2 2i \sum_{a'} \bar{t}_{mn,a'a}^* \bar{r}_{mm,a'b} k_{a'}^{(m)}, \quad (105)$$

$$Y_{\alpha\beta}^{(l)} = \eta^2 2i \sum_{a'} \bar{t}_{ln,a'a}^* \bar{t}_{lm,a'b} k_{a'}^{(l)}, \quad l \neq n, m, \quad (106)$$

and (99) now gives

$$\begin{aligned} & \sum_{a'} \bar{r}_{nn,a'a}^* \bar{t}_{nm,a'b} \frac{k_{a'}^{(n)}}{\sqrt{k_a^{(n)} k_b^{(m)}}} \\ & + \sum_{a'} \bar{t}_{mn,a'a}^* \bar{r}_{mm,a'b} \frac{k_{a'}^{(m)}}{\sqrt{k_a^{(n)} k_b^{(m)}}} \\ & + \sum_{l \neq n, m} \left[\sum_{a'} \bar{t}_{ln,a'a}^* \bar{t}_{lm,a'b} \frac{k_{a'}^{(l)}}{\sqrt{k_a^{(n)} k_b^{(m)}}} \right] = 0. \end{aligned} \quad (107)$$

We can restate Equations (103) and (107) in a clearer matrix notation by defining the diagonal matrices K and Q :

$$K_{mn,aa'} = \delta_{mn} \delta_{aa'} \sqrt{k_a^{(m)}}, \quad (108)$$

$$Q_{mn,aa'} = \delta_{mn} \delta_{aa'} \frac{1}{\sqrt{k_a^{(m)}}}, \quad (109)$$

and then write (103) and (107) in matrix form as

$$(K\bar{S}Q)^\dagger K\bar{S}Q = 1. \quad (110)$$

Thus we have shown that in general current conservation does not imply that the matrix $\bar{S}$ defined by Equation (96) satisfies the standard unitarity relation $\bar{S}^\dagger \bar{S} = 1$, but rather, the more complicated formula (110). In the special case where the outgoing momenta in all the channels are the same, it is easy to see that the condition (110) reduces to the unitarity of $\bar{S}$; however, in our case it does not. Therefore Equation (96), which in the usual case defines a unitary scattering matrix, does not do so for a multi-channel waveguide-scattering geometry. It seems preferable to reserve the term S -matrix for a unitary object; therefore, it is natural to define the generalized S -matrix (unitary for all of the geometries considered) by

$$S = K\bar{S}Q. \quad (111)$$

It is obvious from (110) that S so defined is unitary. This definition is equivalent to defining new reflection and

transmission amplitudes in the same manner as Fisher and Lee [12],

$$r_{nn,a'b} = \bar{r}_{nn,a'b} \sqrt{\frac{k_{a'}^{(n)}}{k_b^{(n)}}}, \quad (112)$$

$$t_{ln,a'b} = \bar{t}_{ln,a'b} \sqrt{\frac{k_{a'}^{(l)}}{k_b^{(n)}}}. \quad (113)$$

These amplitudes can be thought of as the ratios of the amplitudes of the scattered waves to the amplitude of an incoming plane wave, when we normalize all waves to unit longitudinal flux. When expressed in terms of r and t , the scattering waves $\{\psi_{(n,a)}^{(+)}\}$ look as shown in (67) (up to an overall normalization constant).

In terms of these redefined transmission and reflection matrices, the matrix S has the familiar form

$$S = \begin{bmatrix} r_{11} & t_{12} & \cdots & t_{1N_L} \\ t_{21} & r_{22} & \cdots & t_{2N_L} \\ \vdots & \vdots & \ddots & \vdots \\ t_{N_L 1} & t_{N_L 2} & \cdots & r_{N_L N_L} \end{bmatrix}. \quad (114)$$

The unitarity of S then implies the simpler relations

$$r_{nn}^\dagger r_{nn} + \sum_{l \neq n} t_{ln}^\dagger t_{ln} = 1 \quad (115)$$

and

$$r_{nn}^\dagger t_{nm} + t_{mn}^\dagger r_{mm} + \sum_{l \neq n, m} t_{ln}^\dagger t_{lm} = 0. \quad (116)$$

Another set of equations satisfied by the r 's and t 's can be obtained by noting that as a consequence of (110) and (111), $\det(S) \neq 0$, and so $S^\dagger$ is the inverse of S from the right too:

$$SS^\dagger = 1; \quad (117)$$

then, expanding (117), one gets

$$r_{nn}^\dagger r_{nn} + \sum_{l \neq n} t_{nl}^\dagger t_{nl} = 1 \quad (118)$$

and

$$r_{nn}^\dagger t_{mn} + t_{nm}^\dagger r_{mm} + \sum_{l \neq n, m} t_{nl}^\dagger t_{ml} = 0. \quad (119)$$

To summarize, we have found that flux conservation implies that S , rather than $\bar{S}$, is unitary.

• Nonorthogonality of scattering states

We can now proceed to show that the scattering states $\{\psi_{(n,a)}^{(+)}\}$ are not orthogonal. Let us first note that

$$\langle \psi_\alpha^{(-)} | \psi_\beta^{(-)} \rangle = \langle T\psi_\alpha^{(+)} | T\psi_\beta^{(+)} \rangle = \langle \psi_\beta^{(+)} | \psi_\alpha^{(+)} \rangle, \quad (120)$$

which is a consequence of the antiunitarity of T .

In order to define sensibly an orthonormal basis for states which are not square-integrable, it is necessary to consider a

continuum of states, so that delta-function normalization makes sense in terms of integrals over a continuous density of states. Therefore, although in our calculation only the states precisely at ϵ_F come into the dc limit, we must define our states in the larger space of propagating states with variable energy. Thus we consider now two scattering states $\psi_{\epsilon(n,a)}^{(+)}$ and $\psi_{\epsilon'(n',a')}^{(+)}$, where ϵ and ϵ' can refer to states of different energy. If the set $\{\psi_{\epsilon(n,a)}^{(+)}\}$ were orthonormal, we would have

$$\langle \psi_{\epsilon(n,a)}^{(+)} | \psi_{\epsilon'(n',a')}^{(+)} \rangle = \delta(\epsilon - \epsilon') \delta_{(n,a)(n',a')}, \quad (121)$$

which, as a consequence of Equation (120), would imply

$$\langle \psi_{\epsilon(l,b)}^{(-)} | \psi_{\epsilon'(l',b')}^{(-)} \rangle = \delta(\epsilon - \epsilon') \delta_{(l,b)(l',b')}. \quad (122)$$

On the other hand, using (91),

$$\begin{aligned} \langle \psi_{\epsilon(n,a)}^{(+)} | \psi_{\epsilon'(n',a')}^{(+)} \rangle \\ = \sum_{(l,b)(l',b')} \bar{S}_{(l,b)(n,a)}^*(\epsilon) \bar{S}_{(l',b')(n',a')}(\epsilon') \langle \psi_{\epsilon(l,b)}^{(-)} | \psi_{\epsilon'(l',b')}^{(-)} \rangle. \end{aligned} \quad (123)$$

Therefore, if $\{\psi_{\epsilon(n,a)}^{(+)}\}$ were orthonormal, we could substitute (121) and (122) into (123) and obtain

$$\begin{aligned} \delta(\epsilon - \epsilon') \delta_{(n,a)(n',a')} \\ = \sum_{(l,b)} \bar{S}_{(l,b)(n,a)}^*(\epsilon) \bar{S}_{(l,b)(n',a')}(\epsilon) \delta(\epsilon - \epsilon'), \end{aligned} \quad (124)$$

which implies

$$\bar{S}^\dagger(\epsilon) \bar{S}(\epsilon) = 1. \quad (125)$$

In short, we have shown that the orthonormality of the set $\{\psi_{\epsilon(n,a)}^{(+)}\}$ implies that the matrix $\bar{S}$ defined in Equation (96) must be unitary. But we have just shown that current conservation implies that $\bar{S}$ is *not* unitary [it is the matrix S defined by (114) that is unitary.] Therefore $\{\psi_{\epsilon(n,a)}^{(+)}\}$ is not orthonormal. Since states with different energies are certainly orthogonal due to the Hermitian character of the Hamiltonian, we conclude that $\{\psi_{\epsilon(n,a)}^{(+)}\}$ (for a fixed energy) is not an orthogonal set. Langreth and Abrahams [16] assumed that the matrix defined by Equation (96) was unitary; hence, they incorrectly stated that the scattering states were orthogonal. To emphasize this point further, we note that there is no choice of normalization which makes these states orthogonal. Flux conservation implies that states chosen to consist of a single incident wave from infinity and outgoing waves in all the channels cannot be orthogonal.

Appendix B

In Section 4 we studied the current response of a multi-probe system driven by voltages applied to its leads, and obtained Equation (126) below. However, there is a whole class of experiments performed under conditions in which the currents through the leads are fixed and the voltages at the leads are the measured quantities. In this appendix we show a general procedure to obtain the voltage response when the conductance coefficients g_{mn} are known.

• Definition of the problem

The conductance coefficients g_{mn} are defined by the relation

$$I_m = \sum_{n=1}^{N_L} g_{mn} V_n \quad m = 1, 2, \dots, N_L, \quad (126)$$

which can be regarded as a representation of the N_L -dimensional vector equation

$$|I\rangle = \mathbf{g} |V\rangle \quad (127)$$

in the standard basis $\{|e_n\rangle\}$

$$|e_1\rangle = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \dots, |e_{N_L}\rangle = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix}. \quad (128)$$

With this notation $\langle e_n | I \rangle = I_n$ is the current into lead n . On the other hand, following Büttiker [1], we can characterize the voltage response of the system by defining resistance coefficients $R_{m'n',mn}$ as the ratios of the voltage differences between leads m and n to the current flowing from lead m' to lead n' , when all other leads draw no current:

$$R_{m'n',mn} \equiv \frac{V_m - V_n}{I} \quad \begin{cases} I = I_{n'} = -I_{m'}, \\ I_l = 0 \text{ for } l \neq n', m'. \end{cases} \quad (129)$$

It is obvious that the $\{R_{m'n',mn}\}$ should be obtainable from the $\{g_{mn}\}$, since the latter contain all the information concerning the dissipative response of the system to applied voltages in the leads. Naively, in order to compute $R_{m'n',mn}$ one would like to set $I_{n'} = -I_{m'} = I$ and all other currents to zero, i.e.,

$$|I\rangle = I |e_{n'}\rangle - I |e_{m'}\rangle \quad (130)$$

in (127), invert the equation for $|V\rangle$, and finally compute the expression in (129) by taking the difference between V_m and V_n . Nevertheless, it is not possible to proceed in that manner without some further elaboration, since $\mathbf{g}$ is not invertible, as we see below.

• Solution to the problem

The singularity of the matrix $\mathbf{g}$ derives from the constraints imposed on it by two basic features of the currents and voltages in *any* system, namely the arbitrariness in the choice of the zero reference level for the voltages and the conservation of current (Kirchoff's law). To see how this happens, let us define $|a_1\rangle$ to be the unit vector proportional to $(1, 1, \dots, 1)$,

$$|a_1\rangle = \frac{1}{\sqrt{N_L}} (|e_1\rangle + |e_2\rangle + \dots + |e_{N_L}\rangle). \quad (131)$$

With this notation, a shift in the zero voltage reference level corresponds to replacing $|V\rangle$ with $|V\rangle - (\text{const.})|a_1\rangle$. Since upon that replacement the current in (127) has to remain unchanged regardless of the value we choose for the constant, we must have

$$\mathbf{g} | a_1 \rangle = 0; \quad (132)$$

therefore, $| a_1 \rangle$ is an eigenvector of $\mathbf{g}$ with eigenvalue 0. Consequently, given a solution $| V' \rangle$ of (127), there is a whole family of solutions of (127) that differ from $| V' \rangle$ by a multiple of the vector $| a_1 \rangle$. We will assume that 0 is a nondegenerate eigenvalue of $\mathbf{g}$, so only the eigenvector $| a_1 \rangle$ has eigenvalue 0. Therefore it is also true that any two solutions of (127) differ by a multiple of $| a_1 \rangle$. In particular, we will search for the solution $| V' \rangle$ that has no component along $| a_1 \rangle$ (i.e., $| V' \rangle$ perpendicular to $| a_1 \rangle$ or $\langle a_1 | V' \rangle = 0$), and then obtain any other solution $| V \rangle$ by adding $(\text{const.}) | a_1 \rangle$ to the former. The requirement of current conservation $\sum_{n=1}^{N_L} I_n = 0$ also has a simple expression in terms of the notation just defined, namely $\langle a_1 | I \rangle = 0$. In other words, this equation states that all physical $| I \rangle$'s (i.e., currents satisfying Kirchhoff's law) are perpendicular to the vector $| a_1 \rangle$. Since $| I \rangle$ in (127) must satisfy this requirement regardless of what voltages $| V \rangle$ we apply to the leads, we conclude from (127) that

$$\langle a_1 | \mathbf{g} = 0. \quad (133)$$

In short, we have found that the freedom of choice for the zero reference level for the potentials and the requirement of current conservation constraint implies that any possible $\mathbf{g}$ must have the vector $| a_1 \rangle$ as a right and left eigenvector with eigenvalue 0. By going back to Equation (86), we note that the conductance coefficients g_{mn} obtained from the "microscopic theory" for a system in the absence of a magnetic field do indeed satisfy the above constraints [in that context (132) and (133) were seen to be consequences of current conservation and the symmetric character of $\mathbf{g}$]. Furthermore, we have made the observation that for our purposes Equation (127) can be thought of as holding between vectors $| V' \rangle$ and $| I \rangle$ in the $(N_L - 1)$ -dimensional subspace perpendicular to $| a_1 \rangle$. In this subspace $\mathbf{g}$ does not have a zero eigenvalue and therefore can be inverted.

Instead of bringing the matrix g_{mn} into a $1 \oplus (N_L - 1)$ block form and then inverting the $(N_L - 1)$ -dimensional block, it is more convenient to proceed as follows. We found in Section 4 that in the absence of a magnetic field the conductance matrix $\mathbf{g}$ is real and symmetric, so its nonzero eigenvalues $\{\lambda_n\}_{n=2}^{N_L}$ have corresponding eigenvectors $\{| a_n \rangle\}_{n=2}^{N_L}$ that can be taken to be orthonormal. By writing $\mathbf{g}$ in terms of its spectral representation

$$\mathbf{g} = \sum_{n=2}^{N_L} \lambda_n | a_n \rangle \langle a_n | + 0 | a_1 \rangle \langle a_1 |, \quad (134)$$

we see explicitly that even though $\mathbf{g}$ is singular as a transformation in the whole N_L -dimensional space, it is invertible when regarded as a transformation from the $(N_L - 1)$ -dimensional subspace of vectors perpendicular to $| a_1 \rangle$ onto itself. The solution to the equation we want to solve,

$$| I \rangle = \sum_{n=2}^{N_L} \lambda_n | a_n \rangle \langle a_n | V' \rangle, \quad (135)$$

is easily found to be

$$\sum_{n=2}^{N_L} \frac{1}{\lambda_n} | a_n \rangle \langle a_n | I \rangle = | V' \rangle, \quad (136)$$

which is certainly not changed if we subtract 0 from the left-hand side to obtain

$$\left[\sum_{n=2}^{N_L} \frac{1}{\lambda_n} | a_n \rangle \langle a_n | - | a_1 \rangle \langle a_1 | \right] | I \rangle = | V' \rangle. \quad (137)$$

But the matrix in square brackets is the inverse of the N_L -dimensional matrix $\tilde{\mathbf{g}}$ defined by

$$\begin{aligned} \tilde{\mathbf{g}} &= \sum_{n=2}^{N_L} \lambda_n | a_n \rangle \langle a_n | - | a_1 \rangle \langle a_1 | \\ &= \mathbf{g} - | a_1 \rangle \langle a_1 |, \end{aligned} \quad (138)$$

and Equation (137) is what we would have obtained had we started with

$$| I \rangle = \tilde{\mathbf{g}} | V' \rangle \quad (139)$$

instead of (127). Roughly speaking, we have been able to invert Equation (127) in the smaller subspace by resorting to the artifice of defining the nonsingular matrix $\tilde{\mathbf{g}}$ and inverting Equation (139) in the whole space instead. Considering the k th component of (137), we get

$$V'_k = \sum_{l=1}^{N_L} (\tilde{\mathbf{g}}^{-1})_{kl} I_l \quad k = 1, 2, \dots, N_L, \quad (140)$$

and by setting $I_{n'} = -I_{m'} = I$ and $I_l = 0$ for $l \neq n', m'$ in the equation above, we obtain the voltages $\{V'_k\}$ we were looking for

$$V'_k = (\tilde{\mathbf{g}}^{-1})_{kn'} I - (\tilde{\mathbf{g}}^{-1})_{km'} I \quad k = 1, 2, \dots, N_L. \quad (141)$$

In principle the V'_k 's in (129) may differ from the V'_k 's just found by a constant, but of course the physical quantities $R_{m'n',mn}$ only depend on the voltage differences and those are insensitive to the value of that constant. By specializing (141) to the cases $k = m$ and $k = n$, using $V'_m - V'_n = V_m - V_n$ and substituting into the definition (129), we arrive at the final result

$$\begin{aligned} R_{m'n',mn} &= (\tilde{\mathbf{g}}^{-1})_{mn'} + (\tilde{\mathbf{g}}^{-1})_{nm'} \\ &\quad - (\tilde{\mathbf{g}}^{-1})_{mm'} - (\tilde{\mathbf{g}}^{-1})_{nn'}. \end{aligned} \quad (142)$$

To summarize, in order to find the coefficients $R_{m'n',mn}$ given Equation (126), we simply obtain $\tilde{\mathbf{g}}$ from $\mathbf{g}$ by subtraction:

$$\tilde{\mathbf{g}} = \mathbf{g} - \frac{1}{N_L} \begin{bmatrix} 1 & \cdots & 1 \\ \cdots & \cdots & \cdots \\ 1 & \cdots & 1 \end{bmatrix}, \quad (143)$$

and then compute the four elements of $\tilde{\mathbf{g}}^{-1}$ indicated in

(142), which require the evaluation of one $N_L \times N_L$ and four $(N_L - 1) \times (N_L - 1)$ determinants.

Finally, we point out that even though we made use of the symmetric character of $\mathbf{g}$ in writing (134), a property that we do not expect to hold in the presence of a magnetic field, that assumption is not necessary to derive (142). The essential feature for the validity of (142) is that there exists a basis in which $\mathbf{g}$ is represented by a block-diagonal matrix with a zero in the position (1, 1) and a nonsingular $(N - 1) \times (N - 1)$ block. Since Kirchhoff's Law and the freedom to define the zero of voltage imply that $|a_1\rangle$ is always a left and right eigenvector of $\mathbf{g}$ with eigenvalue 0, any basis consisting of $|a_1\rangle$ and a set of basis vectors to the subspace orthogonal to $|a_1\rangle$ will lead to the required form for $\mathbf{g}$. We can then find the inverse transformation to the $(N - 1)$ -dimensional block by inverting the $N \times N$ matrix obtained from $\mathbf{g}$ by replacing the zero in position (1, 1) with a -1 . In basis-independent language, that replacement corresponds to subtracting $|a_1\rangle \langle a_1|$ from $\mathbf{g}$, so the N -dimensional matrix to be inverted is still exactly $\tilde{\mathbf{g}}$ defined in (143), and Equation (142) is valid in all cases.

Büttiker [1] has analyzed the symmetries of four-probe resistance measurements by assuming that Equation (4) is valid even in the presence of a magnetic field B . As noted in our conclusions, this is a substantial assumption, and its range of validity remains to be determined by a microscopic derivation. Büttiker shows that the symmetries of the S -matrix are insufficient to imply that $R_{m'n',mn}(B) = R_{mn,m'n'}(-B)$, but they do imply that the quantities $R_{m'n',mn}(B) \pm R_{mn,m'n'}(B)$ are symmetric (antisymmetric) under field reversal. Accepting the validity of Equation (4), it is a simple exercise to extend those results to a general multi-probe system by using Equation (142). An outline of the proof goes as follows: As a consequence of (4) and the transformation of the S -matrix under time-reversal, the matrix $\mathbf{g}(B)$ goes into its transpose when we reverse the field, and from (143) it is clear that $\tilde{\mathbf{g}}$ also has that property: $\tilde{\mathbf{g}}_{mn}(B) = \tilde{\mathbf{g}}_{nm}(-B)$. Since the determinant of a matrix equals that of its transpose, and

$$A_{mn}[\tilde{\mathbf{g}}(-B)] = A_{mn}[\tilde{\mathbf{g}}^T(B)] = A_{nm}[\tilde{\mathbf{g}}(B)], \quad (144)$$

where $A_{mn}(\tilde{\mathbf{g}})$ is the determinant of the cofactor matrix of the element $\tilde{\mathbf{g}}_{mn}$, one obtains

$$[\tilde{\mathbf{g}}^{-1}(-B)]_{mn} = [\tilde{\mathbf{g}}^{-1}(B)]_{nm}. \quad (145)$$

This result combined with Equation (142) implies the symmetry relations given above.

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