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Electrical linear-response theory in an arbitrary magnetic field: A new Fermi-surface formation

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We develop a novel formulation of dc electrical linear-response theory for a phase-coherent conductor with multiple leads valid in *arbitrarily strong* magnetic field and for a given impurity configuration and measuring geometry. This formulation is convenient for discussion of the quantum Hall effect and mesoscopic transport phenomena. We express the total current response I_m through lead m completely in terms of the voltages V_n applied at the leads, independent of the electric field in the material, i.e., $I_m = \sum_n g_{mn} V_n$. We show that while the current-density response is not in general expressible as a Fermi-surface quantity, the total transport current determined by these conductance coefficients g_{mn} does depend only on the wave functions (or Green functions) at the Fermi surface as $T \to 0$. This yields new and useful Green-function expressions for the g_{mn} and the longitudinal and Hall resistances. When transformed by appropriate applications of scattering theory, these expressions are shown to be equivalent to the relation $g_{mn} = T_{mn}$, where T_{mn} is the sum of all the transmission coefficients between leads m and n, as first obtained by Büttiker on the basis of phenomenological arguments. A brief discussion of the relation between this formula and other proposed Landauer formulas is given. It is noted that the occurrence of the quantum Hall effect is very natural in this formulation and simple conditions on the scattering matrix of the conductor which imply the quantum Hall effect are derived.

I. INTRODUCTION

A reexamination of electrical linear-response theory in an arbitrary magnetic field is of particular interest now due to two major developments in the field of quantum-transport phenomena. The first development is the discovery of a wealth of novel sample-specific and geometry-specific quantum phenomena in small ("mesoscopic") conductors at low temperature.[1] The second is the discovery of the integer quantum Hall effect,[2] which demonstrates that in the two-dimensional quantum limit the Hall resistance shows highly nonlinear and (as the system size goes to infinity) discontinuous dependence on magnetic field.

In the former case, mesoscopic conductors, the first novel effect discovered experimentally was the apparently random dependence of the resistance of a given sample on magnetic field (or carrier density in gated semiconductor systems) which was reproducible in a given sample although differing from sample to sample.[3–6] The samples initially studied were in the diffusive regime, in which the voltage probes are separated by a distance greater than the elastic scattering length l, but the temperature is low enough that inelastic scattering is negligible. It is now understood that the reproducible resistance noise arises from a quantum-interference effect similar to laser speckle whose manifestation in a given sample depends on the particular configuration of impurities;[7,8] the statistical behavior of these (time-independent) fluctuations was shown to have some universal features.[9,10] These measurements also revealed a further initially puzzling observation: although putatively measurements of the longitudinal resistance, the magnetoresistance pattern ("magnetofingerprint") of a given sample was not symmetric in magnetic field. It was subsequently shown that this asymmetry arises from the multiprobe nature of the measurement and that the data do satisfy reciprocity symmetries implied by time-reversal symmetry.[11,12] These results make it clear that in the phase-coherent regime all parts of the sample contribute essentially equally to the fluctuations in the resistance, and simply attaching leads along the wire in the standard geometry does not ensure that the longitudinal resistivity is being measured. This emphasizes the nonlocal nature of the transport measurements in mesoscopic systems, which, for example, leads to a saturation in the resistance fluctuations when the probes are spaced less than an inelastic length apart, at a magnitude corresponding to conductance fluctuations of order e^2/h per phase-coherent volume.[13–18] In addition to the electric resistance, other transport properties of mesoscopic systems should show fluctuating behavior.[19]

More recent experiments have probed the ballistic regime in which bulk elastic scattering is negligible and the resistance arises entirely from the sample geometry. Here novel behavior is observed even in the absence of a magnetic field. For example, in four-probe measurements such samples showed a nonlocal *average* resistance for each bend in the probe geometry,[20] and in two-probe geometries with a constriction (point contact) they showed a dramatic new effect, point-contact resistance quantized in steps of approximately e^2/h (per spin).[21–23]

All of these phenomena arise from the dependence of the linear-response coefficients on specific impurity configurations and/or sample geometries, and an adequate theoretical understanding of such effects requires a formulation of linear-response theory valid for a given system. We provide such a formulation below.

The relevance of our calculation to the quantum Hall effect is somewhat different. The integer quantum Hall effect is typically studied in larger semiconducting samples, and is observed to be relatively insensitive to the measuring geometry and impurity configuration in these systems. In addition, there undeniably exists an adequate theoretical understanding of many features of the effect.[2] Nonetheless, relatively little of this understanding is based upon actual *microscopic* calculations of the Hall resistance of a two-dimensional (2D) quantum-mechanical system, and there appears to be some disagreement in the literature upon appropriate starting points for such a calculation.[24] This is of particular importance when one considers questions relating to the breakdown of the quantization in the region of "extended states" between the plateaus, for which a complete theory does not yet exist. We present an exact formal theory of the Hall resistance, which provides a different and potentially useful starting point for microscopic calculations. In particular, the scattering formulation of the theory, first introduced by Büttiker[12] on the basis of Landauer-type arguments[25] (and which we derive from linear-response theory below), is sufficiently simple that the existence of the quantum Hall effect under rather general conditions can be seen from elementary physical arguments[26,27] (as will be discussed in the final section of the paper).

The most obvious immediate application of our theory is to the intersection of these two areas, transport in mesoscopic systems in a magnetic field, and, in particular, the Hall effect in such systems. This has been a subject of intense experimental interest recently.[28–37] The 2D semiconductor systems that show the quantum Hall effect on the macroscopic scale also show it on a mesoscopic scale, but with generally poorer quantization and with sample-specific fluctuations and resonant effects superimposed.[30,38] The statistical behavior of these fluctuations is not yet completely understood. In addition, gated samples exhibit quantization of the "longitudinal resistance,"[32–34] an effect which follows almost trivially from the scattering formulation of the theory.[27,32,39] Finally, there are the intriguing phenomena of the disappearance (or "quenching") of the low-field Hall effect in ultrathin ballistic samples[28,29,36,37,40] and the coherent electron focusing[31] and "generalized Hall effect,"[35] which have recently been studied in detail in the ballistic semiconductor point-contact systems.

With these motivations, the present work has three major goals. (1) To provide a formulation of electrical linear-response theory in an arbitrary magnetic field, of particular relevance for multiprobe mesoscopic conductors, which is valid for a given sample geometry and a given impurity configuration. (2) To express the theory only in terms of the exact eigenstates of the system (and, equivalently, the exact Green functions). Hence we provide a theoretical starting point for microscopic calculations based only on the exact relations of current conservation and time-reversal symmetry, and containing no physical assumptions about the nature of the states, implicit averaging procedures, etc. other than the important assumption of the approximate validity of the noninteracting-electron model. (3) To rewrite the theory in terms of the exact scattering states in order to make contact with the Landauer-type formulations. In this regard we use the term "Landauer formula" in a general way to denote any expression for the linear-response coefficients in terms of the S matrix of the conductor. We demonstrate the exact equivalence of our linear-response formula to the multiprobe Landauer formula proposed by Büttiker.[12]

There is, of course, an enormous literature on quantum-mechanical linear-response theory, dating back to the original work of Kubo and Greenwood,[41] and our work relates to and builds on various previous calculations. Our analysis of the principal-value term in the conductivity-response function, which results in a Fermi-surface expression for the Hall resistance,[42] is similar in several respects to that of Smrčka and Středa,[42(a)] and the method of making the connection between Green-function expressions and the scattering matrix builds on the previous work of Fisher and Lee,[43] Stone and Szafer,[44] and Kucera and Středa.[45] Our formulation adds important new elements for two reasons.

First, most previous calculations have focused on deriving expressions for the *conductivity,* or conductivity tensor, whereas the quantities which characterize a given system are the spatially varying conductivity-response function $\sigma(x,x')$ (which describes the current *density* response to an electric field) or the *conductance coefficients* (defined below) that describe the total current flowing in and out of the system in response to voltages applied at its boundaries. The conductivity tensor as a set of intensive variables can only be defined as an average property of the system, usually obtained by averaging $\sigma(x,x')$ over the sample volume,[42(a)] or over the impurity configurations of an ensemble of similar systems,[46] or both. Obviously, this is suspect in the mesoscopic regime, where sample-specific fluctuations are important. But there is another basic problem with this procedure: $\sigma(x,x')$ and the conductance coefficients describe different physical properties of the systems and have different behaviors which become particularly important in the presence of a magnetic field. $\sigma(x,x')$ describes both the transport current and the circulating or diagmagnetic currents which always exist in the presence of a magnetic field, whereas the conductance coefficients describe only the total transport currents. We show below that *only* the conductance coefficients are completely described by wave functions at the Fermi surfaces (as $T\rightarrow 0$), whereas $\sigma(x,x')$ depends, in general, on all the states below the Fermi energy. Since it is the conductance coefficients which are measured in standard transport experiments, this shows that the Hall resistance can always be expressed as a Fermi-surface quantity (without any additional assumptions about the existence of states localized near the edges).

The second new feature of our calculation concerns the relationship between the scattering-theoretic approach and linear-response theory. The linear-response theory formulations proposed previously in order to describe a given sample,[43,47,48] such as that of Fisher and Lee,[43] or Langreth and Abrahams,[48] have focused on deriving various versions of the Landauer formula in a *two-probe* geometry, whereas it has now become apparent that a multiprobe formula such as that of Büttiker[12] is necessary to describe the mesoscopic regime. Stone and Szafer have argued in a recent review article that Büttiker's multiprobe Landauer formula is the relevant Landauer formula for describing standard transport experiments.[44] Their conclusion is supported by the success of this formula in describing the observed reciprocity symmetries[11,12] and in quantitatively accounting for the resistance fluctuations of multiprobe microstructures.[13–18] The same review derived the multiprobe formula from linear-response theory in the absence of a magnetic field, by an extension of the arguments used by Fisher and Lee[43] in the two-probe case, but pointed out the nontrivial and crucial nature of the extension to finite magnetic field. Recently, Landauer formulas have been proposed to describe the high-magnetic-field limit on the basis of a nominally two-probe geometry.[49,50] These approaches have been very useful in emphasizing the role of edge states in establishing the quantum Hall effect, and of interedge scattering in its breakdown; however, these formulas have not been connected to a rigorous linear-response calculation, and indeed probably do not provide a full description of the Hall effect and its breakdown.[39,51,52] The calculation that we present below is very different from the calculation of Fisher and Lee[43], or, indeed, *any* of the previous derivations of Landauer formulas from linear-response theory. All previous derivations have started with an expression which was manifestly on the Fermi surface (such an expression arises immediately in the two-probe case, or in the presence of time-reversal symmetry), whereas our derivation starts with the general expression for $\sigma(x,x')$ in a magnetic field, which contains a non-Fermi-surface (principal-value) term. We show that such a term leads to a transport current that is a Fermi-surface quantity, a result which is crucially needed in order to obtain the correct reciprocity symmetries, implied by Büttiker's multiprobe Landauer formula. Thus our derivation provides the final step in proving the equivalence of the scattering-theoretic (Landauer-Büttiker) and standard (Kubo-Greenwood) approaches to linear-response theory. In the final section we derive some general properties of the multiprobe Landauer formula of particular interest and relevance to experiments of high magnetic field, and show that in a simple limit the original Landauer formula,[25] and a trivial multichannel extension of it, is obtained.

Before embarking on the detailed calculations, we discuss some general features of the model and of the calculation. We consider a structure which consists of a finite region connected to N_L perfectly ordered, straight semi-infinite leads (see Fig. 1); in the finite region there may be disorder or particular geometric features which scatter

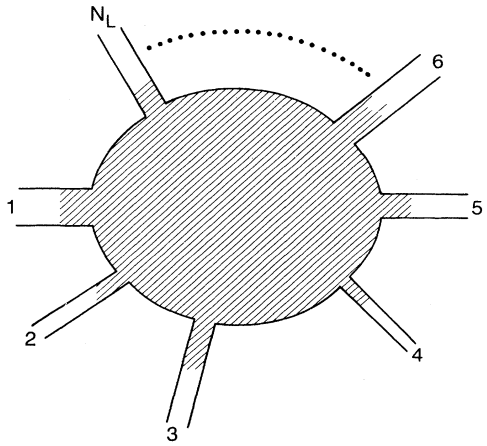

FIG. 1. An arbitrary multiprobe structure. A possibly disordered region (hatched) is connected to N_L straight, ordered leads which are used to feed current or measure voltage.

the electrons (including, of course, the junctions between the leads). The transport throughout the structure is completely coherent, no phase breaking or inelastic scattering within the sample is taken into account. We apply voltages to the perfect leads which are constant in space at frequency Ω, find the current response, and take the limit of the frequency going to zero.

The calculation is *not* performed self-consistently in the sense that the fields resulting from charge imbalances in the perfect leads caused by the current flow are not taken into account. We argue that this is correct because the voltages on the perfect leads are meant to represent the chemical potentials of large phase-randomizing reservoirs; the voltages are not meant to represent the electrostatic potential in a true physical perfect lead (after all, these are not present in the experiment). The perfect leads are a construct for representing the complicated transition from the phase-coherent region of interest to a large reservoir. The chemical potential of a reservoir is changed negligibly by the current flow into the system; thus, to worry about the charge imbalances in the perfect leads implied by our calculation is to take the perfect leads too seriously.[53] A self-consistent linear-response theory has been proposed for two-probe models in connection with derivations of the original Landauer formula,[47,48] but we argue that such calculations are not needed if one does a multiprobe calculation, which then allows the chemical-potential difference *induced* by the current flow to be distinct from the chemical-potential difference of the current source and sink. That the perfect leads in such a model do indeed act like phase-breaking centers, and hence define the boundaries of the phase-coherent region, has been indicated by physical arguments[54] and by numerical simulations.[16] We also neglect self-consistency in the mesoscopic region in the sense that we do not include screening of the charge inhomogeneities predicted to occur within an interacting model.[25] Therefore this theory would not fully describe the current density within the material, but as shown below, in a noninteracting theory the total transport current is insensitive to the de-

tails of the local current density, and this is consistent with experiments in which materials with very different screening lengths show quantitatively similar dc transport behavior.[13,14]

The calculation also satisfies the general constraints that current conservation imposes on any sensible dc transport theory.[55] These are, first of all, that $\nabla\cdot\langle\mathbf{J}(r)\rangle=0$, where $\langle\mathbf{J}(r)\rangle$ is the expectation value of the current density determined by $\int\underline{\sigma}(x,x')\cdot\mathbf{E}(r')dr'$. This, in turn, implies $\nabla_i\nabla_j\sigma_{ij}=0$. Our formulation is shown to satisfy this condition. It is important to realize that current conservation does not imply $\nabla_i\sigma_{ij}=0$ (although this stronger condition holds in the absence of a field), and the conductivity-response tensor need not be divergenceless in order for the total transport current to be determined by the voltages at the boundaries. This will be discussed in more detail below.

Our calculation starts by finding an expression for the nonlocal conductivity, $\underline{\sigma}(x,x')$, in terms of an exact eigenstate basis of the unperturbed Hamiltonian [Sec. II, Eq. (29)]. By using current conservation the total current response (conductance coefficients) are determined simply by integrals of $\underline{\sigma}(x,x')$ over the cross sections of the perfect leads. Next, we express our result for σ in terms of Green functions of the unperturbed system [Sec. III, Eq. (52)]. When these are used to evaluate the conductance coefficients, we show (as discussed above) that only Green functions near the Fermi energy and connecting points on the perfect leads are involved [Sec. IV, Eqs. (75) and (76)]. Finally, we connect the asymptotic form of the Green functions to the transmission coefficients of the scattering problem (Sec. V). Using these relations, the current response is exactly given by Büttiker's multiprobe Landauer formula[12] for arbitrary magnetic field (at zero temperature). A discussion and conclusion (Sec. VI) emphasizing the implications of our work for the quantum Hall effect follows the calculation. The Appendixes contain a discussion of the connection between our work and previous expressions for the spatially averaged conductivity in bulk systems (Appendix A), versions of our main results appropriate for discrete systems that are often used in numerical calculations (Appendix B), and several technical points needed in the main text.

II. LINEAR-RESPONSE THEORY IN AN EXACT EIGENSTATE REPRESENTATION

We consider the Hamiltonian of a system of noninteracting electrons in an arbitrary static potential and in a magnetic field $\mathbf{B}(\mathbf{x})$ characterized by the vector potential $\mathbf{A}(\mathbf{x})$,

$$H_0=\frac{1}{2M}\left[\mathbf{p}-\frac{e}{c}\mathbf{A}(\mathbf{x})\right]^2+U(\mathbf{x})\ . \tag{1}$$

We ignore spin degrees of freedom throughout; the generalization to spin $\frac{1}{2}$ is straightforward. H_0 has a complete, orthonormal set of eigenstates $\psi_\alpha(\mathbf{x})$ with eigenvalues ε_α,

$$\begin{aligned}&\int d\mathbf{x}\,\psi_\alpha^*(\mathbf{x})\psi_\beta(\mathbf{x})=\delta(\alpha-\beta)\ ,\\&\int d\alpha\,\psi_\alpha^*(\mathbf{x})\psi_\alpha(\mathbf{x}')=\delta(\mathbf{x}-\mathbf{x}')\ .\end{aligned} \tag{2}$$

The system that we study is a finite region of arbitrary shape with an arbitrary static potential connected to N_L perfectly ordered, straight infinite leads (Fig. 1). Since we are studying an infinite system, the spectrum is continuous and we therefore use an integral sign to denote both the integration over the continuous quantum number indexing the energy of the states and summation over the discrete quantum numbers which will characterize the propagating states (channels) at fixed energy. The application of a perturbing voltage $V(\mathbf{x},t)$ leads to a total Hamiltonian given by

$$H=H_0+eV(\mathbf{x},t)\ . \tag{3}$$

We have chosen to express the perturbation in the scalar-potential gauge rather than as a vector potential as is often done[44,56] in order to make some steps in the calculation easier (in particular, there is no diamagnetic term to be canceled). For the dc response, we shall consider a slow enough time variation that the magnetic fields associated with $V(\mathbf{x},t)$ are negligible.[44] Note that we will consider the charge of the particles to be positive throughout this calculation.

We take the perturbation $V(\mathbf{x},t)$ to have the form

$$V(\mathbf{x},t)=V(\mathbf{x})\cos(\Omega t)e^{-\delta|t|}\ , \tag{4}$$

which corresponds to an electric field given by

$$\mathbf{E}(\mathbf{x},t)=\mathbf{E}(\mathbf{x})\cos(\Omega t)e^{-\delta|t|}\ , \tag{5a}$$

$$\mathbf{E}(\mathbf{x})=-\nabla V(\mathbf{x})\ . \tag{5b}$$

The only restriction we make on $V(\mathbf{x})$ is that it eventually reach some constant value (in general, different) on each of the leads, so that the electric field in the leads vanishes far enough from the sample. In order to represent a typical "dc" measurement (which is performed at ac frequencies on the order of hertz), we take the rate at which the perturbation is turned on, δ, to zero before taking the frequency of the perturbation, Ω, to zero.[44] This ensures that the system is subjected to many cycles of the perturbation so that the frequency Ω is well defined. Since the electric field vanishes in the leads, its Fourier transform will have a peak at $q=0$ of width approximately $1/L$ (ignoring small-scale fluctuations). Since such fields have a substantial $q=0$ component a net current will flow for arbitrarily small Ω; hence, we have already taken the $q\to0$ limit in the sense of standard linear-response theory.[57] Thus, letting $\mathbf{J}(\mathbf{x},t,\Omega,\delta)$ be the expectation value of the current-density response to V, we wish to calculate

$$\lim_{\Omega\to0}\lim_{\delta\to0}\mathbf{J}(\mathbf{x},t,\Omega,\delta)\ . \tag{6}$$

We calculate the expectation value of the current density by taking the trace of the density matrix multiplied by the current-density operator expressed in the basis of eigenstates introduced above. In the absence of interactions, this approach is completely equivalent to the standard definition of the current-density response in terms of the expectation value of the current-current correlation function[57,58] The current-density operator is

$$\mathbf{J}_{\rm op}(x)=\frac{e}{2M}\left[n(x)\left[\mathbf{p}-\frac{e}{c}\mathbf{A}(x)\right]+\left[\mathbf{p}-\frac{e}{c}\mathbf{A}(x)\right]n(x)\right] . \tag{7}$$

We simplify the notation by introducing the gauge-invariant derivative $\mathbf{D}=\nabla-(ei/\hbar c)\mathbf{A}(\mathbf{x})$ and the double-sided derivative operator defined with respect to two arbitrary functions f and g by

$$f\overleftrightarrow{\mathbf{D}}g=f(\mathbf{x})\mathbf{D}g(\mathbf{x})-g(\mathbf{x})\mathbf{D}^*f(\mathbf{x})=-g\overleftrightarrow{\mathbf{D}}^*f . \tag{8}$$

Then the matrix elements of the current density are

$$[\mathbf{J}_{\rm op}(\mathbf{x})]_{\beta\alpha}=-\frac{ie\hbar}{2M}[\psi^*_\beta(\mathbf{x})\overleftrightarrow{\mathbf{D}}\psi_\alpha(\mathbf{x})]\equiv-\frac{ie\hbar}{2M}\mathbf{W}_{\beta\alpha}(\mathbf{x}) , \tag{9}$$

where we have introduced a reduced current-density operator $\mathbf{W}$. $\mathbf{W}$ has the important symmetry

$$\mathbf{W}_{\alpha\beta}(\mathbf{x})=-\mathbf{W}^*_{\beta\alpha}(\mathbf{x}) . \tag{10a}$$

Introducing the time-reversal operator and denoting by $\mathcal{T}(\beta)$ the time-reversed state corresponding to state β, we have the additional relation

$$\mathbf{W}_{\beta\alpha}(\mathbf{x},\mathbf{B})=\mathbf{W}^*_{\mathcal{T}(\beta)\mathcal{T}(\alpha)}(\mathbf{x},-\mathbf{B}) . \tag{10b}$$

Finally, we note that

$$\nabla'\cdot\mathbf{W}_{\alpha\beta}(\mathbf{x}')=-\frac{2M}{\hbar^2}\varepsilon_{\beta\alpha}\psi^*_\alpha(\mathbf{x}')\psi_\beta(\mathbf{x}') , \tag{11}$$

where $\varepsilon_{\beta\alpha}\equiv\varepsilon_\beta-\varepsilon_\alpha$, which is simply an expression of current conservation.

The density matrix in equilibrium, ρ_0, in terms of the Fermi function $f(\varepsilon)$ is simply

$$\rho_0=\int d\alpha f(\varepsilon_\alpha)|\psi_\alpha\rangle\langle\psi_\alpha| . \tag{12}$$

The time-evolution equation for the full density matrix, $i\hbar\,d\rho/dt=[H,\rho]$, implies that the time-evolution equation for $\rho_1=\rho-\rho_0$ to first order in the perturbation is

$$i\hbar\frac{d\rho_1}{dt}=[H_0,\rho_1(t)]+[H_1(t),\rho_0] , \tag{13}$$

with the boundary condition $\rho_1\to0$ as $t\to-\infty$. Expressing the matrix elements of Eq. (13) in terms of the compact notation

$$f_{\beta\alpha}\equiv f(\varepsilon_\beta)-f(\varepsilon_\alpha) ,$$
$$V_{\alpha\beta}\equiv\int d\mathbf{x}\,\psi^*_\alpha(\mathbf{x})V(\mathbf{x})\psi_\beta(\mathbf{x}) , \tag{14}$$

we find

$$i\hbar\frac{d}{dt}(\rho_1)_{\alpha\beta}=-\varepsilon_{\beta\alpha}(\rho_1)_{\alpha\beta}+ef_{\beta\alpha}V_{\alpha\beta}\cos(\Omega t)e^{-\delta|t|} . \tag{15}$$

This equation and its boundary condition are easily solved using an integrating factor. Evaluating the relevant integral for $t<0$ (of course, working at $t>0$ gives the same result in the static limit) yields the first-order correction to the density matrix,

$$[\rho_1(t<0)]_{\alpha\beta}=\frac{e}{2}f_{\beta\alpha}V_{\alpha\beta}e^{\delta t}\left[\frac{e^{+i\Omega t}}{\varepsilon_{\beta\alpha}-\hbar\Omega+i\hbar\delta}+\frac{e^{-i\Omega t}}{\varepsilon_{\beta\alpha}+\hbar\Omega+i\hbar\delta}\right] . \tag{16}$$

Expressions for the current density result from combining the expression for the current-density operator [Eq. (9)] with the expressions for the density matrix [Eqs. (12) and (16)]. In equilibrium

$$\mathbf{J}_0(\mathbf{x})=\mathrm{Tr}(\rho_0\mathbf{J}_{\rm op})=-\frac{ie\hbar}{2M}\int d\alpha f(\varepsilon_\alpha)\mathbf{W}_{\alpha\alpha}(\mathbf{x})\neq\mathbf{0} . \tag{17}$$

In a non-translationally-invariant system, the current density is nonzero even in equilibrium because the magnetic field generates closed current loops which roughly follow the equipotential contours. These circulating currents correspond to the diamagnetic response of the system.[59] Application of Eq. (11) to Eq. (17) immediately yields $\nabla\cdot\mathbf{J}_0=0$, i.e., no net current flows into or out of the system in response to the magnetic field, as one expects. In Appendix C we show that $\mathbf{J}_0$ does not even generate a net current in any single lead, thus $\mathbf{J}_0(\mathbf{x})$ does not contribute to the transport current and can be neglected in our further calculations.

The first-order response is given by

$$\mathbf{J}_1(\mathbf{x},t)=\mathrm{Tr}[\rho_1(t)\mathbf{J}_{\rm op}(\mathbf{x})]=\int d\alpha\int d\beta[\rho_1(t)]_{\alpha\beta}[\mathbf{J}_{\rm op}(\mathbf{x})]_{\beta\alpha} , \tag{18}$$

which yields

$$\mathbf{J}_1(\mathbf{x},t<0,\Omega,\delta)=-\frac{ie^2\hbar}{4M}\int d\alpha\int d\beta f_{\beta\alpha}V_{\alpha\beta}\mathbf{W}_{\beta\alpha}(\mathbf{x})e^{\delta t}\left[\frac{e^{+i\Omega t}}{\varepsilon_{\beta\alpha}-\hbar\Omega+i\hbar\delta}+\frac{e^{-i\Omega t}}{\varepsilon_{\beta\alpha}+\hbar\Omega+i\hbar\delta}\right] . \tag{19}$$

To make further progress, take the limit as the turn-on rate, δ, goes to zero using

$$\lim_{\delta\to0}\frac{1}{\varepsilon_{\beta\alpha}\pm i\hbar\Omega+i\hbar\delta}=-i\pi\delta(\varepsilon_{\beta\alpha}\pm\hbar\Omega)+\mathbf{P}\left[\frac{1}{\varepsilon_{\beta\alpha}\pm\hbar\Omega}\right] , \tag{20}$$

where P indicates a principal-value integral. Furthermore, we collect the dissipative terms (in phase with $\mathbf{E}$) and the reactive terms (out of phase), yielding

$$\mathbf{J}_1(\mathbf{x},\, t<0,\, \Omega)=-\frac{ie^2\hbar}{4M}\int d\alpha\int d\beta\, f_{\beta\alpha}V_{\alpha\beta}\mathbf{W}_{\beta\alpha}(\mathbf{x})$$

$$\times\left\{\cos(\Omega t)\left[-i\pi\delta(\varepsilon_{\beta\alpha}-\hbar\Omega)-i\pi\delta(\varepsilon_{\beta\alpha}+\hbar\Omega)+\mathrm{P}\left[\frac{1}{\varepsilon_{\beta\alpha}-\hbar\Omega}\right]+\mathrm{P}\left[\frac{1}{\varepsilon_{\beta\alpha}+\hbar\Omega}\right]\right]\right.$$

$$\left.+i\sin(\Omega t)\left[-i\pi\delta(\varepsilon_{\beta\alpha}-\hbar\Omega)+i\pi\delta(\varepsilon_{\beta\alpha}+\hbar\Omega)+\mathrm{P}\left[\frac{1}{\varepsilon_{\beta\alpha}-\hbar\Omega}\right]-\mathrm{P}\left[\frac{1}{\varepsilon_{\beta\alpha}+\hbar\Omega}\right]\right]\right\}. \tag{21}$$

One would like at this point to take the static limit, $\Omega\to 0$. However, the terms involving the δ functions in energy in Eq. (21) are undefined if one takes $\Omega\to 0$ within the integrals. If one were to do this, the δ function would set $\varepsilon_\beta=\varepsilon_\alpha$, so that one would need to evaluate $V_{\alpha\beta}$ for $\alpha=\beta$. Because of the δ-function normalization of the states [Eq. (2)] and the fact that the integral in the definition of $V_{\alpha\beta}$ extends over the perfect leads where $V(x)$ is constant, the matrix element $V_{\alpha\beta}$ is highly singular at $\alpha=\beta$. Thus, taking the $\Omega\to 0$ limit within the integrals involves evaluating the product of a singular factor ($V_{\alpha\beta}$) and zero (from $f_{\beta\alpha}$) which would have to be defined by an additional limiting procedure. We therefore look for a more amenable form for $\mathbf{J}_1$ before taking the $\Omega\to 0$ limit.

If we go back to Eq. (19) and rewrite $V_{\alpha\beta}$ in terms of an integral over the electric field, $\mathbf{E}(\mathbf{x})$, which is nonzero only in a finite region of space because of our boundary condition that the applied voltage is constant on the perfect leads, then the limit as the frequency goes to zero is well defined. In order to make the notation clear, it is convenient to introduce some coordinates in each perfect lead. As shown in Fig. 2, let $\hat{\mathbf{x}}_n$ be a unit vector parallel to lead n and pointing *outward* from the junction region, let y_n be the coordinate perpendicular to $\hat{\mathbf{x}}_n$ [defined so that one has a right-handed coordinate system $(\hat{\mathbf{x}}_n,\hat{\mathbf{y}}_n,\hat{\mathbf{z}}_n)$ with $\hat{\mathbf{z}}_n$ pointing into the page], and let C_n be the cross-section curve of lead n at x_n. Finally, denote by A the finite region bounded by curves C_n. Multiplying Eq. (11) on both sides by $V(\mathbf{x}')f_{\beta\alpha}$ and integrating using the divergence theorem yields

$$f_{\beta\alpha}\int_A d\mathbf{x}'\, V(\mathbf{x}')\psi_\alpha^*(\mathbf{x}')\psi_\beta(\mathbf{x}')=-\frac{\hbar^2}{2M}\frac{f_{\beta\alpha}}{\varepsilon_{\beta\alpha}}\int_A d\mathbf{x}'\,\mathbf{W}_{\alpha\beta}(\mathbf{x}')\cdot\mathbf{E}(\mathbf{x}')-\frac{\hbar^2}{2M}\sum_{n=1}^{N_L}V_n\frac{f_{\beta\alpha}}{\varepsilon_{\beta\alpha}}\int_{C_n}dy_n'\,\mathbf{W}_{\alpha\beta}(\mathbf{x}_n')\cdot\hat{\mathbf{x}}_n\,. \tag{22}$$

The left-hand side of Eq. (22) differs from the quantity $f_{\beta\alpha}V_{\alpha\beta}$, that we need in Eq. (19) only by being an integral over the finite "sample" region; we thus consider the limit of Eq. (22) as $x_n\to\infty$ for all n. Since the electric field is zero in the perfect leads, the first term on the right-hand side of Eq. (22) remains unchanged. For the second term, we show in Appendix D that

$$\lim_{x_n\to\infty}\left[\frac{f_{\beta\alpha}}{\varepsilon_{\beta\alpha}}\int_{C_n}dy_n\,\mathbf{W}_{\alpha\beta}(\mathbf{x}_n)\cdot\hat{\mathbf{x}}_n\right]=0 \tag{23}$$

when interpreted as a distribution for integrals over β. Since we do indeed integrate $f_{\beta\alpha}V_{\alpha\beta}$ over β in Eq. (19), the boundary terms in Eq. (22) can be neglected as the volume of integration goes to infinity. Using Eqs. (22) and (23) in Eq. (19) and taking the $\delta\to 0$ limit as in Eq. (20), we find that

$$\mathbf{J}_1(\mathbf{x},\, t<0,\, \Omega)=\frac{ie^2\hbar^3}{8M^2}\int d\alpha\int d\beta\,\mathbf{W}_{\beta\alpha}(\mathbf{x})\frac{f_{\beta\alpha}}{\varepsilon_{\beta\alpha}}\int_A d\mathbf{x}'\,\mathbf{W}_{\alpha\beta}(\mathbf{x}')\cdot\mathbf{E}(\mathbf{x})$$

$$\times\left\{\cos(\Omega t)\left[-i\pi\delta(\varepsilon_{\beta\alpha}-\hbar\Omega)-i\pi\delta(\varepsilon_{\beta\alpha}+\hbar\Omega)+\mathrm{P}\left[\frac{1}{\varepsilon_{\beta\alpha}-\hbar\Omega}\right]+\mathrm{P}\left[\frac{1}{\varepsilon_{\beta\alpha}+\hbar\Omega}\right]\right]\right.$$

$$\left.+i\sin(\Omega t)\left[-i\pi\delta(\varepsilon_{\beta\alpha}-\hbar\Omega)+i\pi\delta(\varepsilon_{\beta\alpha}+\hbar\Omega)+\mathrm{P}\left[\frac{1}{\varepsilon_{\beta\alpha}-\hbar\Omega}\right]-\mathrm{P}\left[\frac{1}{\varepsilon_{\beta\alpha}+\hbar\Omega}\right]\right]\right\}. \tag{24}$$

Because the integrand on the first line of this equation is obviously bounded at $\varepsilon_{\beta\alpha}=0$, the $\Omega\to 0$ limit is now straightforward. For the δ-function terms we use

$$\lim_{\Omega\to 0}\frac{f(\varepsilon_\alpha\pm\hbar\Omega)-f(\varepsilon_\alpha)}{\pm\hbar\Omega}=+f'(\varepsilon_\alpha)\ , \tag{25}$$

while, for the principal-value terms,

$$\lim_{\Omega\to 0}\mathrm{P}\left[\frac{1}{\varepsilon_{\beta\alpha}\pm\hbar\Omega}\right]=\mathrm{P}\left[\frac{1}{\varepsilon_{\beta\alpha}}\right]\ . \tag{26}$$

This last equation may seem obvious; however, note that the limit implied by the principal-value symbol is actually the $\delta\to 0$ limit, so that naively taking the $\Omega\to 0$ limit in the denominator involves switching the order of the $\delta\to 0$ and $\Omega\to 0$ limits, which is not allowed on physical grounds (as discussed above and in Ref. 44). To overcome this difficulty, it can be shown that Eq. (26) is valid as a relation between distributions. Using these two equations in Eq. (24), we see immediately that the reactive term proportional to $\sin(\Omega t)$ is identically zero.[60] Thus the total dc current-density response is dissipative and is given by

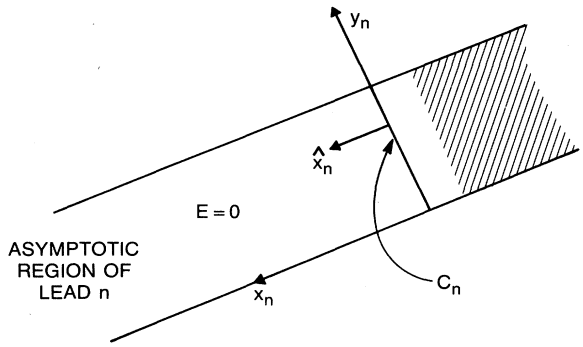

FIG. 2. Asymptotic region of lead n. C_n is a cross-section line in lead n located in the asymptotic region where the electric field is zero. In each lead we define a local coordinate system (x_n,y_n) and an outward pointing unit vector, $\hat{\mathbf{x}}_n$, normal to C_n.

$$\mathbf{J}_1(\mathbf{x})=+\frac{e^2\hbar^3\pi}{4M^2}\int d\alpha\int d\beta\left[f'(\varepsilon_\alpha)\delta(\varepsilon_{\beta\alpha})+\frac{i}{\pi}\frac{f_{\beta\alpha}}{\varepsilon_{\beta\alpha}}\mathrm{P}\left[\frac{1}{\varepsilon_{\beta\alpha}}\right]\right]\mathbf{W}_{\beta\alpha}(\mathbf{x})\int_A d\mathbf{x}'\,\mathbf{W}_{\alpha\beta}(\mathbf{x}')\cdot\mathbf{E}(\mathbf{x}')\ . \tag{27}$$

Expressing this result in terms of the nonlocal response function $\underline{\sigma}(\mathbf{x},\mathbf{x}')$ defined by

$$\mathbf{J}_1(\mathbf{x})=\int d\mathbf{x}'\,\underline{\sigma}(\mathbf{x},\mathbf{x}')\cdot\mathbf{E}(\mathbf{x}')\ , \tag{28}$$

we arrive at the main result of this part of the calculation,

$$\underline{\sigma}(\mathbf{x},\mathbf{x}')=+\frac{e^2\hbar^3\pi}{4M^2}\int d\alpha\int d\beta\left[f'(\varepsilon_\alpha)\delta(\varepsilon_{\beta\alpha})+\frac{i}{\pi}\frac{f_{\beta\alpha}}{\varepsilon_{\beta\alpha}}\mathrm{P}\left[\frac{1}{\varepsilon_{\beta\alpha}}\right]\right]\mathbf{W}_{\beta\alpha}(\mathbf{x})\mathbf{W}_{\alpha\beta}(\mathbf{x}')\ . \tag{29}$$

Using the properties of the current matrix elements given in Eq. (10) we can check explicitly that the response function given in Eq. (29) satisfies the Onsager relations. First, because the time-reversal operator is unitary, the integral over states α can be written as an integral over states $\mathcal{T}(\alpha)$, $\int d\alpha=\int d[\mathcal{T}(\alpha)]$. Second, Eq. (10b) and then Eq. (10a) applied to the current-matrix-element part of Eq. (29) yields

$$\mathbf{W}_{\beta\alpha}(\mathbf{x})\mathbf{W}_{\alpha\beta}(\mathbf{x}')=\mathbf{W}_{\mathcal{T}(\alpha)\mathcal{T}(\beta)}(\mathbf{x},-\mathbf{B})\mathbf{W}_{\mathcal{T}(\beta)\mathcal{T}(\alpha)}(\mathbf{x}',-\mathbf{B})\ . \tag{30}$$

Finally, noting that $\varepsilon_{\mathcal{T}(\alpha)}=\varepsilon_\alpha$, we see that application of time-reversal ($\mathcal{T}$) symmetry has resulted in the interchange of the indices α and β, which can be restored to their original order by interchanging the spatial arguments and tensor indices in the two factors $\mathbf{W}$. Substitution of this relation back into Eq. (29) yields

$$\sigma_{ij}(\mathbf{x},\mathbf{x}',\mathbf{B})=\sigma_{ji}(\mathbf{x}',\mathbf{x},-\mathbf{B})\ , \tag{31}$$

which are the correct Onsager relations for the full conductivity-response function. In addition, by interchanging the indices α and β everywhere in Eq. (29) and noting that the δ-function term is even under this interchange, while the principal-value term is odd, application of time reversal to the product of $\mathbf{W}$'s implies that the δ-function term is symmetric in the magnetic field while the principal-value term is antisymmetric. Therefore the principal-value term is zero at $B=0$, and the conductivity-response function is manifestly dependent only on states near the Fermi surface.

As noted in the Introduction, any sensible transport theory must satisfy current conservation in the static limit, $\nabla\cdot\mathbf{J}=0$, and since $\nabla\cdot\mathbf{J}_0=0$, this implies $\nabla\cdot\mathbf{J}_1=0$. We first check that our Eq. (27) does obey this relation exactly and then discuss the constraints that current conservation places on the response function $\underline{\sigma}(\mathbf{x},\mathbf{x}')$. Using Eq. (11) in Eq. (27),

$$\nabla\cdot\mathbf{J}_1(\mathbf{x})=+\frac{e^2\hbar^3\pi}{4M^2}\int d\alpha\int d\beta\left[f'(\varepsilon_\alpha)\delta(\varepsilon_{\beta\alpha})+\frac{i}{\pi}\frac{f_{\beta\alpha}}{\varepsilon_{\beta\alpha}}\mathrm{P}\left[\frac{1}{\varepsilon_{\beta\alpha}}\right]\right]\frac{2M}{\hbar^2}\varepsilon_{\beta\alpha}\psi_\beta^*(\mathbf{x})\psi_\alpha(\mathbf{x})\int_A d\mathbf{x}'\,\mathbf{W}_{\alpha\beta}(\mathbf{x}')\cdot\mathbf{E}(\mathbf{x}')\ . \tag{32}$$

The δ-function term gives zero immediately. For the principal-value term, we use Eqs. (22) and (23) to rewrite Eq. (32) in terms of matrix elements of the potential:

$$\nabla\cdot\mathbf{J}_1(\mathbf{x})=-i\frac{e^2}{\hbar}\int d\alpha\int d\beta\,\psi_\beta^*(\mathbf{x})\psi_\alpha(\mathbf{x})[f(\varepsilon_\beta)-f(\varepsilon_\alpha)]V_{\alpha\beta}\ . \tag{33}$$

Exchanging the dummy indices α and β in the $f(\varepsilon_\alpha)$ term, we find that

$$\nabla\cdot\mathbf{J}_1(\mathbf{x})=-i\frac{e^2}{\hbar}\int d\beta f(\varepsilon_\beta)\int d\alpha\left[\psi_\beta^*(\mathbf{x})\psi_\alpha(\mathbf{x})\int d\mathbf{x}'\,\psi_\alpha^*(\mathbf{x}')\psi_\beta(\mathbf{x}')V(\mathbf{x}')-\psi_\alpha^*(\mathbf{x})\psi_\beta(\mathbf{x})\int d\mathbf{x}'\,\psi_\beta^*(\mathbf{x}')\psi_\alpha(\mathbf{x}')V(\mathbf{x}')\right]\ . \tag{34}$$

The α integral gives a $\delta(x-x')$ from the completeness relation and thus the two terms on the left-hand side of Eq. (34) cancel identically, yielding the expected answer, $\nabla\cdot\mathbf{J}_1=0$.

Given that the current density satisfies current conservation, what constraint does this put on the response function $\underline{\sigma}$? Without reference to our microscopic expression for $\underline{\sigma}(\mathbf{x},\mathbf{x}')$, one sees from the fact that $\mathbf{E}$ is the gradient of a potential and the divergence theorem that

$$\begin{aligned}\nabla\cdot\mathbf{J}_1&=\int_A d\mathbf{x}'\,\nabla\cdot\underline{\sigma}(\mathbf{x},\mathbf{x}')\cdot\mathbf{E}(\mathbf{x}')\\&=-\int_A d\mathbf{x}'[\nabla\cdot\underline{\sigma}(\mathbf{x},\mathbf{x}')]\cdot\nabla'V(\mathbf{x}')\\&=\int_A d\mathbf{x}'[\nabla\cdot\underline{\sigma}(\mathbf{x},\mathbf{x}')\cdot\nabla']V(\mathbf{x}')\\&\quad-\sum_{n=1}^{N_L}V_n\nabla\cdot\int_{C_n}dy_n'\,\underline{\sigma}(\mathbf{x},\mathbf{x}')\cdot\hat{\mathbf{x}}_n=0\ .\end{aligned} \tag{35}$$

Because the form of the applied potential, $V(x')$, is arbitrary (its magnitude is constrained to be very small by our linear-response assumption), we derive the following independent conditions that must be satisfied by any microscopic expression for $\underline{\sigma}(\mathbf{x},\mathbf{x}')$:

$$\nabla\cdot\underline{\sigma}(\mathbf{x},\mathbf{x}')\cdot\nabla'=0\ , \tag{36a}$$

$$\nabla\cdot\int_{C_n}dy_n'\,\underline{\sigma}(\mathbf{x},\mathbf{x}')\cdot\hat{\mathbf{x}}_n=0\ \text{ for all } n\ . \tag{36b}$$

Using Eqs. (22) and (23), and arguments similar to those used above to show current conservation, it is straightforward to show that the microscopic expression for $\underline{\sigma}(\mathbf{x},\mathbf{x}')$ given in Eq. (29) does indeed satisfy each of these conditions independently.

A crucial technical point to emphasize here is that current conservation alone does *not* imply the stronger condition $\nabla\cdot\underline{\sigma}=\underline{\sigma}\cdot\nabla'=0$ that has been widely discussed in the recent literature.[55] This stronger condition *is* satisfied in the absence of a magnetic field, which is easily seen from our earlier observation that the principal-value term in Eq. (29) is zero at $B=0$ and noting that Eq. (11) applied to the δ-function term immediately yields zero. However, this stronger condition does not hold in the presence of a field. This also can be seen easily, since $\nabla\cdot\underline{\sigma}$ is simply given by Eq. (32) above without the factor $E(x')$ and the integration over x'. This expression is, in general, nonvanishing; we emphasize again that this is not problematic, since it is consistent with current conservation.

This completes our discussion of the current density and the nonlocal response function in terms of the exact eigenstate basis; we now discuss the total transport current through each lead that results from this current density. The current coming out of lead m, I_m is related to the current density and the voltage by

$$I_m=\int_{C_m}dy_m\,\mathbf{J}_1(\mathbf{x}_m)\cdot\hat{\mathbf{x}}_m=\sum_n g_{mn}V_n\ , \tag{37}$$

where we have introduced linear-response coefficients for the current in terms of the voltage, g_{mn}, which we shall refer to as conductance coefficients. The identification of the condition $\nabla\cdot\underline{\sigma}=0$ with current conservation in previous work has led to some confusion in the literature over whether the g_{mn} can be expressed solely in terms of the voltages on the leads for $B\neq0$.[17] We note that the condition $\nabla\cdot\underline{\sigma}$ is only sufficient, but not necessary for this to be the case. Instead, only the weaker condition (36b) (which *is* a consequence of current conservation) is necessary, as we now show. Writing the current density in terms of $\underline{\sigma}$, expressing $\mathbf{E}$ as a gradient of V, and using the divergence theorem, one arrives at

$$\begin{aligned}I_m&=\int_A d\mathbf{x}'\,V(\mathbf{x}')\int_{C_m}dy_m\,\hat{\mathbf{x}}_m\cdot\underline{\sigma}(\mathbf{x},\mathbf{x}')\cdot\nabla'\\&\quad-\sum_{n=1}^{N_L}V_n\int_{C_m}dy_m\int_{C_n}dy_n'\,\hat{\mathbf{x}}_m\cdot\underline{\sigma}(\mathbf{x},\mathbf{x}')\cdot\hat{\mathbf{x}}_n\ .\end{aligned} \tag{38}$$

The first term is zero by Eqs. (31) and (36b), which gives the intuitive result

$$g_{mn}=-\int_{C_m}dy_m\int_{C_n}dy_n'\,\hat{\mathbf{x}}_m\cdot\underline{\sigma}(\mathbf{x},\mathbf{x}')\cdot\hat{\mathbf{x}}_n\ . \tag{39}$$

Hence the conductance coefficient between two leads is simply the "flux" of the conductivity tensor into those leads. For $B=0$ this expression was previously obtained by Kane *et al.*[61] in the multiprobe case.

Using our result for $\underline{\sigma}$, Eq. (29), we obtain the explicit expression

$$g_{mn}=-\frac{e^2\hbar^3\pi}{4M^2}\int d\alpha\int d\beta\left[f'(\varepsilon_\alpha)\delta(\varepsilon_{\beta\alpha})+\frac{i}{\pi}\frac{f_{\beta\alpha}}{\varepsilon_{\beta\alpha}}\mathrm{P}\left[\frac{1}{\varepsilon_{\beta\alpha}}\right]\right]\int_{C_m}dy_m\,\hat{\mathbf{x}}_m\cdot\mathbf{W}_{\beta\alpha}(\mathbf{x}_m)\int_{C_n}dy_n'\,\mathbf{W}_{\alpha\beta}(\mathbf{x}_n')\cdot\hat{\mathbf{x}}_n\ . \tag{40}$$

This equation simplifies considerably in two special cases. First, as noted earlier, symmetry considerations imply that the principal-value term in $\underline{\sigma}(\mathbf{x},\mathbf{x}')$ is zero at $B=0$. Hence, the contribution of the principal-value term in Eq. (40) is zero for $B=0$. Second, in the case of a two-probe structure, g_{mm} completely determines the transport since the potential can be chosen to be zero in one of the leads. Adding the (α,β) term to the (β,α) term using Eqs. (10), we note that the δ-function term picks out the real part of the product of the $\mathbf{W}$'s while the principal-value term picks out the imaginary part. In the expression for the diagonal coefficient g_{mm}, the factor

$$\int_{C_m} dy_m \int_{C_m} dy'_m [\hat{\mathbf{x}}_m \cdot \mathbf{W}_{\beta\alpha}(\mathbf{x}_m)][\mathbf{W}_{\alpha\beta}(\mathbf{x}'_m)\cdot\hat{\mathbf{x}}_m] \quad (41)$$

is real for arbitrary B, so the coefficient g_{mm} depends only on states near the Fermi surface (at the Fermi surface for $T=0$). Thus, without any further work we see that transport in a two-probe structure is determined completely by states near the Fermi energy, and is symmetric in a magnetic field. However, a similar statement does not hold for $\underline{\sigma}(\mathbf{x},\mathbf{x}')$, a result we expect on physical grounds, since we expect circulating currents inside the sample for nonzero B, no matter what measuring geometry is used.

This completes the derivation within the exact eigenstate representation. Our central results are the expressions for the current density, Eq. (27), the response function, Eq. (29), and the conductance coefficients, Eqs. (39) and (40).

III. GREEN-FUNCTION EXPRESSIONS FOR THE RESPONSE FUNCTION $\underline{\sigma}$

In order to make the physics involved in the expressions of the preceding section more transparent, as well as to make quantitative calculations possible, we transform from the exact eigenstate formalism to Green functions. The basic quantities that will enter our expressions are the retarded and advanced one-particle Green functions,

$$G_\varepsilon^{\pm}(\mathbf{x},\mathbf{x}') = \int d\alpha\, \psi_\alpha(\mathbf{x})\psi_\alpha^*(\mathbf{x}')/(\varepsilon-\varepsilon_\alpha \pm i\eta) ,$$

and their sum and difference, which we denote by

$$\Delta G_\varepsilon(\mathbf{x},\mathbf{x}') \equiv G_\varepsilon^+(\mathbf{x},\mathbf{x}') - G_\varepsilon^-(\mathbf{x},\mathbf{x}') = -2\pi i \int d\alpha\, \psi_\alpha(\mathbf{x})\psi_\alpha^*(\mathbf{x}')\delta(\varepsilon-\varepsilon_\alpha) , \quad (42a)$$

$$\Sigma G_\varepsilon(\mathbf{x},\mathbf{x}') \equiv G_\varepsilon^+(\mathbf{x},\mathbf{x}') + G_\varepsilon^-(\mathbf{x},\mathbf{x}') = 2\int d\alpha\, \psi_\alpha(\mathbf{x})\psi_\alpha^*(\mathbf{x}')P\left[\frac{1}{\varepsilon-\varepsilon_\alpha}\right] . \quad (42b)$$

The product of the two $\mathbf{W}$ which enters the expression for the response function in Eq. (29) can be written in terms of eigenstates as

$$\mathbf{W}_{\beta\alpha}(\mathbf{x})\mathbf{W}_{\alpha\beta}(\mathbf{x}') = -\psi_\alpha(\mathbf{x})\psi_\alpha^*(\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'\psi_\beta(\mathbf{x}')\psi_\beta^*(\mathbf{x}) . \quad (43)$$

It is convenient to treat the part of $\underline{\sigma}$ that involves the δ function separately from the part that involves the principal-value integral; we call these parts $\underline{\sigma}_s$ and $\underline{\sigma}_{as}$, respectively, because of their symmetry under reversal of the magnetic field as discussed after Eq. (31). In treating $\underline{\sigma}_s$, we replace the energy ε_α by a dummy variable ε in order to separate out the energy dependence of the Fermi function, obtaining

$$\underline{\sigma}(\mathbf{x},\mathbf{x}') \equiv \frac{e^2\hbar^3\pi}{4M^2}\int d\alpha \int d\beta\, f'(\varepsilon_\alpha)\delta(\varepsilon_\beta-\varepsilon_\alpha)\mathbf{W}_{\beta\alpha}(\mathbf{x})\mathbf{W}_{\alpha\beta}(\mathbf{x}') = \frac{e^2\hbar^3\pi}{4M^2}\int_{-\infty}^{\infty} d\varepsilon\, f'(\varepsilon)\int d\alpha \int d\beta\, \delta(\varepsilon-\varepsilon_\alpha)\delta(\varepsilon-\varepsilon_\beta)\mathbf{W}_{\beta\alpha}(\mathbf{x})\mathbf{W}_{\alpha\beta}(\mathbf{x}') . \quad (44)$$

By using Eq. (43) to replace the $\mathbf{W}$ by eigenstate expressions and then Eqs. (42) to convert to Green functions, we arrive at the desired expression for the Fermi-surface part of the response function,

$$\underline{\sigma}_s(\mathbf{x},\mathbf{x}') = -\frac{e^2\hbar^3}{16\pi M^2}\int_{-\infty}^{\infty} d\varepsilon[-f'(\varepsilon)]\Delta G_\varepsilon(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'\Delta G_\varepsilon(\mathbf{x}',\mathbf{x}) . \quad (45)$$

When averaged over space, assuming a uniform electric field in the sample, this expression yields the well-known Kubo formula for the longitudinal conductivity.[41,58]

The principal-value part of $\underline{\sigma}$ is

$$\underline{\sigma}_{as}(\mathbf{x},\mathbf{x}') \equiv \frac{e^2\hbar^3\pi}{4M^2}\int d\alpha \int d\beta \frac{i}{\pi}\frac{f(\varepsilon_\beta)-f(\varepsilon_\alpha)}{\varepsilon_{\beta\alpha}}\mathbf{P}\left[\frac{1}{\varepsilon_{\beta\alpha}}\right]\mathbf{W}_{\beta\alpha}(\mathbf{x})\mathbf{W}_{\alpha\beta}(\mathbf{x}') . \quad (46)$$

By exchanging α and β in the term involving $f(\varepsilon_\alpha)$ and then replacing ε_β with a dummy variable ε by introducing a δ function, we arrive at

$$\underline{\sigma}_{as}(\mathbf{x},\mathbf{x}') = \frac{ie^2\hbar^3}{4M^2}\int_{-\infty}^{\infty} d\varepsilon\, f(\varepsilon)\int d\alpha \int d\beta \frac{\delta(\varepsilon-\varepsilon_\beta)}{\varepsilon-\varepsilon_\alpha}\mathbf{P}\left[\frac{1}{\varepsilon-\varepsilon_\alpha}\right][\mathbf{W}_{\beta\alpha}(\mathbf{x})\mathbf{W}_{\alpha\beta}(\mathbf{x}')-\mathbf{W}_{\alpha\beta}(\mathbf{x})\mathbf{W}_{\beta\alpha}(\mathbf{x}')] . \quad (47)$$

Note that the dependence on ε can be written more compactly using

$$\frac{1}{\varepsilon-\varepsilon_\alpha}\mathrm{P}\left[\frac{1}{\varepsilon-\varepsilon_\alpha}\right]=-\frac{d}{d\varepsilon}\mathrm{P}\left[\frac{1}{\varepsilon-\varepsilon_\alpha}\right]. \tag{48}$$

Expressing the $\mathbf{W}$ in terms of eigenstates using Eq. (43) and then using the definitions of ΔG_ε and ΣG_ε yields the basic Green-function expression for $\underline{\sigma}_{as}$:

$$\underline{\sigma}_{as}(\mathbf{x},\mathbf{x}')=-\frac{e^2\hbar^3}{16\pi M^2}\int_{-\infty}^{\infty}d\varepsilon\, f(\varepsilon)\left[\frac{d}{d\varepsilon}\Sigma G_\varepsilon(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'\Delta G_\varepsilon(\mathbf{x}',\mathbf{x})-\Delta G_\varepsilon(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'\frac{d}{d\varepsilon}\Sigma G_\varepsilon(\mathbf{x}',\mathbf{x})\right]. \tag{49}$$

In order to combine $\underline{\sigma}_s$ and $\underline{\sigma}_{as}$ into the total response function $\underline{\sigma}$, it is convenient to write out the Green-function expressions in terms of G_ε^+ and G_ε^-. First, for $\underline{\sigma}_{as}$ notice that the $G_\varepsilon^+G_\varepsilon^-$ and $G_\varepsilon^-G_\varepsilon^+$ terms in Eq. (49) form total derivatives with respect to ε. These terms, then, can be integrated by parts, which moves the energy derivative onto the Fermi function; note that the boundary terms vanish because $G_\varepsilon^\pm\to 0$ as $\varepsilon\to-\infty$ while $f(\varepsilon)\to 0$ quickly as $\varepsilon\to\infty$. Thus we have

$$\begin{aligned}\underline{\sigma}_{as}(\mathbf{x},\mathbf{x}')=&\frac{e^2\hbar^3}{16\pi M^2}\int d\varepsilon[-f'(\varepsilon)][G_\varepsilon^+(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'G_\varepsilon^-(\mathbf{x}',\mathbf{x})-G_\varepsilon^-(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'G_\varepsilon^+(\mathbf{x}',\mathbf{x})]\\&-\frac{e^2\hbar^3}{16\pi M^2}\int d\varepsilon\, f(\varepsilon)\left[\frac{d}{d\varepsilon}G_\varepsilon^+(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'G_\varepsilon^+(\mathbf{x}',\mathbf{x})-\frac{d}{d\varepsilon}G_\varepsilon^-(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'G_\varepsilon^-(\mathbf{x}',\mathbf{x})\right.\\&\left.-G_\varepsilon^+(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'\frac{d}{d\varepsilon}G_\varepsilon^+(\mathbf{x}',\mathbf{x})+G_\varepsilon^-(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'\frac{d}{d\varepsilon}G_\varepsilon^-(\mathbf{x}',\mathbf{x})\right].\end{aligned} \tag{50}$$

For $\underline{\sigma}_s$, we leave the $G_\varepsilon^+G_\varepsilon^-$ and $G_\varepsilon^-G_\varepsilon^+$ terms as they are in Eq. (45); however, for the $G_\varepsilon^+G_\varepsilon^+$ and $G_\varepsilon^-G_\varepsilon^-$ terms we integrate by parts so as to cancel two of the terms in Eq. (50). This yields

$$\begin{aligned}\underline{\sigma}_s(\mathbf{x},\mathbf{x}')=&\frac{e^2\hbar^3}{16\pi M^2}\int d\varepsilon[-f'(\varepsilon)][G_\varepsilon^+(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'G_\varepsilon^-(\mathbf{x}',\mathbf{x})+G_\varepsilon^-(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'G_\varepsilon^+(\mathbf{x}',\mathbf{x})]\\&-\frac{e^2\hbar^3}{16\pi M^2}\int d\varepsilon\, f(\varepsilon)\left[\frac{d}{d\varepsilon}G_\varepsilon^+(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'G_\varepsilon^+(\mathbf{x}',\mathbf{x})+\frac{d}{d\varepsilon}G_\varepsilon^-(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'G_\varepsilon^-(\mathbf{x}',\mathbf{x})\right.\\&\left.+G_\varepsilon^+(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'\frac{d}{d\varepsilon}G_\varepsilon^+(\mathbf{x}',\mathbf{x})+G_\varepsilon^-(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'\frac{d}{d\varepsilon}G_\varepsilon^-(\mathbf{x}',\mathbf{x})\right].\end{aligned} \tag{51}$$

Adding Eqs. (50) and (51) to form $\underline{\sigma}=\underline{\sigma}_s+\underline{\sigma}_{as}$, we find that the nonlocal response function in terms of the Green functions is

$$\begin{aligned}\underline{\sigma}(\mathbf{x},\mathbf{x}')=&\frac{e^2\hbar^3}{8\pi M^2}\int d\varepsilon[-f'(\varepsilon)]G_\varepsilon^+(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'G_\varepsilon^-(\mathbf{x}',\mathbf{x})\\&-\frac{e^2\hbar^3}{8\pi M^2}\int d\varepsilon\, f(\varepsilon)\left[\frac{d}{d\varepsilon}G_\varepsilon^+(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'G_\varepsilon^+(\mathbf{x}',\mathbf{x})+G_\varepsilon^-(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'\frac{d}{d\varepsilon}G_\varepsilon^-(\mathbf{x}',\mathbf{x})\right].\end{aligned} \tag{52}$$

As the temperature goes to zero, the limit of Eq. (52) is simply obtained using $f(\varepsilon)\to\Theta(E_F-\varepsilon)$ and $-f'(\varepsilon)\to\delta(\varepsilon-E_F)$.

IV. GREEN-FUNCTION EXPRESSIONS FOR THE CONDUCTANCE COEFFICIENTS

The current-response coefficients, g_{mn}, can be found from Eq. (52) by integrating over the wire cross sections as in Eq. (39). We now show that this leads to an enormous simplification for $m\neq n$ because the terms involving $G_\varepsilon^+G_\varepsilon^+$ or $G_\varepsilon^-G_\varepsilon^-$ in Eq. (52) are identically zero when integrated over the cross sections. To show this, we proceed in two steps. First, we show that these terms are zero in the asymptotic limit $x_m\to\infty$, $x_n\to\infty$, with $m\neq n$. Second, we show that the derivatives of the $G_\varepsilon^+G_\varepsilon^+$ or $G_\varepsilon^-G_\varepsilon^-$ terms are zero and conclude that these terms are zero for any x_m and x_n' (with $m\neq n$). To fix the discussion, we consider a typical term involving $G_\varepsilon^+G_\varepsilon^+$:

$$S(x_m,x_n')\equiv\int_{C_m}dy_m\int_{C_n}dy_n'\frac{d}{d\varepsilon}G_\varepsilon^+(\mathbf{x}_m,\mathbf{x}_n')\times(\overleftrightarrow{\mathbf{D}}^*\cdot\hat{\mathbf{x}}_m)(\overleftrightarrow{\mathbf{D}}'\cdot\hat{\mathbf{x}}_n)G_\varepsilon^+(\mathbf{x}_n',\mathbf{x}_m)\ . \tag{53}$$

In order to discuss the asymptotic behavior of the Green functions most clearly, we present the quantum mechanics of the perfect leads in a particular gauge at this point. We suppose that the magnetic field, B, is perpendicular to the leads and constant in each lead n for $x>x_n$. We choose the gauge to be Landau-like in the asymptotic region,

$$\mathbf{A}(\mathbf{x}_m)=B_m y_m\hat{\mathbf{x}}_m\ . \tag{54}$$

That such a gauge can be chosen for an arbitrary configuration of wires is shown in Appendix E. The eigenstates of an infinite perfect lead are solutions of the Schrödinger equation,

$$\left[\frac{1}{2M}\left[\mathbf{p}-\frac{e}{c}\mathbf{A}\right]^2+U(y)\right]\xi_A(\mathbf{x})=\varepsilon_A\xi_A(\mathbf{x})\ , \tag{55}$$

where A denotes a complete set of quantum numbers. Because of the translational symmetry in the x direction in the Landau gauge, one can write the $\xi_A(\mathbf{x})$ as

$$\xi_a^\pm(\mathbf{x})=\frac{1}{\sqrt{\theta_a}}e^{\pm ik_a x}\chi^\pm_{n_a,k_a}(y)\ . \tag{56}$$

Here, a denotes a complete set of quantum numbers (n_a is the channel number), except for the direction of the wave: $k_a>0$, so that outgoing and incoming states are explicitly labeled $+$ and $-$, respectively. θ_a is the outgoing particle flux through the wire cross section C_m carried by $e^{+ik_a x}\chi^+_{n_a,k_a}(y)$ and is defined in terms of matrix elements of the current-density operator [Eq. (9)] as

$$\theta_a\equiv-\frac{i\hbar}{2M}\int_{C_m}dy_m[e^{+ik_a x}\chi^+_{n_a,k_a}(y)]^*(\overleftrightarrow{\mathbf{D}}\cdot\hat{\mathbf{x}}_m)\times e^{+ik_a x}\chi^+_{n_a,k_a}(y)\ ; \tag{57}$$

note $\theta_a>0$. The χ satisfy the reduced equation

$$\left[-\frac{\hbar^2}{2M}\frac{d^2}{dy^2}+\tfrac{1}{2}\omega_c^2(l_B^2k_a\pm y)^2+U(y)\right]\chi^\pm_{n_a,k_a}(y)=\varepsilon_{n,k_a}\chi^\pm_{n_a,k_a}(y)\ , \tag{58}$$

where $l_B^2\equiv\hbar c/eB$ and $\omega_c\equiv eB/Mc$. We normalize the χ so that $\int dy\,|\chi^\pm_{n_a,k_a}(y)|^2=1$. For a fixed energy $\varepsilon_{n,k_a}=E$, the $\chi^\pm_{n_a,k_a}$ are *not* orthogonal because of the dependence of the reduced Hamiltonian on k_a. Thus, one cannot expand arbitrary functions of y simply by projecting onto the set $\chi(y)$ as one does in the $B=0$ case.[43,44] Note that we have normalized the $\xi^\pm$ so that they carry unit flux; in this way an S matrix defined in terms of these ξ [see Eq. (79)] will be unitary, which will be useful in making the connection to scattering theory in the next section.

The states defined in the preceding paragraph are useful because of a fundamental identity between states at the same energy which we derive from current conservation. For states at the same energy, $\varepsilon_a=\varepsilon_b$, Eq. (11) implies

$$\nabla\cdot\mathbf{W}_{AB}(\mathbf{x})=0,\quad \varepsilon_A=\varepsilon_B\ . \tag{59}$$

This implies that the current matrix element integrated over a cross section of lead m is constant,

$$I_{AB}(x)\equiv\int_{C_m}dy_m\,\hat{\mathbf{x}}_m\cdot\mathbf{W}_{AB}(\mathbf{x})=\text{const},\quad \varepsilon_A=\varepsilon_B\ . \tag{60}$$

Remembering that $\mathbf{W}_{\alpha\beta}(\mathbf{x})$ is proportional to a matrix element of the current operator [Eq. (9)] and that the momentum operator generates translations, we have

$$I_{AB}(x+\Delta x)=\frac{2Mi}{e\hbar}\int_{C_m}dy_m\,\hat{\mathbf{x}}_m\cdot\langle\xi_A|\mathbf{J}_{\text{op}}(x+\Delta x,y)|\xi_B\rangle=\frac{2Mi}{e\hbar}\int_{C_m}dy_m\,\hat{\mathbf{x}}_m\cdot\langle\xi_A|e^{-ip\Delta x/\hbar}\mathbf{J}_{\text{op}}(x,y)e^{+ip\Delta x/\hbar}|\xi_B\rangle\ . \tag{61}$$

Since ξ is chosen to be an eigenstate of the translation operator, $e^{-ip\Delta x/\hbar}$ acting on a ξ simply produces a phase factor,

$$I_{AB}(x+\Delta x)=e^{i(k_B-k_A)\Delta x}I_{AB}(x)\ . \tag{62}$$

For Eqs. (60) and (62) to both be valid, one must have $I_{AB}=0$ whenever $\varepsilon_A=\varepsilon_B$ unless $A=B$. This is the desired identity. It will be of most use to us slightly rewritten in the form

$$\begin{aligned}&\int_{C_m}dy_m\,\xi_a^{\pm*}(\mathbf{x}_m)(\overleftrightarrow{\mathbf{D}}\cdot\hat{\mathbf{x}}_m)\xi_b^\pm(\mathbf{x}_m)=\pm\frac{2Mi}{\hbar}\delta_{ab},\quad \varepsilon_a=\varepsilon_b\\ &\int_{C_m}dy_m\,\xi_a^{+*}(\mathbf{x}_m)(\overleftrightarrow{\mathbf{D}}\cdot\hat{\mathbf{x}}_m)\xi_b^-(\mathbf{x}_m)=0,\quad \varepsilon_a=\varepsilon_b\\ &\int_{C_m}dy_m\,\xi_a^{-*}(\mathbf{x}_m)(\overleftrightarrow{\mathbf{D}}\cdot\hat{\mathbf{x}}_m)\xi_b^+(\mathbf{x}_m)=0\ ,\quad \varepsilon_a=\varepsilon_b\ .\end{aligned} \tag{63}$$

The symbol δ_{ab} means that the states must be exactly the same in all discrete quantum numbers; we have used a Kronecker δ here rather than the Dirac δ used previously because the restriction to equal energies means that none of the remaining quantum numbers is continuous.

The next step is to use the special states and the identity introduced in the preceding two paragraphs to analyze the asymptotic behavior of the Green functions. For convenience of notation, we define a restricted sum over a at energy ε by

$$\sum_a^\varepsilon\equiv\int da\,\delta(\varepsilon-\varepsilon_a)\ .$$

Be definition, the boundary condition on $G_\varepsilon^+(\mathbf{x},\mathbf{x}')$ is that it is outgoing whenever either $\mathbf{x}$ or $\mathbf{x}'$ goes to infinity in

any lead.[62] Choosing $\mathbf{x}$ and $\mathbf{x}'$ in different leads, we then have

$$G_\varepsilon^+(\mathbf{x}_m,\mathbf{x}'_n)\to\sum_a^\varepsilon d_a(\mathbf{x}'_n)\xi_a^+(\mathbf{x}_m)\quad\text{as } x_m\to\infty\ . \tag{64}$$

The asymptotic behavior of $G_\varepsilon^-(\mathbf{x}_m,\mathbf{x}'_n)$ as $x_m\to\infty$ is obtained from Eq. (64) by replacing ξ_a^+ by ξ_a^-. The relation between G_ε^+ and G_ε^-, $G_\varepsilon^+(\mathbf{x}_m,\mathbf{x}'_n)=[G_\varepsilon^-(\mathbf{x}'_n,\mathbf{x}_m)]^*$, yields, then,

$$G_\varepsilon^+(\mathbf{x}_m,\mathbf{x}'_n)\to\sum_c^\varepsilon b_c(\mathbf{x}_m)\xi_c^{-*}(\mathbf{x}'_n)\quad\text{as } x'_n\to\infty\ . \tag{65}$$

Combining Eqs. (64) and (65), we obtain the asymptotic behavior of G_ε^+ as both arguments tend to infinity,

$$G_\varepsilon^+(\mathbf{x}_m,\mathbf{x}'_n)\to\sum_{a,c}^\varepsilon f_{ac}^\varepsilon\xi_a^+(\mathbf{x}_m)\xi_c^{-*}(\mathbf{x}'_n)$$
$$\text{as } x_m,x'_n\to\infty,\quad m\neq n\ . \tag{66}$$

A very similar expression holds for G_ε^-,

$$G_\varepsilon^-(\mathbf{x}_m,\mathbf{x}'_n)\to\sum_{b,d}^\varepsilon(f_{bd}^\varepsilon)^*\xi_b^{+*}(\mathbf{x}_m)\xi_d^-(\mathbf{x}'_n)$$
$$\text{as } x_m,x'_n\to\infty,\quad m\neq n\ . \tag{67}$$

Using the asymptotic behavior of the Green functions, we are now ready to show that the $G_\varepsilon^+G_\varepsilon^+$ and $G_\varepsilon^-G_\varepsilon^-$ terms in $\underline{\sigma}$ [Eq. (52)] do not contribute to the current-response coefficients g_{mn} for $m\neq n$. Using the expansion (66) to evaluate $S(x_m,x'_n)$ defined in Eq. (53), we find that, for $m\neq n$ as $x_m,x'_n\to\infty$,

$$S(x_m,x'_n)\to\sum_{a,b,c,d}^{(\varepsilon)}\int_{C_m}dy_m\int_{C_n}dy'_n\frac{d}{d\varepsilon}[f_{ac}^\varepsilon\xi_a^+(\mathbf{x}_m)\xi_c^{-*}(\mathbf{x}'_n)](\overleftrightarrow{\mathbf{D}}^*\cdot\hat{\mathbf{x}}_m)(\overleftrightarrow{\mathbf{D}}'\cdot\hat{\mathbf{x}}_n)f_{bd}^\varepsilon\xi_b^+(\mathbf{x}'_n)\xi_d^{-*}(\mathbf{x}_m)\ . \tag{68}$$

The energy derivative in the expression for S can be expanded to yield three terms:

$$\frac{d}{d\varepsilon}[f_{ac}^\varepsilon\xi_a^+(\mathbf{x}_m)\xi_c^{-*}(\mathbf{x}'_n)]=\frac{d}{d\varepsilon}(f_{ac}^\varepsilon)\xi_a^+(\mathbf{x}_m)\xi_c^{-*}(\mathbf{x}'_n)+f_{ac}^\varepsilon\frac{d}{d\varepsilon}[\xi_a^+(\mathbf{x}_m)]\xi_c^{-*}(\mathbf{x}'_n)+f_{ac}^\varepsilon\xi_a^+(\mathbf{x}_m)\frac{d}{d\varepsilon}[\xi_c^{-*}(\mathbf{x}'_n)]\ . \tag{69}$$

Using the relation

$$f_1(x)g_1(x')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'f_2(x)g_2(x')$$
$$=-(f_2\overleftrightarrow{\mathbf{D}}f_1)(g_1\overleftrightarrow{\mathbf{D}}'g_2)\ , \tag{70}$$

we see that all three terms which result from using Eq. (69) in Eq. (68) contain one or both of the factors

$$\int_{C_n}dy'_n\,\xi_c^{-*}(\mathbf{x}'_n)(\overleftrightarrow{\mathbf{D}}'\cdot\hat{\mathbf{x}}_n)\xi_b^+(\mathbf{x}'_n)=0\ , \tag{71a}$$

$$\int_{C_m}dy_m\,\xi_d^{-*}(\mathbf{x}_m)(\overleftrightarrow{\mathbf{D}}\cdot\hat{\mathbf{x}}_m)\xi_a^+(\mathbf{x}_m)=0\ . \tag{71b}$$

Both of these factors are equal to zero because of the current-conservation identity (63). Thus we conclude that $S(x_m,x'_n)$ is asymptotically equal to zero,

$$S(x_m,x'_n)\to0\quad\text{as } x_m,x'_n\to\infty,\quad m\neq n\ . \tag{72}$$

Note that if one considered a case where two energy derivatives were present either on the same or different Green functions, there would be terms in which neither factor shown in Eqs. (71) was present; these terms would, in general, be nonzero.

While the asymptotic behavior, Eq. (72), is valuable, we would like to evaluate the current, and hence S, at finite x_m and x'_n. We show in Appendix F that the derivative of terms involving $G_\varepsilon^+G_\varepsilon^+$ and $G_\varepsilon^-G_\varepsilon^-$ with respect to either spatial variable is zero,

$$\frac{\partial}{\partial x_m}S(x_m,x'_n)=\frac{\partial}{\partial x'_n}S(x_m,x'_n)=0\ . \tag{73}$$

Thus, in fact, S is zero for any x_m or x'_n,

$$\int_{C_m}dy_m\int_{C_n}dy'_n\frac{d}{d\varepsilon}G_\varepsilon^+(\mathbf{x}_m,\mathbf{x}'_n)$$
$$\times(\overleftrightarrow{\mathbf{D}}^*\cdot\hat{\mathbf{x}}_m)(\overleftrightarrow{\mathbf{D}}'\cdot\hat{\mathbf{x}}_n)G_\varepsilon^+(\mathbf{x}'_n,\mathbf{x}_m)=0,\quad m\neq n\ . \tag{74}$$

Analogous arguments will hold for any $G_\varepsilon^-G_\varepsilon^-$ term or for terms with the energy derivative on the second Green function.

In showing that the $G_\varepsilon^+G_\varepsilon^+$ and $G_\varepsilon^-G_\varepsilon^-$ terms are zero, our argument depends crucially on the fact that we calculate the conductance not the conductivity, and that we calculate the current response rather than, say, the particle-density response. In fact, a simple generalization of our argument shows that the contribution of the off-Fermi-surface part of the current density to the current through any cross section of the system is zero. The current through any cross section within the system, C_m, can be written in terms of the voltages on the leads using Eqs. (37)–(39). The off-Fermi-surface or circulating part of the current density contributes to the current through terms such as S [Eq. (53)], where C_n are the cross sections in the asymptotic region as before. However, these terms are zero by exactly the argument which leads to Eq. (74), showing that the circulating current through any cross section of the system is zero. In addition to being of use to us here, the identity (74) (and the version demonstrated in Appendix F without the energy derivative) has implications for diagrammatic calculations of conductance fluctuations.[63]

Because terms involving $G_\varepsilon^+G_\varepsilon^+$ or $G_\varepsilon^-G_\varepsilon^-$ do not contribute to the conductance coefficient between different leads, the g_{mn} that result from the $\underline{\sigma}$ in Eq. (52) are

$$g_{mn}=\frac{-e^2\hbar^3}{8\pi M^2}\int d\varepsilon[-f'(\varepsilon)]\int_{C_m}dy_m\int_{C_n}dy'_n\,G^+_\varepsilon(\mathbf{x}_m,\mathbf{x}'_n)(\overleftrightarrow{\mathbf{D}}^*\cdot\hat{\mathbf{x}}_m)(\overleftrightarrow{\mathbf{D}}'\cdot\hat{\mathbf{x}}_n)G^-_\varepsilon(\mathbf{x}'_n,\mathbf{x}_m),\quad m\neq n\ . \tag{75}$$

This is the fundamental equation for the current response in terms of Green functions. For the diagonal part of g, we noted in the preceding section that g_{mm} depends only on states near the Fermi surface because the principal-value contribution is identically zero. Thus, in the notation of this section, the contribution of $\underline{\sigma}_{as}$ to g_{mm} is zero, so that

$$g_{mm}=\frac{e^2\hbar^3}{16\pi M^2}\int d\varepsilon[-f'(\varepsilon)]\int_{C_m}dy_m\int_{C_m}dy'_m\,\Delta G_\varepsilon(\mathbf{x}_m,\mathbf{x}'_m)(\overleftrightarrow{\mathbf{D}}^*\cdot\hat{\mathbf{x}}_m)(\overleftrightarrow{\mathbf{D}}'\cdot\hat{\mathbf{x}}_m)\Delta G_\varepsilon(\mathbf{x}'_m,\mathbf{x}_m)\ . \tag{76}$$

Equations (75) and (76) are the central results of this paper. They show that the conductance coefficients g_{mn} depend only on states near the Fermi level for arbitrary magnetic field or number of leads. Since there exist a variety of numerical and analytic techniques for calculating the Green functions in various microscopic models, these equations provide a natural starting point for calculating the basic linear-response coefficients of particular structures in a magnetic field, exactly what is needed to make contact with experiments in the mesoscopic regime.

Using these expressions for the asymptotic behavior of the Green functions, we can express the conductance coefficients g_{mn} in terms of the asymptotic coefficients f^ε_{ac}. Inserting Eqs. (66) and (67) into Eq. (75), we use the identity (63) to reduce the integrals over C_m and C_n to δ functions and find

$$g_{mn}=\frac{e^2\hbar}{2\pi}\int d\varepsilon[-f'(\varepsilon)]\sum_{a,c}^{\varepsilon}|f^\varepsilon_{ac}|^2,\quad m\neq n\ . \tag{77}$$

An explicit expression for the asymptotic coefficients f^ε_{ac} follows from Eq. (66) by multiplying by appropriate ξ and using the identity (63); the result is

$$f^\varepsilon_{ac}=-\frac{\hbar^2}{4M^2}\int_{C_m}dy_m\int_{C_m}dy'_n\,G^+_\varepsilon(\mathbf{x}_m,\mathbf{x}'_n)\times(\overleftrightarrow{\mathbf{D}}^*\cdot\hat{\mathbf{x}}_m)(\overleftrightarrow{\mathbf{D}}'\cdot\hat{\mathbf{x}}_n)\times\xi^{+*}_a(\mathbf{x}_m)\xi^-_c(\mathbf{x}'_n),\quad m\neq n\ . \tag{78}$$

V. CONNECTION TO SCATTERING THEORY

A very appealing and intuitive way to think about quantum transport is through the connection to a scattering problem as pioneered by Landauer.[25] In this section we transform our result in terms of Green functions into the scattering language. We find that the response coefficients g_{mn} are simply proportional to the total transmission coefficients between the two leads as Büttiker has proposed.[12]

It is not surprising that the asymptotic behavior of the Green functions is closely connected to the transmission amplitudes appearing in the scattering-wave states; such an expression is now well known for zero magnetic field.[43,44] We now derive this connection explicitly for the case of arbitrary magnetic field. Let $\psi^+_{n,a}(\mathbf{x})$ denote the scattering-wave states at fixed energy ε of the Hamiltonian H_0 in Eq. (1), where n,a labels the input lead and input channel [in the sense of Eq. (56)] for the wave; in the asymptotic region,

$$\psi^+_{n,a}(\mathbf{x})\rightarrow\begin{cases}\xi^-_a(\mathbf{x}_n)+\sum_c^{\varepsilon}t_{nn,ca}\xi^+_c(\mathbf{x}_n)\ , & \mathbf{x}\text{ in lead }n\\ \sum_c^{\varepsilon}t_{mn,ca}\xi^+_c(\mathbf{x}_m), & \mathbf{x}\text{ in lead }m\ .\end{cases} \tag{79}$$

Here, $t_{mn,ca}$ denotes the transmission amplitude for going from mode a in lead n to mode c in lead m, and with our choice of normalization for the ξ the $t_{mn,ca}$ form a unitary S matrix. It has been stated previously in the literature[43,44] (including, unfortunately, in a recent article by one of the authors) that the scattering states $\psi^+_{n,a}$ do not form an orthogonal set for any choice of normalization, for these multichannel systems, in which the confining potential extends to infinity. This is incorrect; there is a natural choice of normalization that makes the states orthogonal, even though they are not orthogonal when normalized as in Appendix A of Ref. 44,[64] Thus it is admissible to use the scattering states as the exact eigenstates in Eq. (40), and if one were interested only in making the connection between exact-eigenstate linear-response theory and an S-matrix formulation, one could proceed directly from Eq. (40) using the scattering states to obtain an expression for the g_{mn} in terms of the elements of the S matrix. In Refs. 43 and 44 it was found that such a procedure gave exactly the same results as that obtained using the Green-function expressions; however, the reason for this agreement was unclear since substituting nonorthogonal states into Eq. (40), which assumes orthogonality, was suspect. This minor technical puzzle is now resolved; however, Green-function expressions such as Eqs. (75) and (76) for the g_{mn} are both interesting in their own right and, in general, are more useful for microscopic calculations, so we have chosen to extend the Green-function approach used in Refs. 43 and 44.

To establish the relation between the $t_{mn,ca}$ and the asymptotic coefficients f^ε_{ca} that we are looking for, it is useful to introduce a second set of scattering states corresponding to the same geometrical structure but without any disorder—$U(\mathbf{x})=0$ in Eq. (1). We call these states $\phi^+_{n,a}$ and in the asymptotic region:

$$\phi^+_{n,a}(\mathbf{x})\rightarrow\begin{cases}\xi^-_a(\mathbf{x}_n)+\sum_c^{\varepsilon}t^B_{nn,ca}\xi^+_c(\mathbf{x}_n)\ , & \mathbf{x}\text{ in lead }n\\ \sum_c^{\varepsilon}t^B_{mn,ca}\xi^+_c(\mathbf{x}_m), & \mathbf{x}\text{ in lead }m\end{cases} \tag{80}$$

where the transmission amplitudes for this case are labeled with a B for ballistic. The two sets of states ψ and ϕ are related through the Green function for the complete problem by the standard equation[62]

$$\psi^+_{n,a}(\mathbf{x})=\phi^+_{n,a}(\mathbf{x})+\int_A d\mathbf{x}'\, G^+_\varepsilon(\mathbf{x},\mathbf{x}')U(\mathbf{x}')\phi^+_{n,a}(\mathbf{x}') \ . \tag{81}$$

The integral extends only over the region A because $U(\mathbf{x})=0$ outside of A. The equation of motion of the Green function[62] can be written in the form

$$G^+_\varepsilon(\mathbf{x},\mathbf{x}')U(\mathbf{x}')=\left[\varepsilon+\frac{\hbar^2}{2M}(\mathbf{D}'^*)^2\right]G^+_\varepsilon(\mathbf{x},\mathbf{x}') -\delta(\mathbf{x}-\mathbf{x}') \ , \tag{82}$$

which, when used in the scattering equation, Eq. (81), with $\mathbf{x}$ in A, yields

$$\psi^+_{n,a}(\mathbf{x})=\int_A \mathbf{d}'\mathbf{x}\,\phi^+_{n,a}(\mathbf{x}')\left[\varepsilon+\frac{\hbar^2}{2M}(\mathbf{D}'^*)^2\right] \times G^+_\varepsilon(\mathbf{x},\mathbf{x}'), \quad \mathbf{x} \text{ within } A \ . \tag{83}$$

The formula

$$\int_A d\mathbf{x}[\mathbf{D}^*\cdot\mathbf{F}(\mathbf{x})]f(\mathbf{x})=-\int_A d\mathbf{x}\,\mathbf{F}(\mathbf{x})\cdot\mathbf{D}f(\mathbf{x}) +\int d\mathbf{S}\cdot\mathbf{F}(\mathbf{x})f(\mathbf{x}) \tag{84}$$

allows one to integrate easily by parts. Employing this formula twice, we find

$$\int_A d\mathbf{x}'\,\phi^+_{n,a}(\mathbf{x}')\mathbf{D}'^*\cdot[\mathbf{D}'^*G^+_\varepsilon(\mathbf{x},\mathbf{x}')]=\int_A d\mathbf{x}'\,G^+_\varepsilon(\mathbf{x},\mathbf{x}')\mathbf{D}'^2\phi^+_{n,a}(\mathbf{x})-\int d\mathbf{S}'\cdot[G^+_\varepsilon(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}'\phi^+_{n,a}(\mathbf{x}')] \ . \tag{85}$$

When the first term in this equation is evaluated using the Schrödinger equation for ϕ, and then Eq. (85) is used in Eq. (83), the resulting equation for ψ is

$$\psi^+_{n,a}(\mathbf{x})=-\frac{\hbar^2}{2M}\int d\mathbf{S}'\cdot[G^+_\varepsilon(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}'\phi^+_{n,a}(\mathbf{x}')] \ , \quad \mathbf{x} \text{ within } A \ . \tag{86}$$

Combining the asymptotic behavior of both ϕ [Eq. (80)] and $G^+_\varepsilon(\mathbf{x},\mathbf{x}')$ for fixed $\mathbf{x}$ as $\mathbf{x}'$ tends to infinity [Eq. (65)] with the current-conservation identity [Eq. (63)], we see that only the surface integral in lead n contributes in Eq. (86) because $\phi_{n,a}$ has an incoming wave only in lead n. Thus the final integral equation for $\psi_{n,a}$ in terms of the Green function at the boundary is

$$\psi^+_{n,a}(\mathbf{x})=-\frac{\hbar^2}{2M}\int_{C_n} dy'_n\, G^+_\varepsilon(\mathbf{x},\mathbf{x}'_n)(\overleftrightarrow{\mathbf{D}}'\cdot\hat{\mathbf{x}}_n)\xi_a(\mathbf{x}'_n) \ , \quad \mathbf{x} \text{ within } A \ . \tag{87}$$

The transmission amplitude $t_{mn,ca}$ can be extracted from $\psi_{n,a}$ by simply applying a projection operator suggested by the current-conservation identity [Eq. (63)], yielding the fundamental relation between transmission amplitudes and the Green functions:

$$t_{mn,ca}=-\frac{i\hbar^3}{4M^2}\int_{C_n}dy_m\int_{C_n}dy'_n \times G^+_\varepsilon(\mathbf{x}_m,\mathbf{x}'_n)(\overleftrightarrow{\mathbf{D}}^*\cdot\hat{\mathbf{x}}_m)(\overleftrightarrow{\mathbf{D}}'\cdot\hat{\mathbf{x}}_n)\xi^{+*}_c(\mathbf{x}_m)\xi^-_a(\mathbf{x}'_n) \ , \tag{88}$$

which is valid for all m and n.

For $m\neq n$, comparing to Eq. (78) yields

$$t_{mn,ca}=i\hbar f^\varepsilon_{mn,ca}, \quad m\neq n \ . \tag{89}$$

Using this in Eq. (77) to express the conductance coefficients in terms of the transmission amplitudes, we arrive at the final central result of this paper,

$$g_{mn}=\frac{e^2}{h}\int d\varepsilon[-f'(\varepsilon)]\sum^\varepsilon_{a,c}|t_{mn,ca}|^2, \quad m\neq n \ . \tag{90}$$

The physical fact that no current flows when the voltages on the leads are all the same provides a constraint on the g_{mn}, $\sum_n g_{mn}=0$. On the other hand, unitarity forces a constraint on the total transmitted intensities given by

$$\sum_n T_{mn}(\varepsilon)=N_{\text{chan}}, \quad T_{mn}(\varepsilon)\equiv\sum^\varepsilon_{a,c}|t_{mn,ca}|^2 \tag{91}$$

where N_{chan} is the number of propagating states, called channels, at energy ε. These two constraints fix the diagonal conductance coefficient to be

$$g_{mm}=-\sum_{n\neq m}g_{mn} =-\frac{e^2}{h}\int d\varepsilon[-f'(\varepsilon)][N_{\text{chan}}-T_{mm}(\varepsilon)] \ . \tag{92}$$

The final step is to specialize to the zero-temperature case using $-f'(\varepsilon)\to\delta(\varepsilon-E_F)$; the conductance coefficients per spin are then

$$g_{mn}=\frac{e^2}{h}T_{mn}(E_F), \quad m\neq n \ . \tag{93}$$

At zero temperature, the explicit relation between the current coming out of lead m and the voltage on lead n is, then,

$$I_m=\frac{e^2}{h}\left[-N_{\text{chan}}V_m+\sum_{n=1}^{N_L}T_{mn}V_n\right] , \tag{94}$$

which is the multiprobe Landauer formula as derived by Büttiker.[12]

In order to calculate the resistance, one must apply the constraints for the experimental situation with which one wants to compare and solve Eq. (94) for the voltages in terms of the current. Since Eq. (94) is noninvertible (because the zero of potential is arbitrary), some additional

linear algebra is involved, which is discussed in Appendix B of Stone and Szafer.[44]

VI. CONCLUSIONS

A. The multiprobe Landauer formula and linear-response theory

The simplicity and intuitively appealing nature of the scattering formulation of the linear-response theory [Eq. (94)], as compared to the equivalent exact eigenstate expression [comprised by Eqs. (37), (39), and (40)], suggest that there should be a simple physical argument for Eq. (94). In our opinion, that argument is simply Büttiker's original phenomenological derivation of the multiprobe Landauer formula. For completeness, we summarize that argument briefly here; the original argument can be found in Ref. 12.

Consider a multiprobe conductor of the type shown in Fig. 1, except that instead of the infinite perfect leads one imagines that each lead is attached to an ideal "reservoir." A reservoir in this context has four important properties. (1) It is in equilibrium at a chemical potential μ_n (for the nth lead). (2) It is large enough relative to the conductor and to the chemical-potential differences involved that any steady-state current flowing from the reservoir is negligible deep within the reservoir (so a measurement in the presence of current flow would still yield μ_n). (3) No particle entering the reservoir returns to the conductor without an inelastic (phase-randomizing) event. (4) The interface between the reservoir and the "sample" generates no additional resistance (this can be achieved by adiabatically widening the lead to a large region which is the reservoir).[65]

Suppose now that the N_L chemical potentials $\mu_n \equiv eV_n$ are given some fixed values, which shall be measured from the lowest of those, μ_0. For carriers below μ_0 the net current into all reservoirs must be zero because all incoming and outgoing states are occupied (at $T=0$). The total current injected into reservoir m from reservoir n (summed over all N incoming channels) in the energy interval between μ_n and μ_0 is just

$$I_{mn} = e \sum_a v_a \frac{dn_a}{dE}(\mu_n - \mu_0) \sum_b T_{mn,ab} = (e^2/h) T_{mn}(V_n - V_0) ,$$

where dn_a/dE is the density of states for channel a, and we have used the well-known cancellation of the velocity and 1D density-of-states factors. The current injected into the conductor from reservoir m is, by a similar argument, just $(e^2/h)(N_{\text{chan}} - R_{mm})(V_m - V_0)$; hence, the *total current* I_m *into* the conductor from reservoir m is given by the difference of this term and the total outgoing current, $\sum_{n \neq m} I_{mn}$, which is just Eq. (94) (with $V_0 \equiv 0$). Note that the argument apparently is completely independent of the presence of a magnetic field (since the necessary cancellation of v_a and dn_a/dE still occurs in an arbitrary field). This surprisingly generality led to the question addressed in this work of whether microscopic calculations supported the validity of Eq. (94) at all magnetic fields. We agree with Ref. 12 that the validity of Eq. (94) in arbitrary field is remarkable, and add, given the complexity of the intermediate steps leading to Eq. (94), that it appears that this simple and useful expression would have been very difficult to obtain from a linear-response model in the absence of Büttiker's original arguments.

Büttiker's multiprobe Landauer formula, Eq. (94), was proposed at the end of a period of both controversy and progress in our understanding of the physically relevant Landauer formula. (We remind the reader that we use the term "Landauer formula" generally to denote any expression for the linear-response coefficients in terms of the S matrix of the conductor.) A recent review article[44] describes much of this historical development and we will not reproduce that discussion in the present article. Instead, we will make some comments about the novel features of Eq. (94), which allow a derivation from linear-response theory to succeed, and then discuss simple limits of Eq. (94) in a high magnetic field that emphasize both its relevance to the integer quantum Hall effect and its relation to the original Landauer formula, $g = T/(1-T)$, where T is the total transmission coefficient out of the reservoir serving as current source.

Although, beginning with the work of Engquist and Anderson,[66] earlier work emphasized the importance of the four-probe nature of a (typical) resistance measurement in deriving Landauer formulas,[67] Eq. (94) is the first such formula that treats the current and voltage probes on an equal footing, and hence involves the entire S matrix (scattering into all the probes) instead of just scattering between the current source and sink. Thus, other approaches, by necessity, had to assume that the voltage difference induced by the current flow could be expressed only in terms of the scattering between current source and sink (even though they did not require this induced voltage to be the *same* as that between the source and the sink). There is no reason to believe that such a general expression, which ignores the dynamics of scattering into the voltage probes, should exist in the mesoscopic regime, and, indeed, the experiments on voltage fluctuations,[13,14] nonlocal bend resistance,[20] and the anomalous quantized Hall effect[35] in mesoscopic conductors (as well as many others) clearly demonstrate that the measuring probes can be of crucial importance in this regime.

More importantly, earlier approaches had understood that the chemical-potential difference induced by a current flow was the chemical-potential difference between two reservoirs, adjusted so that no net current flows into them.[66] However, because their approaches ultimately wished to eliminate the scattering into the voltage probes from the final description, they were forced to introduce some physical assumption to characterize the "effective chemical potential" at a point along the conductor. Since the channels in the conductor are, by definition, out of equilibrium in the presence of current flow, this necessitates some hypothesis about equilibration of different channels at the Fermi energy which appeared to have some arbitrariness and lack of generality.[67] Equation (94), on the other hand, allows the equilibration of the measuring reservoirs with the sample

in the presence of current flow to be determined by the (enlarged) scattering matrix of the conductor, removing the need to define an "effective chemical potential" along the conductor. The induced chemical-potential difference is that *between the measuring reservoirs* and is fixed only by the condition that voltage probes draw no current. As long as a voltage measurement is ultimately made by equilibrating with measuring reservoirs, and *one can reasonably well model the scattering into that reservoir,* it is hard to see how Eq. (94) can fail (although it certainly can reduce to simpler descriptions in certain limits, one of which we will discuss below).

It is precisely because Eq. (94) requires no assumptions about equilibrium of carriers within the sample (or in the perfect leads) that it can be derived straightforwardly from linear-response theory. The boundary condition of a large phase-randomizing reservoir is well mimicked by the infinite perfect leads in the linear-response model. As discussed in the Introduction, the effect of the current flow on the assumed equipotential in the leads can and should be ignored because the leads are representing ideal reservoirs which are unaffected by the small current flow. Note, that the chemical potentials of the voltage reservoirs are also unaffected by the current flow; instead they are adjusted externally to cancel that flow. We stress that an understanding of the role of the reservoirs is essential in justifying the boundary conditions imposed in the linear-response calculation and the physical situations to which such calculations can be applied.[12,65] We believe that our calculation, combined with those of Refs. 43 and 44, now establishes the complete equivalence of the Kubo and Landauer approaches as long as the linear-response calculation incorporates the correct boundary conditions (i.e., infinite system with all leads explicitly included).

B. The multiprobe Landauer formula and the quantum Hall effect

As discussed above, a major application of this formulation of linear-response theory is to the integer quantum Hall effect, particularly in mesoscopic systems. Several recent papers have analyzed the quantum Hall effect on the basis of Eq. (94),[26,27,32,68–71] and also on the basis of simpler Landauer formulas in which the probes are not introduced explicitly.[49,50] One of the most basic issues raised [given Eq. (94), which determines the "longitudinal" and "Hall" resistances for any set of measurements on a sample] is what are the necessary and sufficient conditions on the conductance matrix g_{mn} such that one observed a quantized Hall resistance, and/or zero longitudinal resistance, for a given subset of measurements. Our present discussion of this issue will overlap substantially with previous work;[26,27,32,68] however, we note that despite the fact that many specific examples have been analyzed (and, in particular, the four-probe case[26,27,32,68]), no answer to this general question has been demonstrated in the literature. We have been able to prove a number of general properties of Eq. (94) relating to the integer quantum Hall effect. Here we will report the simplest and most relevant of our results, and defer a detailed discussion to a separate publication.[72]

Assume that the sample depicted in Fig. 1 is immersed in a strong perpendicular magnetic field of orientation such that the Lorentz force exerted on the carriers emerging from the leads into the sample pushes them in the clockwise direction. As we have seen above, the transverse wave functions in the perfect leads are pushed towards the edge of the leads by the magnetic field, in a direction determined by the sense of their longitudinal velocity. The magnitude of that velocity, because it is proportional to dE_n/dk, is highest for states with large amplitude nearest the edge. Hence the current is fed into the sample from the perfect leads in edge states localized on the furthest clockwise edge of each lead. In the sample, where there is bulk disorder, the edge states are mixed and are no longer simply those of the leads; nonetheless, if the typical energy of the disordered potential is small compared to $\hbar\omega_c$ and the Fermi energy is far from that of a bulk Landau level, then there are still current-carrying edge states.[72] As Büttiker has emphasized,[27] it will be very difficult for carriers in these edge states to backscatter more than a cyclotron radius, and therefore the clockwise transmission matrices $T_{m+1,m}$ will be very close to their maximum value, N_{chan} (for simplicity in the following discussion, we shall assume the same number of propagating channels N_{chan} in all leads). Labeling the leads of the system in increasing order clockwise as in Fig. 1, we are then led to define the ideal system as that in which all clockwise transmission coefficients $T_{m+1,m}=N_{\text{chan}}$, and all others, including the reflection coefficients R_{mm}, are equal to zero. We use this as our reference state for the breakdown of the quantum Hall effect, and define a localized breakdown as a scattering path directly connecting two leads which are not connected in the ideal system. While the edge-state picture is useful for motivating this starting-point, it is not essential to our results, which only characterize the conditions on the $\underline{g}$ matrix leading to the quantum Hall effect.

A *measuring configuration* exhibits the complete integer quantum Hall effect if all resistances measured on the same side of the current path (a line connecting the current source and sink) are zero (vanishing "longitudinal resistance"), and all resistances measured across the current path give $R_H=(h/e^2)(1/N_{\text{chan}})$ (quantized "Hall resistance"). Although less common than four-probe measurements, two-probe resistance measurements can be done in certain structures[21,73] and yield the quantized Hall-resistance value.[73] We include the two-probe resistances in our analysis as resistances measured across the current path. A *system* exhibits the complete integer quantum Hall effect if this property holds for all choices of current leads, i.e., all measuring configurations.

We have proved the following statements for systems with an arbitrary number of leads, based on an analysis of Eq. (94). (1) The ideal system exhibits the complete quantum Hall effect, and it is the only system exhibiting the complete quantum Hall effect. (2) An arbitrary nonideal system still exhibits the complete quantum Hall effect for all configurations in which the current path does not cross a localized scattering path. (3) A nonideal system in which there is only one localized breakdown, measured

in a configuration in which this scattering path crosses the current path, so that there is a probability of interedge reflection $R=1-T$, has the following properties. (a) All longitudinal resistances measured on the same side of the localized breakdown will be zero. (b) All longitudinal resistances measured across the line of localized breakdown will be equal to $(h/e^2)(1/N_{\rm chan})R/T$. (c) All Hall resistances measured on the same side of the breakdown will be $(h/e^2)(1/N_{\rm chan})$. (d) All Hall resistances measured across the region of breakdown will be equal to the appropriate sum or difference of these longitudinal and quantized Hall resistances.

To illustrate the usefulness and ease of analyzing these questions with Eq. (94), we present a brief proof of statement (1). Equation (94), written in matrix notation as $I=\underline{g}V$ is a linear equation in an N_L-dimensional vector space in a given representation; define the orthonormal basis vectors in this representation to be $\hat{\mathbf{e}}_m$. Feed current into the system through lead n and take it out through lead $n'>n$ and choose units so that this current is unity, i.e., the "current vector' is $I=\hat{\mathbf{e}}_n-\hat{\mathbf{e}}_{n'}$. With resistance measured in units of h/e^2, this configuration shows the complete quantum Hall effect if the solution of Eq. (94) is

$$V_{\rm QH}(n,n')=(1/N_{\rm chan})\sum_{m=n}^{n'-1}\hat{\mathbf{e}}_m \ ,$$

since this has the property of vanishing voltage difference for all leads on a given side of the current path, and voltage difference $1/N_{\rm chan}$ for all leads separated by the current path. In the ideal system, where there is only clockwise transmission, the g matrix is $\underline{g}_{\rm QH}=N_{\rm chan}(\underline{I}-\underline{P}_1)$, where $\underline{I}$ is the identity matrix and $\underline{P}_1$ is the matrix which permutes each basis vector by one step, i.e., $\underline{P}_1\hat{\mathbf{e}}_m=\hat{\mathbf{e}}_{m+1}$. But it then follows by inspection that $V_{\rm QH}$ is a solution of Eq. (94):

$$\underline{g}_{\rm QH}V_{\rm QH}=\sum_{m=n}^{n'-1}\hat{\mathbf{e}}_m-\sum_{m=n+1}^{n'}\hat{\mathbf{e}}_m=\hat{\mathbf{e}}_n-\hat{\mathbf{e}}_{n'} \ .$$

It also follows that $\underline{g}_{\rm QH}$ is the only matrix for which $V_{\rm QH}(n,n')$ is a solution, as any correction to $g_{\rm QH}$ would have to give zero when acting on $V_{\rm QH}$ for all choices of n,n', and it is easy to show that the only such matrix is identically zero. Thus we conclude that the complete quantum Hall effect occurs if and only if electrons injected into the sample ultimately arrive with probability 1 at the contact towards which the magnetic field is most directly driving then; it is easy to see how this might occur in the edge-state picture as discussed in detail by Büttiker.[27]

We will not prove statements (2) or (3) at this time, but pause briefly to discuss statement (3), which has very recently been independently derived by Haug *et al.*,[32] Jain and Kivelson,[39] and in special cases by Büttiker.[27] The striking point is that for this special situation of only a single localized breakdown of the edge states one obtains the original 1D Landauer formula in the one-channel case, and a simple multichannel generalization, which, to our knowledge, has never been proposed before in the literature. This clarifies the point that the original Landauer formula does not necessarily require weakly coupled probes, but rather probes which do not themselves contribute to the longitudinal resistance (that probes do cause resistance in zero field has been shown in the experiments in Ref. 20). In the quantized Hall regime the scattering into the probes is as large as possible, but this is precisely balanced by the flux out of the voltage reservoir along the same edge, and the presence of probes does not result in any net flux reflected back into the current source. Under these circumstances it is only reflection in the sample which contributes to longitudinal resistance, and one has the conditions necessary for the derivation of the one-channel Landauer formula to be valid. For the many-channel case one again must consider the equilibration of the channels, and Eq. (94) leads to a different and simpler result than has been proposed in the literature (see Ref. 44 and references therein) *for this special situation.*

It has been possible very recently to study this particular case experimentally in gated quantum Hall systems.[32–34] These experiments focused on the situation in which $R/T=1$ (exactly one channel is transmitted and one is reflected), so that statement (3) implies a striking new effect—quantization of the longitudinal resistance as well as the Hall resistance. This effect was indeed observed and the correctness of the conclusions following from Eq. (94) were convincingly demonstrated. It is important to note that the samples studied in some of these experiments were hundreds of micrometers across, far from what is normally considered the mesoscopic regime. This emphasizes that Büttiker's multiprobe Landauer formula is relevant to the macroscopic Hall effect, as long as certain phase-coherent scattering processes which should not occur in this length scale are excluded. This will be discussed in more detail elsewhere.[72] We believe that further applications of this multichannel Landauer formula will lead to new insights into quantum-transport phenomena in high magnetic field, in both the mesoscopic and macroscopic regimes.

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APPENDIX A: CONNECTION TO PREVIOUS WORK IN BULK SYSTEMS

Previous linear-response calculations in a magnetic field have dealt with the conductivity tensor of bulk systems without introducing a description of the probes, and have used either impurity averaging[46] or spatial averaging[41,42(a)] as an essential part of the calculation. These formulations should be obtainable in our approach as well, and for specificity we will make contact with the of Smrčka and Středa,[42(a)] which has been used as a start-

ing point for discussions of the quantum Hall effect,[74] and has also been a starting point for deriving a well-known formulation due to Středa,[75] in which the Hall conductivity is not expressed in terms of Fermi-state quantities. The aim of Smrčka and Středa is to find the linear-response tensor, $\underline{L}$, which relates the spatially averaged current density to a constant applied electric field $\mathbf{E}$,

$$\frac{1}{S}\int_A d\mathbf{x}\,\mathbf{J}(\mathbf{x}) \equiv \underline{L}\cdot\mathbf{E}\ , \tag{A1}$$

where S is the length of the region A along the direction of the direction of current flow; we follow Smrčka and Středa in taking $S=1$. The relation between $\underline{L}$ and the conductivity-response function of Eq. (52) above, is then,

$$\underline{L} = \int_A d\mathbf{x}\int_A d\mathbf{x}'\,\bar{\sigma}(\mathbf{x},\mathbf{x}')\ . \tag{A2}$$

The expression for $\underline{L}$ given by Smrčka and Středa involves a trace over a product of Green functions and velocity operators. To arrive at this result we start with our Eq. (52) for the response function and interpret Eq. (A2) as a real-space representation of a trace.

First, integrate the first term in Eq. (52) by parts with respect to energy and use this relation in Eq. (A2) to yield

$$\underline{L} = \frac{-e^2\hbar^3}{8\pi M^2}\int_A d\mathbf{x}\int_A d\mathbf{x}'\int d\varepsilon\, f(\varepsilon)\left[\frac{d}{d\varepsilon}G_\varepsilon^+(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'\Delta G_\varepsilon(\mathbf{x}',\mathbf{x}) - \Delta G_\varepsilon(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'\frac{d}{d\varepsilon}G_\varepsilon^-(\mathbf{x}',\mathbf{x})\right]\ . \tag{A3}$$

Using four sets of complete states in real space, $\int d\mathbf{r}_i\,|\mathbf{r}_i\rangle\langle\mathbf{r}_i|$, and the matrix elements of the current-density operator in real space,

$$\langle\mathbf{r}_i|\mathbf{J}_{\rm op}(\mathbf{x})|\mathbf{r}_2\rangle = -\frac{ie\hbar}{2M}\delta(\mathbf{x}-\mathbf{r}_i)\overleftrightarrow{\mathbf{D}}\delta(\mathbf{x}-\mathbf{r}_2)\ , \tag{A4}$$

we find that $\underline{L}$ expressed as a trace is

$$\underline{L} = -\frac{\hbar}{2\pi}\int_A d\mathbf{x}\int_A d\mathbf{x}'\int d\varepsilon\, f(\varepsilon){\rm Tr}\left[\mathbf{J}_{\rm op}(\mathbf{x})\frac{dG_\varepsilon^+}{d\varepsilon}\mathbf{J}_{\rm op}(\mathbf{x}')\Delta G_\varepsilon - \mathbf{J}_{\rm op}(\mathbf{x})\Delta G_\varepsilon\,\mathbf{J}_{\rm op}(\mathbf{x}')\frac{dG_\varepsilon^-}{d\varepsilon}\right]\ . \tag{A5}$$

Since the operator ΔG_ε can be expressed in terms of the Hamiltonian through $\Delta G_\varepsilon = -2\pi i\delta(\varepsilon - H)$, Eq. (A5) is equivalent to

$$\underline{L} = i\hbar\int_A d\mathbf{x}\int_A d\mathbf{x}'\int d\varepsilon\, f(\varepsilon){\rm Tr}\left[\mathbf{J}_{\rm op}(\mathbf{x})\frac{dG_\varepsilon^+}{d\varepsilon}\mathbf{J}_{\rm op}(\mathbf{x}')\delta(\varepsilon-H) - \mathbf{J}_{\rm op}(\mathbf{x})\delta(\varepsilon-H)\mathbf{J}_{\rm op}(\mathbf{x}')\frac{dG_\varepsilon^-}{d\varepsilon}\right]\ . \tag{A6}$$

The next step is to rewrite the trace over the current-density operator as a trace over the velocity operator. To do this, note that for a general operator A the definitions of a trace and the current-density operator imply that

$$\begin{aligned}\int d\mathbf{x}\,{\rm Tr}[\mathbf{J}_{\rm op}(\mathbf{x})A_{\rm op}] &= \int d\mathbf{x}\int d\mathbf{x}'\int d\alpha\,\langle\mathbf{x}'|\mathbf{J}_{\rm op}(\mathbf{x})|\alpha\rangle\langle\alpha|A_{\rm op}|\mathbf{x}'\rangle \\ &= \frac{e\hbar}{2Mi}\int d\mathbf{x}\int d\mathbf{x}'\int d\alpha[\delta(\mathbf{x}-\mathbf{x}')\mathbf{D}' + \mathbf{D}'\delta(\mathbf{x}'-\mathbf{x})]\psi_\alpha(\mathbf{x})\langle\alpha|A_{\rm op}|\mathbf{x}'\rangle\ .\end{aligned} \tag{A7}$$

The integral over $\mathbf{x}$ can now be performed because of the δ functions; thus, using, in addition, the definition of the velocity operator,

$$\begin{aligned}\int d\mathbf{x}\,{\rm Tr}[\mathbf{J}_{\rm op}(\mathbf{x})A_{\rm op}] &= \frac{e\hbar}{Mi}\int d\mathbf{x}'\int d\alpha\,\mathbf{D}'\psi_\alpha(\mathbf{x}')\langle\alpha|A_{\rm op}|\mathbf{x}'\rangle \\ &= e\int d\mathbf{x}'\int d\alpha\langle\mathbf{x}'|\mathbf{v}_{\rm op}|\alpha\rangle\langle\alpha|A_{\rm op}|\mathbf{x}'\rangle \\ &= e\,{\rm Tr}(\mathbf{v}_{\rm op}A_{\rm op})\ .\end{aligned} \tag{A8}$$

We can use Eq. (A8) to greatly simplify Eq. (A6), and find that

$$\underline{L} = i\hbar e^2\int d\varepsilon\, f(\varepsilon){\rm Tr}\left[\mathbf{v}_{\rm op}\frac{dG_\varepsilon^+}{d\varepsilon}\mathbf{v}_{\rm op}\delta(\varepsilon-H) - \mathbf{v}_{\rm op}\delta(\varepsilon-H)\mathbf{v}_{\rm op}\frac{dG_\varepsilon^-}{d\varepsilon}\right]\ , \tag{A9}$$

which is the result found by Smrčka and Středa [their Eq. (31)]. From this point, all of the subsequent results of Smrčka and Středa can, of course, be derived, including the more standard form of the longitudinal conductivity at zero temperature which dates back to Kubo *et al.*[41,58]

$$L_{xx}=\pi\hbar e^2\mathrm{Tr}[v_x\delta(E_F-H)v_x\delta(E_F-H)]\ , \tag{A10}$$

as well as the more complex expression for the Hall conductivity, which was written in terms of Fermi-surface quantities in Smrčka and Středa,[42(a)] and subsequently transformed into the non-Fermi-surface expression[75] used by Středa in treating the quantum Hall regime. Smrčka and Středa are able to obtain Fermi-surface expressions for these response coefficients because spatial averaging eliminates the circulating currents which are described by non-Fermi-surface terms in Eq. (29) for $\underline{\sigma}(\mathbf{x},\mathbf{x}')$. Thus the spatially averaged conductivity behaves essentially like the conductance coefficients and is a Fermi-surface quantity, whereas (as shown above) the current-density-response function $\underline{\sigma}(\mathbf{x},\mathbf{x}')$ is not, and the failure to distinguish these quantities apparently had led to some confusion in the literature.[24] Previous work has interpreted the Fermi-surface expression for the spatially averaged conductivity in terms of diamagnetic currents flowing at the edges in certain limits.[76–78] Here we emphasize that such an interpretation is not essential to the basic result that the Hall resistance can be expressed as a Fermi-surface quantity; the Fermi-surface states need not be edge states.

APPENDIX B: LATTICE FORM OF THE MAIN RESULTS

In order to perform computations of the resistance of mesoscopic structures, it is often useful to work in a discretized space rather than in continuum space as we have in the main text. In this appendix we therefore describe how to translate our continuum results into the lattice language. We consider a nearest-neighbor 2D tight-binding Hamiltonian on a square lattice with sites labeled by pairs of integers n,m:

$$\begin{aligned}H_0=&\sum_{n,m}\varepsilon_{n,m}|n,m\rangle\langle n,m|\\&-\sum_{n,m}(V^x_{n,m}|n,m\rangle\langle n+1,m|+\mathrm{H.c.})\\&-\sum_{n,m}(V^y_{n,m}|n,m\rangle\langle n,m+1|+\mathrm{H.c.})\ ,\end{aligned} \tag{B1}$$

where the hopping matrix elements are related to the vector potential by

$$\begin{aligned}V^x_{n,m}&=\exp(ieA^x_{n,m}/\hbar c)\ ,\\V^y_{n.m}&=\exp(ieA^y_{n,m}/\hbar c)\ .\end{aligned} \tag{B2}$$

In transcribing the continuum results, the basic quantity we will need to know how to treat is the derivative operator $\overleftrightarrow{\mathbf{D}}$ which is related to the current-density operator [Eq. (9)]. Thus, we first find the velocity operator in our lattice case,

$$\begin{aligned}v^x_{\mathrm{op}}&\equiv\frac{1}{i\hbar}[x_{\mathrm{op}},H_0]\\&=\frac{1}{i\hbar}\sum_{n,m}(V^x_{n,m}|n,m\rangle\langle n+1,m|\\&\qquad-V^{x*}_{n,m}|n+1,m\rangle\langle n,m|)\ ,\end{aligned} \tag{B3}$$

where a similar expression holds for v^y_{op}. The current-density operator is related to the velocity and density operators by

$$\mathbf{J}_{\mathrm{op}}(n,m)=e[n_{\mathrm{op}}(n,m)\mathbf{v}_{\mathrm{op}}+\mathbf{v}_{\mathrm{op}}n_{\mathrm{op}}(n,m)]/2\ .$$

Using $n_{\mathrm{op}}(n,m)=|n,n\rangle\langle n,m|$, this yields

$$\begin{aligned}J^x_{\mathrm{op}}(n,m)=\frac{e}{2i\hbar}(&V^x_{n,m}|n,m\rangle\langle n+1,m|-V^{x*}_{n,m}|n+1,m\rangle\langle n,m|\\&+V^x_{n-1,m}|n-1,m\rangle\langle n,m|-V^{x*}_{n-1,m}|n,m\rangle\langle n-1,m|)\ .\end{aligned} \tag{B4}$$

As in Appendix A [Eq. (A5)], any of our continuum expressions involving $\overleftrightarrow{\mathbf{D}}$ can be interpreted as a trace over operators where J_{op} is substituted for $\overleftrightarrow{\mathbf{D}}$,

$$\begin{aligned}&f(\mathbf{x},\mathbf{x}')\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'g(\mathbf{x}',\mathbf{x})\\&\qquad=-\left[\frac{2Mi}{e\hbar}\right]^2\mathrm{Tr}[\mathbf{J}_{\mathrm{op}}(\mathbf{x})f_{\mathrm{op}}\mathbf{J}_{\mathrm{op}}(\mathbf{x}')g_{\mathrm{op}}]\ .\end{aligned} \tag{B5}$$

To get the corresponding lattice expression, one need only substitute the lattice form of J_{op} [Eq. (B4)]. This is a general prescription for transcribing the continuum results onto the lattice and can be used to interpret our results for the nonlocal response function [Eq. (52)], the current-conservation identity [Eq. (63)], the conductance coefficients [Eqs. (75) and (76)], and the relation between the Green function and the transmission amplitudes [Eq. (88)].

An annoying feature of this general prescription is that it generates cumbersome equations with many terms; since J_{op} has four terms, $\overleftrightarrow{\mathbf{D}}^*\overleftrightarrow{\mathbf{D}}'$ will generate 16 terms. We now show that for the cases where there is an integration over the cross section of the lead, many of the terms are identical and the resulting expressions are considerably simpler. We first introduce an operator closely related to J^x_{op},

$$\begin{aligned}K_{\mathrm{op}}(n)\equiv\frac{e}{i\hbar}\sum_m(&V^x_{n,n}|n,m\rangle\langle n+1,m|\\&-V^{x*}_{n,m}|n+1,m\rangle\langle n,m|)\ .\end{aligned} \tag{B6}$$

Physically, K_{op} represents the current going through the bonds between columns n and $n+1$. Matrix elements of this operator have the two crucial properties of satisfying the current-continuity equation [Eq. (11)] and the current-conservation identity for states in the perfect leads [Eq. (63)]. To show the first of these, we rewrite the Hamiltonian in order to express K_{op} in terms of the Hamiltonian:

$$h_n^{(2)} \equiv \sum_m (V^x_{n,m} |n,m\rangle \langle n+1, m| + V^{x*}_{n-1,m} |n,m\rangle \langle n-1, m|) , \quad \text{(B7a)}$$

$$h_n^{(1)} \equiv \sum_m \varepsilon_{n,m} |n,m\rangle \langle n,m| - \sum_m (V^y_{n,m} |n,m\rangle \langle n, m+1| + \text{H.c.}) , \quad \text{(B7b)}$$

$$H_0 = \sum_n h_n^{(1)} - \sum_n h_n^{(2)} . \quad \text{(B7c)}$$

Introducing eigenstates $|\alpha\rangle$ and $|\beta\rangle$ of H_0 with eigenvalues ε_α and ε_β, we have

$$\langle\beta|[K_{op}(n+1)-K_{op}(n)]|\alpha\rangle = \frac{e}{i\hbar}\langle\beta|[h^{(2)}_{n+1} - (h^{(2)}_{n+1})^+]|\alpha\rangle . \quad \text{(B8)}$$

Using $h^{(2)}_{n+1}$ to act on $|\alpha\rangle$ and $(h^{(2)}_{n+1})^+$ to act on $\langle\beta|$, substituting H_0 and $h^{(1)}$ from Eq. (B7), and cancelling the contributions from $h^{(1)} = (h^{(1)})^+$, we arrive at

$$\langle\beta|[K_{op}(n+1)-K_{op}(n)]|\alpha\rangle = \frac{ie}{\hbar}\langle(\varepsilon_\alpha - \varepsilon_\beta)\sum_m (\langle\beta|n+1, m\rangle\langle n+1, m|\alpha\rangle) . \quad \text{(B9)}$$

This equation is a direct analog of the current-continuity equation, Eq. (11); in particular, if the energies of the states are the same, the matrix element of $K_{op}(n)$ is independent of n.

Turning now to the current-conservation identity in the perfect leads, we use our general prescription to transcribe Eq. (63) and get

$$\sum_m \langle \xi^{\pm *}_a | J^x_{op}(n,m) | \xi^\pm_b \rangle = \pm e\delta_{ab}, \quad \varepsilon_a = \varepsilon_b . \quad \text{(B10)}$$

Using $\sum_m J^x_{op}(n,m) = [K_{op}(n)+K_{op}(n-1)]/2$ and noting that the two K_{op} terms are equal by use of Eq. (B9) yields

$$\langle \xi^{\pm *}_a | K_{op}(n) | \xi^\pm_b \rangle = \pm e\delta_{ab}, \quad \varepsilon_a = \varepsilon_b \quad \text{(B11)}$$

which is the desired identity.

The current-conservation relations for K_{op} that have just been derived can be used to simplify the general expressions for equations involving an integral over a cross section. As an example, we consider the equation for the conductance coefficients, g_{ij}, between different leads i and j, Eq. (75). Our general transcription procedure yields

$$g_{ij} = -\frac{\hbar}{2\pi}\int d\varepsilon[-f'(\varepsilon)] \sum_m \sum_{m'} \text{Tr}[J^x_{op}(n,m) G^+_\varepsilon J^x_{op}(n',m') G^-_\varepsilon], \quad i \neq j \quad \text{(B12)}$$

where (n,m) labels a site in the perfectly ordered part of lead i and (n',m') labels a site in lead j. Substituting K_{op} for $\sum_m J_{op}$, we obtain

$$g_{ij} = -\frac{\hbar}{8\pi}\int d\varepsilon[-f'(\varepsilon)\text{Tr}\{[K_{op}(n)+K_{op}(n-1)]G^+_\varepsilon [K_{op}(n')+K_{op}(n'-1)]G^-_\varepsilon\}, \quad i \neq j . \quad \text{(B13)}$$

Using the equation of motion for the Green function with $i \neq j$ and noting that both Green functions in Eq. (B13) are at the same energy, we find by an argument identical to that used for the current-continuity equation above [Eq. (B9)] that

$$\text{Tr}\{[K_{op}(n)-K_{op}(n-1)]G^+_\varepsilon K_{op}(n')G^-_\varepsilon\} = 0 , \quad n \text{ far from } n' . \quad \text{(B14)}$$

Thus the four terms in Eq. (B13) are the same, yielding

$$g_{ij} = -\frac{\hbar}{2\pi}\int d\varepsilon[-f'(\varepsilon)]\text{Tr}[K_{op}(n)G^+_\varepsilon K_{op}(n')G^-_\varepsilon] , \quad i \neq j . \quad \text{(B15)}$$

Similar simplifications occur in the expression for g_i [Eq. (76)].

Because the connection between the Green function and the transmission coefficients, Eq. (88), is perhaps the most physical route to use in performing a calculation, we give the lattice form of this connection explicitly. For the transmission between different leads, the argument used to arrive at Eq. (B15) yields

$$t_{ij,ca} = -\frac{i\hbar}{e^2}\text{Tr}[K_{op}(n)G^+_\varepsilon K_{op}(n')|\xi^-_a\rangle\langle\xi^+_c|]$$

$$= -\frac{i\hbar}{e^2}\langle\xi^+_c|K_{op}(n)G^+_\varepsilon K_{op}(n')|\xi^-_a\rangle, \quad i \neq j . \quad \text{(B16)}$$

For the reflection coefficients, the δ function in the equation of motion for the Green function introduces some subtleties; we find in this case

$$t_{ii,ca} = -\frac{i\hbar}{e^2}\langle\xi^+_c|K_{op}(n-1)G^+_\varepsilon K_{op}(n)|\xi^-_a\rangle . \quad \text{(B17)}$$

APPENDIX C: THE EQUILIBRIUM CURRENT DENSITY

We show here that the equilibrium current density given in Eq. (17) yields zero total current in each lead. Integrating the current density over a cross section of the lead and using the definition of **W** [Eq. (9)], one finds that the equilibrium current through lead m is

$$I_m^{(0)}=-\frac{ie\hbar}{2M}\int d\alpha\, f(\varepsilon_\alpha)\int_{C_m} dy_m\, \psi_\alpha^*(\mathbf{x}_m)(\overleftrightarrow{\mathbf{D}}\cdot\hat{\mathbf{x}}_m)\psi_\alpha(\mathbf{x}_m)\ . \tag{C1}$$

Rewriting this by introducing two new variables, ε and $\mathbf{x}'_m$, which are then integrated over using δ functions, yields

$$I_m^{(0)}=-\frac{ie\hbar}{2M}\int d\varepsilon\, f(\varepsilon)\int_{C_n} dy_m\int d\alpha\,\delta(\varepsilon_\alpha-\varepsilon)\int d\mathbf{x}'_m\,\delta(\mathbf{x}_m-\mathbf{x}'_m)\psi_\alpha^*(\mathbf{x}'_m)(\overleftrightarrow{\mathbf{D}}\cdot\hat{\mathbf{x}}_m)\psi_\alpha(\mathbf{x}_m)\ , \tag{C2}$$

where $(\overleftrightarrow{\mathbf{D}}\cdot\hat{\mathbf{x}}_m)$ now acts to the left on the δ function. The integral over the states α simply yields the difference between two Green functions [Eq. (42a)], while the δ function can be expressed in terms of a Green function by using the equation of motion.[62] These two operations yield

$$I_m^{(0)}=-\frac{ie\hbar}{2M}\int d\varepsilon\, f(\varepsilon)\int_{C_m} dy_m\int d\mathbf{x}'_m\left[+\frac{\hbar^2}{2M}(\overleftrightarrow{\mathbf{D}}')^2-U(\mathbf{x}'_m)+\varepsilon\right]G_\varepsilon^{\pm}(\mathbf{x}'_m,\mathbf{x}_m)(\overleftrightarrow{\mathbf{D}}\cdot\hat{\mathbf{x}}_m)\Delta G_\varepsilon(\mathbf{x}_m,\mathbf{x}'_m)\ . \tag{C3}$$

Performing the integral over dy_m first, we see that all terms contain either

$$\int_{C_m} dy_m\, G_\varepsilon^+(\overleftrightarrow{\mathbf{D}}\cdot\hat{\mathbf{x}}_m)G_\varepsilon^+$$

or

$$\int_{C_m} dy_m\, G_\varepsilon^-(\overleftrightarrow{\mathbf{D}}\cdot\hat{\mathbf{x}}_m)G_\varepsilon^-\ .$$

Arguments very similar to those in Sec. IV [Eqs. (68)–(72)] show that both of these integrals go to zero as $x_m\to\infty$; we thus conclude that $I_m^{(0)}\to 0$ as $x_m\to\infty$. The fact that the divergence of the current density is zero implies that the current in each lead is constant; hence, $I_m^{(0)}=0$. Furthermore, the current through any cross section, C^*, of the structure is zero, since current conservation implies that the net current into the volume formed by C^* and the lead cross sections is zero, while we have just shown that the current in the leads is zero. This result is expected, of course, and confirms that while there can be circulating current in equilibrium ($G_\varepsilon^+G_\varepsilon^+$ or $G_\varepsilon^-G_\varepsilon^-$ terms), there can be no transport current ($G_\varepsilon^+G_\varepsilon^-$ or $G_\varepsilon^-G_\varepsilon^+$ terms).

APPENDIX D: THE BOUNDARY VALUE OF THE CURRENT OPERATOR AS $x\to\infty$

In rewriting the current density so that the $\Omega\to 0$ limit can be taken, we used the identity

$$\lim_{x_n\to\infty}\left[\frac{f_{\beta\alpha}}{\varepsilon_{\beta\alpha}}\int_{C_n} dy_n\,\mathbf{W}_{\alpha\beta}(\mathbf{x}_n)\cdot\hat{\mathbf{x}}_n\right]=0\ . \tag{D1}$$

We show that this is true in the sense of distributions by considering the integral over state index β with a smooth function $F(\beta)$,

$$Q\equiv\int d\beta\, F(\beta)\frac{f_{\beta\alpha}}{\varepsilon_{\beta\alpha}}\int_{C_n} dy_n\,\psi_\alpha^*(\mathbf{x}_n)(\overleftrightarrow{\mathbf{D}}\cdot\hat{\mathbf{x}}_n)\psi_\beta(\mathbf{x}_n)\ , \tag{D2}$$

where we have used the definition of **W**. Notice that the integral over β commutes with the integral over C_n and that $f_{\beta\alpha}/\varepsilon_{\beta\alpha}$ is a smooth function of β, so that we are led to study simply the integral of $\psi_\beta(\mathbf{x})$ times an arbitrary smooth function of β. In order to analyze the integral, it is convenient to choose the eigenstates to be the scattering-wave states defined in Eq. (79). Because the asymptotic form of the scattering-wave states is known, we can express an integral over these states explicitly in terms of an integral over k or energy,

$$\int d\beta=\sum_{m=1}^{N_L}\sum_{a=1}^{\infty}\int_0^\infty\frac{dk_a}{2\pi}g(\varepsilon_a-\varepsilon_a^{(0)})\Theta(\varepsilon_a-\varepsilon_a^{(0)})\ , \tag{D3}$$

where m labels the leads, a labels the incoming channels in that lead, $g(\varepsilon)$ is the one-dimensional density of states, $\varepsilon_a^{(0)}$ is the threshold energy for mode a, and $\varepsilon_a=\hbar^2k_a^2/2M$. Using Eq. (D3), as well as the asymptotic form of the scattering waves, we find that our integral over β is

$$\begin{aligned}\int d\beta\, G(\beta)\psi_\beta(\mathbf{x}_n)&=\sum_{m=1}^{N_L}\sum_{a=1}^{\infty}\int_0^\infty\frac{dk_a}{2\pi}\tilde{G}(m,a,k_a)\psi^+_{m,a,k_a}(\mathbf{x}_n)\\&=\sum_{m=1}^{N_L}\sum_{a=1}^{\infty}\int_{-\infty}^\infty\frac{dk_a}{2\pi}\tilde{G}(m,a,k_a)\Theta(k_a)\psi^+_{m,a,k_a}(\mathbf{x}_n)\\&\to\sum_{m=1}^{N_L}\sum_{a=1}^{\infty}\int_{-\infty}^\infty\frac{dk_a}{2\pi}\tilde{G}(m,a,k_a)\Theta(k_a)[r^{(1)}_{m,a,k_a}(y_n)e^{+ik_ax_n}+r^{(2)}_{m,a,k_a}(y_n)e^{-ik_ax_n}]\ \text{ as } x_n\to\infty\ ,\end{aligned} \tag{D4}$$

where the functions $r^{(i)}$ involve transmission coefficients and the transverse wave functions. The integral over k_a is simply the Fourier transform of $\tilde{G}\Theta(k_a)r^{(i)}$. Since the worst possible singularity in this product is the discontinuity caused by the Θ function, this Fourier transform decays to zero as $x_n \to \infty$. Thus, we conclude that

$$\int d\beta\, G(\beta)\psi_\beta(\mathbf{x}_n) \to 0 \quad \text{as } x_n \to \infty \tag{D5}$$

for any smooth function G. From this we conclude that $Q \to 0$ as $x_n \to \infty$ [Q defined in Eq. (D2)], and hence that Eq. (D1) is valid in the sense of distributions.

APPENDIX E: CHOOSING A LANDAU GAUGE IN EACH LEAD

In order to apply the results for the quantum mechanics of a perfect lead given in Sec. III to our multiprobe structures, it is necessary to show that one can choose a gauge which is Landau-like in the ordered part of each lead. We have already introduced a coordinate system in each perfect lead, $\hat{\mathbf{x}}_n$ and $\hat{\mathbf{y}}_n$, in connection with the linear response calculation in Sec. I (also see Fig. 2). We start by considering the Landau gauge in the coordinate system in lead 1,

$$\mathbf{A}_1(\mathbf{x}_1) = B_n y_1 \hat{\mathbf{x}}_1, \quad \mathbf{x}_1 \text{ in lead } n \ . \tag{E1}$$

To express $\mathbf{A}$ in the Landau gauge appropriate to lead n which makes an angle θ_n with lead 1, one needs to apply a gauge transformation,

$$\mathbf{A}_n(\mathbf{x}_1) = \mathbf{A}_1(\mathbf{x}_1) + \nabla f_n(\mathbf{x}_1) \ , \tag{E2}$$

with f_n given by

$$f_n(\mathbf{x}_1) = -B_n x_1 y_1 \sin^2\theta_n + \tfrac{1}{4} B_n (y_1^2 - x_1^2)\sin(2\theta_n) \ . \tag{E3}$$

A straightforward computation using $x_1 = x_n\cos\theta_n - y_n\sin\theta_n$ and $y_1 = x_1\sin\theta_n + y_n\cos\theta_n$ shows that $\mathbf{A}_n(\mathbf{x}_n) = B_n y_n \hat{\mathbf{x}}_n$ in lead n.

In a multilead structure, one wants to apply the transformation (E3) so that it only affects lead n. Therefore, define a generalized smooth step function $\zeta_n(\mathbf{x})$ by

$$\zeta_n(\mathbf{x}) = \begin{cases} 1, & \mathbf{x} \text{ in ordered part of lead } n \ , \\ 0, & \mathbf{x} \text{ in lead } m \neq n \ , \\ \text{smooth interpolation for } \mathbf{x}, & \text{elsewhere} \ . \end{cases} \tag{E4}$$

Now the function $\zeta_n(\mathbf{x}_1)f_n(\mathbf{x}_1)$ generates a gauge transformation which turns the vector potential only in lead n. Clearly, then, by applying the gauge transformation generated by

$$f(\mathbf{x}_1) = \sum_{n=2}^{N_L} \zeta_n(\mathbf{x}_1) f_n(\mathbf{x}_1) \tag{E5}$$

to the starting gauge in Eq. (E1), one arrives at a gauge which is Landau-like in the ordered part of each lead, allowing one to use the results for the quantum mechanics of a perfect lead as in Sec. III.

APPENDIX F: SPATIAL DERIVATIVES OF $G_\varepsilon^+ G_\varepsilon^+$ TERMS

In Sec. III we showed that the contribution of the $G_\varepsilon^+ G_\varepsilon^+$ and $G_\varepsilon^- G_\varepsilon^-$ terms in $\underline{\sigma}$ [Eq. (52)] to the conductance coefficients g_{mn} is zero as x_m and x_n' tend to infinity for $m \neq n$, Eq. (72). However, in any practical calculation the conductance coefficients must be evaluated at finite x_m and x_n'. In this appendix we show that the spatial derivatives of the $G_\varepsilon^+ G_\varepsilon^+$ and $G_\varepsilon^- G_\varepsilon^-$ terms are zero, so that these terms must be zero for all x_m and x_n'. To be specific, we will work with $S(x_m, x_n')$ defined in Eq. (53); in analyzing $S(x_m, x_n')$, it is convenient to start by analyzing a term without the energy derivative, which we denote $R(x_m, x_n')$,

$$R(x_m, x_n') \equiv \int_{C_m} dy_m \int_{C_n} dy_n'\, G_\varepsilon^+(\mathbf{x}_m, \mathbf{x}_n') \times (\overleftrightarrow{\mathbf{D}}^* \cdot \hat{\mathbf{x}}_m)(\overleftrightarrow{\mathbf{D}}' \cdot \hat{\mathbf{x}}_n) G_\varepsilon^+(\mathbf{x}_n', \mathbf{x}_m) \ . \tag{F1}$$

The asymptotic analysis presented in the text [as in arriving at Eq. (68)] implies that, for $m \neq n$ as $x_m, x_n' \to \infty$,

$$R(x_m, x_n') \to \sum_{a,b,c,d}^{(\varepsilon)} \int_{C_m} dy_m \int_{C_n} dy_n'\, f_{ac}^\varepsilon \xi_a^+(\mathbf{x}_m) \xi_c^{-*}(\mathbf{x}_n') (\overleftrightarrow{\mathbf{D}}^* \cdot \hat{\mathbf{x}}_m)(\overleftrightarrow{\mathbf{D}}' \cdot \hat{\mathbf{x}}_n) f_{bd}^\varepsilon \xi_b^+(\mathbf{x}_n') \xi_d^{-*}(\mathbf{x}_m) \ . \tag{F2}$$

Using Eqs. (70) and (71), we conclude that $R(x_m, x_a')$, like $S(x_m, x_n')$, vanishes asymptotically,

$$R(x_m, x_n') \to 0 \ . \tag{F3}$$

Some simplifying notation,

$$D_x = (\mathbf{D} \cdot \hat{\mathbf{x}}_m) \ ,$$

$$G = G_\varepsilon^+(\mathbf{x}_m, \mathbf{x}_n'), \quad \bar{G} \equiv G_\varepsilon^+(\mathbf{x}_n', \mathbf{x}_m) \ ,$$

$$\frac{\partial}{\partial x_m} = D_x + \frac{ie}{\hbar c} A_x \ ,$$

allows one to write the derivative of R in the compact form

$$\frac{\partial}{\partial x_m} R(x_m, x_n') = \int_{C_m} dy_m \int_{C_n} dy_n' (G D_x^{*2} - D_x^2 G)(\overleftrightarrow{\mathbf{D}}' \cdot \hat{\mathbf{x}}_n)\bar{G} \ . \tag{F4}$$

Using the equation of motion for the Green function *when* $m \neq n$,

$$\left[\varepsilon + \frac{\hbar^2}{2M}(D_x^2 + D_y^2) - U(x,y)\right] G_\varepsilon^+(\mathbf{x}_m, \mathbf{x}_n') = 0 \ , \tag{F5}$$

we replace the x derivatives in Eq. (F4) with y derivatives

$$\frac{\partial}{\partial x_m} R(x_m,x_n') = \int_{C_n} dy_m \int_{C_n} dy_n' (-GD_y^{*2} + D_y^2 G)(\vec{\mathbf{D}}' \cdot \hat{\mathbf{x}}_n)\bar{G} \ , \tag{F6}$$

where the explicit dependence on ε or $U(x,y)$ has canceled out between the two terms. Because the Green function vanishes at the ends of the curve C_m, integrating the D_y^* term by parts twice exactly cancels the D_y term; hence,

$$\frac{\partial}{\partial x_m} R(x_m,x_n') = 0 \ . \tag{F7}$$

A similar argument shows that the derivative of R with respect to x_n' is also zero. Using the asymptotic behavior (F3), we conclude that R is zero,

$$\int_{C_m} dy_m \int_{C_n} dy_n' \, G_\varepsilon^+(\mathbf{x}_m,\mathbf{x}_n') \times (\vec{\mathbf{D}}^* \cdot \hat{\mathbf{x}}_m)(\vec{\mathbf{D}}' \cdot \hat{\mathbf{x}}_n) G_\varepsilon^+(\mathbf{x}_n',\mathbf{x}_m) = 0, \quad m \neq n \ . \tag{F8}$$

Turning now to the term with the energy derivative, $S(x_m,x_n')$ defined in Eq. (53), we write out the energy derivative as a limit and find

$$\frac{\partial}{\partial x_m} S(x_m,x_n') = \lim_{\Delta \to 0} \left[\frac{\partial}{\partial x_m} \int_{C_m} dy_m \int_{C_n} dy_n' \frac{G_{\varepsilon+\Delta} - G_\varepsilon}{\Delta} (\vec{\mathbf{D}}^* \cdot \hat{\mathbf{x}}_m)(\vec{\mathbf{D}}' \cdot \hat{\mathbf{x}}_n) \bar{G}_\varepsilon \right] . \tag{F9}$$

Using the previous result for $R(x_m,x_n')$, this immediately simplifies to

$$\frac{\partial}{\partial x_m} S(x_m,x_n') = \lim_{\Delta \to 0} \left[\frac{1}{\Delta} \frac{\partial}{\partial x_m} \int_{C_m} dy_m \int_{C_n} dy_n' \, G_{\varepsilon+\Delta} (\vec{\mathbf{D}}^* \cdot \hat{\mathbf{x}}_m)(\vec{\mathbf{D}}' \cdot \hat{\mathbf{x}}_n) \bar{G}_\varepsilon \right], \quad m \neq n \ . \tag{F10}$$

Treating ∂/∂_m as before, we note that now the energies in the equations for the two Green functions $G_{\varepsilon+\Delta}$ and $\bar{G}$ do not cancel, and in contrast to the null result obtained above we are left with

$$\frac{\partial}{\partial x_m} S(x_m,x_n') = \lim_{\Delta \to 0} \left[\frac{1}{\Delta} \int_{C_m} dy_m \int_{C_n} dy_n' \, \Delta [G_{\varepsilon+\Delta} (\vec{\mathbf{D}}' \cdot \hat{\mathbf{x}}_n) \bar{G}_\varepsilon] \right] = \int_{C_m} dy_m \int_{C_n} dy_n' \, G_\varepsilon (\vec{\mathbf{D}}' \cdot \hat{\mathbf{x}}_n) \bar{G}_\varepsilon \ . \tag{F11}$$

Using the asymptotic behavior of G_ε and $\bar{G}_\varepsilon$ as $x_n' \to \infty$, Eqs. (64) and (65), and the current-conservation identity (63), we conclude by an argument similar to that in the text that

$$\frac{\partial}{\partial x_m} S(x_m,x_n') \to 0 \ \text{ as } x_n' \to \infty \ \text{ for any } x_m \quad (m \neq n) \ . \tag{F12}$$

We are thus led to study the second derivative of S with respect to x_m and x_n',

$$\frac{\partial^2}{\partial x_n' \partial x_m} S(x_m,x_n') = \frac{\partial}{\partial x_n'} \int_{C_m} dy_m \int_{C_n} dy_n' G_\varepsilon (\vec{\mathbf{D}}' \cdot \hat{\mathbf{x}}_n) \bar{G}_\varepsilon \ , \quad m \neq n \ . \tag{F13}$$

Proceeding in exactly the same way with $\partial/\partial x_n'$ as with $\partial/\partial x_m$, we find that

$$\frac{\partial^2}{\partial x_n' \partial x_m} S(x_m,x_n') = 0, \quad m \neq n \ . \tag{F14}$$

From this equation combined with the asymptotic behavior in Eq. (F12), we conclude that $(\partial/\partial x_m) S(x_m,x_n') = 0$. A similar argument shows that the derivative with respect to x_n' is zero. Combining these results with the asymptotic behavior of S [Eq. (72)], we arrive at the conclusion that S itself is equal to zero for $m \neq n$, Eq. (74).

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[59]The diamagnetic response of mesoscopic systems is discussed in, e.g., A. G. Aronov, A. Yu. Zyuzin, and B. Z. Spivak, Pis'ma Zk. Eksp. Teor. Fiz. **43**, 431 (1986) [JETP Lett. **43**, 555 (1986)]; C. L. Kane, R. A. Serota, and P. A. Lee, in Ref. 55; N. Trivedi and D. A. Browne, Phys. Rev. B **38**, 9581 (1988); O. D. Cheishvilli, Pis'ma Zh. Eksp. Teor. Fiz. **48**, 206

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[60]Working with an applied vector potential, the authors of Ref. 44 expressed the reactive response in a form which does not obviously vanish as $\omega \rightarrow 0$. In fact, one can use the identity (23) to show that the expression for the reactive response in Ref. 44 is zero [A. Szafer (private communication)].

[61]C. L. Kane, R. A. Serota, and P. A. Lee, in Ref. 55.

[62]A. Messiah, *Quantum Mechanics* (Wiley, New York, 1958), pp. 825–828.

[63]When calculating higher moments of the conductivity as was done by Lee and Stone (Ref. 10) and by Al'tshuler and Shklovskii (reference given below) using the symmetrical formulation of the Kubo tensor, one is led to consider diagrams arising from the G^+G^+ terms, such as the three- and four-diffuson diagrams evaluated in Ref. 10, and, in fact, one finds that such diagrams are not identically zero. Al'tshuler and Shklovskii argued that such diagrams may be neglected and a more detailed proof of this was given by Kane *et al.* (Ref. 55), who showed that the sum of all such contributions must vanish to leading order in $(k_F l)^{-1}$ in the weak-disorder limit. Our result shows that such terms vanish for each impurity configuration, independent of the degree of disorder; hence such diagrams must cancel to all orders. The fundamental origin of this exact cancellation is the identity (63), which implies that the asymptotic behavior of terms of the form G^+G^+ or G^-G^- does not allow them to carry net current into or out of the system. The numerical value for the two-probe conductance fluctuations quoted in Ref. 10 and by Al'tshuler and Shklowskii agree and are correct; however, the three- and four-diffuson diagrams evaluated in Ref. 10 could have been omitted. The exact cancellation of such contributions also simplifies the calculation of higher moments of the conductance (B. L. Al'tshuler and B. I. Shklovskii, Zh. Eksp. Teor. Fiz. **91**, 220 (1986) [Sov. Phys.—JETP **64**, 127 (1986)]).

[64]Appendix A of Ref. 44 noted that to define the orthogonality relations for these states one had to consider states with differing energies as well as the different channels which propagate at the same energy. It was then shown that if one attempted to normalize the states so that the orthogonality relations were of the form $\langle \psi^+_{\varepsilon,n,a} | \psi^+_{\varepsilon',n',a'} \rangle = \delta(\varepsilon - \varepsilon')\delta_{na,n'a'}$, then the unitarity of the S matrix contradicted this assumed orthogonality. Recently, it has been pointed out that if one assumes an orthogonality relation of the form $\langle \psi^+_{\varepsilon,n,a} | \psi^+_{\varepsilon',n',a'} \rangle = \delta(k_{an} - k_{a'n'})\delta_{na,n'a'}$, no such contradiction ensues [A. Kriman (private communication)]. An explicit proof of the orthogonality of the scattering states, assuming this normalization, has subsequently been constructed [A. Kriman, A. Szafer, and A. D. Stone (unpublished)].

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