Twisted boundary conditions and transport in disordered systems

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Condensed matter systems are usually characterized by their response to external fields. The Kubo linear response theory is the standard theoretical tool used to analyze it. In order to obtain transport quantities with this method, we generally need to know both the eigenvalues and the eigenfunctions. This article discusses another methodological approach which in some cases allows one to obtain some characteristics of the dc dissipative transport from the response to a gauge field in a multiply connected geometry. This avoids the need of the eigenstates to characterize the transport properties which are directly read off the behavior of the energy spectrum. This method is applied to the problem of transport in metals and Anderson insulators. © *1997 American Institute of Physics.* [S0022-2488(97)01304-2]

I. INTRODUCTION

Among the various ways to characterize the state of matter, the response to an external electric field constitutes one of the major probes. It might be either the dc or the ac responses measuring the dissipative or reactive parts, the optical spectrum, etc.

The basic formalism used in order to express these transport coefficients is the Kubo linear response theory. It involves the knowledge of the expectation value of a current–current correlation function. This means that already in the simplest cases (e.g., a gas of noninteracting electrons moving in a random potential) we need to know both the energy spectrum and the eigenfunctions. The latter are difficult to evaluate, where in some cases, for instance, a semi-classical approximation can be used.

This methodological problem inherent to the Kubo linear response theory can be avoided in certain cases which shall be discussed further by considering the same system closed on itself and submitted to twisted boundary conditions. Then, the usual sum rules involving off-diagonal matrix elements (e.g., the Thomas–Reiche–Kuhn sum rule) have to be generalized and it is possible to express Kubo correlation functions in terms of the sensitivity of the energy levels to an applied gauge field.

A. Equivalence between an Aharonov–Bohm flux and a twist of the boundary conditions

To set up the problem, we consider the example of one electron of mass M moving on a ring of length L and radius R. The Hamiltonian is $H(0)=(p^2/2M)+V$ and $V(x)$ is a potential which might, for instance, describe the effect of disorder. To obtain the energy spectrum, we must impose boundary conditions. Single valuedness of the wave functions $\psi(x)$ requires $\psi(x+L)=\psi(x)$. Twisted boundary conditions (TBC) are defined through the generalization $\psi(x+L)=e^{i\phi}\psi(x)$, where ϕ is a real parameter. It is possible to get rid of the phase factor by a suitable gauge transformation. This modifies the Hamiltonian $H(0)$ into:

$$H(\phi)=\frac{1}{2M}\left(p+\frac{\hbar\phi}{L}\right)^2+V(x). \tag{1}$$

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$H(\phi)$ describes the motion of an electron on a ring pierced by an Aharonov–Bohm (AB) magnetic flux Φ defined by the vector potential $A_\theta = \Phi/L$ and the physical nature of the twist parameter ϕ is given in that case by $\phi = \Phi/\Phi_0 \equiv (e/h)\,\Phi$. The eigenenergies E_n of the twisted Hamiltonian in Eq. (1) do depend on ϕ and their curvature at $\phi = 0$ is given by the (nonperturbative) expression:

$$\left.\frac{\partial^2 E_n}{\partial \phi^2}\right|_{\phi=0} = \frac{\hbar^2}{2ML^2}\left(1 + \frac{2}{M}\sum_{l\neq n}\frac{|\langle l|p_x|n\rangle|^2}{e_n - e_l}\right), \tag{2}$$

where $(|n\rangle, e_n)$ describe the eigenstates of $H(0)$.

B. The f-sum rule

The combination on the rhs of Eq. (2) does appear in another context, namely, the Thomas–Reiche–Kuhn sum rule (or f-sum rule).[1] It might be useful to rederive it here. Consider the Hamiltonian $H(0)$ on the real line (the 3d generalization is straightforward), and the eigenbasis $(|n\rangle, e_n)$. Using the commutator $[x, H_0] = (i\hbar/M)\,p_x$, we may write $i\hbar/M\,\langle n|p_x|l\rangle = (e_l - e_n) \times \langle n|x|l\rangle$ so that:

$$\sum_{l\neq n}\frac{|\langle l|p_x|n\rangle|^2}{e_n - e_l} = \frac{M}{2i\hbar}\sum_{l\neq n}\left[\langle l|p_x|n\rangle\langle n|x|l\rangle - \langle l|x|n\rangle\langle n|p_x|l\rangle\right]. \tag{3}$$

We can extend the sum on the rhs to all states $|n\rangle$ since $\langle n|p_x|n\rangle = 0$ in the absence of applied magnetic field (time reversal invariance). Then,

$$\frac{2}{M}\sum_{l\neq n}\frac{|\langle l|p_x|n\rangle|^2}{e_n - e_l} = \frac{1}{i\hbar}\langle l|[p_x, x]|l\rangle = -1 \tag{4}$$

(for suitably normalized eigenstates). Equation (4) is the formulation of the f-sum rule, and the $f_{ln} \equiv (2/M)[|\langle l|p_x|n\rangle|^2/(e_n - e_l)]$ are the oscillator strengths.[1] The puzzling result is the following. The proof of the f-sum rule relies only on the commutation relation $[p_x, x] = -i\hbar$. We could therefore expect that it will work as well for the TBC case so that the curvature $\partial^2 E_n/\partial\phi^2|_{\phi=0} = 0$ for any state. However, in the multiply connected geometry considered for TBC, the position operator x is not single valued and therefore is not admissible so that the usual proof of the f-sum rule cannot be used. This point is crucial and will be at the heart of the subsequent discussion. Roughly speaking, it might be formulated in the following way using the language of metals and insulators. A metallic system is characterized by *delocalized states* such that the f-sum rule is not fulfilled in the multiply connected geometry and therefore the twist curvature is nonzero. On the other hand, an insulator is characterized by (exponentially) *localized states* such that it is always possible to build (even for multiply connected geometries) an effective position operator. The f-sum rule is then fulfilled and the curvature is zero (up to exponentially small corrections with the system size).[2] Therefore, the behavior of the appropriate curvature is the hallmark characterizing localized or extended states. The remainder of this article is a declination of this theme for the physical situation of the Anderson metal–insulator transition where the curvature is related to the dc residual electrical conductance.[3]

II. TRANSPORT IN DISORDERED METALS: THE THOULESS CURVATURE

A. The Kubo linear response theory

Consider a d-dimensional gas of volume L^d of noninteracting electrons moving in a random potential $V(r)$ in the absence of magnetic field. The (one particle) Hamiltonian is $H(0)$. According to Kubo, the expression of the residual (T=0), dc conductivity Re $\sigma_{ii}(\omega=0,T=0)\equiv\sigma$ is given by the trace

$$\sigma=\frac{e^2\hbar}{\pi M^2 L^d}\mathrm{Tr}(\Im G_0{}^+(E_f)p_i\Im G_0{}^+(E_f)p_i), \tag{5}$$

where p_i is the momentum along the i-direction and $\Im G_0{}^+(E)$ is the imaginary part of the resolvent operator $G_0{}^+(E)=[1/E-H(0)+i\eta]\,(\eta\to 0^+)$ associated with $H(0)$. The relation between the conductance G_d and the conductivity is $G_d=\sigma L^{d-2}$. Due to the impurity potential $V(r)$, both G_d and σ are random variables. A large part of the activity in the field of Mesoscopic Quantum Physics during the last years has been devoted to the calculation of the various moments of σ mainly in the weakly disordered (metallic) regime but also for Anderson insulators.[4] The average conductivity $\langle\sigma\rangle$ for weakly disordered metals is calculated to low orders in the small parameter $1/k_f l$, where l is the *elastic* mean free path and k_f the Fermi wave vector. The zeroth order (including the so called diffusion modes) gives the Drude expression: $\langle\sigma\rangle=ne^2\tau/M$. To that order the average conductance $\langle G_d\rangle$ can be formally expressed (in units of e^2/h) as the ratio of two characteristic energies as $\langle G_d\rangle=(e^2/h)(E_c/\Delta)$, where $E_c\equiv\hbar D/L^2$ is referred to the Thouless energy and $\Delta\equiv 1/L^d\rho(E_f)$ is the mean level spacing . The diffusion constant D is related to $\langle\sigma\rangle$ by the Einstein relation $\langle\sigma\rangle=e^2D\rho(E_f)$ and $\rho(E_f)$ is the density of states at the Fermi energy. This formal way of writing $\langle G_d\rangle$ corresponds to the standard physical picture of block scaling[5] and diffusion motion (random walk) of the electronic wavepackets. The next order in $1/k_f l$ leads to the weak localization corrections (cooperon diagrams) which are at the basis of the scaling theory of localization.[6]

B. The Thouless curvature

The Kubo formula [Eq. (5)] for the conductivity requires the knowledge of the eigenfunctions of the Hamiltonian $H(0)$. To see it, rewrite σ under the form:

$$\sigma=\frac{\pi e^2\hbar}{M^2L^d}\sum_{n,m}|\langle n|p_i|m\rangle|^2\delta(E_f-\epsilon_n)\,\delta(E_f-\epsilon_m). \tag{6}$$

Since we shall be interested in the behavior of finite size systems, it is worth mentioning under which conditions Eq. (6) is derived. We consider a finite size system in a box with a discrete energy spectrum. The applied constant electric field is described by a harmonic vector potential in the limit $\omega\to 0$. A finite conductivity is the result of transitions induced by the (ω-dependent) electric field between levels separated by $\hbar\omega$, so that keeping the system finite and taking the limit $\omega\to 0$, the conductivity vanishes. In order to obtain a finite response, two methods are usually considered. One is to take the thermodynamic limit first (for finite ω) so that the spectrum becomes continuous. Then, the limit $\omega\to 0$ gives a finite conductivity. The other method, usually considered for finite size mesoscopic systems consists of assuming the existence of a weak coupling between the system and external reservoirs through leads and contacts. This coupling is described phenomenologically by an energy γ over which the energy levels are spread out such that $\hbar\omega\gg\gamma\gg\Delta$ in order for the transitions between the levels to be induced by the electric field only and not by the coupling to the leads. Finally, we consider the limits $\gamma\to 0$ and then $\omega\to 0$. Both methods are equivalent and represent nothing more than a way to regularize the sum in Eq. (6). Keeping this in mind, and taking the limits as prescribed above we obtain:

$$\sigma = \frac{\pi e^2 \hbar}{M^2} L^d \rho^2(E_f) |\langle n(E_f)|p_i|m(E_f)\rangle|^2, \tag{7}$$

where the matrix element is between off-diagonal states (diagonal ones are zero) with the same energy E_f. This requires a degenerate Fermi surface and the knowledge of the eigenfunctions at the Fermi energy.

Consider now twisting the boundary conditions of the system along, say, the x direction, leaving the boundary conditions unchanged in the other directions. The curvature of the energy levels is given by Eq. (2). Let us now see how this curvature might be related to the conductivity σ. The main steps of the original derivation of Edwards and Thouless[7] are the following. Define the dimensionless quantity $g_T = (1/\Delta)(\partial^2 E_n/\partial\phi^2)|_{\phi=0}$, where the energy E_n is the closest to the Fermi energy. Due to the disordered potential, g_T is a random variable. We assume the matrix elements of the momentum to be uncorrelated with the energies. This, as we shall see, is correct within the Random Matrix Theory (RMT) description of weakly disordered metals. Replacing the squared matrix element by its average over the disorder, we obtain:

$$g_T = \frac{\hbar^2}{2ML^2\Delta}\left[1 + \frac{2}{M}\langle |p_x|^2\rangle \sum_{m\neq n} \frac{1}{\epsilon_n - \epsilon_m}\right]. \tag{8}$$

Then, we assume for the average conductivity the Drude expression and using $\tau = (M/\hbar k_f)^2 D$ gives $\langle |p_x|^2\rangle = M\Delta k_f l$. From Eq. (8) we obtain

$$g_T = \frac{\hbar^2}{2ML^2\Delta}\left[1 + 2\Delta k_f l \sum_{m\neq n} \frac{1}{\epsilon_n - \epsilon_m}\right].$$

The remaining random sum is zero on average. It is likely to be dominated by the smallest denominator, i.e., typically of the order of the inverse mean level spacing Δ. Assuming the energy levels to be uncorrelated (which is incorrect for weakly disordered metals) , the sum in Eq. (8) has a Cauchy distribution with a width π/Δ, and $g_T = (\hbar^2/2ML^2\Delta)[1 + 2\pi k_f l]$. For weakly disordered metals, $k_f l \gg 1$, so that $(\hbar^2/ML^2\Delta)\,\pi k_f l = \pi(E_c/\Delta)$. Therefore, the typical curvature g_T is (in units of e^2/h) the Drude average conductance obtained from the Kubo formula.

This derivation is based on assumptions which are not well justified or even incorrect. I would like to present a slightly different argumentation independent of some of the previous assumptions. First, I define the Thouless curvature g_T by the quantity

$$g_T = \frac{1}{2}\frac{\partial^2}{\partial\phi^2} N(E_f, \phi)|_{\phi=0}, \tag{9}$$

where $N(E_f, \phi)$ is the density of states integrated up to the Fermi energy. This has the advantage of defining the curvature as a trace. Using

$$N(E_f, \phi) = \int \frac{1}{\pi} d\epsilon f(\epsilon) \Im \text{ Tr } G^+(\epsilon, \phi) \ ,$$

where $f(\epsilon)$ is the Fermi–Dirac distribution and $G^+(\epsilon, \phi)$ the resolvent operator, we obtain:

$$g_T = \frac{1}{\pi}\frac{\hbar^2}{2ML^2}\int d\epsilon f(\epsilon) \Im \text{ Tr}\left[(G^+(\epsilon,0))^2 + \frac{2}{M} G^+(\epsilon,0) p_x G^+(\epsilon,0) p_x G^+(\epsilon,0)\right]$$

$$= -\frac{1}{\pi}\frac{\hbar^2}{2ML^2}\int d\epsilon f(\epsilon)\frac{\partial}{\partial\epsilon} \Im \text{ Tr}\left[G^+(\epsilon,0) + \frac{1}{M} G^+(\epsilon,0) p_x G^+(\epsilon,0) p_x\right]$$

which after an integration by parts gives

$$g_T = -\sum_n \delta(\epsilon_n - E_f)\frac{\partial^2 \epsilon_n}{\partial \phi^2}\bigg|_{\phi=0}. \tag{10}$$

I shall take g_T given by Eq. (9) as an operational definition of the Thouless curvature. It is already clear from that definition that g_T cannot be reduced to the Kubo expression [Eq. (5)] for the conductivity; they are different quantities. For instance, unlike the conductivity σ, the average of the curvature g_T over disorder is zero. To see it, let us rewrite g_T using Eq. (2). Then,

$$\langle g_T \rangle = \frac{\hbar^2}{2ML^2}(-\rho(E_f) + \langle I \rangle),$$

where

$$\langle I \rangle \equiv \frac{1}{M}\int \frac{1}{\pi} d\epsilon f'(\epsilon) \mathrm{Im} \sum_{p_1,p_2} p_1 \cdot p_2 \left\langle \frac{\partial}{\partial \epsilon} \langle p_1 | G_0^+(\epsilon) | p_2 \rangle \right\rangle = \frac{1}{M}\frac{\partial}{\partial E_f}\left(\frac{1}{3} p_f^2 \rho(E_f)\right) = +\rho(E_f)$$

and therefore $\langle g_T \rangle = 0$. This result is nothing but a derivation of the compressibility sum rule.[8,9] Nevertheless, g_T contains information about transport properties of the system and in particular as we shall see now, its second moment is proportional to the square of the average (Drude) conductivity. To calculate $\langle g_T^2 \rangle$, consider the quantity $\delta N(E,\phi) \equiv N(E,\phi) - N(E,0)$. Expanding $\delta N(E,\phi)$ up to the fourth order in ϕ gives

$$g_T^2 = \frac{1}{24}\frac{\partial^4}{\partial \phi^4} \delta N^2(E_f,\phi)|_{\phi=0} \tag{11}$$

so that we need to calculate $\langle \delta N^2(E_f,\phi) \rangle$ which describes the fluctuation of the number of levels in a band of width E around the Fermi level. It has been obtained for $\phi = 0$ (Ref. 10) by assuming that the energy spectrum of a weakly disordered system is well described by the RMT.[11] The validity of this assumption for energies $\Delta \ll E \ll E_c$ has been thoroughly discussed in the literature.[4] It corresponds to the physical situation where diffusive electronic wavepackets explore ergodically the whole (finite size) system, i.e., for times $t \gg \tau_D = L^2/D$. In that limit, the spatial dependence of the solutions of the diffusion equation does not contribute to the diffuson and cooperon diagrams so that only the zero mode ($q = 0$) remains. This regime sometimes called zero-dimensional could have been obtained directly by setting $d = 0$ in the solution of the diffusion equation. The RMT assumption is different from those used in the original derivation of the Thouless formula.[7] It takes into account the correlation between the energy levels which leads to the level repulsion characteristic of the Wigner–Dyson distribution. The extension of this calculation to $\phi \neq 0$ gives:

$$\langle \delta N^2(E,\phi) \rangle = \frac{1}{2\pi^2}\left[\ln\left(1 + \left(\frac{E}{\Delta}\right)^2\right) + \ln\left(1 + \frac{E^2}{(\Delta + 4E_c\phi^2)^2}\right)\right]. \tag{12}$$

Together with Eq. (11) it gives $\langle g_T^2 \rangle = (6/\pi^2)(E_c/\Delta)^2$. Using the Drude expression for the average conductance $\langle g \rangle$ we obtain:

$$\frac{e^2}{h}\langle g_T^2 \rangle^{1/2} = \frac{\sqrt{6}}{\pi}\langle g \rangle \tag{13}$$

which establishes the Thouless relation.

III. THE SCATTERING DESCRIPTION OF TRANSPORT

So far, we have seen how to describe the average Drude conductivity from the curvature of the energy levels with respect to a twist of the boundary conditions. This description is limited to the Drude approximation and does not apply, for instance, to higher order corrections leading to weak localization effects and eventually to the Anderson metal–insulator transition. The aim of this section is to derive another expression of the Kubo formula [Eq. (5)], in terms of the response to an AB flux where the thermodynamic limit is taken from the very beginning so that there is no need to consider a frequency dependent electric field.

Consider a large electronic system with a continuous energy spectrum submitted to a time-dependent AB flux of the form $\Phi(t/T)$ where T is some characteristic time scale. For instance, $\Phi(t/T)=-Vt$ describes a constant voltage V and $T=h/eV$ is the Bloch period. This looks very much like the Greenwood[12] description of the dissipative conductance. But the latter applies to finite size systems where the adiabatic theorem can be used to study the motion of the energy levels with $\Phi(t/T)$. Here, this option does not exist since we consider a continuous spectrum. The interaction of electrons with the AB flux is conveniently described using the on-shell scattering matrix $S(E,\Phi)$, for which there is a continuous version of the adiabatic theorem. In a scattering description,[13] there is a characteristic time, the Wigner time delay $t_W(E)$, which tells us about the time required by a wave packet to sweep off the scattering potential. In the limit $T\gg t_W(E)$, an incident wavepacket of energy E interacts essentially with a stationary (time-independent) flux line. Hence, our adiabatic expansion will be in terms of the small parameter $t_W(E)/T$.

The basic setup of the scattering description for the case of an AB flux has been described elsewhere.[14] To be self-contained I shall present the main results. The scattering states $|\Psi_\alpha{}^{\pm}(E)\rangle$ are eigenstates of the total Hamiltonian at energy E; α (assumed to be a discrete variable for the sake of simplicity) describes the scattering channels at that energy and $\pm$ defines ingoing and outgoing states. The S matrix is then defined by $S=\int dE\Sigma_\alpha|\Psi_\alpha{}^{+}(E)\rangle\langle\Psi_\alpha{}^{-}(E)|$. The following relation holds:

$$\delta \ln \mathrm{Det}\, S(E)=-2i\pi\, \mathrm{Tr}_E \delta H, \tag{14}$$

where $S(E)$ is the S matrix restricted to the energy shell E and Tr_E is defined for any operator A by

$$\mathrm{Tr}_E A=\sum_\alpha \langle\Psi_\alpha{}^{+}(E)|A|\Psi_\alpha{}^{+}(E)\rangle. \tag{15}$$

The variation δH of the Hamiltonian is due to a variation of the scattering potential—here the AB flux. Defining the total phase shift $\eta(E)$ by $\ln \mathrm{Det}\, S(E)=2i\eta(E)$ we rewrite Eq. (14) as $\delta\eta(E)=-\pi\, \mathrm{Tr}_E\delta H$.

Bearing in mind these preliminary definitions, we write the Hamiltonian under the form $H(\Phi(t))=H(\Phi(0))+V(t)$ which defines the scattering potential $V(t)$ and with $\Phi(0)=\lim_{T\to\infty}\Phi(t/T)$. We assume that initially the system is in an eigenstate $(|\phi_a\rangle,E_a)$ of the time independent Hamiltonian $H(\Phi(0))$ and we write the state of the system $|\Psi(t)\rangle$ at time t as

$$|\Psi(t)\rangle=|\phi_a\rangle+|\delta\Psi(t)\rangle \tag{16}$$

which defines $|\delta\Psi(t)\rangle$. The Schrödinger equation can now be rewritten

$$|\delta\Psi(t)\rangle=\frac{1}{E_a-H(t)+i\eta}\left[V(t)|\phi_a\rangle-i\hbar\frac{\partial}{\partial t}|\delta\Psi(t)\rangle\right] \tag{17}$$

where $\eta\to 0^+$. For a slowly varying perturbation, we can as a first approximation neglect the second term in the bracket. The validity of this approximation can be checked doing the change of

variable $s=t/T$. Then, the second term appears to be proportional to $1/T$ and is negligible in the adiabatic limit $T\to\infty$. Equation (17) can be solved iteratively and gives to lowest order $|\delta\Psi(t)\rangle_{ad}=G^+(E_a,t)V(t)|\phi_a\rangle$ so that $|\Psi(t)\rangle_{ad}=(1+G^+(E_a,t)V(t))|\phi_a\rangle$ or equivalently:

$$|\Psi(t)\rangle_{ad}=\frac{i\eta}{E_a-H(t)+i\eta}|\phi_a\rangle \tag{18}$$

which according to the Lippman Schwinger equation shows that $|\Psi(t)\rangle_{ad}$ is nothing but a scattering state $|\Psi_a{}^+(E_a,t)\rangle$ at energy E_a of the Hamiltonian $H(\Phi(t))$ where t is taken as a fixed parameter. This defines the adiabatic states as the scattering states due to the potential $V(t)$ with a fixed t.

To obtain the first order correction to the adiabatic approximation, we insert the expression of $|\delta\Psi(t)\rangle_{ad}$ into Eq. (17):

$$|\delta\Psi(t)\rangle_1=G^+(E_a,t)(V(t)|\phi_a\rangle-i\hbar\frac{\partial}{\partial t}|\Psi_a{}^+(E_a,t)\rangle). \tag{19}$$

Since the scattering states are eigenstates of the Hamiltonian $H(\Phi(t))$ with energy E_a, they obey the corresponding Schrödinger equation so that

$$\frac{\partial}{\partial t}|\Psi_\alpha{}^+(E_a,t)\rangle=\mathscr{P}G^+(E_a,t)\dot{H}|\Psi_a{}^+(E_a,t)\rangle, \tag{20}$$

where $\mathscr{P}G^+(E_a,t)=1/[E_a-H(t)]$ and $\dot{H}$ is the time derivative of $H(\Phi(t))$. This gives:

$$|\Psi(t)\rangle_1=(1+2i\hbar G^+(E_a,t)\mathscr{P}G^+(E_a,t)\dot{H})|\Psi_a{}^-(E_a,t)\rangle \tag{21}$$

for the first correction to the adiabatic approximation. It is rather straightforward to check that it is proportional to $1/T$. This describes the energy exchange between the system and the external source, here the potential $V(t)$. It has been considered to study various problems including the calculation of the friction force[15] and of the mobility of heavy impurities in Fermi liquids.[16] Equation (21) is the starting point of our calculation of the Kubo linear response coefficients.

The expectation value of a given operator A can be written

$$\langle A\rangle={}_1\langle\Psi(t)|A|\Psi(t)\rangle_1=\langle\Psi_a{}^+(E_a)|A|\Psi_a{}^+(E_a)\rangle+\sigma_A\dot{\phi}, \tag{22}$$

where the first term is the thermodynamic response associated with A (magnetization, persistent currents...), while the second term deals with the energy exchange within the adiabatic approximation and defines a Kubo response coefficient σ_A. It is a complex number whose real part describes dissipation and the imaginary part is related to the reactive response.

From now on I shall focus on the electrical dissipative conductance. This approach has been extended to the case where there is, in addition, a uniform magnetic field in order to obtain the Hall conductance within this formalism.[17] The dissipative conductance corresponds to the particular case where the operator A is the total current I flowing in the system and where $\Phi(t/T)$ is a time dependent AB magnetic flux. Therefore, $\langle I\rangle=-\langle\partial H/\partial\Phi\rangle$ and Φ is $\Phi(0)=\lim_{T\to\infty}\Phi(t/T)$. To lowest order in $1/T$, we obtain from (21) and (22):

$$G_a=-\frac{e^2}{\pi\hbar}\Im\left\langle\Psi_a{}^+(E_a)\left|\frac{\partial H}{\partial\phi}(G^+(E_a))^2\frac{\partial H}{\partial\phi}\right|\Psi_a{}^+(E_a)\right\rangle, \tag{23}$$

where $\phi \equiv (e/h)\,\Phi(0)$ and the scattering states are obtained in the limit $T \to \infty$. To obtain the dissipative conductance G_d, we have to sum over the filled states with the Fermi–Dirac distribution $f(E)$. It gives $G_d = \int dE f(E) \Sigma_a \delta(E - E_a) G_a$. Using $\delta(E - E_a) = 1/\pi \langle \Psi_a{}^+(E_a) | \Im G^+(E) | \Psi_a{}^+(E_a) \rangle$, we obtain:

$$G_d = -\frac{e^2}{\pi h} \int dE f(E) \mathrm{Tr}_E \left(\Im G^+(E) \frac{\partial H}{\partial \phi} \Im (G^+(E))^2 \frac{\partial H}{\partial \phi} \right). \tag{24}$$

Using the cyclicity of the trace, the identity $(G^+(E))^2 = -(\partial/\partial E)\, G^+(E)$ and performing an integration by parts, we obtain at $T = 0$, where $\partial f(E)/\partial E = -\delta(E - E_f)$

$$G_d = \frac{e^2}{\pi h}\, \mathrm{Tr}_{E_f} \left(\Im G^+(E_f) \frac{\partial H}{\partial \phi} \Im G^+(E_f) \frac{\partial H}{\partial \phi} \right) \tag{25}$$

which is the standard Kubo expression for the conductance. Since $\Im G^+(E_f) \propto \delta(E_f - H)$, we obtain, as expected, $G_d \propto \rho^2(E_f)$. To connect Eq. (26) to Eq. (5) for the conductivity, we consider the expression (1) for the Hamiltonian in the presence of an AB flux which corresponds to a given direction, say x, and $\partial H/\partial \phi \,|_{\phi = 0} = (\hbar/ML)\, p_x$. Then,

$$G_d = \frac{e^2 \hbar}{\pi M^2 L^2}\, \mathrm{Tr}_{E_f} (\Im G^+(E_f) p_x \Im G^+(E_f) p_x), \tag{26}$$

which, using $G_d = \sigma L^{d-2}$, gives back Eq. (5).

A. Connection with the scattering phase shift

The total current is given to the lowest (adiabatic) approximation by

$$I_{ad} = \left(\frac{dE}{d\Phi} \right)_{ad} = \int dE_a f(E_a) \left\langle \Psi_a{}^+(E_a) \left| \frac{\partial H}{\partial \Phi} \right| \Psi_a{}^+(E_a) \right\rangle. \tag{27}$$

Using Eq. (14), it is rewritten at $T = 0$:

$$I_{ad}(\Phi(0)) = \frac{e}{\pi h} \int_0^{E_f} dE \frac{\partial}{\partial \phi} \eta(E, \phi(0)). \tag{28}$$

This is the expression of the (thermodynamic) persistent current flowing in the system due to the AB flux line[14] in terms of the total scattering phase shift $\eta(E, \phi(0))$.

The first order correction is obtained by inserting Eq. (21) into the expression of the current:

$$_1\left\langle \Psi(t) \left| \frac{\partial H}{\partial \Phi} \right| \Psi(t) \right\rangle_1 = -\frac{1}{\pi} \frac{\partial}{\partial \Phi} \eta(E_a, \Phi(0)) + \frac{2\hbar}{\pi} \frac{d\Phi}{dt} \frac{\partial}{\partial E_a} \left(\frac{\partial}{\partial \Phi} \eta(E_a, \Phi(0)) \right)^2.$$

Therefore, the total current is given to that approximation by

$$I(\Phi) = I_{ad}(\Phi(0)) + \frac{2\hbar}{\pi} \frac{d\Phi}{dt} \left(\frac{\partial}{\partial \Phi} \eta(E_F, \Phi(0)) \right)^2. \tag{29}$$

From Eq. (22) we identify the dissipative conductance G_d

$$G_d = \frac{1}{\pi^2} \frac{e^2}{h} \left(\frac{\partial}{\partial \phi} \eta(E_f, \phi(0)) \right)^2, \tag{30}$$

which is equivalent to Eq. (26), thus establishing the description of the dissipative transport in terms of the scattering phase shift.

I did consider here the limit of noninteracting electrons, but a formally identical scattering description applies as well to a Fermi liquid.[18]

IV. DISTRIBUTION FUNCTION OF THE CURVATURE; GENERALIZATION OF THE THOULESS RELATION

G_d has been calculated in the limit of an infinite system and in order to compare with our previous results in Section II, we need an equivalent expression for finite size. For a large system, the relation between the variation $\delta E_n(\phi) \equiv E_n(\phi) - E_n(0)$ of the energy levels and the total phase shift $\eta(E,\phi)$ evaluated in a narrow energy window around E_n is[19] $\pi \delta E_n(\phi) = \Delta\, \eta(E,\phi)$, where Δ^{-1} is the density of states near the energy E. This is a consequence of Eq. (14). Then, for a large but finite system, the dissipative conductance can be rewritten:

$$G_d = \frac{e^2}{h} \frac{1}{\Delta^2} \overline{\left(\frac{\partial E_n}{\partial \phi} \right)^2} \Bigg|_{E_n = E_f}, \tag{31}$$

where $\overline{\ldots}$ is an average over ϕ and the energy E_n is close to the Fermi level. Relation (31) is important in two respects. First, it allows one to write the Kubo formula for a finite size system in terms of the behavior of the energy levels as a function of an AB flux. Second, unlike the Thouless curvature [Eq. (9)], it is not restricted to the Drude term. In principle, it could be used as well to evaluate the whole distribution function of the conductance and higher orders in $1/k_f l$ for the average. The first interesting point in comparing these two expressions is that at the Drude level they should already be connected since both of them are different formulations of $\sigma = ne^2\tau/M$. This means that for a given system there is a relation[20] between the typical curvature $\sqrt{\langle g_T^2 \rangle}$ of the energy levels evaluated at $\phi = 0$ and $g_d = (1/\Delta^2)\langle (\partial E_n/\partial \phi)^2 \rangle$, where $G_d \equiv (e^2/h)\, g_d$. Such a relation is not obvious between a local quantity (the curvature) measured at $\phi = 0$ and a global one averaged over the whole energy curves $E_n(\phi)$. The aim of this section is to discuss this connection and its generality.

We consider first the distribution function $P(c)$ of the curvature $c \equiv \partial^2 E_n/\partial \phi^2 \,|_{\phi=0}$. We saw that, assuming the energy levels to be uncorrelated, $P(c)$ has a Cauchy distribution $P(c) = (1/\pi)[\gamma_0/(\gamma_0^2 + c^2)]$, where the width γ_0, obtained from Eq. (8), is $\gamma_0 = (2\pi\hbar^2/M^2L^2)(\langle |p_x|^2 \rangle/\Delta)$. However, the energy levels in a weakly disordered metal are correlated so that the curvature distribution is no longer Cauchy. The form of $P(c)$ was extensively studied[21] in the search of quantum signatures of chaos in the parametric motion of energy levels. For various systems (random matrices, quantum kicked tops,...), the tail of the curvature distribution was found to be $P(c) \sim 1/c^{2+\beta}$ for large c. The exact form of the distribution has been first approximated by Zakrzewski and Delande[22] by fitting their numerical results for various models with chaotic spectra. It is given by the modified Cauchy form:

$$P_\beta(c) = \frac{N_\beta}{(\gamma_\beta^2 + c^2)^{1/2(\beta+2)}}, \tag{32}$$

where N_β is a normalization constant and $\beta = 1$ if the system is time reversal invariant, $\beta = 2$ if this symmetry is broken and $\beta = 4$ if there is Kramers degeneracy. Von Oppen[23] succeeded in demonstrating that Eq. (32) is indeed exact for the Gaussian unitary ensemble of hermitian matrices ($\beta = 2$). Recent numerical results[24] have extended the validity of the distribution $P_\beta(c)$ to metallic spectra perturbed by an AB flux. In particular, in the limit $\phi \to 0$ here considered, where the spectrum is time reversal invariant ($\beta = 1$), the form (33) has been obtained analytically by Fyodorov and Sommers.[25]

The following simple argument shows, at least for the tail of P_β, how the modified Cauchy distribution is derived from the Wigner–Dyson assumption. Within the RMT description of the energy spectrum, the distribution $P_\beta(s)$ of the distance s (in units of the mean level spacing Δ) between neighboring levels is given by $P_\beta(s) \sim s^\beta$ for small s. In the presence of a perturbation ϕ, the separation $s(\phi)$ of an isolated pair of neighboring levels might be written $s(\phi) = \sqrt{s^2 + \phi^2} \sim s + \phi^2/2s$ (for $s \to 0$), so that the curvature $c \sim 1/s$. Using $P_\beta(s)ds = P_\beta(c)dc$, we obtain $P_\beta(c) \sim 1/(c^{2+\beta})$ (for large c). The immediate consequence of the expression of $P_\beta(c)$ is the divergence of the second moment of the curvature for the case of an AB flux around $\phi = 0$. Therefore, this moment cannot be used to evaluate a conductance even for the Drude term. In the previous derivation leading to Eq. (13), we did consider a smeared curvature [Eq. (9)] insensitive to the exact form of the curvature distribution. But in order to compare (for a discrete energy spectrum) between the curvature g_T of the levels (at $\phi = 0$) and g_d, we have to take into account the exact expression of $P_\beta(c)$. It is worth emphasizing that the divergence of $\langle c^2 \rangle$ is a nonperturbative result, $\langle c^2(\phi) \propto {E_c}^2 \ln(\Delta/E_c\phi^2)$ for small ϕ ($\phi \ll \sqrt{\Delta/E_c} \ll 1$).[26] Therefore, it cannot be obtained from the unitary case (where $\langle c^2 \rangle$ is finite) by taking the limit $\phi \to 0$. Since the second moment of the curvature diverges due to the $1/c^3$, tail one can choose $\langle |c_n(0)| \rangle$ instead to define the conductance as $g_T = \langle |c_n(0)| \rangle / \Delta$.[27] Using the distribution $P_\beta(c)$, we obtain $g_T = \gamma_1/\Delta$ for $\beta = 1$ and $g_T = (2/\pi)(\gamma_2/\Delta)$ for $\beta = 2$. The unexpected result is that the coefficient γ_β entering the expression of $P_\beta(c)$ and defining the natural scaling of the curvature is

$$\gamma_\beta = \pi\beta \frac{\overline{\langle i^2(\phi) \rangle}}{\Delta} = \frac{\pi\beta}{\Delta} \overline{\left\langle \left(\frac{\partial E_n}{\partial \phi} \right)^2 \right\rangle}, \tag{33}$$

where $\langle \ldots \rangle$ and $\overline{\ldots}$ are averages taken, respectively, over the disorder (or the energies) and the flux ϕ. For the case where ϕ is an AB flux, we obtain therefore a relation[20] between the Thouless average curvature $g_T = \langle |c_n(0)| \rangle / \Delta$ and the expression (31) averaged over the disorder

$$g_T = 2\pi g_d. \tag{34}$$

This relation has the universality of the RMT,[28] i.e., it does not depend on the microscopic details of the physical problem. It is also more general than the relation (13) between g_T and the Drude conductance, since Eq. (34) holds beyond the range of validity of RMT when weak localization corrections ($\propto \Delta/E_c$) are taken into account.[25]

Eq. (34) applies to problems other than transport in disordered systems.[29,30] But for the latter, it can be considered as a characterization of metallic systems with delocalized wave functions. The equality (34) between a curvature and the Kubo conductance is a result of the RMT. For instance it does not hold either in ballistic or in localized systems. Section V will provide such an example in a one dimensional disordered system.

V. RELATION BETWEEN THE LANDAUER AND THOULESS CONDUCTANCES

There is another very popular description of the conductance introduced by Landauer.[31] It connects transport to the scattering properties of disordered systems connected to reservoirs through ideal leads. The system is characterized by an S-matrix, but unlike the derivation of Section III, here the S-matrix refers to the whole finite system as a scatterer and not to a time-dependent AB flux. The Landauer conductance g'_L is given by

$$g'_L = \frac{e^2}{h} \frac{T}{1-T}, \tag{35}$$

where $T=\Sigma_i|t_i|^2$ is the sum of the transmission probabilities $T_i=|t_i|^2$ of each available channel i. g_L' diverges for a perfectly transmitting sample where $T=1$. There is a related formula derived from microscopic linear response theory[32] which gives $g_L=(e^2/h)\,T$. It was subsequently generalized to the multichannel case by Fisher and Lee[33] under the form $g_L=(e^2/h)\,\Sigma_i|t_i|^2=(e^2/h)\,\mathrm{Tr}\,tt^\dagger$, where t is the transmission matrix. The discrepancy between this relation and the Landauer formula can be understood in the following way.[34] The conductance g_L' is obtained from the system alone, i.e., for a voltage being the difference of chemical potential of the ideal leads. It corresponds to a four probe terminal measurement.[35] In contrast, the conductance $g_L=(e^2/h)\,T$ is finite for a finite perfect sample. It corresponds to a two terminal measurement where the voltage is the difference of the chemical potentials in the incoherent reservoirs, i.e., when the voltage probes are separated by more than the phase coherence length L_ϕ, so that the leads serve both as current and voltage probes. For a perfect scatterer ($T=1$), it remains the finite conductance of the leads, i.e., the contact resistance given by the total number of channels (in units of e^2/h). In a 1d geometry, these two conductances are related. The two probe resistance $R=(h/e^2)(1/T)$ is the total resistance of the circuit made of the contact resistance h/e^2 due to the leads and $(h/e^2)[(1-T)/T]$ of the system itself such that $1/T=1+(1-T)/T$, i.e., $g_L'^{-1}+(h/e^2)=g_L^{-1}$. In the general multichannel case, the four probe Landauer conductance g_L' is more difficult to define since it depends on the geometry of the system, i.e., on the exact microscopic details of the contacts between the leads and the system. Since the Thouless curvature g_T or the Kubo expression g_d are independent of these details, we shall be interested in the relation between these curvatures and g_L.

The relationship between g_L' and the Thouless curvature has been discussed by Anderson and Lee.[36] In a strictly 1d geometry, these authors found that the Thouless conductance is not proportional to g_L but instead to its square root. This result was subsequently criticized. I would like to show that their result is indeed correct provided we replace g_L' by g_L. Therefore the Thouless curvature g_T is not the conductance in a 1d geometry as in the metallic case but one must choose instead g_d given by Eq. (31), i.e., the average of the square of the persistent currents. The breaking of the proportionality between g_T and g_d given by Eq. (34) is a consequence of the fact that we are outside the range of validity of RMT for a localized 1d system. To obtain back the relation (34) and therefore g_T proportional to g_L, we must go to the limit of a large number of coupled channels as studied numerically.[37]

Let us turn back to the 1d geometry discussed by Anderson and Lee. In that case the S-matrix is 2×2 and it is possible to define instead another (Hermitian) matrix M given in terms of the reflection and transmission amplitudes r and t by:

$$M=\begin{pmatrix} \dfrac{1}{t} & -\dfrac{r}{t} \\ -\dfrac{r^*}{t^*} & \dfrac{1}{t^*} \end{pmatrix}$$

which couples the right channels

$$\Psi_R=\begin{pmatrix} i_R \\ o_R \end{pmatrix}$$

to the left channels

$$\Psi_L=\begin{pmatrix} o_L \\ i_L \end{pmatrix}$$

such that $\Psi_R = M\Psi_L$. The energy spectrum of the system with twisted boundary conditions is obtained by solving $M\Psi = \lambda\Psi$, where $\lambda = e^{\pm i\phi}$, i.e., by closing as usual the system on itself with a fictitious AB flux. The density of states $n(E)$ is given by the relation $n(E) = (1/\pi)(d\theta/dE)$, where $\theta = \Im \ln \mathrm{Det}\, S(E,\phi)$ is the counting function. Then, g_T and g_d are obtained by means of Eqs. (9) and (30), i.e.,

$$g_T = \frac{1}{2\pi} \left. \frac{\partial^2 \theta}{\partial \phi^2} \right|_{\phi=0} \tag{36}$$

and

$$g_d = \frac{1}{\pi^2} \overline{\left(\frac{\partial \theta}{\partial \phi} \right)^2}, \tag{37}$$

where $\overline{\ldots}$ is an average over ϕ. The relation between θ and ϕ is obtained as follows. Notice first that Tr M is representation independent. By definition of the twisted boundary conditions, $e^{\pm i\phi}$ are eigenvalues of M and therefore Tr $M = 2\cos\phi$. On the other hand, using the explicit expression of M we have Tr $M = 2\,\mathrm{Re}(1/t)$, where $t = |t|e^{i\theta}$ is the transmission amplitude with a phase $\theta(E)$ which follows directly from the relation between the matrices S and M. Therefore, Tr $M = 2|t|^{-1}\cos\theta$ and

$$\cos\phi = |t(E)|^{-1} \cos\theta(E,\phi). \tag{38}$$

The Kubo conductance g_d is then obtained directly from Eq. (37), $g_d = (1/\pi^2)\, g_L$. But from Eq. (36), we have $g_T = (1/2\pi)\sqrt{g_L}$ as found by Anderson and Lee.[38] Again, this result is not surprising for an insulator. The new result here is that it is possible to relate the Landauer conductance and the conductance g_d expressed also in terms of TBC.

VI. CONCLUSION

I have shown in this article how to obtain information about the transport properties of disordered and noninteracting systems without evaluating the full Kubo linear response coefficients as given by Eq. (5). We obtained various expressions for transport quantities in terms of the parametric motion of the energy levels with respect to a twist of boundary conditions for the system in a nonsimply connected geometry. In the metallic regime of a weakly disordered system, we can describe the energy spectrum by means of the RMT. There, the Thouless curvature g_T, the typical value g_d of the persistent currents and the Landauer conductance g_L do coincide up to the correction of weak localization. For an Anderson insulator, g_L and g_d are linearly related but are proportional to the square root of the Thouless curvature. The range of applicability of these relations is wider than the Anderson problem of a disordered metal and were successfully applied not only to the study of Quantum Chaotic systems but also to Quantum Hall systems.[39]

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