

Conductance and Statistical Properties of Metallic Spectra

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We present a new expression of the dissipative conductance and study under which conditions it is equal to the Thouless conductance defined as the curvature of the energy levels for a change of the boundary conditions. This equality is related to the transition between different classes of universality of random matrices.

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In this Letter we study the connection between statistical properties of the energy spectrum of metals and the dissipation. This problem was first considered by Thouless [1] who argued that the electrical conductance can be related to the sensitivity of the energy spectrum to a change of the boundary conditions.

This relation between a transport quantity and a property of the equilibrium spectrum is not obvious. On the one hand, the conductance g_d is the *dissipative* quantity given by the Kubo formula. On the other hand, the sensitivity of the energy levels to the boundary conditions may be characterized as follows. Let the wave function ψ obey the general boundary condition, $\psi(x+L) = \psi(x)e^{i\phi}$. Then, at small ϕ the energy levels move quadratically. The individual level curvature at the origin ($\phi=0$) is easily found from perturbation theory. It is given by

$$\frac{1}{2} \left(\frac{\partial^2 E_n}{\partial \phi^2} \right)_{\phi=0} = \frac{\hbar^2}{2mL^2} + \frac{\hbar^2}{mL^2} \sum_{l \neq n} \frac{|\langle l | p_x | n \rangle|^2}{E_n - E_l}, \quad (1)$$

where E_n is a single level energy and p_x the momentum along the x direction. For a metallic system, i.e., in the presence of disorder, this curvature is a random quantity. Let us denote by g_c its typical value measured in units of the mean level spacing Δ :

$$g_c = \frac{1}{\Delta} \left\langle \left(\frac{\partial^2 E_n}{\partial \phi^2} \right)_{\phi=0}^2 \right\rangle^{1/2}, \quad (2)$$

where $\langle \dots \rangle$ represents an average over the disorder.

The fundamental relation $g_d = g_c$ between g_d , a transport quantity, and g_c , an equilibrium quantity, is known as the Thouless formula. Its derivation uses two assumptions. One of them is to assume in Eq. (1) that the energy levels are uncorrelated. This is not the case in metallic systems [2]. The second approximation consists in replacing the nondiagonal matrix element of p_x in Eq. (1) by its diagonal contribution at the Fermi level which is proportional to the Kubo conductivity.

In this Letter, we go beyond the above approximations to derive this relation in the metallic regime. In addition, we show that this problem is related to the transition between universality classes of random matrices in the presence of time-reversal symmetry breaking. First, we propose a new expression of the dissipative conductance g_d based on scattering theory and compare it to the Kubo

formula. Then we examine under which conditions this quantity is related to the curvature of the levels. To that purpose, we describe the statistics of the energy levels versus ϕ in terms of the random matrix theory and relate the conductance to the transition between the so-called Gaussian orthogonal ensemble and the Gaussian unitary ensemble, in the presence of time-reversal symmetry breaking.

In order to calculate the dissipative conductance g_d , we consider a ring threaded by an Aharonov-Bohm flux Φ . There it is known, using a gauge transformation, that the energy spectrum coincides with the one at zero flux provided we make the change $\psi(x+L) = \psi(x)e^{2i\pi\Phi/\Phi_0}$, where $\Phi_0 = h/e$ is the flux quantum. This flux Φ is thus a physical realization of the perturbation parameter $\phi = 2\pi\Phi/\Phi_0$. This geometry was recently considered to study the persistent currents for a stationary flux in the mesoscopic limit [3-6]. It is also a paradigm used to calculate the dissipative conductivity σ when the flux Φ is time dependent [7,8]. The standard derivation of σ is based on a perturbation calculation for a discrete spectrum. Then, a phenomenological coupling to a reservoir is introduced to smear out the energy spectrum and is taken to zero at the end of the calculation before the thermodynamic limit is considered. Here, we start from a continuous spectrum and propose a description in terms of the scattering phase shift [5]. We consider the case of a *time-dependent* flux of the form $\Phi(t/T)$, where T is some characteristic time scale, and we calculate the current $I(\Phi)$ flowing in the ring, in perturbation theory with the parameter $1/T$ [9]. In the scattering approach, since the thermodynamic limit is taken at the very beginning, the spectrum is a continuum at the scale of \hbar/T . To show the connection between the two approaches, we first notice that in the limit $V \rightarrow \infty$ of an infinite volume, it is always possible to associate with any solution $|n\rangle$ of energy E of the Hamiltonian at zero flux a solution $|n'\rangle$ in the presence of the flux at the same energy. These two stationary eigenstates differ in the asymptotic limit only by a phase shift, so that there exists an operator $S(E, \phi)$ defined by $|n'\rangle = S(E, \phi)|n\rangle$. S is the on-shell scattering matrix. The scattering phase shift $\eta(z, \phi)$ is then the function obtained from the $S_+(z, \phi)$ matrix describing outgoing waves by $\eta(z, \phi) = \text{Im} \ln \text{Det} S_+(z, \phi)$. The relation between the flux-dependent energy levels $E(\phi)$ and

$\eta(\phi)$ is then given by $E(\phi)/\Delta = \eta(\phi)$. Moreover, the Friedel sum rule connects the variation $\delta\eta$ of the phase shift to the one δN of the number of states.

An adiabatic limit can be found which corresponds to the zeroth-order approximation $T \rightarrow \infty$. It describes the situation of a stationary flux. The persistent current flowing in the ring is then known to be given by the sum of the currents carried by the filled energy levels $I_{\text{ad}}(\Phi) = -\sum_n \partial E_n / \partial \phi$. It can also be expressed [5] in terms of the total scattering phase shift as $I_{\text{ad}}(\Phi) = (1/\pi\Phi_0) \times \int_0^{E_f} dE \partial_\phi \eta(E, \phi)$.

We now consider the first-order correction in $1/T$. It describes energy exchange between the system and the external flux source and gives the first off-diagonal correction to the S_+ matrix. The corresponding current $I_1(\Phi)$ is given by

$$I_1(\Phi(t)) = \frac{2\hbar}{\pi} \frac{d\Phi}{dt} \left[\frac{\partial}{\partial \Phi} \eta(E_f, \Phi) \right]^2 + O\left(\frac{1}{T}\right)^2. \quad (3)$$

It allows us to identify a conductance G_d given by

$$G_d = \frac{1}{\pi^2} \frac{e^2}{h} \left[\frac{\partial}{\partial \phi} \eta(E_f, \phi) \right]^2. \quad (4)$$

This expression of the conductance and the adiabatic expansion of the current in powers of $1/T$ contains the Kubo formula for the dissipative conductivity. A detailed description of this is discussed in [9]. But let us present an outline of it. The expression of G_d is proportional to the square of the contribution at the Fermi level of the persistent current [5] $d\eta(E_f, \phi)/d\phi = (\pi\Phi_0/\Delta)i(E_f)$. Moreover, the current $i(E_f)$ is by definition related to the diagonal matrix element of p_x through $i(E_f) = (e/mL)\langle n|p_x|n\rangle$, where $|n\rangle$ describes eigenstates at the Fermi level. The dissipative conductance G_d is then rewritten as $G_d = (2\pi e^2 \hbar/m^2)n^2(E_f)L^{2d-2}|\langle n|p_x|n\rangle|^2$, where $n(E_f)$ is the density of states at E_f . Ohm's law $G_d = \sigma L^{d-2}$ allows us therefore to identify the conductivity, $\sigma = (e^2 \hbar/m^2)n^2(E_f)L^d|\langle n|p_x|n\rangle|^2$. This expression coincides exactly with those obtained through the Kubo formula. Nevertheless, it is worth noticing that the conductance G_d given by Eq. (4) is more general. First, it is time dependent since the flux Φ is. For $\Phi(t) = -Vt$, which describes the simplest situation of an applied emf, G_d is, like η , a periodic function of time with period $\hbar/2eV$. The Kubo expression is then obtained from Eq. (4) by taking the time or the flux average. This procedure can be compared to the usual linear response derivation as shown in [9].

In order to make the connection between the statistical properties of the energy spectrum and dissipation and to derive the Thouless relation, we will consider now the dimensionless conductance $g_d = \langle \overline{G_d} \rangle$, where the angular brackets and the overbar represent, respectively, averages over the disorder and the flux (or the time), so that

$$g_d = \left\langle \left[\frac{\partial}{\partial \phi} N(E_f, \phi) \right]^2 \right\rangle, \quad (5)$$

where we have used the Friedel sum rule $\pi\delta N = \delta\eta$ which relates the variation of the number of states to the total phase shift. From now on, we will express all the quantities in terms of δN . Equation (5) is remarkable since it relates the dissipation to a characteristic of the spectrum. We see that g_d measures a global, Φ -averaged, property of the spectrum, while g_c given by Eq. (2) measures a local, $\Phi \rightarrow 0$, property. We are now in a position to relate these two quantities.

To that purpose, we assume the following expression for the correlation function of δN :

$$\langle \delta N(E_f, \phi) \delta N(E_f, \phi') \rangle = D \left[\frac{\phi - \phi'}{2} \right] + D \left[\frac{\phi + \phi'}{2} \right]. \quad (6)$$

This assumption is equivalent to assuming that the harmonics of $\delta N(\phi)$ are not correlated. This was shown explicitly for noninteracting electrons in the metallic limit $k_f l \gg 1$ by means of a microscopic calculation [4] and more generally observed numerically [3]. Taking Eq. (6) into account, we have

$$\left\langle \left[\frac{\partial}{\partial \phi} N(E_f, \phi) \right]^2 \right\rangle = \frac{1}{4} \left[\left[\frac{\partial^2 D}{\partial \phi^2} \right]_\phi - \left[\frac{\partial^2 D}{\partial \phi^2} \right]_{\phi=0} \right]. \quad (7)$$

Since D is a periodic function of ϕ , we obtain $g_d = -\frac{1}{4} (\partial^2 D / \partial \phi^2)_{\phi=0}$. From Eq. (6) we have $\langle \delta N^2(\phi) \rangle = D(0) + D(\phi)$ and then

$$g_d = -\frac{1}{4} \frac{\partial^2}{\partial \phi^2} \langle \delta N^2(E_f, \phi) \rangle \Big|_{\phi=0}. \quad (8)$$

Similarly, from Eqs. (2) and (6), we obtain

$$g_c^2 = \frac{1}{8} \frac{\partial^4}{\partial \phi^4} \langle \delta N^2(E_f, \phi) \rangle \Big|_{\phi=0} \quad (9)$$

so that for small ϕ we can write the expansion

$$\langle \delta N^2(\phi) \rangle = \langle \delta N^2(0) \rangle - 2g_d \phi^2 + \frac{1}{3} g_c^2 \phi^4. \quad (10)$$

On the other hand, by definition of g_c [Eq. (2)], the levels typically shift as

$$\delta E_{\text{typ}}(\phi)/\Delta = \frac{1}{2} g_c \phi^2. \quad (11)$$

So far, we have expressed in terms of the two parameters g_d and g_c , the variation of the two quantities $\langle \delta N^2(\phi) \rangle$ and $\delta E_{\text{typ}}(\phi)$ which characterize the statistical properties of the spectrum. $\langle \delta N^2 \rangle$ is the fluctuation of the number N of particles at fixed chemical potential E_f . This quantity measures the rigidity of the spectrum [2]. We show now that the flux variations of these two quantities $\langle \delta N^2(\phi) \rangle$ and $\delta E_{\text{typ}}(\phi)$ are driven by a *unique* parameter. At this stage, it is the only requirement to establish that g_d and g_c are proportional.

To that purpose, we describe the statistical properties of the energy spectrum of the metal by means of the random matrix theory (RMT). First, let us underline its main features [10]. The energy spectrum of such a complex system can be described by an ensemble of Hamil-

tonian matrices H whose elements H_{ij} are independent random variables with a Gaussian distribution of variance $v^2 = \langle H_{ij}^2 \rangle$ and zero average. We assume implicitly, but it is worthwhile to notice, that in the thermodynamic limit $V \rightarrow \infty$, where the RMT assumptions are best justified, the spectrum has a continuous part so that the energy levels can be related to the scattering phase shift. This prevents, for instance, considering the case of a localized spectrum.

For a time-reversal invariant system described by the Gaussian orthogonal ensemble (GOE), the Hamiltonian matrices have real symmetric elements. When the time-reversal symmetry is broken, for instance in the presence of a magnetic field or an Aharonov-Bohm flux, the Hamiltonian matrices become complex Hermitean. The corresponding ensemble is the Gaussian unitary ensemble (GUE). The transition between these two ensembles, orthogonal ($\alpha=0$) and unitary ($\alpha=1$), has been considered by Pandey and Mehta [11] by means of an interpolating ensemble of the form $H = H(S) + iaH(A)$, where $H(S)$ and $H(A)$ are real symmetric and antisymmetric matrices of dimension d and variance v^2 . They have shown that the transition between GOE and GUE is driven by the single parameter va/Δ [12]. For a Gaussian matrix of size d and variance v^2 , the mean level spacing is given by $\Delta = v/\sqrt{d}$ so that the parameter which drives the transition is the combination da^2 . This means that generally, all the correlation functions depend only on this scaling parameter. This result, which may appear natural in the context of the RMT, has a fundamental consequence in our physical problem.

Our last step is to make the connection between the physical problem and the description of the time-reversal symmetry breaking in the RMT. First the question arises whether the RMT provides a good description of a metal or not. By using a supersymmetric description of the Hamiltonian of a disordered metal and reducing it to a nonlinear σ model field theory, Efetov [13] was able to derive the various correlation functions of the energy levels. He found them identical to those derived from the RMT in the two limits $\alpha=0$ and $\alpha=1$. But, in principle, they can also be calculated in the crossover regime of interest here. This, in addition to recent numerical calculations [14], shows the reliability of the RMT to describe a metal. Now to describe the crossover at finite α , we know, on the one hand, that for small values of α , the typical energy shift varies like da^2 . On the other hand, at small flux, the energy levels vary as $g_c \phi^2$ [Eq. (11)]. This suggests [14] the identification of the parameter da^2 with $g_c \phi^2$ [15]. Then for a metallic ring the transition between the GOE and GUE due to a flux Φ is driven by the unique parameter $g_c \phi^2$ which depends only on the characteristics of the Hamiltonian matrix. All the statistical properties of the spectrum thus depend on the single parameter $g_c \phi^2$. This tells us first, that in the expansion of $\langle \delta N^2(\phi) \rangle$ in Eq. (10), the fourth-order term is proportional to the square of the second-order term, and second,

that the small flux behavior of $\langle \delta N^2(\phi) \rangle$ and δE_{typ} must be characterized by the same parameter. As a result, we deduce

$$g_d = a g_c, \quad (12)$$

which can also be rewritten as

$$\overline{\left\langle \left(\frac{\partial E}{\partial \phi} \right)^2 \right\rangle} = \pi^2 a \Delta \left\langle \left(\frac{\partial^2 E}{\partial \phi^2} \right)^2 \right\rangle_{\phi=0}^{1/2} \quad (13)$$

This is the central result of this Letter. It establishes the Thouless relation between the typical curvature g_c of the energy levels and the dissipative conductance g_d . From Eq. (13), it can also be seen as a relation between the typical zero flux curvature which is a local quantity and the flux average of $\langle (\partial E / \partial \phi)^2 \rangle$ which contains information about the flux dependence of the energy levels at any value of ϕ .

Let us now summarize the main results established in this Letter. First, we have shown how the dissipative conductance g_d depends only on the phase shift at the Fermi energy, which is proportional to the diagonal matrix element of p_λ . By describing the energy spectrum of a metallic ring threaded by an Aharonov-Bohm flux with the random matrix theory, we showed that the dissipative conductance is proportional to the typical zero-flux curvature of the energy levels. This establishes the well-known Thouless result with less restrictive assumptions. Nevertheless, our study cannot discriminate between various microscopic models (for instance independent or interacting electrons) but contains them through the parameter a . All of our results can be rewritten in terms of the scattering phase shift η instead of the number of states and then apply also to the situation of an interacting electron gas described by a Fermi liquid theory.

The dissipation in the system is completely characterized by the nature of the transition between the orthogonal (GOE) to the unitary (GUE) ensembles. The quadratic term in Eq. (10) is negative. This is the signature of the well-known result that the energy spectrum becomes more rigid in the absence of time-reversal symmetry.

Our results could be of some interest to describe properties of so-called "quantum chaotic" systems. All these calculations depend on the assumption that in the thermodynamic limit, the spectra for zero and nonzero fluxes are similar. This supposes that both of them contain a continuous part and that $g_c \gg 1$. Therefore we cannot describe within our approach extreme situations such as the Anderson localization transition or in the presence of a genuine magnetic field, the transition to a spectrum of Landau levels.

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