

The Thouless formula: From disordered to chaotic spectra

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A new expression of the dissipative dc conductance is presented in terms of the scattering phase shift by a time dependent Aharonov–Bohm flux line. It is then related to the Thouless conductance defined as the curvature of the energy levels under a change of the boundary conditions. The relation between these two conductances is found to be universal for all systems obeying Wigner–Dyson statistics. This provides a new characterization of quantum chaotic systems.

1. Introduction

In this article, I would first like to discuss the problem of the quantum transport in condensed matter systems. I will restrict myself to the study of zero temperature, dc transport coefficients in weakly disordered metallic systems, i.e. the residual conductivity (or conductance). Among the different approaches to this problem I will focus especially on those first derived by Edwards and Thouless [1] presenting the conductance g as a measure of the sensitivity of the energy levels to a change of boundary conditions. Section 2 contains the main line of the original derivation. Section 3 contains a new derivation of the dissipative dc conductance in terms of the scattering phase shift by a time dependent Aharonov–Bohm flux line. Its relation to the Kubo formulation will be outlined. Starting from this new expression, we will prove the Thouless formula in great generality for the metallic regime (section 4) [2]. The universality of this result will be defined as well as the generalization of the Thouless approach to characterize chaotic energy spectra. This will help us to precise the range of validity of the random matrix theory (RMT) description and to conclude finally (section 5) on the deviations from this regime near a localization transition and for ballistic or non-ergodic systems.

2. The Thouless expression for the dc conductance

Consider a d -dimensional cubic sample of volume L^d made out of a

disordered metal, characterized by its elastic mean free path ℓ describing the role of the impurities and by the Fermi wavevector k_f . We assume that we have a good metal, i.e. that the condition $k_f \ell \gg 1$ is realized. Moreover, we will ignore throughout this analysis the role of Coulomb interactions between the electrons.

The quantum mechanics of this system is well described by the one electron Hamiltonian $H_0 = p^2/2m + V(r)$, where $V(r)$ represents the scattering potential by the impurities.

Suppose now that instead of the periodic boundary conditions usually considered for the wavefunction, we make the following choice:

$$\psi(x + L) = \psi(x) e^{i\phi}, \quad (1)$$

where ϕ is a real parameter. For the sake of simplicity, we apply the transformation (1) in one direction only but this could be generalized. A simple gauge transformation shows that the spectrum of H_0 with boundary conditions (1) is identical to those obtained by imposing periodic boundary conditions but with the new Hamiltonian

$$H(\phi) = \frac{1}{2m} \left(p_x + \frac{\hbar\phi}{L} \right)^2 + V(x) \quad (2)$$

instead of $H_0 = H(\phi = 0)$. The individual energy levels are now clearly functions of ϕ and their curvature at $\phi = 0$ is given by

$$\frac{1}{2} \left(\frac{\partial^2 E_n}{\partial \phi^2} \right)_{\phi=0} = \frac{\hbar^2}{2mL^2} + \frac{\hbar^2}{m^2 L^2} \sum_{l \neq n} \frac{|\langle l | p_x | n \rangle|^2}{E_n - E_l}. \quad (3)$$

In eq. (3), the states $(|n\rangle, E_n)$ characterize the spectrum of H_0 . Due to the disorder, these curvatures are random quantities. Let us now define g_T as the typical curvature at $\phi = 0$ measured in units of the mean level spacing Δ ,

$$g_T = \frac{1}{\Delta} \left\langle \left(\frac{\partial^2 E_n}{\partial \phi^2} \right)_{\phi=0}^2 \right\rangle^{1/2}, \quad (4)$$

where $\langle \dots \rangle$ represents an average over the impurity potential. g_T is a dimensionless quantity known as the Thouless parameter.

Before going further, let us give a physical realization of the parameter ϕ . By closing the system on itself (ring geometry) and piercing it by a Aharonov-Bohm magnetic flux line Φ , we obtain a system whose 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 is the geometry considered to study the persistent currents for a stationary flux in the mesoscopic limit [3]. To go further along the original argument of Edwards and Thouless, we shall make now two assumptions about the sum of random variables which appears on the right hand side of eq. (3).

(i) The mean square value of the matrix element of p_x in eq. (3) does not depend strongly on the energy difference $E_n - E_j$. We can then replace it by the expression obtained from the Kubo formula. This gives

$$\langle |\langle l | p_x | n \rangle|^2 \rangle = m\Delta k_f \ell. \quad (5)$$

(ii) It remains in eq. (3) the sum over the states of the inverse of the energy differences. This sum is likely to be dominated by the largest term corresponding to a denominator of order Δ . This result is exact if the levels are uncorrelated.

These two assumptions allow to rewrite g_T as

$$g_T = \frac{\hbar^2}{2m\Delta L^2} (1 + k_f \ell).$$

In the metallic regime here considered, $k_f \ell \gg 1$, it reduces to

$$g_T = \frac{1}{\Delta} \frac{\hbar D}{L^2} = \frac{\hbar}{e^2} \sigma L^{d-2}, \quad (6)$$

where $D = (1/d)v_f \ell$ is the diffusion constant and σ the usual Drude conductivity. The Thouless number g_T then appears as the dimensionless conductance expressed by Ohm's law, eq. (6). But the two assumptions used are quite restricting, since for instance energy levels of metallic systems are correlated.

3. Scattering formulation of the dissipative transport

The standard derivation of the dc conductivity σ is based on a perturbation calculation for a discrete spectrum (Kubo approach). 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 [4,5]. Here, we start from a continuous spectrum and propose a description in terms of the scattering phase shift [6]. 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 with the parameter $1/T$ [7]. The other time scale entering this

perturbation expansion and small compared to T is provided by the Wigner time delay $t_w(E)$ which measures the time required by a wavepacket to sweep off the scattering potential. We then assume $T \gg t_w(E)$ so that an incident wavepacket interacts essentially with a stationary flux line. This describes completely our adiabatic limit.

To zeroth order, $I_0(\Phi)$ describes simply the current flowing in the open system. It can be expressed [6] in terms of the total scattering phase shift as

$$I_0(\Phi) = \frac{1}{\pi\Phi_0} \int_0^{E_f} dE \partial_\phi \eta(E, \phi),$$

where $\eta(E, \phi) = \text{Im}(\ln(\text{Det } S(E, \phi)))$ is the total scattering phase shift and $S(E, \phi)$ is the on-shell scattering matrix.

The first order correction in $1/T$ describes the 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

$$I_1(\Phi(t)) = \frac{2\hbar}{\pi} \frac{d\Phi}{dt} \left(\frac{\partial}{\partial \Phi} \eta(E_f, \Phi) \right)^2 + \mathcal{O}\left(\frac{1}{T}\right)^2. \tag{7}$$

It allows to identify a conductance G_d given by

$$G_d = \frac{1}{\pi^2} \frac{e^2}{h} \left(\frac{\partial}{\partial \Phi} \eta(E_f, \Phi) \right)^2. \tag{8}$$

The Kubo expression is then obtained from eq. (8) by taking the time or the flux average. This procedure can be compared to the usual linear response derivation as shown in ref. [7].

4. The Thouless formula [2]

In order to make the connexion 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 $\langle \dots \rangle$ and $\overline{\dots}$ represent respectively averages over the disorder and the flux (or the time) so that

$$g_d = \left\langle \overline{\left(\frac{\partial}{\partial \Phi} N(E_f, \Phi) \right)^2} \right\rangle, \tag{9}$$

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 . The eq. (9) 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_T given by eq. (4) 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 :

$$\langle \delta N(E_f, \phi) \delta N(E_f, \phi') \rangle = D(\frac{1}{2}(\phi - \phi')) + D(\frac{1}{2}(\phi + \phi')). \quad (10)$$

This is equivalent as assuming that the harmonics of $\delta N(\phi)$ are not correlated. This can be shown explicitly for non-interacting electrons in the metallic limit $k_f \ell \gg 1$ by means of a microscopic calculation [8] and more generally observed numerically [9]. Taking eq. (10) into account, we have

$$\left\langle \left(\frac{\partial}{\partial \phi} N(E_f, \phi) \right)^2 \right\rangle = \frac{1}{4} \left[\left(\frac{\partial^2 D}{\partial \phi^2} \right)_{\phi} - \left(\frac{\partial^2 D}{\partial \phi^2} \right)_{\phi=0} \right]. \quad (11)$$

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. (10) we have $\langle \delta N^2(\phi) \rangle = D(0) + D(\phi)$ and then

$$g_d = -\frac{1}{4} \frac{\partial^2}{\partial \phi^2} \langle \delta N^2(E_f, \phi) \rangle |_{\phi=0}. \quad (12)$$

Similarly, from eqs. (4) and (10), we obtain for g_T ,

$$g_T^2 = \frac{1}{8} \frac{\partial^4}{\partial \phi^4} \langle \delta N^2(E_f, \phi) \rangle |_{\phi=0}, \quad (13)$$

so that for small ϕ , we can write the expansion

$$\langle \delta N^2(\phi) \rangle = \langle \delta N^2(0) \rangle - 2g_d \phi^2 + \frac{1}{3} g_T^2 \phi^4. \quad (14)$$

This quantity measures the rigidity of the spectrum [8].

To go further, we describe the statistical properties of the energy spectrum of the metals by means of the random matrix theory (RMT) [10].

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.

Our last step is to make the connexion between our 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 non-linear σ model field theory, Efetov [11] 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, orthogonal and unitary. But, in principle, they can also be calculated in the crossover regime of interest here. This in addition with recent numerical calculations [12], shows the reliability of the RMT to describe a metal.

The transition between those two ensembles, orthogonal and unitary, has been considered by Pandey and Mehta [13] by means of an interpolating ensemble. They have shown that the transition between GOE and GUE is driven by a single parameter which can be identified here as $g_T \phi^2$. This means that generally, all the correlation functions depend only on this scaling parameter. This result, which might appear natural in the context of the RMT, has a fundamental consequence in our physical problem. This tells us that in the expansion of $\langle \delta N^2(\phi) \rangle$ in eq. (14), the fourth order term is proportional to the square of the second order term. As a result, we deduce

$$g_d = a g_T. \quad (15)$$

The constant a is universal, i.e. does not depend on the model considered as long as it can be described by the RMT. To calculate it, we can use for instance the expression of Altshuler and Shklovskii [8] for the fluctuation of the energy levels. It is calculated from a microscopic theory in perturbation with the parameter $(k_f \ell)^{-1}$, using a diagrammatic technique where only one class of diagrams is considered. It can be generalized to include the role of ϕ and we have [12]

$$\langle \delta N^2(E, \phi) \rangle = \frac{1}{2\pi^2} \left[\ln \left(1 + \left(\frac{E}{\Delta} \right)^2 \right) + \ln \left(1 + \frac{E^2}{(\Delta + 4E_c \phi^2)^2} \right) \right], \quad (16)$$

for $\Delta \leq E \leq E_c$, where $E_c = \hbar D/L^2$ is the Thouless energy identified in eq. (6). By inserting eq. (16) into eqs. (12) and (13), one obtains $g_d = (1/\pi^2)E_c/\Delta$ and $g_T = (\sqrt{6}/\pi)(E_c/\Delta)$. Therefore $a = 1/\pi\sqrt{6}$. It could have been calculated in an equivalent way by using directly the RMT.

5. Generalisation to quantum chaotic spectra

The analysis we developed to establish the Thouless formula in the context of metallic disordered mesoscopic systems can be extended to study the energy spectra of quantum systems which are classically chaotic. The idea is to consider the response of these systems to a change of boundary conditions of the type given by eq. (1). Then for billiards, the parameter ϕ has the meaning of an Aharonov–Bohm magnetic flux line piercing it. For more complicated systems, like for instance the quantum kicked rotator, ϕ has a different meaning. But for all these cases it is important to note that although the introduction of the parameter ϕ does not affect the classical motion (it is clear for a Aharonov–Bohm flux line), it modifies the energy spectrum and breaks the time reversal symmetry. The system is therefore driven from the orthogonal to the unitary ensemble. Usually, the RMT describes these spectra by the distribution function $P(s)$ of the spacing between neighbouring levels or the associated correlation functions for a given symmetry ensemble GOE or GUE. Here, by means of our generalised Thouless formula, we propose to study *how the energy levels depend on the parameter ϕ* . It is then possible to measure the typical curvature of these levels for $\phi = 0$ which corresponds to g_T and the average over ϕ of the square of the slopes of the energy levels which is a measure of g_d . Within the range of validity of the RMT, the ratio g_d/g_T is universal and again given by the constant $1/\pi\sqrt{6}$. This provides us with a clear criterion for the domain of applicability of the RMT.

For the case of disordered systems, there are certainly deviations from this universal behavior both in the ballistic regime (clean systems) and near an Anderson metal–insulator transition. Also for chaotic systems, there should be similar deviations. For instance for the quantum kicked rotator when chaotic diffusion is quantum mechanically suppressed and replaced by Anderson-like localisation in phase space.

6. Conclusion

I have presented here a new expression for the dissipative dc conductance related to the total scattering phase shift associated to a time dependent Aharonov–Bohm flux line. By assuming that the energy spectrum of a disordered metal can be described within the framework of RMT, I 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. The constant of proportionality is universal,

i.e. does not depend on the microscopic model considered as long as we stay within the RMT approximation. This leads to a natural extension of these results to quantum systems which are classically chaotic, and allows us to identify also for these cases a new universal regime. All these calculations depend on the assumption that in the thermodynamic limit, the spectra for zero and non-zero fluxes are similar. This supposes that both of them contain a continuous part and that $g_T \gg 1$.

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