

Fourier's Law for Quasi One-Dimensional Chaotic Quantum Systems

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Abstract

We derive Fourier's law for a completely coherent quasi one-dimensional chaotic quantum system coupled locally to two heat baths at different temperatures. We solve the master equation to first order in the temperature difference. We show that the heat conductance can be expressed as a thermodynamic equilibrium coefficient taken at some intermediate temperature. We use that expression to show that for temperatures large compared to the mean level spacing of the system, the heat conductance is inversely proportional to the level density and, thus, inversely proportional to the length of the system.

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1 Introduction

In classical physics, Fourier's law states that the heat conductance is inversely proportional to the length L of a physical system. For a system S coupled at either end to two reservoirs at different temperatures T_1 and T_2 with $T_2 > T_1$, the heat conductance C is defined by writing the heat current through the system as $C(T_2 - T_1)$. The law $C \propto L^{-1}$ is intuitively obvious when one thinks of C^{-1} as the resistance of a macroscopic system against heat (i.e., phonon) transport. The system can be thought of as consisting of building blocks each

with its own resistivity against heat transport. The resistance is the sum of these resistivities and grows linearly with L , resulting in $C \propto 1/L$.

Does that law also apply when S is a quantum system? The argument just given suggests that the answer depends on the degree of coherence of the system. Consider, for instance, a system consisting of K building blocks of length l each so that $L = Kl$, and assume that at the interface between neighboring blocks the system is coupled to the outside world so that quantum coherence between neighboring blocks is destroyed. Then the classical argument given above applies and C is inversely proportional to L .

Here we are interested in the heat conductance of a fully coherent quasi one-dimensional quantum system S . No sources of decoherence are present other than the decoherence due to the coupling of S to the reservoirs at either of its ends. Phonons travel coherently from one end of S to the other. Because of that coherence, the inverse heat conductance cannot be calculated by adding the resistivities of individual blocks in the manner described above, and it is not clear why C should be proportional to L^{-1} . The example of electron transport through mesoscopic samples coupled to two external leads actually suggests independence of C on L . That is seen as follows. At sufficiently low temperature, electron transport is fully coherent [1]. The electrical conductance cannot be calculated by adding the resistivities of parts of the system. Rather, for non-interacting electrons the conductance as given by the Landauer-Büttiker formula is the sum of squares of elements of the scattering matrix, i.e., of the quantum-mechanical transition amplitudes connecting the two leads. That formula embodies full quantum coherence of the mesoscopic system. The elements of the scattering matrix do not display a systematic dependence on the length of the system. Thus, the analogy with electron transport suggests that in a fully coherent system, C should be independent of L . On the other hand, numerical studies of several small quantum systems (typically spin chains) coupled to two reservoirs strongly suggest that C is indeed inversely proportional to the length of the system [2, 3, 4].

In the present paper we offer an analytical resolution of the resulting paradox. We focus attention on chaotic quantum systems. We thereby exclude both integrable systems and disordered systems with localization. We do so because it is known that some integrable systems do not comply with Fourier's law. Moreover, it is clear that in disordered systems with localization, the heat conductance decreases exponentially with length. We later identify those of our assumptions that fail for localized systems. Starting from the master equation which describes the coupling of a quantum system to two reservoirs (heat baths) at different temperatures, we use a perturbation expansion in the temperature difference to derive in first order an expression for the heat current. We show that the heat conductance C in that expression can be written as a thermodynamic equilibrium coefficient calculated at some intermediate temperature T_0 even when the conducting system itself is not in thermodynamic equilibrium. We show for a wide class of quantum systems that except for a normalization factor, the resulting expression for C is indeed independent of L as suggested by the analogy with mesoscopic electron transport. The normalization factor

has the form $1/\sum_m \exp[-E_m/(k_B T_0)]$ typical for equilibrium systems. Here E_m are the eigenenergies of the system S and k_B is the Boltzmann constant. It is easily seen that the sum over m is linear in the total level density of S and, thus, grows linearly with L . For C that yields an inverse dependence on L in agreement with the results reported in Refs. [2, 3].

Work on the heat conductance in quantum mechanics has a long history, starting with Refs. [5, 6, 7], and many papers thereafter. The length dependence of the heat conductance C and the influence of quantum coherence on the value of C were discussed in none of these early works, however. In the related electrical-conductance problem, the importance of quantum coherence was recognized only in the 1980s [1]. During the last decade Fourier's law in quantum mechanics has been intensely studied, especially for quantum spin chains. In addition to the papers cited above we mention Refs. [8, 9, 10, 11] and the review [4] where further references may be found. The present paper is based on a random-matrix model. The results derived within that model and obtained as ensemble averages are generically valid for quasi one-dimensional chaotic quantum systems.

2 Master Equation

We consider two heat baths (reservoirs) labeled 1 and 2 with temperatures T_1 and $T_2 \geq T_1$ coupled to a quantum system S . The Hamiltonian H_S of the system has eigenfunctions $|m\rangle$ and eigenvalues E_m . The occupation probabilities of the states $|m\rangle$ are denoted by P_m . The stationary state of the system S is described by the master equation

$$\sum_m (W_{nm}^{(1)}(T_1) + W_{nm}^{(2)}(T_2))P_m = \left(\sum_m (W_{mn}^{(1)}(T_1) + W_{mn}^{(2)}(T_2)) \right) P_n . \quad (1)$$

The derivation and conditions of validity of Eq. (1) have been thoroughly discussed in the literature, see for instance Ref. [12]. To fix our notation, we give a brief derivation of Eq. (1) in the Appendix. We will show that the P_m are uniquely determined and, for $T_1 \neq T_2$, in general differ from an equilibrium distribution. We will use Eq. (1) to calculate the stationary heat current and, from that, Fourier's law and an expression for the heat conductance. In doing so we exclude systems and/or couplings with pathological properties. Examples would be a system consisting of two uncoupled parts, or a localized system, or a system with coupling matrices $W_{mn}^{(i)}$ where at least one is close to diagonal in the eigenvalue representation of H_S .

It is clear from the outset that within the framework of Eq. (1) a temperature gradient within the system S cannot exist since the temperature of the system S is defined in terms of the occupation probabilities P_m and these are the same throughout the system. That fact reflects quantum coherence throughout the system S . This statement does not preclude the possibility that a suitably defined local energy expectation value possesses a non-zero gradient, however.

For such a situation to arise, the P_m must differ from the thermodynamic equilibrium values in Eq. (4) below.

Explicit values of the coupling matrix elements $W_{mn}^{(i)}(T_i)$ with $i = 1, 2$ are worked out in the Appendix. According to Eq. (53) these obey

$$W_{nm}^{(i)}(T_i) = X_{nm}^{(i)} \exp\{(\beta_i/2)(E_m - E_n)\} \quad (2)$$

where $\beta_i = 1/T_i$. We put the Boltzmann constant equal to unity. Here $X_{nm}^{(i)}$ is real, independent of temperature and, in contrast to $W_{mn}^{(i)}$, symmetric, $X_{nm}^{(i)} = X_{mn}^{(i)}$. Eq. (2) implies

$$W_{nm}^{(i)}(T_i) = \exp[\beta_i(E_m - E_n)]W_{mn}^{(i)}(T_i) . \quad (3)$$

Eq. (3) immediately yields the form of the normalized solutions P_n of Eq. (1) for the equilibrium case, $T_1 = T_2 = T$. With $\beta = 1/T$ these are given by

$$P_n^{\text{eq}} = \frac{\exp[-\beta E_n]}{\sum_m \exp[-\beta E_m]} . \quad (4)$$

The equilibrium distribution (4) is independent of the values of the elements of the coupling matrices $X^{(i)}$. Can such independence also be expected for the non-equilibrium case $T_1 \neq T_2$? For simplicity we take $X^{(1)} = X^{(2)} = X$ and note that the matrix X is symmetric. Eq. (1) takes the form

$$\sum_m X_{nm} \left\{ \left(\exp[(\beta_1/2)(E_m - E_n)] + \exp[(\beta_2/2)(E_m - E_n)] \right) P_m - \left(\exp[(\beta_1/2)(E_n - E_m)] + \exp[(\beta_2/2)(E_n - E_m)] \right) P_n \right\} = 0 . \quad (5)$$

For this equation to hold independently of the values of the X_{mn} , each of the coefficients multiplying X_{mn} must, in general, vanish individually. It is seen immediately that that is possible only for $T_1 = T_2$. The developments in Sections 3.1 and 3.2 below show that the argument is somewhat simplistic and must be refined. Nevertheless we conclude that in the non-equilibrium case the values of the occupation probabilities P_m depend, in general, on the values of the $X_{mn}^{(i)}$.

To determine the stationary heat current I through the system S we multiply Eq. (1) with E_n and sum over n . We obtain

$$\begin{aligned} \sum_{mn} E_n W_{nm}^{(1)}(T_1) P_m - \sum_{mn} E_n W_{mn}^{(1)}(T_1) P_n \\ = - \sum_{mn} E_n W_{nm}^{(2)}(T_2) P_m + \sum_{mn} E_n W_{mn}^{(2)}(T_2) P_n . \end{aligned} \quad (6)$$

Eq. (6) expresses energy conservation. We interpret the negative left- and the positive right-hand side of Eq. (6) as the heat current I (energy per unit time transferred to the system from bath 2 or from the system to bath 1, respectively). That interpretation is in keeping with the fact that the master equation (1) is the stationary form of a more general equation for the time derivative of the occupation probabilities P_m of the states m .

3 Perturbation Expansion

According to Fourier's law, the heat current I is proportional to the temperature difference between the two heat baths. This suggests using a perturbative approach in powers of $\delta T = (1/2)(T_2 - T_1) > 0$. We accordingly expand the quantities appearing in Eq. (1) around some intermediate temperature T_0 that obeys $T_1 < T_0 < T_2$ in powers of δT up to and including terms linear in δT . The choice of T_0 plays an important role in the calculation.

Expanding the coefficients $W^{(i)}(T_i)$ at T_0 in powers of $\delta T = (1/2)(T_2 - T_1)$, we use

$$\frac{\partial W_{nm}^{(i)}}{\partial T} = \frac{1}{2T^2}(E_n - E_m)W_{nm}^{(i)} , \quad (7)$$

see Eq. (2). We likewise expand the solutions P_m of Eq. (1) around the equilibrium solution (4) at $T = T_0$, omitting the normalization factor,

$$P_m = \exp[-\beta_0 E_m](1 + \delta P_m) \quad (8)$$

where $\beta_0 = 1/T_0$. By definition of the equilibrium solution, the terms of zeroth order in δT in Eq. (1) mutually cancel. For $i = 1, 2$ we define the real symmetric matrices

$$B_{mn}^{(i)} = \exp[-(\beta_0/2)(E_m + E_n)]X_{mn}^{(i)} . \quad (9)$$

and the vectors

$$A_m^{(i)} = \frac{1}{T_0^2} \sum_n (E_m - E_n) B_{mn}^{(i)} . \quad (10)$$

We note that

$$\sum_m A_m^{(i)} = 0 . \quad (11)$$

The master equation takes the form

$$\sum_i (-)^i A_n^{(i)} \delta T + \sum_i \sum_m B_{nm}^{(i)} \delta P_m - \left(\sum_i \sum_m B_{nm}^{(i)} \right) \delta P_n = 0 . \quad (12)$$

This is a set of inhomogeneous linear equations for the unknown quantities δP_n . The homogeneous equations possess the non-trivial (equilibrium) solution $\delta P_n = 1$ (all n). According to Eq. (11) the inhomogeneity is orthogonal upon that solution. Therefore, the inhomogeneous equations possess a unique solution δP_m with

$$\sum_m \delta P_m = 0 . \quad (13)$$

That is the solution we study in the sequel.

We consider consecutively three cases: (i) The coupling matrix elements are equal, $X_{mn}^{(1)} = X_{mn}^{(2)}$; (ii) the coupling matrix elements are similar, $X_{mn}^{(1)} = aX_{mn}^{(2)}$ with $a > 0$; (iii) the coupling matrix elements are dissimilar so that neither case (i) nor case (ii) applies.

3.1 Symmetric Coupling

For the symmetric case with equal couplings, $X_{mn}^{(1)} = X_{mn}^{(2)} = X_{mn}$, we choose the intermediate temperature

$$T_0 = \frac{1}{2} (T_1 + T_2) . \quad (14)$$

We have $B_{mn}^{(1)} = B_{mn}^{(2)} = B_{mn}$ so that $\sum_i (-)^i A_m^{(i)} = 0$ for all m . Therefore, the solution of Eq. (12) vanishes identically, and the solution of the master equation (1) is given by the equilibrium solution (4) with $1/\beta$ taken at $T = T_0$ even in the non-equilibrium case $T_1 \neq T_2$, up to and including linear terms in δT . The system S is in thermal equilibrium at the mean temperature T_0 . There cannot exist a gradient in the local expectation value of the energy. A non-vanishing non-equilibrium solution of the master equation (1) must be of second order in δT .

An explicit expression for the heat current is obtained by using for P_m the equilibrium solution (including the normalization factor) and by expanding the left-hand side of Eq. (6) up to terms linear in δT . That gives

$$I = \frac{1}{\sum_n \exp[-\beta_0 E_n]} \left(\frac{1}{2T_0^2} \sum_{mn} (E_m - E_n)^2 B_{mn} \right) \delta T . \quad (15)$$

This, in a very general form, is Fourier's law. The heat conductance is given by an equilibrium property of the system: The coefficient $\sum_{mn} (E_m - E_n)^2 B_{mn}$ is calculated at the equilibrium temperature T_0 . The choice (14) of T_0 is justified by hindsight: It is easy to check that for a different choice, we do not find $\delta P_m = 0$ for all m . That shows the importance of the choice of T_0 : Apparent deviations from thermal equilibrium indicated by nonvanishing δP_m s may only be caused by an improper choice of T_0 .

3.2 Similar Couplings

We turn to case (ii) where $X_{mn}^{(1)} = aX_{mn}^{(2)}$ with $a > 0$. Again, the choice of T_0 is important to minimize apparent (but unreal) deviations of the system from thermal equilibrium. Thus we write

$$T_0 = \alpha T_1 + (1 - \alpha) T_2 \quad (16)$$

with $0 < \alpha < 1$ and determine α from the condition that the solutions δP_m of the linearized master equation (12) vanish. That equation now takes the form

$$[-2(1 - \alpha)A_n^{(1)} + 2\alpha A_n^{(2)}] \delta T + \sum_i \sum_m B_{nm}^{(i)} \delta P_m - \left(\sum_i \sum_m B_{nm}^{(i)} \right) \delta P_n = 0 . \quad (17)$$

Because of the definition (10) and the condition $X_{mn}^{(1)} = aX_{mn}^{(2)}$ the inhomogeneity vanishes if we choose $\alpha = a/(1 + a)$ and, thus,

$$T_0 = \frac{1}{1 + a} (aT_1 + T_2) . \quad (18)$$

Thus, the system S is in thermal equilibrium at the temperature T_0 given by Eq. (18). The equilibrium temperature is shifted away from the arithmetic mean of T_1 and T_2 toward the temperature of the heat bath with the stronger coupling to the system. That is physically very plausible. The heat current is given by

$$\begin{aligned} I &= \frac{1}{\sum_n \exp[-\beta_0 E_n]} \left(\frac{1}{2T_0^2} \frac{2}{1+a} \sum_{mn} (E_m - E_n)^2 B_{mn}^{(1)} \right) \delta T \\ &= \frac{1}{\sum_n \exp[-\beta_0 E_n]} \left(\frac{1}{2T_0^2} \frac{2a}{1+a} \sum_{mn} (E_m - E_n)^2 B_{mn}^{(2)} \right) \delta T . \end{aligned} \quad (19)$$

The same conclusions as in Section 3.1 apply: The system is in thermal equilibrium at temperature T_0 . The heat conductance is evaluated at the equilibrium temperature. A gradient of the local energy expectation value and deviations from equilibrium must be of second order in δT .

3.3 Dissimilar Couplings

In the case of dissimilar couplings we expect that the difference will be rather small and statistical in nature. Indeed, the derivation of the master equation in the Appendix is based upon the assumption that the operators $Q^{(i)}$ that couple the system S to either heat bath are local operators that act on either end of S . In describing such coupling operators explicitly, it is commonly assumed that they are made up of local position and momentum operators. For chaotic systems we expect the matrices $X^{(1)}$ and $X^{(2)}$ to be similar. It is not difficult, however, to imagine systems where the matrices $X^{(1)}$ and $X^{(2)}$ differ strongly. That is the case, for instance, for localized systems. Then $X^{(1)}$ couples most strongly to states localized near one end of the sample. Such states do not couple significantly to $X^{(2)}$ at the other end, and conversely for $X^{(2)}$. A drastic and systematic difference between the two coupling matrices invalidates our treatment.

The case of dissimilar couplings is more complicated than the cases of equal and similar couplings and requires some algebra. It turns out that the occupation probabilities P_m differ from an equilibrium distribution. However, it is possible to define a temperature T_0 such that the heat conductance is given by an equilibrium expression calculated at T_0 .

We use the ansatz Eq. (16) and obtain Eq. (17). But now the inhomogeneity in Eq. (17) does not vanish for any value of α , and it is necessary to determine the solutions $\delta P_m \propto \delta T$ of that equation. We define $B_{nm} = \sum_i B_{nm}^{(i)}$ and the real symmetric matrix $\tilde{B}_{nm} = B_{nm} - \delta_{nm} \sum_k B_{nk}$. Eq. (17) takes the form

$$[-2(1-\alpha)A_n^{(1)} + 2\alpha A_n^{(2)}]\delta T + \sum_m \tilde{B}_{nm} \delta P_m = 0 . \quad (20)$$

We have $\sum_m \tilde{B}_{nm} = 0$. Therefore, the matrix \tilde{B}_{nm} possesses one vanishing eigenvalue, λ_1 say, with associated eigenvector $\{1, 1, \dots, 1\}^T$. The matrix \tilde{B}

can be diagonalized by a real orthogonal matrix \mathcal{O} ,

$$[\mathcal{O}\tilde{B}\mathcal{O}^T]_{mn} = \delta_{mn}\lambda_m. \quad (21)$$

The eigenvector $\{1, 1, \dots, 1\}^T$ occupies the first column of the matrix \mathcal{O}^T , and the vector $\{1, 1, \dots, 1\}$ occupies the first row of the matrix \mathcal{O} . We assume that all eigenvalues λ_m with $m \geq 2$ differ from zero. We multiply Eq. (20) from the left with the matrix \mathcal{O} , define the vectors $\tilde{A}_m^{(i)} = \sum_k \mathcal{O}_{mk} A_k^{(i)}$ and $\delta\tilde{P}_m = \sum_k \mathcal{O}_{mk} \delta P_k$, and observe that $\tilde{A}_1^{(i)} = 0$ (see Eq. (11)) and that $\delta\tilde{P}_1 = 0$ (see Eq. (13)). For $m \geq 2$ that yields

$$[-2(1-\alpha)\tilde{A}_m^{(1)} + 2\alpha\tilde{A}_m^{(2)}]\delta T = \lambda_m \delta\tilde{P}_m. \quad (22)$$

Solving for $\delta\tilde{P}_m$ and transforming back to δP_m we find

$$\delta P_m = \delta T \sum_n \left(\sum_{k \geq 2} \mathcal{O}_{km} \frac{1}{\lambda_k} \mathcal{O}_{kn} \right) [-2(1-\alpha)A_n^{(1)} + 2\alpha A_n^{(2)}]. \quad (23)$$

In order to use that result in Eq. (8), we normalize the solutions defined by Eq. (8) so that $\sum_m P_m = 1$ and expand the resulting expression in powers of δP_m , keeping only terms up to first order. For P_m that yields

$$P_m = \frac{\exp[-\beta_0 E_m]}{\sum_n \exp[-\beta_0 E_n]} \left(1 + \delta P_m - \frac{\sum_k \exp[-\beta_0 E_k] \delta P_k}{\sum_l \exp[-\beta_0 E_l]} \right). \quad (24)$$

Insertion of Eqs. (23) into (24) gives the occupation probabilities of the states m . The solutions δP_m do not vanish identically for any choice of α , and there is no choice of temperature T_0 for which the system would be in thermal equilibrium. Thus, the local expectation value of the energy may not be the same throughout the system, and it may possess a non-zero gradient. We have not investigated that possibility.

We turn to the heat current I defined in Eq. (6). In terms of the solutions (23) I is given by

$$\begin{aligned} I &= \frac{1}{\sum_n \exp[-\beta_0 E_n]} \left(\frac{\delta T}{2T_0^2} 2(1-\alpha) \sum_{mn} (E_m - E_n)^2 B_{mn}^{(1)} \right. \\ &\quad \left. - \sum_{mn} (E_m - E_n) B_{mn}^{(1)} \delta P_n \right) \\ &= \frac{1}{\sum_n \exp[-\beta_0 E_n]} \left(\frac{\delta T}{2T_0^2} 2\alpha \sum_{mn} (E_m - E_n)^2 B_{mn}^{(2)} \right. \\ &\quad \left. - \sum_{mn} (E_m - E_n) B_{mn}^{(2)} \delta P_n \right). \end{aligned} \quad (25)$$

To simplify these expressions we consider the last term in the first of Eqs. (25). With the help of Eqs. (11) and (23) that term can be written as

$$\sum_{mn} (E_m - E_n) B_{mn}^{(1)} \delta P_n = 2T_0^2 \delta T \left(\alpha \sum_{k \geq 2} \tilde{A}_k^{(1)} \frac{1}{\lambda_k} \tilde{A}_k^{(2)} - (1-\alpha) \sum_{k \geq 2} \tilde{A}_k^{(1)} \frac{1}{\lambda_k} \tilde{A}_k^{(1)} \right). \quad (26)$$

For equal couplings we have $\tilde{A}_k^{(1)} = \tilde{A}_k^{(2)}$ and the right-hand side of Eq. (26) vanishes for $\alpha = 1/2$. For similar couplings we have $\tilde{A}_k^{(1)} = a\tilde{A}_k^{(2)}$ and the right-hand side of Eq. (26) vanishes for $\alpha = 1/(1+a)$. In the present case of dissimilar couplings, the expression in big round brackets is linear in α and, therefore, vanishes at some uniquely defined value α_1 . That value defines via Eq. (16) a temperature $T_0^{(1)}$. We expect that $T_0^{(1)}$ obeys $T_1 \leq T_0^{(1)} \leq T_2$ and that, therefore, α_1 obeys $0 \leq \alpha_1 \leq 1$. Values of α_1 outside the interval $[0, 1]$ would be physically implausible. Similar considerations apply to the second of Eqs. (25). Again there exists a value of α_2 and an associated temperature $T_0^{(2)}$ for which the term linear in δP_n vanishes. We cannot prove, however, that $\alpha_2 = \alpha_1$, or that $T_0^{(1)} = T_0^{(2)}$.

Choosing $T_0 = T_0^{(1)}$ in the first and $T_0 = T_0^{(2)}$ in the second of Eqs. (25) we obtain for the heat current

$$\begin{aligned} I &= \frac{1}{\sum_n \exp[-\beta_0^{(1)} E_n]} \left(\frac{1}{(T_0^{(1)})^2} (1 - \alpha_1) \sum_{mn} (E_m - E_n)^2 B_{mn}^{(1)}(T_0^{(1)}) \right) \delta T \\ &= \frac{1}{\sum_n \exp[-\beta_0^{(2)} E_n]} \left(\frac{1}{(T_0^{(2)})^2} \alpha_2 \sum_{mn} (E_m - E_n)^2 B_{mn}^{(2)}(T_0^{(2)}) \right) \delta T . \end{aligned} \quad (27)$$

In these equations, the coefficients $B^{(i)}$ are taken at the temperatures $T_0^{(i)}$ with $i = 1, 2$, and $\beta^{(i)} = 1/T_0^{(i)}$. We cannot show that $T_0^{(1)} = T_0^{(2)}$ although that would be physically most plausible. The heat conductance in both expressions (27) is evaluated at some equilibrium temperature $T_0^{(i)}$ even though the system is not in equilibrium.

4 Length Dependence of the Heat Conductance

In Section 3 we have shown that in Fourier's law,

$$I = C \delta T , \quad (28)$$

the heat conductance C can always be written as an equilibrium coefficient of the form

$$C = \frac{\gamma}{T_0^2} \frac{1}{\sum_m \exp[-\beta_0 E_m]} \sum_{mn} (E_m - E_n)^2 \exp[-(\beta_0/2)(E_m + E_n)] X_{mn} . \quad (29)$$

That expression may be viewed as a special case of the Green-Kubo formula [5, 6]. Here γ is a numerical coefficient of order unity, and T_0 is a suitably defined temperature. The symmetric matrix X_{mn} describes the coupling of the quantum system S to one of the two heat baths. We now investigate how the heat conductance C depends on the length L of the system S . We consider a linear chain or a piece of wire or some other quasilinear system, all of length L . We model the system in terms of random matrices, thereby assuming that it is chaotic. We show that for any such device, coupled at either end to heat baths

with different temperatures, the heat conductance is inversely proportional to L as is the case in classical physics, and as is found to be the case for small spin chains [2, 3, 4].

To this end we rewrite the terms appearing in Eq. (29), using the definition (9),

$$\begin{aligned}
\sum_m \exp[-\beta_0 E_m] &= \int dE \exp[-\beta_0 E] \sum_m \delta(E - E_m) , \\
\sum_{mn} (E_m - E_n)^2 B_{mn} &= \sum_{mn} (E_m - E_n)^2 \exp[-\beta_0(E_m + E_n)] X_{mn} \\
&= \int d\varepsilon_1 \int d\varepsilon_2 (\varepsilon_1 - \varepsilon_2)^2 \exp[-\beta_0(\varepsilon_1 + \varepsilon_2)] \\
&\quad \times 2\pi A_0 \exp[(\varepsilon_1 - \varepsilon_2)^2 / \Delta^2] \\
&\quad \times \sum_{mn} |Q_{mn}|^2 \delta(\varepsilon_1 - E_m) \delta(\varepsilon_2 - E_n) . \quad (30)
\end{aligned}$$

We have used Eqs. (2) and (53) and written the expressions appearing in the heat conductance C in terms of length-independent energy integrals, in terms of $|Q_{mn}|^2$, and in terms of $\delta(E - E_m)$. The constant A_0 measures the strength of the coupling of the system to the heat bath, see Eq. (46). By definition the operator Q couples the surface of the system S locally to the heat bath and does not depend on L . Any length dependence of the terms in Eq. (30) is due to sums involving $\delta(E - E_m)$. Such sums appear differently in the first and in the second of Eqs. (30). In the first, the level density $\sum_m \delta(E - E_m)$ itself appears as an independent factor while in the second, the sums involve the squared matrix element $|Q_{mn}|^2$ of Q . In condensed-matter physics, expressions of similar form are referred to as the local density of states and in nuclear physics, as the strength function of the operator Q . It is obvious and confirmed below that the density of states appearing in the first of Eqs. (30) increases linearly with the length L of the system S . It remains to show that the length dependence of the last term in the second of Eqs. (30) is negligible. We do so for a large class of quasi one-dimensional systems S .

We exploit the fact that Q is local, i.e., it acts only on one surface of S . Let P denote an orthogonal projector obeying $P = P^\dagger = P^2$ that projects onto a suitably chosen set of states on that surface such that $Q_{mn} = \langle m|Q|n\rangle = \langle mP|Q|Pn\rangle$. We investigate the length dependence of the expression

$$\sum_m |Pm\rangle \delta(E - E_m) \langle mP| = -\frac{1}{\pi} P \Im \frac{1}{E^+ - H_S} P \quad (31)$$

where E^+ carries an infinitesimal positive imaginary increment and where H_S is the Hamiltonian of S . Expression (31) differs from the expression for the total level density

$$\rho(E) = \sum_m \delta(E - E_m) = -\frac{1}{\pi} \Im \text{Trace} \frac{1}{E^+ - H_S} . \quad (32)$$

We show that the projector P in Eq. (31) has a profound influence on the length dependence.

To model the length dependence of S we think of S as consisting of K blocks of fixed length l each, labelled by a running index $k = 1, \dots, K$. The length of S is then given by $K = Lk$, and the dependence on length is converted into a dependence on K . For H_S we use a matrix representation. Let $H^{(k)}$ be the Hamiltonian matrix for block k . Only neighboring blocks are coupled by Hamiltonian matrices $W^{(kk+1)}$, and we have

$$H_S = \begin{pmatrix} H^{(1)} & W^{(12)} & 0 & 0 & \dots \\ W^{(12)} & H^{(2)} & W^{(23)} & 0 & \dots \\ 0 & W^{(23)} & H^{(3)} & W^{(34)} & \dots \\ 0 & 0 & W^{(34)} & H^{(4)} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} \quad (33)$$

where the upper indices range from 1 to k .

Let the block with $k = 1$ carry the surface on which Q acts. Then we have $PH_S P = PH^{(1)}P$. In the first block, we introduce a complete set of orthonormal basis states $|\mu\rangle$ where $\mu = 1, 2, \dots$. The basis is chosen such that only the first n states are surface states so that $P|\mu\rangle = 0$ for $\mu > n$. Then $P = \sum_{\mu=1}^n |\mu\rangle\langle\mu|$. Instead of the strength function in Eq. (31) we consider

$$-\frac{1}{\pi} \langle 1 | \Im \frac{1}{E^+ - H_S} | 1 \rangle. \quad (34)$$

Without loss of generality we confine ourselves here to the diagonal element of the propagator with respect to the state with $\mu = 1$. That choice is arbitrary, any other value of μ with $\mu \leq n$ would give the same result. We consider only diagonal elements because the non-diagonal elements vanish on average as a consequence of the statistical assumptions introduced below. With $E_1 = \langle 1 | H^{(1)} | 1 \rangle$ and $V_\nu = H_{1\nu}^{(1)}$ for $\nu \geq 2$, the matrix $H^{(1)}$ in Eq. (33) is explicitly written as

$$H^{(1)} = \begin{pmatrix} E_1 & V_\rho \\ V_\nu & H_{\nu\rho}^{(1)} \end{pmatrix}. \quad (35)$$

Here $\nu, \rho \geq 2$. We put $E_1 = 0$ and comment on that choice below.

Analytical progress is possible upon introducing statistical assumptions on the matrix elements of H_S . We assume that the matrices $H^{(k)}$ with $k = 1, 2, \dots, k$ are uncorrelated and are members each of the Gaussian Orthogonal Ensemble (GOE) of random matrices of dimension N , with the limit $N \rightarrow \infty$ eventually taken [13]. Ensemble averages are denoted by angular brackets. The matrix elements are Gaussian-distributed random variables with mean values zero and for $k, l, m = 1, 2, \dots, K$ obey

$$\begin{aligned} \langle H_{\mu\nu}^{(k)} H_{\mu'\nu'}^{(l)} \rangle &= (1 - \delta_{1k}) \delta_{kl} \frac{\lambda^2}{N} (\delta_{\mu\nu'} \delta_{\nu\mu'} + \delta_{\mu\mu'} \delta_{\nu\nu'}) , \\ \langle W_{\mu\rho}^{kl} W_{\mu'\rho'}^{k'l'} \rangle &= \frac{w^2}{N} (\delta_{kk'} \delta_{ll'} + \delta_{kl'} \delta_{lk'}) (\delta_{\mu\mu'} \delta_{\rho\rho'} + \delta_{\mu\rho'} \delta_{\mu'\rho}) , \\ \langle H_{\rho\sigma}^{(k)} W_{\rho'\sigma'}^{(lm)} \rangle &= 0 . \end{aligned} \quad (36)$$

Because of these assumptions the average spectrum of each of the matrices $H^{(k)}$ with $k \geq 2$ has for $N \rightarrow \infty$ the shape of a semicircle with radius 2λ . The coupling between neighboring blocks mediated by the matrices W is characterized by the strength parameter w . It is physically obvious that $w \leq \lambda$. For the first block we introduce a special notation. We assume that the first of Eqs. (36) applies in form also to the case where $k = l = 1$ but does so only for $\mu, \nu, \mu', \nu' \geq 2$. We assume that the V_μ in Eq. (35) are Gaussian random variables with mean value zero, not correlated with the other matrix elements, and obey $\langle V_\mu V_\nu \rangle = v^2 \delta_{\mu\nu}$. We do so in order to display explicitly the role of the coupling of the surface state to the rest of the system, without any restrictions on the value of v^2 . For $N \rightarrow \infty$ the spectrum of $H^{(1)}$ is also of semicircular form but the surface state plays a distinct role.

The random-matrix model introduced in Eqs. (36) describes the generic properties of chaotic quasi one-dimensional quantum systems. It is the most general model we can think of to describe such systems. The same model has been widely used to describe electron transport through disordered mesoscopic samples [14, 15].

We work out the ensemble averages of expressions (32) and (34) in the framework of the random-matrix model defined in Eqs. (36). To this end we calculate the average Green function $G(E) = \langle (E^+ - H_S)^{-1} \rangle$ of the system. Because of the Gaussian distribution of the elements of H_S , that function obeys for $N \rightarrow \infty$ the Pastur equation [16]

$$EG(E) = 1 + \langle H_S G(E) H_S \rangle G(E) . \quad (37)$$

In view of our statistical assumptions, all non-diagonal elements of $G(E)$ (with respect to both block index k and running index μ) vanish. We write $G_{\mu\mu}^{(k)}(E)$ for the diagonal elements in block k and define $G^{(k)} = (1/N) \sum_\mu G_{\mu\mu}^{(k)}$. In block 1 the sum runs from $\mu = 2$. We consider the matrix element $G_{11}^{(1)}(E)$ separately because the expression in Eq. (34) is given by $(-1/\pi) \Im G_{11}^{(1)}(E)$. According to Eq. (37) we have for $N \gg 1$ and $k = 1, 2, \dots, K$ and with $G^{(0)} = 0 = G^{(K+1)}$

$$\begin{aligned} EG_{11}^{(1)}(E) &= 1 + v^2 N G^1 G_{11}^{(1)} , \\ EG^{(k)}(E) &= 1 + [\lambda^2 G^{(k)} + w^2 G^{(k-1)} + w^2 G^{(k+1)}] G^{(k)} . \end{aligned} \quad (38)$$

Therefore, $G_{11}^{(1)}(E)$ is given by

$$G_{11}^{(1)}(E) = \frac{1}{E - v^2 N G^{(1)}} . \quad (39)$$

We observe that the factor Nv^2 represents the total strength of the coupling of the surface state $|1\rangle$ to the system S . Since the state $|1\rangle$ couples only to states in block 1, that strength is independent of the length of S . The complex propagator $G^{(1)}$ is obtained by solving the second set of Eqs. (38).

We solve these equations approximately. For $K \gg 1$ and k somewhere in the middle of the range $[1, K]$, the form of H_S in Eq. (33) suggests that $G^{(k)}$

changes slowly with k . We accordingly put $G^{(k)} = G^{(k-1)} = G^{(k+1)}$. With

$$(\lambda')^2 = \lambda^2 + 2w^2 \quad (40)$$

the resulting quadratic equation for $G^{(k)}$ yields

$$\lambda' G^{(k)}(E) = \frac{E}{2\lambda'} - i\sqrt{1 - \left(\frac{E}{2\lambda'}\right)^2}. \quad (41)$$

The average spectrum in block k , proportional to the imaginary part of $G^{(k)}$, retains the form of the semicircle. However, the range $4\lambda'$ of the spectrum is increased compared to the value 4λ that applies without coupling to the neighboring blocks ($W = 0$). The increase is independent of K , i.e., of the length of the system.

For blocks near the either end of the system, i.e., k -values close to 1 or K , the form of H_S in Eq. (33) and the form of Eqs. (38) suggest that the solutions retain the form (41) but with values of λ' that are smaller than given in Eq. (40). That statement is supported by taking $K = 2$ in which case we find $(\lambda')^2 = \lambda^2 + w^2$. We conclude that the solutions of Eqs. (38) yield average spectra of approximately semicircular shape with ranges λ' that lie between $\sqrt{\lambda^2 + w^2}$ and $\sqrt{\lambda^2 + 2w^2}$ and that are independent of K . An estimate of the range ΔE of the spectrum of H_S confirms that conclusion. We use that $\Delta E \approx \sqrt{(1/(KN))\text{Trace}(H_S)^2}$. For $N \gg K \gg 1$ we obtain $\Delta E \approx \sqrt{\lambda^2 + 2w^2}$, a result that is independent of K and consistent with the values for λ' just mentioned.

Using the form (41) for $G^{(1)}(E)$ in expression (34) and putting in $G^{(1)}(E)$ the energy argument equal to zero for simplicity we obtain

$$-\frac{1}{\pi} \Im \frac{1}{E + iv^2 N/\lambda}. \quad (42)$$

The width $2v^2 N/\lambda$ of the strength function of the state $|1\rangle$ is essentially given by the total strength Nv^2 of the coupling of that state to the system S divided by the range of the spectrum of S . That is a physically very plausible result. Neither Nv^2 nor λ' depend on the length of the system. The result (42) can easily be extended by taking into account the full form of the propagator in Eq. (41) and by dropping the assumption $E_1 = 0$. Instead of the form (42) one obtains an expression of Breit–Wigner form centered at E_1 with a width and a level shift due to the imaginary and the real parts of $G^{(1)}$, respectively. That expression is also independent of K . The same statement obviously applies to the full expression (31).

We compare this result with the total level density of S given by Eq. (32). From the definition of $G^{(k)}$ it follows that

$$\langle \rho(E) \rangle = -\frac{N}{\pi} \Im \sum_k G^{(k)}(E) \quad (43)$$

and, with $G^{(k)}(E)$ almost independent of k , $\langle \rho(E) \rangle \propto K \propto L$. We conclude that the double sum in the numerator of Eq. (29) is independent of L while the single sum in the denominator is linear in L . As a result the heat conductance C is inversely proportional to L .

5 Summary and Conclusions

For a completely coherent chaotic quasi one-dimensional quantum system coupled to two heat baths at different temperatures, we have solved the master equation up to first order in the temperature difference and obtained Fourier's law. For equal or similar couplings at both ends of the system we have shown that the heat conductance C in Fourier's law can always be written as an equilibrium coefficient. In the case of dissimilar couplings the same statement holds generically for chaotic systems but not, for instance, for localized systems.

We have used that result to investigate the dependence of C on the length L of the quantum system. Intuitive arguments based on quantum coherence and the analogy with electron transport through mesoscopic systems both suggest that C be independent of L , in contrast to numerical evidence [2, 3] showing that $C \propto L^{-1}$. We have resolved that discrepancy by showing that aside from a normalization factor, C is indeed independent of L . The entire length dependence of C is found to be due to the normalization factor and determined by the density of states. The latter increases linearly with L and yields $C \propto L^{-1}$.

The length dependence of the remaining term in C is determined by that of the last factor in Eq. (30). That factor bears a close analogy to the spreading width in nuclear physics and to the local density of states in condensed-matter physics. In both cases, it is known that the values are not affected when the dimension of the system is increased. In the present case, we have used a random-matrix approach to model the length dependence. That approach yields generic results [13] (exceptions have measure zero with respect to the probability measure that defines the random-matrix ensemble). We have also used the essential fact that the coupling to the heat baths is local and linked to the surface. We have shown that that fact guarantees the length-independence of the relevant term in Eq. (30).

Having resolved the discrepancy, we may turn the question around and ask: Why does electron transport in mesoscopic systems not show a similar length dependence due to a normalization factor? The answer lies in the temperatures at which heat transport and electron transport are considered. To insure quantum coherence, electron transport is experimentally studied close to zero Kelvin. At such low temperature, only the lowest eigenvalues E_m of the system would contribute to C . The random-matrix model we use is viable only when the density of states is sufficiently high, i.e., when the temperature T_0 at which C is evaluated, is very much larger than the mean level spacing near the ground state. The random-matrix model is not expected to account correctly for effects near the end points of the spectrum.

Although C is inversely proportional to L in both classical and quantum

physics, the causes for that dependence are seen to be strikingly different. In classical physics and for systems of macroscopic size, lack of quantum coherence causes the total resistance to be the sum of the resistivities of subsystems and, thus, $C \propto L^{-1}$. For a fully coherent quantum system, the inverse length dependence of C is due to the linear increase with L of the level density of the system.

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Appendix: Derivation of the Master Equation

In Ref. [17], the master equation for a quantum system coupled to a single heat bath was derived. Here we use the same derivation for a quantum system coupled to two heat baths with temperatures T_1 and T_2 to obtain Eq. (1). We only sketch those parts of the derivation that differ from Ref. [17] and do not repeat here the discussion of the conditions under which the derivation holds. These are the same as in Ref. [17].

The quantum system S has Hamiltonian H_S , eigenvalues E_m , and eigenfunctions $|m\rangle$, with $m = 1, 2, \dots$. With $i = 1, 2$ the two baths have Hamiltonians H_i , eigenvalues $\varepsilon_a^{(i)}$ and eigenfunctions $|ia\rangle$, respectively, with $a = 1, 2, \dots$. The coupling between each of the baths $i = 1, 2$ and the system has the form $W^{(i)} = Q^{(i)}V^{(i)}$. Here $Q^{(i)}$ are local operators that act on either end of the system S while the $V_{ab}^{(i)}$ are uncorrelated random matrices to be specified below. The total Hamiltonian is

$$\begin{aligned} \mathcal{H} &= H_S + H_1 + H_2 + \sum_i W^{(i)} \\ &= H_0 + W . \end{aligned} \tag{44}$$

To define the ensemble we consider case (II) of Ref. [17] and assume that the $W^{(i)}$ are Gaussian-distributed random variables with zero mean values and second moments given by

$$\begin{aligned} \overline{\langle mia | W^{(i)} | nib \rangle \langle pic | W^{(i)} | qid \rangle} &= [\delta_{mp}\delta_{nq}\delta_{ac}\delta_{bd} + \delta_{mq}\delta_{np}\delta_{ad}\delta_{bc}] \\ &\quad \times |Q_{mn}^{(i)}|^2 \overline{(V_{ab}^{(i)})^2} , \quad i = 1, 2 , \\ \overline{\langle 1am | W^{(1)} | 1bn \rangle \langle 2cp | W^{(2)} | 2dq \rangle} &= 0 . \end{aligned} \tag{45}$$

The overbar denotes the average over the ensemble. The second of Eqs. (45) shows that $W^{(1)}$ and $W^{(2)}$ are uncorrelated. In the first of Eqs. (45) we assume standard random-matrix properties. We assume that the coupling of the system S to the heat bath described by the matrices $Q^{(i)}$ acts only on the (left or right) surface of the system and not on its volume. For the matrices $V^{(i)}$ we assume

as in Ref. [17] that with $i = 1, 2$

$$\overline{[V_{ab}^{(i)}]^2} = A_0^{(i)} [\rho^{(i)}(\varepsilon_a) \rho^{(i)}(\varepsilon_b)]^{-1/2} \exp[-(\varepsilon_a^{(i)} - \varepsilon_b^{(i)})^2 / (2\Delta_i^2)] \quad (46)$$

where $A_0^{(i)}$ and Δ_i are constants and where

$$\rho^{(i)}(\varepsilon) \approx \rho_0^{(i)} \exp(\beta_i \varepsilon) \quad (47)$$

is the level density and $\beta_i = 1/T_i$ the inverse temperature of the heat bath labelled (i).

The sum $\sum_i W^{(i)}$ is also a Gaussian random variable with mean value zero. This fact suffices to derive for the average density matrix $\overline{\rho(t, t')}$ of the total system governed by \mathcal{H} the integral equation

$$\overline{\rho(t, t')} = \overline{U(t)} \rho(0, 0) \overline{U^\dagger(t)} + \int_0^t d\tau \int_0^{\tau'} d\tau' \overline{U(t - \tau)} \overline{W \rho(\tau, \tau') W} \overline{U^\dagger(t' - \tau')} . \quad (48)$$

The averaged time-evolution operator obeys

$$\begin{aligned} \overline{U(t)} &= \exp[-iH_0 t] - \int_0^t dt_1 \int_0^{t_1} dt_2 \exp[-iH_0(t - t_1)] \\ &\quad \times \overline{W \exp[-iH_0(t_1 - t_2)] W} \overline{U(t_2)} . \end{aligned} \quad (49)$$

With the help of the assumptions (45) it is easily seen that

$$\begin{aligned} \langle m1a2b | \overline{U(t)} | n1c2d \rangle \\ = \delta_{mn} \delta_{ac} \delta_{bd} \exp[-i(E_m + \varepsilon_a^{(1)} + \varepsilon_b^{(2)})t - (1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t] \Theta(t) \end{aligned} \quad (50)$$

where $\Theta(t)$ is the Heaviside function and where

$$\Gamma_{ma}^{(i)} = 2\pi \sum_{nb} \overline{\langle mia | W^{(i)} | nib \rangle^2} \delta(E_m + \varepsilon_a^{(i)} - E_n - \varepsilon_b^{(i)}) , \quad i = 1, 2 . \quad (51)$$

In Eq. (50) the sum of two Γ 's appears because $W^{(1)}$ and $W^{(2)}$ are uncorrelated and may cause different damping.

We take the trace of Eq. (48) with respect to both heat baths and obtain

$$\begin{aligned} \sum_{ab} \langle m1a2b | \overline{\rho(t, t')} | n1a2b \rangle &= \sum_{ab} \exp[-i(E_m t - E_n t')] \\ &\quad \times \exp[-i(\varepsilon_a^{(1)} + \varepsilon_b^{(2)})(t - t')] \\ &\quad \times \exp[-(1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t - (1/2)(\Gamma_{na}^{(1)} + \Gamma_{nb}^{(2)})t'] \\ &\quad \times \langle m1a2b | \rho(0, 0) | n1a2b \rangle \\ &+ \delta_{mn} \sum_{ab} \int_0^t d\tau \int_0^{\tau'} d\tau' \exp[-i(E_m + \varepsilon_a^{(1)} + \varepsilon_b^{(2)})(t - \tau)] \end{aligned}$$

$$\begin{aligned}
& \times \exp[-(1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})(t - \tau)] \\
& \times \left(\sum_{nc} |\langle m1a2b | W^{(1)} | n1c2b \rangle|^2 \langle n1c2b | \overline{\rho(\tau, \tau')} | n1c2b \rangle \right. \\
& \left. + \sum_{nd} |\langle m1a2b | W^{(2)} | n1a2d \rangle|^2 \langle n1a2d | \overline{\rho(\tau, \tau')} | n1a2d \rangle \right) \\
& \times \exp[i(E_m + \varepsilon_a^{(1)} + \varepsilon_b^{(2)})(t' - \tau')] \\
& \times \exp[-(1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})(t' - \tau')] . \tag{52}
\end{aligned}$$

The Kronecker delta on the right-hand side of Eq. (52) follows from the first of Eqs. (45). Eq. (52) shows that the nondiagonal elements of the reduced density matrix of system S decay exponentially in time. Therefore, we focus attention on the diagonal elements with $m = n$, for $t = t'$ denoted by $P_n(t)$. We differentiate Eq. (52) with respect to t and t' . In the resulting gain terms we use the weak-coupling assumption and the resulting Markov approximation. We make use of Eqs. (46) and (47). With

$$W_{nm}^{(i)}(T_i) = 2\pi A_0^{(i)} |Q_{nm}^{(i)}|^2 \exp[-(E_n - E_m)^2 / (2\Delta_i^2)] \exp[(1/2)\beta_i(E_m - E_n)] \tag{53}$$

that yields Eqs. (1) and (2).

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