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. Due to this 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 [2–4].

In this paper we offer an analytical resolution of the resulting paradox. We focus our 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 $1/\sum_m \exp[-E_m/(k_BT_0)]$ 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 [2, 3].

Work on the heat conductance in quantum mechanics has a long history, starting with [5–7], 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 [8–11] and the review [4] where further references may be found. This 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

\[
\sum_m \left( W^{(1)}_{mn}(T_1) + W^{(2)}_{mn}(T_2) \right) P_m = \left( \sum_m \left( W^{(1)}_{mn}(T_1) + W^{(2)}_{mn}(T_2) \right) \right) P_m.
\]

(1)

The derivation and conditions of validity of equation (1) have been thoroughly discussed in the literature, see for instance [12]. To fix our notation, we give a brief derivation of equation (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 equation (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 equation (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 equation (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 equation (A.10) these obey

\[
W_{mn}^{(i)}(T_i) = X_{mn}^{(i)} \exp\left[ (\beta_i/2)(E_m - E_n) \right],
\]

(2)

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

\[
W_{mn}^{(i)}(T_i) = \exp[\beta_i(E_m - E_n)] X_{mn}^{(i)}(T_i).
\]

(3)

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

\[
P_{\text{eq}}^n = \frac{\exp[-\beta E_n]}{\sum_m \exp[-\beta E_m]}.
\]

(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. Equation (1) takes the form

\[
\sum_m X_{mn} \left( \exp[\beta_1(E_m - E_n)] + \exp[\beta_2(E_m - E_n)] \right) P_m
\]

\[
- \left( \exp[\beta_1(E_n - E_m)] + \exp[\beta_2(E_n - E_m)] \right) P_n \right) = 0.
\]

(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 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 equation (1) with $E_n$ and sum over $n$. We obtain

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

Equation (6) expresses energy conservation. We interpret the negative left- and the positive right-hand side of equation (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 equation (1) around some intermediate temperature $T_0$ that obeys $T_1 < T_0 < T_2$ in powers of $\delta T$ up to and including terms linear in $\delta T$. 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

$$
\frac{\partial W(i)}{\partial T} = \frac{1}{2T^2} (E_n - E_m) W^{(i)} ,
$$

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

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

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

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

and the vectors

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

We note that

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

The master equation takes the form

$$
\sum_i (-)^i A_i^{(i)} \delta T + \sum_i \sum_m B_{mn}^{(i)} \delta P_m - \left( \sum_i \sum_m B_{mn}^{(i)} \right) \delta P_n = 0.
$$

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

$$
\sum_m \delta P_m = 0.
$$

That is the solution we study in what follows.
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, $X_{mn}^{(1)} = a X_{mn}^{(2)}$ with $a > 0$; and (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 $T_0 = \frac{1}{2} (T_1 + T_2)$.\(^{(14)}\)

We have $B_{mn}^{(1)} = B_{mn}^{(2)} = B_{mn}$ so that $\sum_j (-)^j A_j^{(i)} = 0$ for all $m$. Therefore, the solution of equation (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 $\delta T$. 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 $\delta T$.\(^{(15)}\)

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 equation (6) up to terms linear in $\delta T$. That gives

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

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 $\delta P_m$’s may only be caused by an improper choice of $T_0$.

3.2. Similar couplings

We turn to case (ii) where $X_{mn}^{(1)} = a X_{mn}^{(2)}$ 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

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

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

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

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

$$ T_0 = \frac{1}{1 + a} (a T_1 + T_2). $$

Thus, the system $S$ is in thermal equilibrium at the temperature $T_0$ given by equation (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

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

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

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

\[ [-2(1 - \alpha) A^{(1)}_m + 2\alpha A^{(2)}_m] \delta T + \sum_m \tilde{B}_{mn} \delta P_m = 0. \] (20)

We have \( \sum_m \tilde{B}_{nm} = 0 \). Therefore, the matrix \( \tilde{B}_{mn} \) possesses one vanishing eigenvalue, say \( \lambda_1 \), with the associated eigenvector \( \{1, 1, \ldots, 1\}^T \). The matrix \( \tilde{B} \) can be diagonalized by a real orthogonal matrix \( O \),

\[ O \tilde{B} O^T \delta m = \delta_{mn} \lambda_m. \] (21)

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

\[ [-2(1 - \alpha) \tilde{A}_m^{(1)} + 2\alpha \tilde{A}_m^{(2)}] \delta T = \lambda_m \delta \tilde{P}_m. \] (22)
Solving for $\delta P_m$ and transforming back to $\delta P_m$ we find

$$\delta P_m = \delta T \sum_n \left( \sum_{k \geq 2} \left( \sum_{n} \Omega_{kn} \frac{1}{\lambda_k} \right) \right) \left[ -2(1 - \alpha) A_n^{(1)} + 2 \alpha A_n^{(2)} \right].$$  

(23)

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

$$P_m = \frac{\exp[-\beta_0 E_m]}{\sum_n \exp[-\beta_0 E_n]} \left( 1 + \delta P_m - \frac{\sum_n \exp[-\beta_0 E_n] \delta P_n}{\sum_n \exp[-\beta_0 E_n]} \right).$$  

(24)

Insertion of equation (23) into (24) gives the occupation probabilities of the states $m$. The solutions $\delta P_m$ do not vanish identically for any choice of $\alpha$, 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 equation (6). In terms of the solutions (23) $I$ is given by

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

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

(25)

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

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

(26)

For equal couplings we have $\tilde{A}_k^{(1)} = \tilde{A}_k^{(2)}$ and the right-hand side of equation (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 equation (26) vanishes for $\alpha = 1/(1 + \alpha)$. In the present case of dissimilar couplings, the expression in big round brackets is linear in $\alpha$ and, therefore, vanishes at some uniquely defined value $\alpha_1$. That value defines via equation (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, $\alpha_1$ obeys $0 \leq \alpha_1 \leq 1$. Values of $\alpha_1$ outside the interval $[0, 1]$ would be physically implausible. Similar considerations apply to the second of equations (25). Again there exists a value of $\alpha_2$ and an associated temperature $T_{0}^{(2)}$ for which the term linear in $\delta P_n$ 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 equations (25) we obtain for the heat current

$$I = \frac{1}{\sum_n \exp[-\beta_0 E_n]} \left( \frac{1}{\langle T_0^{(1)} \rangle} \right) (1 - \alpha_1) \sum_{mn} (E_m - E_n)^2 B_{mn}^{(1)} (T_{0}^{(1)}) \delta T$$

$$= \frac{1}{\sum_n \exp[-\beta_0 E_n]} \left( \frac{1}{\langle T_0^{(2)} \rangle} \right) \alpha_2 \sum_{mn} (E_m - E_n)^2 B_{mn}^{(2)} (T_{0}^{(2)}) \delta T.$$  

(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,
\[ I = C \delta T, \]
the heat conductance \( C \) can always be written as an equilibrium coefficient of the form
\[ C = \gamma T_0^2 \sum_m \exp[-\beta_0 E_m] \sum_{mn} (E_m - E_n)^3 \exp[-(\beta_0/2)(E_m + E_n)]X_{mn}. \]
That expression may be viewed as a special case of the Green–Kubo formula [5, 6]. Here \( \gamma \) 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 [2–4].

To this end we rewrite the terms appearing in equation (29), using definition (9):
\[ \sum_m \exp[-\beta_0 E_m] = \int dE \exp[-\beta_0 E] \sum_mE, \]
\[ \sum_{mn} (E_m - E_n)^2 B_{mn} = \sum_{mn} (E_m - E_n)^2 \exp[-\beta_0 (E_m + E_n)]X_{mn} \]
\[ = \int d\epsilon_1 \int d\epsilon_2 (\epsilon_1 - \epsilon_2)^2 \exp[-\beta_0 (\epsilon_1 + \epsilon_2)]2\pi A_0 \exp[(\epsilon_1 - \epsilon_2)^2/\Delta^2] \times \sum_{mn} |Q_{mn}|^2 \delta(\epsilon_1 - E_m)\delta(\epsilon_2 - E_n). \]
We have used equations (2) and (A.10) 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 equation (A.3). 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 equation (30) is due to sums involving \( \delta(E - E_m) \). Such sums appear differently in the first and in the second of equations (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 equations (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 equations (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
\[ \sum_m |Pm\rangle \delta(E - E_m)\langle mP| = -\frac{1}{\pi} P \sum_{E^\dagger - H_S} P \]
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 equation (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, labeled by a running index $k = 1, \ldots, K$. The length of $S$ is then given by $L = K l$, 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

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

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 $P H_S P = P H^{(1)} P$. In the first block, we introduce a complete set of orthonormal basis states $|\mu\rangle$ where $\mu = 1, 2, \ldots$. 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 equation (31) we consider

$$-\frac{1}{\pi} \sum_{\mu=1}^{n} \frac{1}{E^* - H_S} |\mu\rangle \langle 1|. \quad (34)$$

Without loss of generality we confine ourselves here to the diagonal element of the propagator with respect to the state with $\mu = 1$. Any other value of $\mu$ 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 $V_\nu = H^{(1)}_{\nu\nu}$ for $\nu \geq 2$, the matrix $H^{(1)}$ in equation (33) is explicitly written as

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

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 $k = 1, 2, \ldots, K$ are uncorrelated and are members each of the Gaussian orthogonal ensemble (GOE) of random matrices of dimension $N$, with the limit $N \to \infty$ eventually taken [13]. Ensemble averages are denoted by angular brackets. The matrix elements are Gaussian-distributed random variables with mean values zero and for $k, l, m = 1, 2, \ldots, K$ obey

$$\langle H^{(k)}_{\mu\nu} H^{(k')}_{\mu'\nu'} \rangle = \lambda^2 N \frac{1}{N} \delta_{\mu\mu'} \delta_{\nu\nu'} + \delta_{\mu\mu'} \delta_{\nu\nu'},$$

$$\langle W^{(k)}_{\mu\rho} W^{(k')}_{\mu'\rho'} \rangle = \frac{w^2}{N} \delta_{kk'} \delta_{\mu\rho'} \delta_{\mu'\rho} + \delta_{\mu'\rho} \delta_{\mu\rho'} \delta_{\nu'\nu},$$

$$\langle H^{(k)}_{\mu\nu} W^{(k')}_{\rho\nu} \rangle = 0. \quad (36)$$

Because of these assumptions the average spectrum of each of the matrices $H^{(k)}$ with $k \geq 2$ has for $N \to \infty$ the shape of a semicircle with radius $2\lambda$. 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 equations (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 $V_\mu$ in equation (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 $N \to \infty$ the spectrum of $H^{(1)}$ is also of semicircular form but the surface state plays a distinct role.

The random-matrix model introduced in equations (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 equations (36). To this end we calculate the average Green’s 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 $N \to \infty$ the Pastur equation [16]

$$EG(E) = 1 + \langle H_S G(E) H_S \rangle G(E). \tag{37}$$

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

$$EG^{(1)}_{11}(E) = 1 + v^2 NG^{(1)}_{11},$$

$$EG^{(k)}(E) = 1 + [\lambda^2 G^{(k)} + w^2 G^{(k-1)} + w^2 G^{(k+1)}] G^{(k)}.$$ \tag{38}

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

$$G^{(1)}_{11}(E) = \frac{1}{E - v^2 NG^{(1)}}. \tag{39}$$

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 equations (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 equation (33) suggests that $G^{(k)}$ changes slowly with $k$. We accordingly put $G^{(k)} = G^{(k-1)} = G^{(k+1)}$. With

$$(\lambda')^2 = \lambda^2 + 2w^2 \tag{40}$$

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

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

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 $4\lambda$ 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 either end of the system, i.e. $k$-values close to 1 or $K$, the form of $H_S$ in equation (33) and the form of equations (38) suggest that the solutions retain the form (41) but with values of $\lambda'$ that are smaller than given in equation (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 equations (38) yield average spectra of approximately semicircular shape with ranges $\lambda'$ 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 $\Delta E$ 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 $\lambda'$ 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

$$-\frac{1}{\pi} \sum_k G(k)(E).$$

The width $2\sqrt{N/\lambda}$ of the strength function of the state $|1\rangle$ is essentially given by the total strength $N\sqrt{\lambda}$ 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 $N\sqrt{\lambda}$ nor $\lambda'$ depend on the length of the system. Result (42) can easily be extended by taking into account the full form of the propagator in equation (41) and by dropping the assumption $E_1 = 0$. Instead of the form (42) one obtains an expression of the 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 equation (32). From the definition of $G(k)$ it follows that

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

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 equation (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 equation (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 this fact guarantees the length independence of the relevant term in equation (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 ensure quantum coherence, electron transport is experimentally studied close to 0 K. 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 endpoints 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 [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 equation (1). We only sketch those parts of the derivation that differ from [17] and do not repeat here the discussion of the conditions under which the derivation holds. These are the same as in [17].

The quantum system $S$ has Hamiltonian $H_S$, eigenvalues $E_m$, and eigenfunctions $|m\rangle$, with $m = 1, 2, \ldots$. With $i = 1, 2$ the two baths have Hamiltonians $H_i$, eigenvalues $\epsilon_{ia}$ and eigenfunctions $|ia\rangle$, respectively, with $a = 1, 2, \ldots$. 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 $V^{(i)}_{ab}$ are uncorrelated random matrices to be specified below. The total Hamiltonian is

$$H = H_S + H_1 + H_2 + \sum_i W^{(i)}$$

$$= H_0 + W. \quad (A.1)$$
To define the ensemble we consider case (II) of [17] and assume that the \( W^{(i)} \) are Gaussian-distributed random variables with zero mean values and second moments given by

\[
\langle m | W^{(i)} | n b \rangle (q i c | W^{(i)} | q i d) = [\delta_{ma} \delta_{ab} \delta_{cd} + \delta_{mb} \delta_{ac} \delta_{bd}] \times |Q_{mn}^{(i)}|^2 (V_{ab}^{(i)})^2, \quad i = 1, 2.
\]

The overbar denotes the average over the ensemble. The second of equations (A.2) shows that \( W^{(1)} \) and \( W^{(2)} \) are uncorrelated. In the first of equations (A.2) 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 [17] that with \( i = 1, 2 \)

\[
\left[ V_{ab}^{(i)} \right]^2 = A_0^{(i)} [\rho^{(i)}(\varepsilon_a) \rho^{(i)}(\varepsilon_b)]^{-1/2} \exp \left[ -\left( \varepsilon_a^{(i)} - \varepsilon_b^{(i)} \right)^2 / (2\Delta_i^2) \right]
\]

where \( A_0^{(i)} \) and \( \Delta_i \) are constants and where

\[
\rho^{(i)}(\varepsilon) \approx \rho_0^{(i)} \exp(\beta_i \varepsilon)
\]

is the level density and \( \beta_i = 1/T \) the inverse temperature of the heat bath labeled \( (i) \).

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

\[
\rho(t, t') = U(t) \rho(0, 0) U^\dagger(t) + \int_0^t \! dt \int_0^{t'} \! dt' U(t - \tau) W \rho(\tau, \tau') W^\dagger U(t' - \tau').
\]

The averaged time-evolution operator obeys

\[
\overline{U(t)} = \exp[-i\mathcal{H}_0 t] - \int_0^t \! dt_1 \int_0^{t_1} \! dt_2 \exp[-i\mathcal{H}_0 (t - t_1)]
\times \overline{W} \exp[-i\mathcal{H}_0 (t_1 - t_2)] \overline{W} U(t_2).
\]

With the help of the assumptions (A.2) it is easily seen that

\[
\langle m 1 a 2 b | \overline{U(t)} | n 1 c 2 d \rangle = \delta_{ma} \delta_{ac} \delta_{bd} \exp \left[ -i(E_m + \varepsilon_a^{(1)} + \varepsilon_b^{(2)})t - (1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t \right] \Theta(t)
\]

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

\[
\Gamma_{ma}^{(i)} = 2\pi \sum_{ab} \langle m a | W^{(i)} | n b \rangle^2 \delta(E_m + \varepsilon_a^{(1)} - E_n - \varepsilon_b^{(1)}), \quad i = 1, 2.
\]

In equation (A.7) the sum of two \( \Gamma \)'s appears because \( W^{(1)} \) and \( W^{(2)} \) are uncorrelated and may cause different damping.

We take the trace of equation (A.5) with respect to both heat baths and obtain

\[
\sum_{ab} \langle m 1 a 2 b | \rho(t, t') | n 1 a 2 b \rangle = \sum_{ab} \exp[-i(E_m t - E_n t') \exp \left[ -i(\varepsilon_a^{(1)} + \varepsilon_b^{(2)})t - (1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t \right] \sum_{ab} \rho(0, 0) | n 1 a 2 b \rangle
\times \exp \left[ -(1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t - (1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t' \right] \langle m 1 a 2 b | \rho(t, t') | n 1 a 2 b \rangle
\times \exp \left[ -(1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t - (1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t' \right]
\]

\[
+ \delta_{mn} \sum_{ab} \int_0^t \! dt \int_0^{t'} \! dt' \exp \left[ -i(E_m + \varepsilon_a^{(1)} + \varepsilon_b^{(2)})t - (1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t \right]
\times \exp \left[ -(1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t - (1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t' \right]
\]

\[
\times \exp \left[ -i(E_m + \varepsilon_a^{(1)} + \varepsilon_b^{(2)})t - (1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t \right]
\]

\[
\times \exp \left[ -(1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t - (1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t' \right]
\]

\[
\times \exp \left[ -i(E_m + \varepsilon_a^{(1)} + \varepsilon_b^{(2)})t - (1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t \right]
\]

\[
\times \exp \left[ -(1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t - (1/2)(\Gamma_{ma}^{(1)} + \Gamma_{mb}^{(2)})t' \right]
\]
\[
\times \left( \sum_{nc} \langle m1a2b \mid W^{(1)} \mid n1c2b \rangle^2 \langle n1c2b \mid \rho(\tau, \tau') \mid n1c2b \rangle + \sum_{nd} \langle m1a2b \mid W^{(2)} \mid n1a2d \rangle^2 \langle n1a2d \mid \rho(\tau, \tau') \mid n1a2d \rangle \right)
\times \exp \left[ i (E_m + \varepsilon_a^{(1)} + \varepsilon_b^{(2)}) (t' - \tau') \right] \exp \left[ -\frac{1}{2} (\Gamma_m^{(1)} + \Gamma_m^{(2)}) (t' - \tau') \right].
\]

Equation (A.9) shows that the nondiagonal elements of the reduced density matrix of the 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 equation (A.9) 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 equations (A.3) and (A.4). With

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

that yields equations (1) and (2).

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