Fourier's law: Insight from a simple derivation

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The onset of Fourier's law in a one-dimensional quantum system is addressed via a simple model of weakly coupled quantum systems in contact with thermal baths at their edges. Using analytical arguments we show that the crossover from the ballistic (invalid Fourier's law) to diffusive (valid Fourier's law) regimes is characterized by a thermal length scale, which is directly related to the profile of the local temperature. In the same vein, dephasing is shown to give rise to classical Fourier's law, similarly to the onset of Ohm's law in mesoscopic conductors.

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I. INTRODUCTION

Fourier's law of heat conduction [1] states that when a system is subject to a temperature difference, a uniform temperature gradient $\nabla T(\mathbf{r})$ ensues in its interior, and the heat current density $\mathbf{j}(\mathbf{r})$ is proportional to that gradient, $\mathbf{j}(\mathbf{r}) = -k\nabla T(\mathbf{r})$. The proportionality constant k is called thermal conductivity and could be position dependent.

Although this law is almost two centuries old, a general demonstration, or a set of conditions for its validity in the general case, is still lacking [2,3]. The problem has recently received renewed attention, both theoretically [4,5] and experimentally [6], especially in quantum systems, due to the growing interest in energy transport at the nanoscale, whose understanding is an important step toward utilizing nanostructures for possible energy applications [7–9].

The difficulty in proving this law from first principles is twofold. For one, a local temperature (in an inherently out-of-equilibrium situation) needs to be defined. Second, a local heat current needs to be calculated and these two quantities need to be compared. Both of these quantities are difficult to evaluate for the simple reason that they are usually neither well defined (like the case of the local temperature [10,11]) nor their definition is unique (for the case of the heat current [12]). In the quantum case, an additional complication arises which is related to the fact that the size of the Hilbert space of a given system generally increases exponentially with system size [13], so that the problem easily becomes computationally very demanding.

In recent years, several models have been put forward where Fourier's law has been studied microscopically [14–27], all of which employ in some way the idea of local equilibrium. The local temperature is usually either calculated from the expectation value of some local energy operator [16,23,28,29], or a uniform temperature gradient is assumed to exist [12]. An alternative route is to study the energy diffusion in closed systems (i.e., without thermal baths) [30], or to study a system with self-consistent reservoirs [22,25,26].

In Ref. [5], the present authors utilized a novel scheme from the theory of open quantum systems [13] to calculate the local temperature and the onset of Fourier's law in electronic quantum wires. The main findings were that for a ballistic system Fourier's law is invalid, and the temperature is constant along the wire. A temperature gradient develops as disorder is introduced in the wire, eventually leading to the onset of Fourier's law. These results, however, relied on numerical simulations and no simple analytical form could be deduced.

In this paper we aim at calculating analytically both the local temperature and the heat current for a model one-dimensional quantum system. Our results indicate that Fourier's law is related to a thermal length scale, either quantum (localization length) or classical (dephasing length), which is reflected in the local temperature profile. Fourier's law is then valid only if this thermal scale is smaller than the system length. In particular, dephasing gives rise to a classical Fourier's law, similarly to the onset of Ohm's law in mesoscopic conductors.

II. MODEL

We consider a set of N weakly connected identical subsystems, S_n. Each subsystem S_n has its own Hamiltonian $\mathcal{H}_n = \Sigma_k \epsilon_k |k^{(n)}\rangle\langle k^{(n)}|$, where $|k^{(n)}\rangle$ are the many-body state vectors of S_n. The subsystems are connected via a tunneling Hamiltonian $\mathcal{H}_{n,n+1} = \Sigma_{k,k'} V_{kk'} |k^{(n)}\rangle\langle k^{(n+1)}| + \text{H.c.}$ The full Hamiltonian is then $\mathcal{H} = \Sigma_n (\mathcal{H}_n + \mathcal{H}_{n,n+1})$.

Here we assume that only the left-most and right-most subsystems (S_L and S_R) are connected to external environments, and are consequently held at temperatures T_L and T_R, respectively. The other subsystems are not coupled to an external environment, and hence transitions between states in the central subsystems have to be mediated by the edge subsystems. The model is schematically depicted in Fig. 1.

III. LOCAL TEMPERATURE

The aim of the calculation is to evaluate the local temperature of S_n as a function of T_L, T_R, and n—which serves

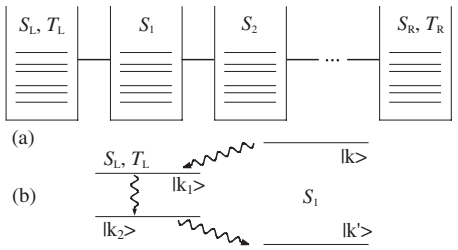

FIG. 1. (a) Schematic representation of the model. The system consists of identical, weakly connected subsystems. The left- and right-most subsystems are held at temperatures T_L and T_R, respectively. (b) Representation of the transition process in S_1 (see text).

as a position variable. The main *assumption* of the model is that the tunneling interaction is weak enough so that each subsystem is in a local thermal equilibrium at a certain temperature T_n, described below.

Let us start by considering only $\mathcal{H}_L$ and a single additional subsystem $\mathcal{H}_1$. By stating that S_L is maintained at a temperature T_L, we assume that it is in a local thermal equilibrium. Like the finiteness of the system, this implies that momentum is not conserved. Due to the external environment (which determines the temperature), there are transitions between different states k and k', which are defined via the scattering rates $W^{(L)}_{k\to k'}$. The statistical meaning of the temperature is that there is a single number T_L, which characterizes all the different transitions by a single rule of detailed balance. This means that regardless of k and k', the transition rates obey $\frac{W^{(L)}_{k\to k'}}{W^{(L)}_{k'\to k}}=\exp(-\frac{\Delta\epsilon_{kk'}}{T_L})$ (taking $k_B=\hbar=1$ throughout the paper), where $\Delta\epsilon_{kk'}=\epsilon_{k'}-\epsilon_k$.

Now consider the system S_1. Since S_1 is described in the energy basis, a transition between states in S_1 is an inelastic process, which (in the absence of interactions) requires the presence of an environment. Since the only subsystem in contact with an environment is S_L, for a particle in a state k in S_1 to scatter to a different state k' in S_1, a scattering event to some state k_1 in S_L has to first occur. From that state, another transition will occur to a state k_2 in S_L and a final transition to k' [this process is depicted in Fig. 1(b)]. Thus, the transition rate in S_1 is given by

$$W^{(1)}_{k\to k'}=\sum_{k_1,k_2}\Gamma^{1\to L}_{k\to k_1}W^{(L)}_{k_1\to k_2}\Gamma^{L\to 1}_{k_2\to k'}, \tag{1}$$

where $\Gamma^{n\to n+1}_{k\to k'}$ is a transition probability from the state k in n to the state k' in n', and is therefore proportional to the overlap between $|k^{(n)}\rangle$ and $|k'^{(n')}\rangle$, and hence to $|V_{kk'}|^2$ (in similarity to the Fermi golden rule). We now assume that the main contribution comes from states of the same energy, and for simplicity we take a uniform tunneling Hamiltonian, i.e., $V_{kk}=V$, which yields $\Gamma^{n\to n+1}_{k\to k'}=\Gamma\,\delta_{kk'}$. This implies

$$W^{(1)}_{k\to k'}=\gamma W^{(L)}_{k\to k'}, \tag{2}$$

where $\gamma=\Gamma^2$ [note that in our notation states labeled by k may belong to different subsystems, denoted by the upper index (n)]. Now, the temperature of S_1 may be obtained from the detailed balance of S_1, via $\frac{W^{(1)}_{k\to k'}}{W^{(1)}_{k'\to k}}=\exp(-\frac{\Delta\epsilon_{kk'}}{T_1})$. Employing Eq. (1), the γ prefactor cancels and we find that $T_1=T_L$. This is a simple manifestation of the fact that two systems in contact with each other equilibrate.

The next step is to consider a chain of N subsystems, still only connected to the single S_L. The goal now is to find the temperature of S_n. One can repeat the procedure described above, with the only change being that n intermediate, neighboring system transitions occur before the particles have a transition event at S_L. Therefore, a simple generalization gives $W^{(n)}_{k\to k'}=\gamma^n W^{(L)}_{k\to k'}$, which again gives $T_n=T_L$. This argument is valid to lowest order in γ, which physically corresponds to including only sequential tunneling processes.

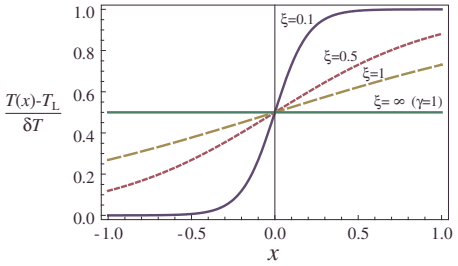

FIG. 2. (Color online) The (normalized) local temperature $[T(x)-T_L]/\delta T$ as a function of the position variable x. This figure should be compared with Fig. 1 of Ref. [5].

By considering the addition of the right-most system S_R and the edge of the N-long chain, one similarly obtains

$$W^{(n)}_{k\to k'}=\gamma^n W^{(L)}_{k\to k'}+\gamma^{N-n}W^{(R)}_{k\to k'}. \tag{3}$$

In this case, however, due to the presence of the right temperature T_R one cannot simply cancel out the prefactor, and the expression for T_L becomes more complex. In order to make progress, we assume that $T_R=T_L+\delta T$, $\delta T\ll T_L$, and assume that the transition rates take the form $W^{(L,R)}_{k\to k'}\propto\exp(-\frac{\Delta\epsilon_{kk'}}{2T_{L,R}})$ (a simple form in agreement with the assumption that S_L and S_R are at equilibrium). Substituting back into Eq. (2) and taking the first order in δT, we find (after some algebraic manipulation)

$$T_n\approx T_L+\delta T\frac{1}{1+\gamma^{2n-N}}. \tag{4}$$

Defining a position variable $x=\frac{2n}{N}-1$ we obtain $T(x)=\frac{1}{1+\exp(-x/\xi)}$, where $\xi=(N\,|\log\,\gamma|)^{-1}$ is the "thermal length" that defines the length-scale over which there is an (approximately) uniform temperature gradient.

In Fig. 2 we plot $[T(x)-T_L]/\delta T$ (which scales from 0 to 1) as a function of position variable x, for different values of $\xi=0.1,0.5,1$ and $\xi=\infty$, which corresponds to $\gamma=1$. For small values of γ (and hence of ξ), most of the temperature change is close to the middle of the wire. In those regions, a uniform temperature gradient is indeed developed, and hence Fourier's conjecture is valid. When $\gamma=1$ the temperature is uniform in the wire, no temperature gradient ensues. This figure should be compared with Fig. 1 of Ref. [5], which shows similar features, albeit obtained from a microscopic model (with no *a priori* assumptions).

We note that while strictly speaking the case $\gamma=1$ is beyond the above perturbation analysis, this result is still valid. This is because in the $\gamma=1$ case all the wave functions are delocalized and span the entire system. Thus, S_L and S_R have the same weight in the transition rates of S_n regardless of n, giving rise to a uniform temperature (which is just $T_n=T_L+\frac{1}{2}\delta T$ for a small temperature difference).

IV. HEAT CURRENT

The next step toward understanding Fourier's law in our model system is to calculate the heat current. If the subsystems are weakly coupled to each other, the local energy is

naturally defined [12] as $E_n=\langle \mathcal{H}_n \rangle$. From the continuity equation [5,12], one has a simple expression for the heat current, $j_n=-\Gamma(E_{n+1}-E_n)$ (taking the distance between the subsystems to be $a=1$). This definition for the heat current could be understood by noting that (under the assumption of a constant Γ) ΓE_{n+1} is simply the rate of energy flow from S_{n+1} to S_n, and vice versa, and thus j_n defined above describes the net energy flow between S_{n+1} and S_n per unit time, i.e., the heat current.

To calculate j_n, we assume that for each subsystem S_n we can define the probability $P_k^{(n)}$ to find the system in the state $|k^{(n)}\rangle$. Then, we have $E_n=\Sigma_k \epsilon_k P_k^{(n)}$, and for the heat current

$$\begin{aligned} j_n &= -\Gamma \sum_k \epsilon_k (P_k^{(n+1)} - P_k^{(n)}) \\ &\approx -\Gamma \sum_k \epsilon_k \frac{\partial P_k^{(n)}}{\partial n} \\ &= -\Gamma \sum_k \epsilon_k \frac{\partial P_k^{(n)}}{\partial T_n} \frac{\partial T_n}{\partial n}. \end{aligned} \tag{5}$$

Since we are assuming local thermal equilibrium, it follows that $P_k^{(n)} \propto \exp(-\epsilon_k / T_n)$, and hence $\frac{\partial P_k^{(n)}}{\partial T_n} = \frac{\epsilon_k}{T_n^2} P_k^{(n)}$. This gives for the heat current,

$$j_n = -\Gamma \sum_k \left(\frac{\epsilon_k^2 P_k^{(n)}}{T_n^2} \right) \nabla T(n) = -\kappa_n \nabla T(n), \tag{6}$$

where $\kappa = \frac{\Gamma \langle \epsilon^2 \rangle}{T_n^2}$, in agreement with the standard expectations [31,32]. Note that j is proportional to the temperature gradient, and hence the thermal conductance scales as L^{-1}, as required by Fourier's law. However, since the local temperature itself has a length dependence, the above rule strictly applies only within the thermal length $\xi/2$ from the center of the wire. Since in experiments the measured thermal conductivity κ is a global property (that is, an average of κ over the entire length of the sample) finite-size effects may take place and give unusual scaling for $\kappa(L)$ [6].

The fact that this simple model exhibits Fourier's law at weak coupling can also be understood by comparing it to the results of Ref. [32], in which a general form of Fourier's law is derived for a general system which obeys three conditions. Our model satisfies these conditions, and hence one indeed expects it to display Fourier's law.

However, we stress that the existence of a temperature gradient does not necessarily imply "normal" heat conduction. While in the system described here we have shown that the two are connected, in other systems, the nonlinear nature of the interactions may give rise to a finite temperature gradient but anomalous conductance [33].

V. DEPHASING

Up to now we have assumed that there is contact between the chain and the external environment only at the edges of the chain. Let us discuss the effect of local environments acting along the chain, which may result in the dephasing of the wave functions (in real systems this may be caused by, e.g., inelastic scattering off low-energy phonons). We thus introduce a length scale L_ϕ, which characterizes the length over which the wave function retains its phase. If $L_\phi > N$ then the dephasing has no effect, and Fourier's law is valid in its form of Eq. (4). However, in the case $L_\phi < N$, there is a new natural division of the system into subsystems of length L_ϕ [34]. Again, we assume that each of these subsystems is in local equilibrium, and interacts weakly with the neighboring subsystem. However, as opposed to the case discussed above, there is no coherent tunneling between the subsystems, but rather classical transport between them. Thus, the rate equations for the occupation probabilities in the subsystems may be written as [35]

$$\dot{P}_k^{(n)} = \Gamma_\phi (P_k^{(n+1)} - P_k^{(n)}) + \Gamma_\phi (P_k^{(n-1)} - P_k^{(n)}), \tag{7}$$

where, for simplicity, we have assumed that the transitions are between states of similar energies. Here $n=1,2,\ldots,N_\phi$ is the index of the subsystem, and the constant Γ_ϕ describes a typical transition rate between subsystems defined via the division to L_ϕ subsystems, and should in principal be determined microscopically.

Equation (7), along with the boundary conditions $P_k^{(\mathrm{L,R})} = P_{k,\mathrm{eqilibrium}}^{(\mathrm{L,R})} \propto \exp(-\epsilon_k / T_{\mathrm{L,R}})$, has a simple solution for its steady state, given by $P_k^{(n)} = P_k^{(\mathrm{L})} + \frac{n}{N}(P_k^{(\mathrm{R})} - P_k^{(\mathrm{L})})$. Assuming that $P_k^{(n)} \propto \exp(-\epsilon_k / T_n)$ and in the limit $T_\mathrm{R} - T_\mathrm{L} = \delta T \ll T_\mathrm{L}$ one obtains a linear form for the local temperature, $T_n \approx T_\mathrm{L} + \frac{n}{N}\delta T$. We thus conclude that *dephasing brings about the classical form of Fourier's law*. Explicit examples can be found in, e.g., Refs. [22,26], where local dephasing was introduced (in a quantum harmonic lattice and electronic system, respectively) by means of local external baths, giving rise to Fourier's law and a linear temperature profile.

It is also useful to consider the analogy between the effect of dephasing on the local temperature and on the resistance of a one-dimensional wire consisting of localized subsystems (i.e., an Anderson insulator) [36]. In the absence of dephasing ($L_\phi > N$) the resistance is exponential in the wire length, $R \sim \exp(N/\xi_{\mathrm{loc}})$, where ξ_{loc} is the localization length. However, when $L_\phi < N$, the resistances of different subsystems of length L_ϕ [each with a resistance of $R_\phi \sim \exp(L_\phi/\xi_{\mathrm{loc}})$] are connected in series, resulting in a linear dependence of the resistance on length, $R \sim R_\phi L / L_\phi$, i.e., classical Ohm's law. This crossover from a classical to a quantum regime is similar to what was demonstrated above in the case of Fourier's law.

VI. DISCUSSION

In summary, we have presented a simple model where the local temperature and heat currents may be evaluated analytically. We have shown that the onset of Fourier's law requires the presence of a local thermal equilibrium at each subsystem that constitutes the full system. It breaks down in the case of strong coupling between the subsystems. In that case, the temperature is constant throughout the sample. Including dephasing processes brings about a classical form of Fourier's law, in similarity to the onset of Ohm's law for the resistance.

The generality of these results may be understood by the following arguments. Consider a one-dimensional system held at a temperature difference δT. Now, the system may be broken into the smallest possible subsystems (S_n in the above calculation). If each such subsystem has a unique temperature which defines the relaxation rates between all the states in the subsystem, then the system is in local thermal equilibrium, and Fourier's law is valid. If not, the system may be coarse grained to generate larger subsystems, and again for each subsystem a local temperature is sought. If local thermal equilibrium is eventually obtained, then the number of coarse-grained subsystems describes the effective length of the system, and along with the interaction between the subsystems, it gives the thermal length ξ which determines the length scale for a uniform temperature gradient to ensue. However, if the coarse-graining procedure reaches the scale of the system, only a single temperature can be defined. In that case, the temperature is uniform across the sample, the thermal conductivity diverges, and Fourier's law is invalid. A similar phenomenon occurs in the presence of dephasing, where the role of the (quantum) thermal length is played by the dephasing length.

Recently, a crossover from ballistic to diffusive thermal transport was shown numerically to appear in a system with self-consistent reservoirs [25]. The crossover was determined from a length scale related to the coupling between the system and the baths, in a similar fashion to the dephasing length L_ϕ discussed above. Our results are in agreement with (and thus provide an intuitive explanation for) the numerical observations in Ref. [25]. However, there are indications that in certain models there is no length-dependent crossover [33]. Therefore, whether the onset of Fourier's law is always a crossover phenomenon seems to depend on the specific model and a satisfactory answer to this question has yet to be found.

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