

# Reconstructing Fourier's law from disorder in quantum wires

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The theory of open quantum systems is used to study the local temperature and heat currents in metallic nanowires connected to leads at different temperatures. We show that for ballistic wires the local temperature is almost uniform along the wire and Fourier's law is invalid. By gradually increasing disorder, a uniform temperature gradient ensues inside the wire and the thermal current linearly relates to this local temperature gradient, in agreement with Fourier's law. Finally, we show that while disorder is responsible for the onset of Fourier's law, the nonequilibrium energy distribution function is determined solely by the heat baths.

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## I. INTRODUCTION

The search for a microscopic derivation of Fourier's law,<sup>1</sup> or even a microscopic demonstration of it, is still a major theoretical challenge.<sup>2,3</sup> In recent years, the problem seems more relevant than ever due to both the continuous miniaturization of electronic devices and the need for alternative energy sources. Both these trends require better understanding of fundamental processes of energy transport in nanoscale systems. Following, there have been many theoretical studies of Fourier's law in various systems, both classical and quantum.<sup>4–15</sup> In the quantum regime, attention has been focused mainly on small spin chains<sup>4,9,16,17</sup> or quantum harmonic oscillators.<sup>10,18</sup>

However, little is known on the energy transport in nanoscale *electronic* quantum systems. This is true even for noninteracting electrons. One of the reasons for this is that in order to demonstrate the validity—or violation—of Fourier's law one needs to (i) define a local temperature out of equilibrium and show that it develops a uniform gradient, (ii) evaluate the local heat current, and (iii) show proportionality between these two quantities. The first task is especially difficult since temperature is a global equilibrium property, and it is not clear if a “local temperature” can be defined at all when the system is out of equilibrium.<sup>19</sup> For this reason, recent studies of the origin of Fourier's law either use a phenomenological definition of local temperature (as an expectation value of a local energy operator<sup>4,16,20</sup>) or assume that a temperature gradient is already present.<sup>21</sup> An alternative route is to study the energy diffusion in closed systems (i.e., without thermal baths)<sup>22</sup> or to study a system with self-consistent reservoirs.<sup>10,14</sup>

An additional reason that renders calculation of energy transport in electronic systems a formidable task is the fact that the size of the Hilbert space scales exponentially with the number of electrons (even for noninteracting ones), making numerical calculations very demanding. This is why previous numerical calculations on heat transport in quantum systems usually refer to very small systems, typically of the order of ten spins (see, however, Ref. 23).

Here we report a calculation of energy transport in electronic quantum wires that overcomes both the above issues. It is based on solving the quantum master equation for noninteracting electrons in the presence of dissipative baths

(held at different temperatures) in the Markov approximation. We use a recently suggested method<sup>24,25</sup> to map the many-electron problem to an effective single-particle system, which allows calculations for systems orders of magnitude larger than in previous studies and enables us to define a local temperature which is directly accessible experimentally, even out of equilibrium. We will discuss at the end of this paper the possible role of interactions and work in this direction.

## II. MODEL

The system consists of a linear chain bonded to small leads, which are connected to thermal baths held at different temperatures (upper panel of Fig. 1).<sup>24,25</sup> A similar setup was used for spin chains in, e.g., Ref. 26. The Hamiltonian of the system is given by  $\mathcal{H} = \mathcal{H}_L + \mathcal{H}_R + \mathcal{H}_d + \mathcal{H}_c$ , where  $\mathcal{H}_{L,R,d} = \sum_{i \in L,R,d} \epsilon_i c_i^\dagger c_i - t \sum_{\langle i,j \rangle \in L,R,d} (c_i^\dagger c_j + \text{H.c.})$  are the tight-binding Hamiltonians of the left lead ( $L$ ), right lead ( $R$ ), and wire ( $d$ ) (of length  $L_d$ ), respectively ( $t$  is the hopping integral, which serves as the energy scale hereafter).  $\mathcal{H}_c = (g_L c_L^\dagger c_{d,0} + g_R c_R^\dagger c_{d,L_d} + \text{H.c.})$  describes the coupling between the left (right) lead to the wire.  $c_{L(R)}^\dagger$  are creation operators for an electron at the point of contact between the left (right) lead and the wire, and  $c_{d,0}$  ( $c_{d,L_d}$ ) destroys an electron at the leftmost (right-most) sites of the wire. The on-site energies  $\epsilon_i$  are randomly drawn from a uniform distribution  $U[-W/2, W/2]$ , with  $W$  being the disorder strength. The lattice constant is taken to be  $a=1$ , and we consider here spinless electrons.

The quantity of interest, from which the required information (such as local temperature, heat current, etc.) may be extracted, is the single-particle density matrix, defined by  $\rho = \sum_{kk'} \rho_{kk'} |k\rangle \langle k'|$ , where  $\rho_{kk'} = \text{Tr}(c_k^\dagger c_{k'} \rho_{MB})$ ,  $\rho_{MB}$  is the full many-body density matrix, and  $|k\rangle$  are the single-particle states. In Refs. 24 and 25 it was shown that  $\rho$  obeys a master equation<sup>27</sup> (setting  $\hbar=1$ ),

$$\dot{\rho} = -i[\mathcal{H}, \rho] + \mathcal{L}_L[\rho] + \mathcal{L}_R[\rho] \equiv \hat{\mathcal{L}}[\rho], \quad (1)$$

where  $\mathcal{L}_{L(R)}[\rho]$  are superoperators acting on the density matrix, describing the left (right) thermal baths, held at temperature  $T_{L(R)}$ , and in contact with the left (right)-most side of the leads (solid lines in the upper panel of Fig. 1). The superop-

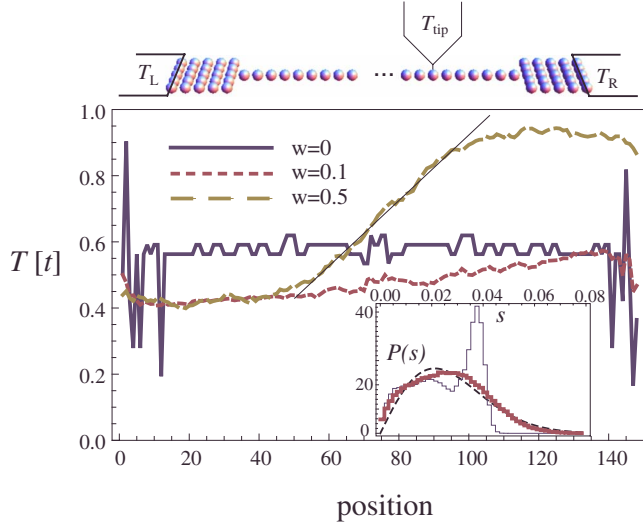


FIG. 1. (Color online) Local temperature as a function of position along the wire. The local temperature is calculated for three different values of disorder,  $W=0$  (solid),  $0.1$  (small dashes), and  $0.5$  (large dashes). For clean wires ( $W=0$ ) the temperature is uniform, and a uniform temperature gradient builds up as the disorder increases. The solid line is a guide for the eyes, pointing out the region from which the local thermal conductivity is calculated (Fig. 2 and text below). Upper panel: geometry of the model system. The solid lines at the edges correspond to the contact area of the thermal baths. Inset: energy-level spacing distribution for  $W=0.1$  (thin line) and  $W=0.5$  (thick line) and the Wigner-Dyson distribution (dashed line), marking the onset of chaos.

erators are defined in the Lindblad form<sup>27,28</sup> via  $V$  operators,  $\mathcal{L}[\rho] = \sum_{k,k'} (-\frac{1}{2}\{V_{kk'}^\dagger V_{kk'}, \rho\} + V_{kk'} \rho V_{kk'}^\dagger)$ , with  $\{\cdot, \cdot\}$  being the anticommutator. The  $V$  operators are generalized to account for the different baths and are given by<sup>25,26</sup>  $V_{kk'}^{(L,R)} = \sqrt{\gamma_{kk'}^{(L,R)} f_D^{(L,R)}(\epsilon_k)} |k\rangle\langle k'|$ , where  $f_D^{(L,R)}(\epsilon_k) = 1 / [\exp(\frac{\epsilon_k - \mu}{k_B T_{L,R}}) + 1]$  are the Fermi distributions of the left and right leads, with  $\mu$  as the chemical potential. The coefficients  $\gamma_{kk'}^{(L,R)} = |\sum_{\mathbf{r}_i \in S_{L,R}} \psi_k(\mathbf{r}_i) \gamma_0 \psi_{k'}^*(\mathbf{r}_i)|$  (where  $\psi_k(r)$  are the single-particle wave functions) describe the overlap between the single-particle states  $|k\rangle$  and  $|k'\rangle$  over the region of contact  $S_{L(R)}$  between the left (right) baths and the corresponding junction leads, shown by the solid lines in the upper panel of Fig. 1.  $\gamma_0$  describes the strength of electron-phonon (bath) interaction. The form above can be derived from first principles by tracing out the bath degrees of freedom, with the latter formed by a dense spectrum of boson excitations (e.g., phonons), which interact *locally* with electrons at the edges of the system.

### III. LOCAL TEMPERATURE

The nonequilibrium steady state of the system is given by the solution of the equation  $\hat{\mathcal{L}}[\rho] = 0$ . In order to calculate the local temperature, we attach a third thermal bath (described by an additional term  $\mathcal{L}_{\text{tip}}(r)[\rho]$  in the master equation) which is connected to a given position  $r$  of the wire and serves as an external probe (upper panel of Fig. 1). The re-

sulting equation for the steady state with the inclusion of this probe now reads  $[\hat{\mathcal{L}} + \mathcal{L}_{\text{tip}}(r)][\rho] = 0$ . The temperature  $T_{\text{tip}}$  of the additional operator is changed, and the resulting local density,  $n(r) = \sum_k \rho_{kk} |\psi_k(r)|^2$ , is compared to that obtained without the additional operator.<sup>29</sup> We then define the local temperature as that  $T_{\text{tip}}$  for which there is minimal change in the local density.<sup>25</sup> Physically, this corresponds to placing a local temperature probe in close proximity to the wire.<sup>30</sup> When the probe has the same local temperature of the wire, there is no net heat flow between them, and thus the local properties of the wire are unchanged.

Figure 1 shows the local temperature profile along a chain of length  $L_d = 150$ . The numerical parameters are the following: lead dimensions  $L_x = L_y = 3$ , temperature of the left and right leads is  $T_L = 0.1$  and  $T_R = 1$ , respectively, and electron number  $n_E = 56$  (corresponding to one third filling). The disorder strength is  $W=0$  (solid line),  $W=0.1$  (small dashes), and  $W=0.5$  (large dashes) and averaged over 500 realizations of disorder (all calculations in this paper were performed over a wide range of parameters, yielding similar conclusions). One can see several features from Fig. 1. The most prominent feature is the fact that for clean ( $W=0$ ) and weakly disordered ( $W=0.1$ ) wires, the temperature hardly changes along the wire. This is evidence that Fourier's law is violated under these conditions. Instead, a uniform temperature gradient at the center of the wire is recovered for large disorder ( $W=0.5$ ). Note that the local temperature is roughly constant up to a "thermal length" from the contacts. This length is determined by the coupling between the wire and the leads, and we have found in our simulations that with increasing wire length, the region of uniform temperature gradient increases and the thermal length remains constant.

In some systems the onset of Fourier's law seems to coincide with that of chaos<sup>4,18</sup> while in others this is not the case.<sup>5,7</sup> It is thus of interest to determine the relation between Fourier's law and chaos in the present context. In order to do so, we plot in the inset of Fig. 1 the distribution function  $P(s)$  for the level spacing  $s$  of neighboring single-particle energy levels for  $W=0.1$  (thin line) and  $W=0.5$  (thick line). The dashed line is the Wigner-Dyson distribution,  $P_{\text{WD}}(s) = s \exp(-\alpha s^2)$  (where  $\alpha$  is some constant), which is conjectured to correspond to the onset of quantum chaos.<sup>31</sup> As seen, the distribution for weak disorder shows features reminiscent of the ordered system and is very different from the Wigner-Dyson distribution. Accordingly, Fourier's law is invalid. On the other hand, for strong disorder we see both agreement with the Wigner-Dyson distribution and a uniform temperature gradient at the center of the wire, suggesting that indeed these have the same physical origin.<sup>32</sup>

### IV. HEAT CURRENT

The next step in validating Fourier's law comes from calculating the local heat current  $j(r)$  and evaluating the thermal conductivity  $\kappa$  such that  $j(r) = -\kappa(r) \nabla T(r)$ . It is clear that for a uniform temperature profile (as that of a clean wire), a finite heat current results in a divergent  $\kappa$ . On the other hand, for the system presented here one expects that the heat current is always finite, since energy is always injected and

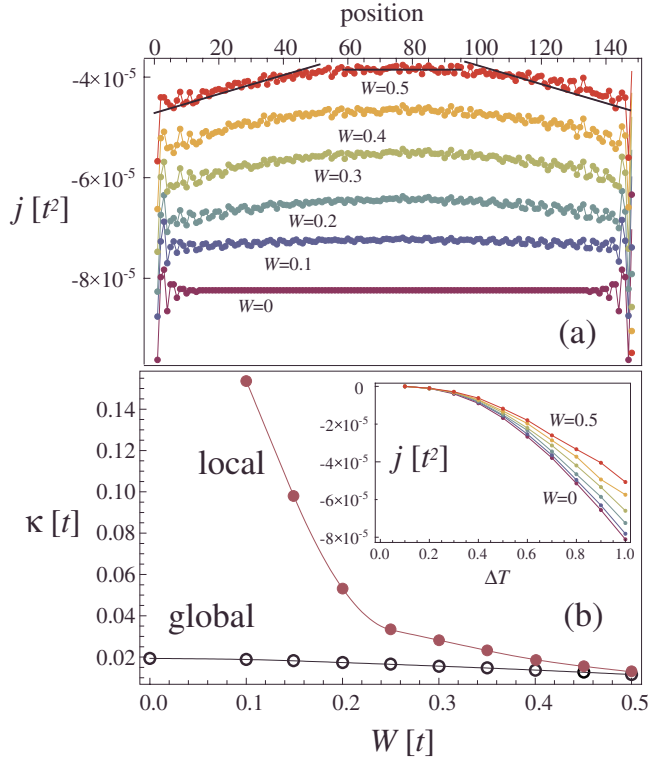


FIG. 2. (Color online) Local heat current and thermal conductivity. (a) Local heat current  $j$  as a function of position for different disorder strengths,  $W=0, 0.1, \dots, 0.5$ . The current is largest close to the leads, where the contact with the heat baths is located. The solid line on  $W=0.5$  is a guide for the eyes. (b) Local (solid circles) and global (empty circles) thermal conductivities as a function of disorder. The two tend to the same value only with increasing disorder when Fourier's law becomes valid. Inset: averaged heat current as a function of temperature difference  $\Delta T$  for different disorder strengths. From the linear regime of these curves the global thermal conductivity was evaluated.

extracted from the system. It is thus natural to define a global thermal conductivity,  $K = -\frac{L\bar{j}}{T_R - T_L}$ , where  $\bar{j}$  is the heat current averaged over the whole wire. Following this definition, it is evident that  $K = \bar{\kappa}$  (where  $\bar{\kappa}$  is the average over the wire of the local thermal conductivity defined via Fourier's law) only when Fourier's law is valid. This definition thus gives us a mean to point to the onset of Fourier's law.

To make this argument substantial one must calculate the local heat current. Due to the noninteracting form of the Hamiltonian of the system we can define the heat current operator via a time derivative of the local energy operator  $\hat{\mathcal{H}}_i$ , i.e.,  $\frac{d\hat{\mathcal{H}}_i}{dt} = \hat{j}_{i-1} - \hat{j}_i$  (in units of  $t^2$ , taking  $\hbar=1$ ).<sup>21,33</sup> The local energy operator in the wire is defined as  $\mathcal{H}_i = \epsilon_i |i\rangle\langle i| - \frac{1}{2}t(|i\rangle\langle i+1| + |i\rangle\langle i-1| + \text{H.c.})$ . The time derivative of a general operator  $\hat{O}$  under the Lindblad formalism is given by<sup>28</sup>  $\frac{d\hat{O}}{dt} = i[\mathcal{H}, \hat{O}] + \sum_{kk'} (-\frac{1}{2}\{V_{kk}^\dagger, V_{kk'}\}, \hat{O}\} + V_{kk}^\dagger \hat{O} V_{kk'})$ . From this relation one may find  $\hat{j}_i$  and calculate its expectation value,  $j_i$ .

In Fig. 2(a)  $j_i$  is plotted as a function of position along the wire (same parameters as in Fig. 1) for different values of disorder  $W=0, 0.1, \dots, 0.5$ . Note that in the central region of the wire the heat current is uniform and increases at a dis-

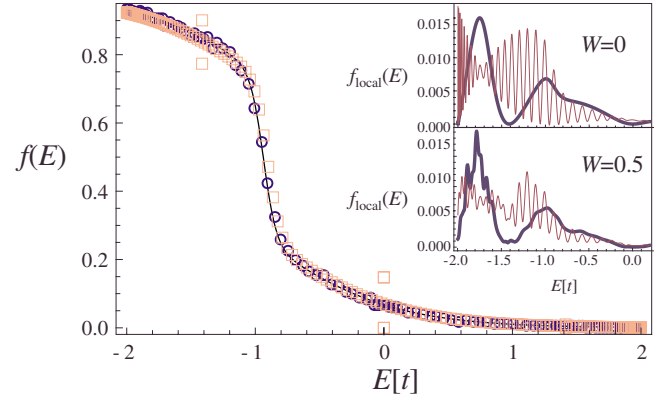


FIG. 3. (Color online) Global electron distribution functions with and without disorder. The distribution function is evaluated for a clean wire (squares) and disordered wire,  $W=0.5$  (circles). The thick line corresponds to an average distribution  $f(E) = \frac{1}{2}[f_L(E) + f_R(E)]$ , where  $f_{L(R)}(E)$  is the Fermi distribution of the left (right) lead with the corresponding temperature. Inset: the local electron distribution function at the edge of the wire (thick line) and the center of the wire (thin line) for a clean system (upper panel) and a disordered system (lower panel).

tance of the order of the thermal length of the leads (solid lines in the  $W=0.5$  curve are guides for the eyes) due to the contact with the heat baths. The inset of Fig. 2(b) shows the averaged heat current (over the whole wire) as a function of temperature difference  $\Delta T = T_R - T_L$  for different values of disorder. From the linear regime one can extract the global  $K$ , shown by empty circles in Fig. 2(b) as a function of disorder. On the other hand, one can extract the averaged local  $\kappa$  by using the local heat current [Fig. 2(a)] and the local temperature (from Fig. 1), calculated and averaged over sites close to the center of the wire, in the region where the temperature profile is linear, i.e., with a uniform temperature gradient, and the heat current is constant [solid lines in Figs. 1 and 2(a)]. The values of the local  $\kappa$  are shown as filled circles in Fig. 2(b) and exhibit a divergence for clean wires. Only at large disorder, the two definitions of thermal conductivity coincide, pointing to the onset of Fourier's law. We note that in our calculations we find the (averaged) heat current to be inversely proportional to the wire length, which, along with a uniform temperature gradient, implies that the (local) thermal conductivity is constant.

In order to further determine the role of disorder, we study the local and global electron energy distribution functions, both of which can be measured experimentally.<sup>34</sup> In terms of the density matrix, the global distribution function is simply  $f(E_k) = \rho_{kk}$  and the local distribution function is given by  $f_{\text{loc}}(E_k, r) = |\psi_k(r)|^2 \rho_{kk}$ . Figure 3 shows the distribution function for the clean wire ( $W=0$ , squares) and disordered wire ( $W=0.5$ , circles) (same parameters as in Fig. 1) as a function of energy. As seen, there is hardly a difference between the two functions. The solid line is the curve  $f(E) = \frac{1}{2}[f_L(E) + f_R(E)]$ , where  $f_{L(R)}(E)$  is the Fermi distribution of the left (right) lead with the corresponding temperature. The excellent agreement between the numerical curves and the averaged density suggests that one cannot consider the wire as a system with an effective temperature  $T_{\text{eff}} = \frac{1}{2}(T_L + T_R)$  but

rather it is the distribution function itself that is averaged and that disorder does not affect the distribution function.

In the inset of Fig. 3 we plot the local distribution function for the clean and disordered wires at the left edge of the wire (thick line) and at the center of the wire (thin line). Again, the curves for clean and disordered wires are very similar. We thus conclude that in our geometry, in contrast to mesoscopic wires,<sup>34</sup> one cannot attribute to the local distribution a simple position dependence even in the presence of disorder.

These findings show that the energy distribution function is only determined by the boundary conditions, namely, those provided by the bath operators and not by the local structure (i.e., the Hamiltonian). On the other hand, the nature of heat transport is determined solely by the microscopic character of the Hamiltonian. This implies that Fourier's law cannot be validated from measuring the local distribution function. It also suggests that one cannot map between models of coherent disorder and models of self-consistent baths.<sup>10,14</sup> The latter inherently introduce dephasing into the dynamics and imply local equilibrium and Fourier's law. Coherent disorder (such as that introduced here), on the other hand, does not, and one cannot *a priori* say whether Fourier's law is valid or not. Finally, these findings indicate that while one may use Hamiltonian (closed) systems to evaluate the linear-response thermal conductivity, the general nonequilibrium properties induced by finite temperature gradients need to be determined using models of open systems.

## V. SUMMARY

In this paper we have studied the onset of Fourier's law in a model system of one-dimensional noninteracting tight-binding electrons. Using the theory of open quantum systems<sup>24,25</sup> we have studied the electron wire under the non-equilibrium situation in which it is held at two different temperatures at its edges. We calculated the local temperature, heat current, and distribution functions for different values of (diagonal) disorder in the wire. Our main findings are as follows. For a clean wire, the temperature is uniform along the wire, and thus Fourier's law is invalid. Upon increasing disorder, a uniform temperature *gradient* evolves in the bulk of the wire, eventually giving rise to a fully developed Fourier's law. Thus, we conclude that Fourier's law is a cross-over phenomenon in this system.<sup>35</sup> Finally, we find that, as

opposed to the temperature profile, the energy distribution function is independent of disorder (even the local distribution function) and it is determined solely by the boundary conditions.

One question naturally arises. What is the origin of Fourier's law and its relation to the disorder strength? A naive answer would be that the onset of Fourier's law is related to the localization length. Once the localization length (determined from the disorder strength) crosses the sample length, then states become localized and weakly coupled. However, from examining the localization length in our model (by numerically calculating the inverse participation ratio), we find that at disorder strengths at which the onset of Fourier's law was observed (i.e., a fully developed temperature gradient), the localization length is already smaller than the wire length (by a factor of  $\sim 4$ ). We thus conjecture that there is another length scale that plays a role here, which is the length scale at which a *local* equilibrium can be defined (see Ref. 36). Its relation to the localization length is yet to be determined and we leave this for future studies.

One possible way to verify Fourier's law is to study the local temperature which can be measured experimentally.<sup>30</sup> Relevant experimental systems for which our predictions may be tested can be, e.g., carbon nanotubes,<sup>37</sup> quantum point contacts,<sup>38</sup> atomic-size metallic wires,<sup>39</sup> or silicon nanowires,<sup>40,41</sup> where measurements of thermal conductance and thermopower have already been demonstrated. A different route is to measure the length dependence of the thermal conductivity, as was recently applied to nanotubes.<sup>42</sup>

Finally we note that the above theory did not include the effects of electron interactions. However, since disorder also affects interacting systems, we expect that our conclusions may be valid also in the interacting case. While for some quasi-one-dimensional systems electron interactions may not be very important, it is nevertheless of interest to find out whether electron interactions alone suffice for the validity of Fourier's law even in clean wires. To resolve this issue one must employ a more elaborate method that can encompass both interactions and environments.<sup>43</sup> Such studies are currently underway.

## ACKNOWLEDGMENT

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