Emergence of Fourier’s law of heat transport in quantum electron systems

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The microscopic origins of Fourier’s venerable law of thermal transport in quantum electron systems has remained somewhat of a mystery, given that previous derivations were forced to invoke intrinsic scattering rates far exceeding those occurring in real systems. We propose an alternative hypothesis, namely, that Fourier’s law emerges naturally if many quantum states participate in the transport of heat across the system. We test this hypothesis systematically in a graphene flake junction, and show that the temperature distribution becomes nearly classical when the broadening of the individual quantum states of the flake exceeds their energetic separation. We develop a thermal resistor network model to investigate the scaling of the sample and contact thermal resistances, and show that the latter is consistent with classical thermal transport theory in the limit of large level broadening.

I. INTRODUCTION

As the dimensions of an electronic device are reduced, the power consumption, and concomitant heat generation, increases. Therefore, a detailed understanding of heat transport at the nanoscale is critical for the future development of stable high-density integrated circuits. Fourier’s law of heat conduction is an empirical relationship stating that the flow of heat is linearly related to an applied temperature gradient via a geometry independent, but material dependent, thermal conductivity.

Although Fourier’s law accurately describes heat transport in macroscopic samples, at the nanoscale heat is carried by quantum excitations (e.g., electrons, phonons, etc.) which are generally strongly influenced by the microscopic details of a system. For instance, violations of Fourier’s law have been observed in graphene nanoribbons, where the system could be tuned between the ballistic phonon regime and the diffusive regime by altering the edge state disorder. Violations in carbon nanotubes have also been observed. In this work, we utilize a state-of-the-art nonequilibrium quantum description of heat transport to investigate the onset of Fourier’s law in a nanoscale device.

II. THEORY OF LOCAL TEMPERATURE MEASUREMENT

Fourier’s law for the heat current density \( J_q = -\kappa \nabla T \) establishes a local linear relationship between an applied
FIG. 1. Classical (panels a,d) and quantum temperature profiles of a graphene flake under thermal bias for two contact geometries. The hot electrode (red) is held at 110K and the cold electrode (dark blue) is held at 90K, where red and blue squares indicate the carbon atoms covalently bonded to the hot and cold electrodes, respectively. In contact type I (upper panels), only the left and right edges of the flake couple to the electrodes, while in contact type II, the coupling to the electrodes wraps around three edges each, leading to three times stronger coupling to the electrodes. The quantum calculations are at Fermi energies $\mu_0 = -0.1\text{eV}$ (b,e) and $-0.6\text{eV}$ (c,f), relative to the Dirac point. The quantum temperature distributions for contact type I exhibit strong oscillations that depend sensitively on $\mu_0$, while for contact type II, the temperature distributions resemble pixelated versions of the classical distribution.

The local temperature distribution of a nonequilibrium quantum system is defined by introducing a floating thermoelectric probe\cite{3,4,10,11}. The probe exchanges charge and heat with the system via a local coupling until it reaches equilibrium with the system:

$$I_p^{(0)} = 0, \quad \nu = 0, 1, \quad (1)$$

where $-eI_p^{(0)}$ and $I_p^{(1)}$ are the electric current and heat current, respectively, flowing into the probe. The probe is then in local equilibrium with a quantum system which is itself out of equilibrium.

In the linear-response regime, for a thermal bias applied between electrodes 1 and 2, forming an open electric circuit, the heat current into electrode $\alpha$ is given by

$$I_\alpha^{(1)} = \sum_\beta \tilde{\kappa}_{\alpha\beta}(T_\beta - T_\alpha), \quad (2)$$

where $\alpha$ and $\beta$ label one of the three electrodes (1, 2, or the probe). Solving this set of linear equations, we arrive at the local temperature distribution\cite{3}

$$T_p(x, y) = \frac{\tilde{\kappa}_{p1}(x, y)T_1 + \tilde{\kappa}_{p2}(x, y)T_2 + \kappa_{p0}T_0}{\tilde{\kappa}_{p1}(x, y) + \tilde{\kappa}_{p2}(x, y) + \kappa_{p0}}. \quad (3)$$

Here $\tilde{\kappa}_{p\beta}(x, y)$ is the position-dependent thermal conductance between electrode $\beta$ and the probe, and $\kappa_{p0}$ is the thermal coupling of the probe to the ambient environment at temperature $T_0$.

In the absence of an external magnetic field, the effec-
tive two-terminal thermal conductances are given by\[8\]

\[
\tilde{\kappa}_{\alpha\beta} = \frac{1}{T} \left[ \mathcal{L}^{(2)}_{\alpha\beta} - \left( \frac{\mathcal{L}^{(1)}_{\alpha\beta}}{\tilde{\mathcal{L}}^{(0)}_{\alpha\beta}} \right)^2 \right] - \mathcal{L}^{(0)}_{\alpha\beta} \left( \frac{\mathcal{L}^{(1)}_{\alpha\gamma} \mathcal{L}^{(1)}_{\gamma\beta}}{\tilde{\mathcal{L}}^{(0)}_{\alpha\gamma} \tilde{\mathcal{L}}^{(0)}_{\gamma\beta}} + \frac{\mathcal{L}^{(1)}_{\alpha\beta} \mathcal{L}^{(1)}_{\beta\gamma} \mathcal{L}^{(1)}_{\gamma\alpha}}{\tilde{\mathcal{L}}^{(0)}_{\alpha\beta} \tilde{\mathcal{L}}^{(0)}_{\gamma\alpha} \tilde{\mathcal{L}}^{(0)}_{\gamma\beta}} \right),
\]

where \(\mathcal{L}^{(p)}_{\alpha\beta}\) in an Onsager linear response function\[12\],

\[
\mathcal{L}^{(p)}_{\alpha\beta} = \mathcal{L}^{(0)}_{\alpha\beta} + \frac{\mathcal{L}^{(0)}_{\alpha\gamma} \mathcal{L}^{(0)}_{\gamma\beta}}{\tilde{\mathcal{L}}^{(0)}_{\alpha\gamma} + \tilde{\mathcal{L}}^{(0)}_{\gamma\beta}},
\]

and

\[
\frac{1}{\mathcal{L}^{(0)}} = \frac{1}{\mathcal{L}^{(0)}_{12}} + \frac{1}{\mathcal{L}^{(0)}_{13}} + \frac{1}{\mathcal{L}^{(0)}_{23}}.
\]

Following the methods of Refs. \[13\]–\[15\], the linear-response coefficients may be calculated in the elastic tunneling regime as

\[
\mathcal{L}^{(p)}_{\alpha\beta}(\mu) = \frac{1}{\hbar} \int dE \left( E - \mu \right)^p \left( - \frac{\partial f}{\partial E} \right) T_{\alpha\beta}(E),
\]

where \(f(E)\) is the equilibrium Fermi-Dirac distribution, and \(T_{\alpha\beta}(E)\) is the transmission probability from contact \(\beta\) to contact \(\alpha\) for an electron of energy \(E\), which may be found using the usual nonequilibrium Green’s function (NEGF) methods. The details of our computational methods may be found in the Supporting Information.

In the simulations discussed below, we consider an ideal broad-band probe with perfect spatial resolution coupled weakly to the system.\[22\] Furthermore, we assume \(\kappa_{\alpha\beta} \ll \tilde{\kappa}_{p1}, \tilde{\kappa}_{p2}\), so that we can unambiguously determine the fundamental value of the local temperature in the nonequilibrium system. Any actual scanning probe won’t achieve this resolution; instead a convolution between the intrinsic profile and the probe’s resolution will be measured. The advantage of considering a probe in this limit is that we can investigate the onset of Fourier’s law without the complications introduced by the probe’s apex wavefunction geometry.

### III. RESULTS FOR \(T_p(x, y)\) IN GRAPHENE NANOJUNCTIONS

We investigate heat transport and temperature distributions in a graphene flake coupled to two macroscopic metal electrodes under a thermal bias. The electrodes are covalently bonded to the edges of the graphene flake. See Supporting Information for details of the model.

#### A. Emergence of Fourier’s law

The classical temperature distribution for a graphene flake with two different contact geometries is shown in panels a and d of Fig. 1. The behavior predicted by Fourier’s law is clearly visible in the characteristic linear temperature gradient across the sample from the hot to the cold electrode. This behavior is to be contrasted with the temperature distributions calculated using quantum heat transport theory, shown in panels b, c, e, and f. Figs. 1b, c show the electron temperature distributions for two different values of the Fermi energy (\(\mu_0 = -0.1eV, -0.6eV\) relative to the Dirac point) for contact type I, where the hot and cold electrodes are covalently bonded to the right and left edges of the graphene flake at the sites indicated by red squares. The temperature exhibits large quantum oscillations\[10\] that depend sensitively on the Fermi energy \(\mu_0\), obscuring any possible resemblance to the classical temperature distribution shown in Fig. 1a. The electron temperature distributions for contact type II are shown for the same two values of \(\mu_0\) in Figs. 1e, e. In this case, although there are atomistic deviations from Fourier’s law, nonetheless the resemblance to the classical distribution shown in Fig. 1a is unmistakable, and there is not a strong dependence on \(\mu_0\).

The different nature of thermal transport for contact types I and II can be understood by considering the density of states (DOS) \(g(E)\) of the system, shown in Fig. 2. For contact type I, \(g(E)\) exhibits a sequence of well-defined peaks, corresponding to the energy eigenfunctions of the graphene flake broadened by coupling to the leads. In constrast, contact type II, where the broadening is three times as large, has a smooth, almost featureless DOS for \(E < 1.2eV\). A sharply-peaked DOS indicates that the system is in the resonant-tunneling regime where thermal transport is controlled by the wavefunction of a single resonant state [or a few (nearly) degenerate states], while a smooth DOS indicates that many quantum states contribute to thermal transport, so that quantum oscillations tend to average out. We find that a necessary and sufficient condition to recover Fourier’s law is that many (nondegenerate) quantum states contribute with comparable strength to the thermal transport. When transport occurs in or near the resonant-tunneling regime, on the other hand, there is no classical limit for the temperature distribution.

We note that for nanostructures amenable to simulation (a few hundred atoms or less), a very large coupling to the electrodes is necessary to push the system out of the resonant-tunneling regime, and we speculate that this may be the reason why attempts to study the quantum to classical crossover in electron thermal transport via simulation have so far proven problematic. Thermal transport experiments are routinely conducted with much larger quantum systems, however, where this condition is well satisfied.

A direct test of Fourier’s law involves not only the temperature distribution but also the heat current density \(J_q\), which may be calculated using NEGF methods (see Supporting Information). The simulated heat flow patterns are shown in Fig. 3 for both classical and quantum
thermal transport in both contact geometries. The quantum heat flow in contact type I bears little relation to the classical flow, but instead exhibits vortices and fine structure that is strongly energy dependent, similar to the local charge current structure\(^1\). In contrast, the quantum heat flow in contact type II is nearly classical, except that it is concentrated along the C—C bonds, which serve as conducting channels. The heat flow patterns shown in Fig. 3 confirm that the crossover to the classical thermal transport regime requires many quantum states of the graphene flake to contribute comparably (smooth DOS).

B. Thermal resistor network model

The thermal conductivity \(\kappa\) in Fourier’s law is material dependent but dimensionally independent. In the regime of quantum transport\(^\text{17}\), linear response theory instead treats the thermal conductance (also traditionally denoted by the symbol \(\kappa\)), which depends in detail on the dimensions and structure of the conductor. In order to investigate the cross-over between these regimes, we develop a thermal circuit model and apply it to the temperature profiles calculated using our theory.

The temperature probe acts as a third terminal in the thermoelectric circuit, and affects the thermal conductance between the hot and cold electrodes. Starting from Eq. (2), the heat current flowing into electrode 1 may be expressed as

\[
I_1^{(1)} = \tilde{\kappa}_{12}(T_2 - T_1),
\]

where the thermal conductance between source and drain in the presence of the thermal probe is

\[
\tilde{\kappa}_{12} = \tilde{\kappa}_{12} + \frac{\tilde{\kappa}_{p1}\tilde{\kappa}_{p2}}{\tilde{\kappa}_{p1} + \tilde{\kappa}_{p2}},
\]

The thermal resistance of the junction may be written
FIG. 4. Thermal resistance values as a function of Fermi energy $\mu_0$ for four different sized hexagonal graphene flake junctions with contact type II, where $N$ is the number of atoms in the flake. $R_s$ is the sample thermal resistance and $R_1$ and $R_2$ are the contact thermal resistances, defined in Eqs. (11)–(13), respectively. The contact resistances are nearly universal in this transport regime: $R_1, R_2 \approx \frac{R_0}{N_c}$, where $R_0$ is the thermal resistance quantum and $N_c$ is the number of atoms bonded to each contact. The sample thermal resistance $R_s$ is inversely correlated with the density of states per unit area times the sample length, $g(\mu_0)L$, as expected based on semiclassical Boltzmann transport theory.

The contact resistances $R_1$, $R_2$, and sample thermal resistance $R_s$ are shown for four different sized graphene flakes with contact type II as a function of Fermi energy in Fig. 4. Here $N$ is the number of atoms in the hexagonal flake. The resistances are normalized by the quantum of thermal resistance $R_0 = \frac{3h}{\pi^2 k_B^2 T_0} \approx 1.2 \times 10^9 K/W$ at $T_0=100K$. For these junctions, the contact resistances exhibit nearly universal behavior

$$R_{\text{th}} \equiv \frac{1}{\kappa_{12}} = R_s + R_1 + R_2,$$

where $R_s$ is the “intrinsic” thermal resistance of the system, and $R_1$ and $R_2$ are thermal contact resistances associated with the interfaces between electrodes 1 and 2, respectively, and the quantum system.

The individual resistances in the network are defined as follows:

$$R_s = \frac{|T_{1s} - T_{2s}|}{|I_1^{(1)}|},$$

(11)

$$R_1 = \frac{|T_1 - T_{1s}|}{|I_1^{(1)}|},$$

(12)

$$R_2 = \frac{|T_{2s} - T_2|}{|I_2^{(1)}|},$$

(13)

where $T_{\alpha s}$ is the temperature averaged over the atoms bonded to electrode $\alpha$.

The contact resistances $R_1, R_2$, and sample thermal resistance $R_s$ are shown for four different sized graphene flakes with contact type II as a function of Fermi energy in Fig. 4. Here $N$ is the number of atoms in the hexagonal flake. The resistances are normalized by the quantum of thermal resistance $R_0 = \frac{3h}{\pi^2 k_B^2 T_0} \approx 1.2 \times 10^9 K/W$ at $T_0=100K$. For these junctions, the contact resistances exhibit nearly universal behavior

$$R_1, R_2 \approx \frac{R_0}{N_c},$$

(14)

where $N_c$ is the number of atoms bonded to each contact, with only small deviations that decrease in amplitude with increasing flake size.

To study the crossover to the classical transport regime, it is useful to compare the sample thermal resistance $R_s$ to the classical result derived from a two-dimensional Boltzmann equation in the relaxation-time
approximation

\[ R_{cl} = \frac{2R_0}{\hbar L g(\mu_0) v_F}. \]  

(15)

where \( g(E) \) is the density of states per unit area of the graphene flake, \( v_F \) is the Fermi velocity, and we have set the scattering time \( \tau = L/v_F \) for these ballistic conductors, where \( L \) is the distance between the source and drain electrodes. Note that these hexagonal flakes have equal width and length, so the geometric factor in \( R_{cl} \) is unity. Eq. (15) implies that near the Dirac point in graphene, where \( v_F \approx \text{const.} \), \( R_{cl} \propto 1/g(\mu_0)L \). Fig. 1 shows that indeed the variations of \( R_s \) with Fermi energy are correlated with the variations of \( 1/g(\mu_0)L \) for various flake sizes, confirming the classical nature of transport in junctions with contact type II. An improved fit might be obtained by including the variation of \( v_F \) with \( \mu_0 \), which is important far from the Dirac point.

Although the temperature distribution can approach the classical limit in some cases via coarse graining, the thermal resistor network model is found to be quantitatively consistent with Fourier’s law only for the nearly classical transport regime, where multiple resonances contribute to the transport. In the quantum transport regime, where individual resonances are important, the contact resistances are not universal, but exhibit large oscillations as well, making the identification of a “sample thermal resistance” problematic.

IV. CONCLUSIONS

Thermal transport in quantum electron systems was investigated, and the crossover from the quantum transport regime to the classical transport regime, where Fourier’s law holds sway, was analyzed. In the quantum regime of electron thermal transport, the local temperature distributions exhibit large oscillations due to quantum interference (see Fig. 1h,c), and the heat flow pattern exhibits vortices and other nonclassical features (see Fig. 3b), while in the classical regime, the heat flow is laminar (see Fig. 3d) and the temperature drops monotonically from the hot to the cold electrode (see Fig. 3e,f).

A satisfactory understanding of the quantum to classical crossover in electron thermal transport has been lacking for a number of years. Perhaps the most promising explanation advanced early on was in terms of dephasing of the electron waves: for sufficiently large inelastic scattering in the system, the electron thermal transport becomes classical. However, many nanostructures of interest for technology, such as graphene, have very weak inelastic scattering, and the origin of Fourier’s law cannot be explained in such systems by this mechanism.

In this article, it was shown that a sufficient condition for a quantum electron system to cross over into the classical thermal transport regime is for the broadening of the energy levels of the system to exceed their separation, so that the DOS becomes smooth. In this limit, the transport involves contributions from multiple resonances above and below the Fermi level, so that interference effects average out. This condition is challenging to achieve in simulations, requiring almost the entire edge of the largest 2D system studied to be covalently bonded to one of the two electrodes (see Fig. 1d–f). For smaller systems, unphysically large electrode coupling would be required to reach the classical regime. However, for the larger systems routinely studied in experiments, it may be quite typical for thermal transport to occur in the classical regime, since the level spacing scales inversely with the system size.

In addition to recovering a nearly classical temperature profile in the limit where the DOS is smooth, it was also shown that the thermal resistance of the junction could be explained using a thermal resistor network model consistent with Fourier’s law in this limit. The contact thermal resistances were found to take on universal quantized values, while the sample thermal resistance was found to be inversely proportional to the DOS per unit area times the sample length, as expected based on semiclassical Boltzmann transport theory (see Fig. 4). In contrast, in the quantum regime, where thermal transport occurs predominantly via a single energy eigenstate (or a few closely-spaced states near the Fermi level), the thermal resistor network model was not found to be useful in analyzing the transport. In this sense, coarse graining of the temperature distribution due to limited spatial resolution of the probe, which leads in many cases to a rather classical temperature profile, is not sufficient to explain the onset of Fourier’s law, since the underlying thermal transport remains quantum mechanical.

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V. APPENDIX

We utilize a standard nonequilibrium Green’s function (NEGF) framework to describe the quantum transport through a three-terminal junction composed of a graphene flake coupled to source and drain electrodes, and a scanning probe. We focus on transport in the elastic cotunneling regime, where the linear response coefficients may be calculated from the transmission coefficients \( T_{\alpha\beta}(E) \) using Eq. (7). The transmission function may be expressed in terms of the junction Green’s functions as

\[ T_{\alpha\beta}(E) = \text{Tr} \left\{ \Gamma^\alpha(E)G^\tau(E)\Gamma^{\beta}(E)G^{\alpha}(E) \right\}, \]  

(16)
where $\Gamma^\alpha(E)$ is the tunneling-width matrix for lead $\alpha$ and $G^\nu(E)$ and $G^a$ are the retarded and advanced Green’s functions of the junction, respectively. In the general many-body problem $G(E)$ must be approximated. In the context of the examples discussed here we consider an effective single-particle description such that
\[
G^\nu(E) = (SE - H - \Sigma^r_T)^{-1},
\]
where $H$ is the Hamiltonian of the nanostructure, $S$ is an overlap matrix which reduces to the identity matrix in an orthonormal basis, and $\Sigma_T$ is the tunneling self-energy.

The tunneling-width matrix for contact $\alpha$ (source, drain, or probe) may be expressed as
\[
[\Gamma^\alpha(E)]_{nm} = 2\pi\sum_{k\in\alpha} V_{nk}V_{mk}^* \delta(E - \epsilon_k),
\]
where $n$ and $m$ label $\pi$-orbitals within the graphene flake, and $V_{nk}$ is the coupling matrix element between orbital $n$ of the graphene and a single-particle energy eigenstate of energy $\epsilon_k$ in electrode $\alpha$. The thermal probe is treated as an ideal broad-band probe with perfect spatial resolution
\[
\Gamma^p = \gamma_p \delta(x - x_p),
\]
while the coupling to the hot and cold electrodes is taken to be diagonal in the graphene atomic basis with a per-band broad-band coupling strength of $3eV$. In the broad-band limit, the tunneling self-energy is a constant matrix given by
\[
\Sigma^r_T = -\frac{i}{2} \sum_\alpha \Gamma^\alpha.
\]

In the low-energy regime (i.e., near the Dirac point), a simple tight-binding Hamiltonian has been shown to accurately describe the $\pi$-band dispersion of graphene\cite{66}. The Hamiltonian of the graphene flake is taken as
\[
H_{\text{graphene}} = \sum_{\langle ij \rangle} t_{ij} d_i^\dagger d_j + H.c.,
\]
where $t = -2.7eV$ is the nearest-neighbor hopping matrix element between 2p$_z$ carbon orbitals of the graphene flake with lattice constant of 2.5Å, and $d_i^\dagger$ creates an electron on the $i$th 2p$_z$ orbital.

The heat current density plotted in Fig. 3 is given within NEGF theory by
\[
J_q = \frac{\hbar}{2m} \int dE \left( E - \mu_0 \right) \left( \nabla - \nabla' \right) G^<(x, x'; E),
\]
where $G^<$ is the Keldysh lesser Green’s function (see, e.g., Ref.\cite{1} for its definition).

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