Steady-State Heat Transport: Ballistic-to-Diffusive with Fourier’s Law

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It is “common knowledge” that Fourier’s law does not capture ballistic phonon effects, which are important when the length of a material is similar to the phonon mean-free-path. Using an approach borrowed from electron transport, we demonstrate that Fourier’s law and the heat equation do capture ballistic effects, including temperature jumps at the contacts, and are thus applicable on all length scales. The key is to apply the proper boundary conditions to the heat equation. Simple analytical solutions are derived, for steady-state heat transport that reproduce the results of the Boltzmann transport equation.

I. INTRODUCTION

Quasi-ballistic phonon transport can impact the thermal response of materials on the nano-scale and even on the micro-scale, given that phonon mean-free-paths (MFP) can span from ~1 nm to >10 μm. This point was illustrated in bulk Si, where molecular dynamics simulations showed that roughly half the heat is carried by phonons with MFP greater than 1 μm [1]. Thus, ballistic phonon effects can impact a variety of problems related to thermal transport, such as: a reduced heat carrying capability of thin films [2, 3], the analysis of experiments probing short time and length scales (e.g., time/frequency-domain thermoreflectance) [4, 5], heating in small electronic devices [6], and they can provide a route to extract the MFP distribution of materials [7, 8].

Traditionally, thermal transport problems are investigated using Fourier’s law \( I_Q = -\kappa \nabla T \) combined with the heat equation \( \nabla^2 T = 0 \), where \( I_Q \) is the heat current, \( T \) the temperature and \( \kappa \) the thermal conductivity. While this approach is simple and tractable, it is commonly assumed that it omits ballistic transport effects and can only be applied when the length of the thermal conductor \( L \) is much greater than the phonon MFP. To include ballistic effects one typically resorts to more sophisticated approaches, including: Monte-Carlo simulations [9], molecular dynamics [10–12] or the phonon Boltzmann transport equation (BTE) [13, 20]. A salient feature observed with these more advanced methods is a temperature discontinuity at the boundaries with the contacts, which occurs even in the case of ideal contacts with no added interface resistance. These temperature jumps at the boundaries are signatures of quasi-ballistic phonon transport [15–17], and do not arise when employing diffusive-type equations such as the heat equation. On the one hand, traditional approaches are easy to solve but omit ballistic effects. On the other hand, sophisticated theory and modeling can capture quasi-ballistic transport but can be difficult to solve. We note that the existence of sophisticated numerical solutions does not diminish the importance of accurate and physically intuitive analytical approaches that capture the essential physics.

It is well known that Fick’s law describes carrier diffusion in semiconductors regions that are short in comparison to the MFP. This is implicit in Shockley’s 1962 treatment of carrier transport [21]. Much later, it was discovered that Fick’s law reproduces the numerical results of the BTE [22], with the explanation in terms of the McKelvey-Shockley flux theory provided by [23, 24]. Small signal a.c. solutions of the flux equations also agree well with numerical solutions of the BTE [25].

In this work, we use the McKelvey-Shockley flux method to solve 1D steady-state heat transport. We obtain simple analytical solutions that are applicable on all length scales, from ballistic to diffusive transport regimes, and can easily reproduce numerical results of the phonon BTE including temperature jumps at the contacts. Importantly, we demonstrate that the McKelvey-Shockley flux equations can effortlessly be recast into traditional diffusive equations, namely Fourier’s law and the heat equation — exactly. As we will show, the key is to use the correct physical boundary conditions. The outline of this paper is as follows: in Section II we describe our approach to heat transport, an example is studied in Section III, Section IV shows a derivation of familiar heat transport equations that include ballistic effects, Section V discusses how to treat energy-dependent mean-free-paths using our simple approach and finally we summarize our findings in Section VI.

II. THEORETICAL APPROACH

For this work, we borrow an approach originally developed for electronic transport that is applicable on all length scales, the McKelvey-Shockley flux method [21, 25], and adapt it for phonon/heat transport. We assume steady-state 1D transport along \( x \) with an infinite \( y-z \) plane. The essence of this approach is to (i) describe phonons in terms of fluxes (i.e. phonon density times average velocity along the transport direction) and (ii) categorize all phonons into two components: forward and backward fluxes. The governing equations of the
McKelvey-Shockley flux method are \[27\]:

\[
\frac{dF^+(x, \epsilon)}{dx} = \frac{F^+(x, \epsilon)}{\lambda(\epsilon)} - \frac{F^-(x, \epsilon)}{\lambda(\epsilon)}, \quad (1)
\]

\[
\frac{dF^-(x, \epsilon)}{dx} = \frac{F^+(x, \epsilon)}{\lambda(\epsilon)} - \frac{F^-(x, \epsilon)}{\lambda(\epsilon)}, \quad (2)
\]

where \(F^+/F^-\) are the forward/backward phonon fluxes [units: # phonons m\(^{-2}\)s\(^{-1}\)eV\(^{-1}\)], \(\lambda(\epsilon)\) is the mean-free-path for backscattering and \(\epsilon\) is the phonon energy. The above coupled equations describe the evolution of each flux type, which can scatter to/from the opposite flux component. \(\lambda(\epsilon)\) governs the scattering, and is defined as the average distance travelled along \(x\) by a phonon with energy \(\epsilon\) before scattering into an opposite moving state. Note that the McKelvey-Shockley flux method can be derived from the BTE \[27\]. The boundary conditions are:

\[
F^+(x = 0^+, \epsilon) = F_0^+(\epsilon), \quad (3)
\]

\[
F^-(x = L^-, \epsilon) = F_0^- (\epsilon), \quad (4)
\]

where \(L\) is the length of the thermal conductor. Thus one needs to specify the injected phonon fluxes at both ends: \(F^+\) on the left side \((x = 0^+)\) and \(F^-\) on the right side \((x = L^-)\). The McKelvey-Shockley flux method described by Eqs. (3-4), forms the basis for our approach to heat transport (see Fig. 1).

The total heat current \(I_Q^{\text{tot}}\) and heat density \(Q^{\text{tot}}\) are written as:

\[
I_Q^{\text{tot}} = \int_0^\infty \epsilon \left[ F^+(x, \epsilon) - F^-(x, \epsilon) \right] \, d\epsilon, \quad [\text{W m}^{-2}]
\]

\[
Q^{\text{tot}}(x) = \int_0^\infty \epsilon \left[ \frac{F^+(x, \epsilon)}{v_x^+} + \frac{F^-(x, \epsilon)}{v_x^-} \right] \, d\epsilon, \quad [\text{J m}^{-3}]
\]

where \(F = F^+ - F^-\) is the net phonon flux, \(n = (F^+ + F^-)/v_x^+\) is the phonon density and \(v_x^+/v_x^-\) is the average \(x\)-projected velocity (defined as \(v_x^+ = \sum_{k,v_x>0} v_x \delta (\epsilon - \epsilon_k)/\sum_{k,v_x>0} \delta (\epsilon - \epsilon_k)\)). The heat current and heat density correspond to multiplying the net phonon flux and the phonon density, respectively, by the energy \(\epsilon\) carried by each phonon (and integrating over all phonon energies). From the above definitions, we can directly replace \(F^+\) in the McKelvey-Shockley flux equations (Eqs. (1-2)) by \(\epsilon I_Q^\pm = \epsilon F^\pm\), as we will assume from this point on unless otherwise stated. In addition, to ease the notation we will drop the explicit dependence on \(\epsilon\) in \(I_Q^\pm\), \(\lambda\) and \(v_x^\pm\), although keep in mind that a final integration over energy is required (Eqs. (5-6)).

Equations (1) and (2) comprise a simple BTE in which the forward and reverse fluxes have been integrated over angle. This particular discretization is especially effective in handling the correct physical boundary conditions, where a flux is injected from each side. Inside the device, the carrier distribution can be very far from equilibrium, but each half of the distribution is at equilibrium with its originating contact as it is injected and scattering gradually mixes both flux components. In the limiting case of purely ballistic transport, each half of the distribution is in equilibrium with its originating contact. More complicated discretizations are possible and sometimes necessary, but we will demonstrate the effectiveness of these simple equations in the remainder of the paper.

III. EXAMPLE: HEAT TRANSPORT IN A DIELECTRIC FILM

Having presented the McKelvey-Shockley flux method adapted for heat transport, we will now demonstrate this approach with an example. We will consider steady-state thermal transport across a dielectric film of length \(L\) (the electronic contribution to thermal transport can be neglected), contacted by two ideal thermalizing contacts each at their respective temperatures \(T_L\) (left contact) and \(T_R\) (right contact), as shown in Fig. 2(a). "Ideal contacts" in this context assumes that \((i)\) each contact is in thermal equilibrium, with phonon statistics given by the Bose-Einstein distribution, and \((ii)\) the interfaces are reflectionless, thus phonons are not scattered at the contacts. While perfect contacts are assumed in this paper, this is not a fundamental limitation of our approach, as we will discuss later.

We begin by subtracting the flux equations (1 and 2):

\[
dI_Q/dx = 0.
\]

This is the energy balance equation, or equivalently the first law of thermodynamics, which states that under steady-state conditions the heat current \(I_Q\) is a constant along \(x\). Using this relation with Eqs. (3-4), we have

\[
\frac{dI_Q^-(x)}{dx} = \frac{dI_Q^+(x)}{dx} = -\frac{I_Q}{\lambda}.
\]

It is straightforward to show that \(I_Q^+(x)\) and \(I_Q^-(x)\) have
If the contacts are in equilibrium, then the injected heat currents from the contacts can be written as

\[
I_{Q,0}^+ = \frac{M}{h} f_{\text{BE}}(T_L), \quad I_{Q,L}^+ = \frac{M}{h} f_{\text{BE}}(T_R),
\]

where \(M(\epsilon)\) is the distribution of modes of the thermal conductor (depends only on the phonon dispersion) \([28, 29]\), \(f_{\text{BE}}\) is the Bose-Einstein occupation function and \(h\) is Planck’s constant. Inserting these expressions into Eq. (11), we obtain:

\[
I_Q = \frac{M}{h} \left( \frac{\lambda}{\lambda + L} \right) \left[ f_{\text{BE}}(T_L) - f_{\text{BE}}(T_R) \right] \Delta T,
\]

where \(K = K^\text{ball} \tau\) is the thermal conductance, \(K^\text{ball}\) is the ballistic thermal conductance \([30]\). Note that Eq. (15) applies in the case of a small \(\Delta T\), while Eq. (14) does not have this limitation. The total heat current is calculated by integrating over energy (Eq. [1]). The above expressions for \(I_Q\) are applicable on all length scales, and span from ballistic to diffusive transport regimes. The transmission coefficient controls the length dependence of the heat current. In the ballistic limit \(L \ll \lambda, \tau \rightarrow 1\) and \(I_Q\) is independent of length. Note that in this limit \(I_Q\) is equal to the known expression in the Casimir limit (see Appendix A). In the diffusive limit \(L \gg \lambda, \tau \approx \lambda/L\) and \(I_Q \propto 1/L\), as expected from classical scaling. Eq. (14) is identical to \(I_Q\) obtained with the Landauer approach \([30, 31]\). One advantage of the McKelvey-Shockley flux method, versus Landauer, is that it provides spatial information on the heat transport properties.

Eq. (6) shows that the heat density is the sum \(I^+_{Q} + I^-_{Q}\) divided by the average forward projected velocity \(v^+\). Often it is desirable to replace heat density by temperature. It is important to note that in small structures (compared to \(\lambda\)) the phonon distribution may be highly nonequilibrium and the definition of temperature, an equilibrium quantity, is ambiguous (no such problem arises with \(I_Q\) and \(Q\)). Assuming a small applied \(\Delta T = T_L - T_R\) ensures the thermal conductor remains near equilibrium, where temperature is well defined. In this case, we can rewrite heat density in terms of temperature using \(\delta Q = C_V \delta T\), where \(C_V\) is the volumetric heat capacity. And, we can expand the heat currents \(I^\pm_{Q}(x) = I^\pm_{Q,eq} + \delta I^\pm_{Q}(x)\) due to a small difference in contact temperatures \(\Delta T\), where \(I^\pm_{Q,eq} = I^\pm_{Q,eq}\) is simply the equilibrium heat current arising from a reference background temperature, chosen as \(T_R\) in this case. Rewriting \(Q\) in terms of \(T\) and we find:

\[
\delta T^\pm(x) = \frac{2 \delta I^\pm_{Q}(x)}{C_V v^+_x},
\]

\[
T(x) = \left[ \frac{\delta T^+(x) + \delta T^-(x)}{2} \right] + T_R.
\]
The temperature profile inside the thermal conductor is proportional to the sum of $\delta I^+_Q$ and $\delta I^-_Q$ or equivalently the average of $\delta T^+(x)$ and $\delta T^-(x)$, and is presented in Fig. 2(c). We see that $T(x)$ varies linearly inside the thermal conductor, and that there are discrete temperature drops at the boundaries. We can use Eqs. (16-17) with Eqs. (9-10) to determine the temperatures at the boundaries:

$$T(0^+) = (2 - T) \frac{T_L}{2} + T \frac{2T_R}{L}, \quad (18)$$
$$T(L^-) = T \frac{T_L}{2} + (2 - T) \frac{T_R}{2}, \quad (19)$$

where the relation $T_L = T_R + 2\delta I^+_{Q,0}/C_V v^+_x$ was used (the factor of two appears since the forward and backward heat currents are equal in the contacts). The boundary temperatures $T(0^+)/T(L^-)$ are weighted averages of the contact temperatures, that depend on $T$. When $T \to 0$ (diffusive limit), the “interior” boundary temperatures tend to the contact temperatures (classical result), and when $T \to 1$ (ballistic limit) the boundary temperatures tend to the average of the contact temperatures (constant $T(x)$ inside the material) [32]. From Eqs. (18-19), we can extract the value of the temperature jumps at the contacts ($\delta T_c$). $\delta T_c$ is found to be identical at both left and right contacts:

$$\delta T_c = \frac{T}{2} (T_L - T_R), \quad (20)$$
$$= \frac{I_Q R^{ball}}{2}, \quad (21)$$

where $R^{ball} = 1/K^{ball}$ is the ballistic thermal resistance with $K^{ball} = C_V v^+_x/2$. We find the temperature jumps are simply proportional to the transmission, which depends on $L$ and $\lambda$, and can be interpreted as an intrinsic contact resistance. The temperature jumps do not occur because the contact interfaces scatter phonons, since we assume reflectionless contacts. Rather, it is because we specify the injected heat currents $I^+_{Q,0}/I^-_{Q,0}$ at one end of the thermal conductor while the opposite ends are “floating” boundaries that depend on $\lambda$ and $L$ (as shown in Fig. 2(b)). Once the forward and backward heat currents are added to obtain temperature, discrete drops are observed at the boundaries.

In this work we have assumed perfectly thermalizing contacts that are in equilibrium, which allows us to extract a simple analytical expression for the temperature jumps. In general one must specify the injected heat currents at the boundaries, which in principle can originate from an adjacent material that need not be in equilibrium.

In Fig. 3 we compare our simple model (lines) to the numerical solutions of the BTE (symbols), in the case of diamond films of length $L = 0.1 \mu m$, $1 \mu m$, $10 \mu m$. Using the effective $\lambda$ values reported in [15] for $T = 77, 300 K$, we find our simple analytical model adequately reproduces the results of the BTE, including the linear temperature profiles and the temperature jumps at the contacts. We note that phonons in a material typically have a broad distribution of $\lambda$, and in general using a constant $\lambda$ may lead to significant errors (in this case $\delta T_c$ should be obtained by evaluating $\lambda$ and $T$ at each energy and integrating over energy following Eqs. (5-6), as discussed in Section V).

To summarize, writing the phonon BTE in the McKelvey-Shockley form (Eqs. (1) and (2)) leads to very accurate solutions for the class of problems considered in this section. In the next section, we will show that exactly the same solutions can be obtained by solving the traditional diffusion equation – if the appropriate boundary conditions are used.

IV. FOURIER’S LAW AND HEAT EQUATION

In this section, we demonstrate how the McKelvey-Shockley flux equations can be rewritten into familiar ex-
pressions for heat transport, that yield exactly the same results. By adding Eq. (1) and Eq. (2) (replacing \( I^\pm \) by \( I_Q^\pm \)) and using the relation \( Q = (I_Q^+ + I_Q^-)/v^+_x \), we obtain

\[
I_Q = -D_{ph} \frac{dQ(x)}{dx} = -\kappa \frac{dT(x)}{dx},
\]

where

\[
D_{ph} = \lambda v^+_x/2, \quad \kappa = C_V D_{ph},
\]

\( D_{ph} \) is the phonon diffusion coefficient and \( \kappa \) is the bulk thermal conductivity (see Appendix B). Eq. (23) is Fourier’s law, and comes out directly from the Mckelvey-Shockley flux method, without making any assumption on \( L \) relative to \( \lambda \). This indicates that the ballistic transport physics contained in the Mckelvey-Shockley flux method are also included in Fourier’s law. By combining Fourier’s law with the energy balance equation (Eq. (7)), we find the heat equation:

\[
\frac{d^2Q(x)}{dx^2} = \frac{d^2T(x)}{dx^2} = 0,
\]

where we assumed the material parameters are position-independent. Fourier’s law has been derived from the BTE [1], by assuming that the phonons at each \( x \) were locally at thermodynamic equilibrium. We find no such assumption is necessary. The key to capturing ballistic transport effects with Fourier’s law is to use the correct physical boundary conditions.

Traditionally, the contact temperatures \( T_L/T_R \) are used as the boundary conditions, however the Mckelvey-Shockley flux method shows it is the injected heat currents that are the physical boundary conditions (Eqns. (3-4)). Stated differently, the BTE is first order in space; it requires one boundary condition in space. Alternatively, we can specify the incoming part of the distribution at the contacts. Specifying the contact temperatures as the physical boundary conditions (Eqns. (3-4)) shows that \( \frac{dT}{dx} \) is reduced, due to the temperature jumps at the boundaries, and is equivalent to replacing \( L \) by \( L + \lambda \). As transport becomes more ballistic, the temperature jumps increase and the absolute temperature gradient inside the thermal conductor decreases. If one assumed \( \frac{dT}{dx} = (T_L - T_R)/L \) for all \( L \), then a reduction in the expected \( I_Q \) could be interpreted as a reduction in the thermal conductivity. This introduces the concept of apparent thermal conductivity, which is mathematically defined as \( \kappa_{app} = \kappa \cdot L/(L + \lambda) \) [22]. Our analysis shows that, physically, ballistic transport does not change the bulk thermal conductivity of the material at any length scale – as long as \( \lambda \) is independent of energy.

Solving the heat equation (Eq. (20)) is straightforward, and simply gives a linear temperature profile

\[
T(x) = T(0^+) \left[ 1 - \frac{x}{L} \right] + T(L^-) \left[ \frac{x}{L} \right].
\]

Inserting this solution into Eqns. (27-28), we can determine \( T(0^+) \) and \( T(L^-) \), which in this case (equilibrium contacts) are equal to Eqns. (18-19). With equilibrium contacts, applying the above boundary conditions is equivalent to replacing the contact temperatures \( T_L \) and \( T_R \) by the “interior” boundary temperatures \( T(0^+) \) and \( T(L^-) \). We note that using Eqns. (18-19) with Eq. (21), \( T(0^+) \) and \( T(L^-) \) can also be rewritten as

\[
T(0^+) = T_L - \frac{P_{ball} I_Q}{2},
\]

\[
T(L^-) = T_R + \frac{P_{ball} I_Q}{2}.
\]

With a given \( T(x) \), we can calculate the heat current using Fourier’s law (Eq. (23)):

\[
I_Q = \kappa \left[ \frac{T(0^+) - T(L^-)}{L} \right],
\]

\[
= \kappa \left[ \frac{T_L - T_R}{L + \lambda} \right].
\]

Note the correct usage of Fourier’s law implies evaluating the gradient of \( T \) using the “interior” boundary temperatures and not the contact temperatures. This expression for heat current is applicable on all length scales, and is equal to Eq. (15). In the diffusive limit \( (L \gg \lambda) \), we have \( I_Q = \kappa (T_L - T_R)/L \), the classical result; in the ballistic limit \( (L \ll \lambda) \), we have \( I_Q = \kappa (T_L - T_R)/\lambda \) and the heat current is independent of \( L \). Eq. (33) shows that \( dT/dx \) is reduced, due to the temperature jumps at the boundaries, and is equivalent to replacing \( L \) by \( L + \lambda \). As transport becomes more ballistic, the temperature jumps increase and the absolute temperature gradient inside the thermal conductor decreases. If one assumed \( dT/dx = (T_L - T_R)/L \) for all \( L \), then a reduction in the expected \( I_Q \) could be interpreted as a reduction in the thermal conductivity. This introduces the concept of apparent thermal conductivity, which is mathematically defined as \( \kappa_{app} = \kappa \cdot L/(L + \lambda) \) [22]. Our analysis shows that, physically, ballistic transport reduces \( dT/dx \) and does not change the bulk thermal conductivity of the material at any length scale – as long as \( \lambda \) is independent of energy.

V. DISCUSSION

In Section II, we validated our approach by comparing our solutions to the numerical results of the BTE where a constant \( \lambda \) was used. In general, the MFP of phonons in a given material can span orders of magnitude [1], and may not be well represented by a single MFP.
Specifically, we calculate the cross-plane thermal resistance using the “simple” approach presented in this paper. Next, we investigate the impact of an energy-dependent \([30]\), using an energy-dependent MFP. From the full phonon dispersion we obtained and the correct \(\lambda\) (markers). From the full phonon dispersion we obtain \(M(\epsilon)\) and \(v_\epsilon^+(\epsilon)\), and including Umklapp, defect and boundary scattering we extract \(\lambda(\epsilon)\) (procedure detailed in the supplemental of \([33]\)). With this model, we can reproduce the lattice thermal conductivity of bulk silicon within 15\% error from 5 K to 300 K.

FIG. 4: (Color online) Cross-plane thermal resistance, \(R_{th} = (T_L - T_R)/I_{Q}^*\), of a silicon film versus length (film thickness). Dashed line: \(R_{th}\) calculated using an energy-dependent MFP that includes Umklapp, defect and boundary scatterings, and was calibrated to experimental data. Solid line: \(R_{th}\) calculated using a constant average bulk MFP. Markers: \(R_{th}\) calculated from the phonon BTE, within the Landauer approach \([30]\), using an energy-dependent MFP.

How does the temperature profile change when using an energy-dependent \(\lambda(\epsilon)\)? According to Eq. \([6]\) and the definition of heat capacity \(\delta Q(x, \epsilon) = C_V(\epsilon) \delta T(x, \epsilon)\), the energy-averaged temperature at any point \(x\) is given by:

\[
\delta T(x) = \frac{\int_0^\infty C_V(\epsilon) \delta T(x, \epsilon) d\epsilon}{\int_0^\infty C_V(\epsilon) d\epsilon},
\]

where

\[
C_V(\epsilon) = \epsilon \left[ \frac{2M(\epsilon)}{h v_\epsilon^+(\epsilon)} \right] \frac{\partial f_{BE}(\epsilon)}{\partial T}.
\]

Note that \(C_V = \int_0^\infty C_V(\epsilon) d\epsilon\), and that the term in brackets is simply the phonon density of states \([30]\). From the temperature profile given by Eq. \([29]\), we only need to compute the energy-averaged temperatures \(T(0^+) = \delta T(0^+) + T_R\) and \(T(L^-) = \delta T(L^-) + T_R\) with Eq. \([34]\). A straight line connecting both points corresponds to the correct energy-averaged temperature profile. \(\delta T(0^+, \epsilon)\) and \(\delta T(L^-, \epsilon)\) are both related to the temperature jump \(\delta T_c(\epsilon)\) at the contacts (Eq. \([20]\)) and thus \(\lambda(\epsilon)\). Hence, if \(M(\epsilon), v_\epsilon^+(\epsilon)\) and \(\lambda(\epsilon)\) are known (using full phonon dispersions and energy-dependent scattering rates), performing detailed modeling within the simple approach described in this paper boils down to evaluating one integral in energy to extract the energy-averaged \(\delta T\) or \(\mathcal{T}\). From this the temperature profile corresponds to a straight line joining \(T(0^+)\) and \(T(L^-)\). Note that if \(\lambda\) is a constant, then \(\delta T\) does not depend on energy, evaluating Eq. \([34]\) is trivial, and \(M(\epsilon)\) and \(v_\epsilon^+(\epsilon)\) do not need to be specified.

VI. SUMMARY

In summary, using the McKelvey-Shockley flux method we derived simple analytical solutions for \(T(x)\) and \(I_Q\), that contain ballistic phonon effects. Our solutions compare well to the results of the phonon BTE, including temperature jumps (\(\delta T_c\)) at the boundaries. Importantly, our approach can be rewritten exactly as Fourier’s law and the heat equation. Using the correct boundary conditions, we show that Fourier’s law and the heat equation capture ballistic effects and are thus applicable on all length scales. The nature of \(\delta T_c\) is discussed, and found to be effectively modeled by introducing a contact resistance equal to the ballistic thermal resistance. This approach can provide quantitatively accurate results using an energy-dependent \(\lambda\) with a full phonon dispersion, which was shown to be important for silicon films. The work presented in this paper may prove useful in extending finite-element heat transfer tools to capture ballistic effects and analyzing experiments probing short length and time scales, such as TDTR. For the latter, a time-dependent McKelvey-Shockley flux method is needed, which we find can be recast as the hyperbolic heat equation with the appropriate boundary conditions (to be presented in future work).
Acknowledgments

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Appendix A: Heat current in the Casimir limit

In this appendix we show how our derived expression for heat current (Eq. 14), in the ballistic phonon limit, reduces to the known result in the Casimir limit. Starting from Eq. (14), we assume purely ballistic transport, meaning \( \lambda \gg L \) and \( T \to 1 \), which gives

\[
I_Q^{\text{tot}} = \int_0^\infty \epsilon \frac{M(\epsilon)}{h} [f_{\text{BE}}(\epsilon, T_L) - f_{\text{BE}}(\epsilon, T_R)] \, d\epsilon, \tag{A1}
\]

where we have integrated over energy to obtain the total heat current (using Eq. 3). With a linear phonon dispersion, as is commonly assumed in the Casimir limit, the distribution of modes is [29]:

\[
M(\epsilon) = \frac{3\pi\epsilon^2}{h^2 v_g^2}, \tag{A2}
\]

where \( v_g \) is the group velocity and the factor of three is for the three acoustic branches. Inserting Eq. (A2) and the expression for \( f_{\text{BE}} \) into Eq. (A1), we find

\[
I_Q^{\text{tot}} = \frac{3\pi}{h^2 v_g^2} \int_0^\infty \left[ \frac{\epsilon^3}{e^{\epsilon/k_BT_L} - 1} - \frac{\epsilon^3}{e^{\epsilon/k_BT_R} - 1} \right] \, d\epsilon, \tag{A3}
\]

where \( k_B \) is Boltzmann’s constant. Defining a new variable \( y = \epsilon/k_BT_L \), Eq. (A3) becomes:

\[
I_Q^{\text{tot}} = \frac{3\pi k_B^4}{h^4 v_g^2} (T_L^4 - T_R^4) \int_0^\infty \frac{y^3}{e^y - 1} \, dy, \tag{A4}
\]

One can show that the integral is equal to \( \pi^4/15 \), which gives the known result for heat current in the Casimir limit [15]:

\[
I_Q^{\text{tot}} = \sigma (T_L^4 - T_R^4), \tag{A5}
\]

\[
\sigma = \frac{\pi^5 k_B^4}{5h^4 v_g^2}, \tag{A6}
\]

where \( \sigma \) is the Stefan-Boltzmann constant for phonons. Note the above expression is valid at temperatures much less than the Debye temperature of the material.

Appendix B: Traditional expression for thermal conductivity

The expression for bulk thermal conductivity derived from the approach presented in this work is (see Eq. 25): 

\[
\kappa = C_V \lambda v_g^+ / 2, \tag{B1}
\]

where \( C_V \) is the heat capacity, \( \lambda \) the mean-free-path for backscattering and \( v_g^+ \) is the average \( x \)-projected velocity of the forward moving carriers. The commonly encountered relation for thermal conductivity is

\[
\kappa = C_V l v_g / 3, \tag{B2}
\]

where \( l \) is the mean-free-path and \( v_g \) the group velocity. We can show that both Eq. (B1) and Eq. (B2) are identical, in the case of an isotropic phonon dispersion (note our approach applies in the case of any full phonon dispersion). In [34], it is shown that \( v_g^+ = v_g/2 \) and \( \lambda = (4/3) l \). Inserting these relations into Eq. (B1), one directly finds Eq. (B2).

Appendix C: Boundary conditions for temperature

In this note we demonstrate how to derive Eqns. (27-28). Our starting point is Fourier’s law, which we showed is applicable on all length scales (Eq. (23)). By subtracting Eqns. (C1) from (C2) and evaluating \( x = 0^+ \), we obtain

\[
2I_{Q,0}^+ = -\kappa \left. \frac{dT}{dx} \right|_{0^+} + v_g^+ Q(0^+). \tag{C3}
\]

By subtracting Eqns. (C1) from (C2) and evaluating \( x = L^- \), we obtain

\[
2I_{Q,L}^- = \kappa \left. \frac{dT}{dx} \right|_{L^-} + v_g^+ Q(L^-). \tag{C4}
\]

Since we assume the applied temperature difference across the contacts \( \Delta T = T_L - T_R \) is small, the heat currents can be expanded as \( I_Q^+(x) = \delta I_Q^+(x) + I_Q^{\text{eq}} \), where \( I_Q^{\text{eq}} = I_{Q,0}^+ + I_{Q,0}^- \) is the equilibrium heat current associated with a reference background temperature (chosen as \( T_R \) in this case) and \( \delta I_Q^+(x) \) is a correction due to \( \Delta T \). Rewriting Eqns. (C3) and (C4) in terms of the injected heat fluxes due to \( \Delta T \) and using the definition for heat capacity \( C_V (\delta Q = C_V \delta T) \), we find:

\[
2 \delta I_{Q,0}^+ = -\kappa \left. \frac{d(\delta T)}{dx} \right|_{0^+} + C_V v_g^+ \delta T(0^+), \tag{C5}
\]

\[
2 \delta I_{Q,L}^- = \kappa \left. \frac{d(\delta T)}{dx} \right|_{L^-} + C_V v_g^+ \delta T(L^-), \tag{C6}
\]
where \( T(x) = \delta T(x) + T_R \). The above equations relate the injected heat currents at the boundaries to the temperature (and its gradient) at the boundaries, and represent the correct physical boundary conditions for the heat equation and Fourier’s law.

Note that Eqs. (C5-C6) are applicable even when the contacts are not in equilibrium. If the contacts are in equilibrium, then \( \delta I_{Q,0}^+ \) and \( \delta I_{Q,L}^- \) can be obtained by expanding Eqs. (12-13):

\[
I^+_{Q,0} = \epsilon \frac{M}{h} \left[ f_{BE}(T_R) + \frac{\partial f_{BE}}{\partial T} \Delta T \right] \quad (C7)
\]

\[
I_{Q,0}^+ = I_{Q,eq}^+ + \delta I_{Q,0}^+ \quad (C7)
\]

\[
I^-_{Q,L} = \epsilon \frac{M}{h} f_{BE}(T_R) \quad (C8)
\]

By choosing \( T_R \) as the reference temperature, we have \( \delta I_{Q,L} = 0 \).

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