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**ON THE EQUATIONS AND BOUNDARY CONDITIONS GOVERNING
PHONON-MEDIATED HEAT TRANSFER IN THE SMALL MEAN FREE PATH LIMIT.
AN ASYMPTOTIC SOLUTION OF THE BOLTZMANN EQUATION**

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ABSTRACT

Using an asymptotic solution procedure, we construct solutions of the Boltzmann transport equation in the relaxation-time approximation in the limit of small Knudsen number, $Kn \ll 1$, to obtain continuum equations and boundary conditions governing phonon-mediated heat transfer in this limit. Our results show that, in the bulk, heat transfer is governed by the Fourier law of heat conduction, as expected. However, this description does not hold within distances on the order of a few mean free paths from the boundary; fortunately, this deviation from Fourier behavior can be captured by a universal boundary-layer solution of the Boltzmann equation that depends only on the material model and the phonon-boundary interaction model (Boltzmann boundary condition). Boundary conditions for the Fourier description follow from matching this inner solution to the outer (Fourier) solution. This procedure shows that the traditional no-jump boundary conditions are appropriate only to zeroth order in Kn . Solution to first order in Kn shows that the Fourier law needs to be complemented by jump boundary conditions with jump coefficients that depend on the material model and the phonon-boundary interaction model. In this work, we calculate these coefficients and the form of the jump conditions for an adiabatic-diffuse and a prescribed-temperature boundary in contact with a constant-relaxation-time material. Extension of this work to variable relaxation-time models is straightforward and will be discussed elsewhere. Our results are validated via comparisons with low-variance deviational Monte Carlo simulations.

INTRODUCTION

The field of phonon transport has recently received considerable attention in the context of microscale solid state heat transfer. Transport at the device scale, namely involving lengthscales larger than 10nm, is of particular interest in many engineering applications. At these scales, a kinetic-theory approach based on the Boltzmann transport equation (BTE) [1] is preferable to atomistic approaches that become computationally intractable.

Over the years, a number of computational methods for solving the BTE have been developed [2–6]. Unfortunately, when characteristic lengthscales become much larger than the phonon mean free path (the limit of small mean free path is approached), phonon transport becomes collision dominated and Boltzmann-based descriptions become stiff, adversely affecting the computational efficiency of numerical solution methods. For example, time-explicit methods become very expensive, because characteristic timescales become diffusive and thus very long compared to the timestep required for accurate solution. Moreover, resolution at the free path scale implies that the number of computational cells or computational particles required for these simulations becomes very large.

In this paper, we address some of these limitations but also seek to improve our fundamental understanding of microscale transport processes by developing an asymptotic method for solving the Boltzmann equation in the small mean free path limit $Kn \leq 0.1$. In this regime, we expect that the classical Fourier description will provide a good approximation to the solution, with kinetic effects becoming increasingly important as Kn increases.

The asymptotic analysis provides a method for *rigorously* deriving the modifications required to the Fourier description so that the latter can continue to provide solutions for continuum fields that are consistent with the Boltzmann equation and thus can be used as a means of effectively solving the Boltzmann equation much more efficiently than direct numerical methods of solution. Such expansions have been used by Sone and co-workers [7, 8] to derive the continuum equations and boundary conditions describing rarefied gas dynamics.

BACKGROUND

We start by recalling the Boltzmann equation for phonon transport in the relaxation time approximation

$$\frac{\partial f}{\partial t} + \mathbf{V}_g \cdot \nabla_{\mathbf{x}'} f = \frac{f^{\text{loc}} - f}{\tau(\omega, p, T)} \quad (1)$$

where f refers to the occupation number of the phonon states, $\mathbf{V}_g(\omega, p)$ to the group velocity, ω to the frequency, p to the polarization, T to the temperature and f^{loc} to an equilibrium distribution defined by energy conservation considerations (refer for instance to [4, 9] for details on the definition of f^{loc}).

In this work we consider steady problems. Assuming small deviations from equilibrium at temperature T_{eq} , the steady-state Boltzmann equation reads

$$\mathbf{V}_g \cdot \nabla_{\mathbf{x}'} f^{\text{d}} = \frac{\mathcal{L}(f^{\text{d}}) - f^{\text{d}}}{\tau(\omega, p, T_{\text{eq}})} \quad (2)$$

where $f^{\text{d}} = (f - f^{\text{eq}})$, with $f^{\text{eq}} = [\exp(\hbar\omega/k_b T_{\text{eq}}) - 1]^{-1}$, and

$$\mathcal{L}(f^{\text{d}})(\omega, p) = \frac{\int_{\omega, \Omega, p} \frac{\hbar\omega f^{\text{d}}}{\tau} \frac{D}{4\pi} d^2\Omega d\omega \frac{df^{\text{eq}}}{dT}}{C_\tau} \quad (3)$$

In the above expression,

$$C_\tau = \int_{\omega, p} \frac{D\hbar\omega}{\tau} \frac{df^{\text{eq}}}{dT} d\omega \quad (4)$$

where

$$\frac{df^{\text{eq}}}{dT} = \frac{\hbar\omega}{4k_b T_{\text{eq}}^2 \sinh\left(\frac{\hbar\omega}{2k_b T_{\text{eq}}}\right)}. \quad (5)$$

In the above, Ω and $d^2\Omega$ respectively refer to the unit vector defining the direction of propagation of a particle and to the dif-

ferential solid angle, expressed as $\sin(\theta)d\theta d\phi$ in spherical coordinates. The density of states is given by

$$D = D(\omega, p) = \frac{k(\omega, p)^2}{2\pi^2 V_g(\omega, p)} \quad (6)$$

In the interest of compactness, in the above expressions and in what follows, we use a single integral symbol to denote both integrals over multiple variables and sum over polarization.

In this study, in the interest of simplicity, we will only consider the single (constant) mean free path case, denoted by $\Lambda = V_g \tau$, where $\tau = \text{const.}$ and $V_g = \|\mathbf{V}_g\| = \text{const.}$. Although this assumption is usually considered to be very restrictive, extension to the variable mean free path case can be readily obtained [10]. This is further discussed in the Conclusion section. The Knudsen number is defined by $\text{Kn} = \Lambda/L$ where L is the characteristic dimension of the system.

ASYMPTOTIC ANALYSIS

Introducing the dimensionless coordinate $\mathbf{x} = \mathbf{x}'/L$ as well as the function

$$\Phi = \frac{f^{\text{d}}}{df^{\text{eq}}/dT} \quad (7)$$

and

$$\Xi(\omega, p) = \frac{\hbar\omega D(\omega, p)}{4\pi} \frac{df^{\text{eq}}}{dT} \quad (8)$$

we write the Boltzmann equation in the form

$$\Omega \cdot \nabla_{\mathbf{x}} \Phi = \frac{\mathcal{L}(\Phi) - \Phi}{\text{Kn}} \quad (9)$$

Using the parameters introduced above and the single mean free path assumption, the scattering operator can be expressed in the form

$$\mathcal{L}(\Phi) = \frac{\int_{\omega, \Omega, p} \frac{\Xi}{\tau} \Phi d^2\Omega d\omega}{C_\tau} \quad (10)$$

It should then be noted that equation (9) is independent of the frequency ω and polarization p (except in the integral expression of (10)). As a direct consequence, the function Φ is also independent of ω and p , that is, it only depends on Ω and \mathbf{x} . The Boltzmann equation can therefore be written in the form

$$\Omega \cdot \nabla_{\mathbf{x}} \Phi = \frac{\int_{\Omega} \Phi / (4\pi) d^2\Omega - \Phi}{\text{Kn}} \quad (11)$$

The usual macroscopic quantities of interest such as temperature, energy density and heat flux can be calculated from

$$T_{\text{tot}} = T_{\text{eq}} + \frac{1}{4\pi} \int_{\Omega} \Phi d^2\Omega = T_{\text{eq}} + T(\mathbf{x}) \quad (12)$$

$$E_{\text{tot}} = E_{\text{eq}} + \int_{\omega,p} \Xi(\omega,p) d\omega \int_{\Omega} \Phi d^2\Omega \quad (13)$$

$$\mathbf{J} = \int_{\omega,p} \Xi(\omega,p) V_g(\omega,p) d\omega \int_{\Omega} \Phi \Omega d^2\Omega \quad (14)$$

We will refer to $T(\mathbf{x})$ as the deviational temperature, since it represents deviation from the equilibrium temperature T_{eq} .

Bulk solution

The asymptotic solution relies on a ‘‘Hilbert-type’’ [11] expansion of the solution Φ of the form

$$\Phi = \sum_{n=0}^{\infty} \text{Kn}^n \Phi_n \quad (15)$$

Given the nature of the proposed solution, similar expansions can be written for the temperature and the heat flux fields

$$T = \sum_{n=0}^{\infty} \text{Kn}^n T_n \quad (16)$$

$$\mathbf{J} = \sum_{n=0}^{\infty} \text{Kn}^n \mathbf{J}_n \quad (17)$$

In this section, we only consider solutions far from any boundary. As will be shown below, close to the boundary, kinetic effects become important due to the incompatibility of the bulk solution with the kinetic (Boltzmann) boundary condition and a separate, boundary layer analysis is required.

We denote $\Phi_G = \sum \text{Kn}^n \Phi_{Gn}$ the bulk solution, anticipating that $\Phi = \Phi_G + \Phi_K$, where Φ_K is the kinetic boundary layer solution that is zero in the bulk and will be similarly expanded later.

When the expansion for Φ_G is inserted in the Boltzmann equation we obtain

$$\Omega \cdot \nabla_{\mathbf{x}} \sum_{n=0}^{\infty} \text{Kn}^{n+1} \Phi_{Gn} = \sum_{n=0}^{\infty} \text{Kn}^n [\mathcal{L}(\Phi_{Gn}) - \Phi_{Gn}] \quad (18)$$

By equating terms of the same order (Kn^1 and higher powers), we obtain the following relationship for all $n \geq 0$

$$\Omega \cdot \nabla_{\mathbf{x}} \Phi_{Gn} = \mathcal{L}(\Phi_{Gn+1}) - \Phi_{Gn+1}. \quad (19)$$

In addition, considering the two terms of order 0 in the right hand side of (18), we find that Φ_{G0} is determined by the solution of the equation

$$\Phi_{G0} = \mathcal{L}(\Phi_{G0}) = \frac{\int_{\omega,\Omega,p} \frac{\Xi}{\tau} \frac{d f^{\text{eq}}}{dT} \Phi_{G0} d^2\Omega d\omega}{C_{\tau}}. \quad (20)$$

From this equation we deduce that Φ_{G0} is a function that depends on \mathbf{x} only, since this is the case for $\mathcal{L}(\Phi_{G0})$. We note here that any function that only depends on \mathbf{x} is a solution. Additionally, since $\Phi_{G0} = \Phi_{G0}(\mathbf{x})$, we find that the zeroth order deviational bulk temperature is given by

$$T_{G0}(\mathbf{x}) = \frac{1}{4\pi} \int_{\Omega} \Phi_{G0}(\mathbf{x}) d^2\Omega = \Phi_{G0}(\mathbf{x}). \quad (21)$$

At this stage, the spatial dependence of Φ_{G0} is undetermined. The additional information needed will be inferred from the application of a solvability condition to Φ_{G1} .

An expression for the order 1 solution can be found using (19)

$$\Phi_{G1} = \mathcal{L}(\Phi_{G1}) - \Omega \cdot \nabla_{\mathbf{x}} \Phi_{G0} \quad (22)$$

A necessary condition for Φ_{G1} to be the order 1 solution is to be equal to the sum of $-\Omega \cdot \nabla_{\mathbf{x}} \Phi_{G0}$ and a function that only depends on \mathbf{x} . Reciprocally, if we write $\Phi_{G1} = \Phi_{e1} - \Omega \cdot \nabla_{\mathbf{x}} \Phi_{G0}$ with $\Phi_{e1} = \Phi_{e1}(\mathbf{x})$, then it follows that Φ_{G1} is solution of (22). Since the temperature associated with Φ_{G1} is exactly Φ_{e1} , we can write $\Phi_{G1} = T_{G1} - \Omega \cdot \nabla_{\mathbf{x}} T_{G0}$.

Finally, order 2 may be derived following the same procedure. Equation

$$\Omega \cdot \nabla_{\mathbf{x}} \Phi_{G1} = \mathcal{L}(\Phi_{G2}) - \Phi_{G2} \quad (23)$$

implies

$$\Phi_{G2} = \mathcal{L}(\Phi_{G2}) - \Omega \cdot \nabla_{\mathbf{x}} T_{G1} + \Omega \cdot \nabla_{\mathbf{x}} (\Omega \cdot \nabla_{\mathbf{x}} T_{G0}) \quad (24)$$

In the following section, we show that the temperature associated with Φ_{G2} is $\mathcal{L}(\Phi_{G2}) = T_{G2}$. We will show it by deriving the governing equation for T_0 .

Governing equation for the temperature field

The solvability condition required to determine Φ_{Gn} is a statement of energy conservation, namely

$$\int_{\omega,p} 4\pi \frac{\Xi}{\tau} \mathcal{L}(\Phi) d\omega = \int_{\omega,p,\Omega} \frac{\Xi}{\tau} \Phi d\omega d^2\Omega \quad (25)$$

Writing this relationship for each order results in

$$\int_{\omega,p} 4\pi \frac{\Xi}{\tau} \mathcal{L}(\Phi_{Gn+1}) d\omega = \int_{\omega,p,\Omega} \frac{\Xi}{\tau} \Phi_{Gn+1} d\omega d^2\Omega \quad (26)$$

for any n and implies

$$\int_{\omega,p,\Omega} \Xi V_g \Omega \cdot \nabla_{\mathbf{x}} \Phi_{Gn} d\omega d^2\Omega = 0 \quad (27)$$

If we apply this relationship to Φ_{G1} , we then obtain

$$\int_{\omega,p,\Omega} \Xi V_g \Omega \cdot \nabla_{\mathbf{x}} (T_{G1} - \Omega \cdot \nabla_{\mathbf{x}} T_{G0}) d\omega d^2\Omega = 0 \quad (28)$$

which implies

$$\nabla_{\mathbf{x}}^2 T_{G0} = 0 \quad (29)$$

This concludes the proof that the 0-th order temperature field obeys the steady state heat equation. It can also be shown that the subsequent order terms similarly obey the heat equation [10]. In other words, for order 1, the highest order considered here, the temperature field in the bulk, $T_{G1}(\mathbf{x})$, obeys

$$\nabla_{\mathbf{x}}^2 T_{G1} = 0 \quad (30)$$

To this order, the *fundamental difference* compared to the macroscopic heat conduction description derived from a continuum point of view, or even Chapman-Enskog type expansions showing [12] that to first order the heat flux is proportional to the temperature gradient (and thus the temperature field obeys the Laplace equation) *resides in the boundary conditions*. A more thorough discussion can be found in the Conclusion section. Below we consider in detail one type of boundary, namely a prescribed-temperature boundary.

Boundary conditions associated with prescribed temperature boundaries

The term prescribed temperature boundary is typically used to describe a boundary approximating a black-body, absorbing incoming phonons and emitting phonons from an equilibrium (isotropic) distribution at a given temperature. In other words, the Boltzmann boundary condition associated with such a boundary at deviational temperature T_b is a Bose-Einstein (equilibrium) distribution at the wall temperature, denoted here by

$f^{\text{eq}}(\omega; T_{\text{eq}} + T_b)$. In the linearized case, the incoming distribution of deviational particles is therefore

$$f_b = T_b \frac{df^{\text{eq}}}{dT} \quad (31)$$

or simply, in terms of quantity Φ defined in (7)

$$\Phi_b = T_b \quad (32)$$

Here we assume that the boundary is flat; boundary curvature will be considered in a future publication. Without loss of generality we assume that the boundary is located at $x_1 = 0$ and with an inward normal pointing in the positive x_1 direction.

We note that Φ_{G0} is isotropic and is thus able to match Φ_b provided we set

$$T_{G0} = T_b \quad (33)$$

at the boundary. Therefore, **at order 0, the solution to the Boltzmann equation with prescribed temperature boundaries is given by the heat equation complemented by the usual Dirichlet boundary conditions** and no boundary layer correction is required ($\Phi_{K0} = 0$).

This situation changes at order 1. The order 1 distribution $\Phi_{G1} = T_{G1} - \Omega \cdot \nabla_{\mathbf{x}} T_{G0}$ is not isotropic due to the gradient of T_{G0} . As a consequence, there is a mismatch between the order 1 solution and the boundary condition (which has been satisfied by Φ_{G0} and is thus zero for all subsequent orders). This mismatch can be corrected by introducing a boundary layer term Φ_{K1} .

Let us write the problem that Φ_{K1} satisfies. First, by linearity, Φ_{K1} is a solution of the Boltzmann equation with one spatial dimension. Introducing the stretched coordinate $\eta = x_1/Kn$, the Boltzmann equation for Φ_{K1} becomes

$$\cos(\theta) \frac{\partial \Phi_{K1}}{\partial \eta} = \mathcal{L}(\Phi_{K1}) - \Phi_{K1} \quad (34)$$

where θ is the polar angle taken with respect to x_1 . The associated boundary condition is

$$\Phi_{K1}|_{\eta=0} + \Phi_{G1}|_{\eta=0} = 0, \quad (35)$$

which translates into the following relation

$$\Phi_{K1}|_{\eta=0} = -T_{G1}|_{\eta=0} + \Omega \cdot \nabla_{\mathbf{x}} T_{G0} \quad (36)$$

The term $\nabla_x T_{G0}$ is known from the order 0 solution. The term $T_{G1}|_{\eta=0}$ is unknown and determined by the fact that there exists only one value for $T_{G1}|_{\eta=0}$ such that Φ_{K1} tends to 0 for $\eta \rightarrow \infty$ [14]. This determination proceeds by decomposing Φ_{K1} into three components

$$\Phi_{K1} = \Phi_{K1,1} + \Phi_{K1,2} + \Phi_{K1,3} \quad (37)$$

where each of $\Phi_{K1,i}$, $i = 1, 2, 3$ is the solution to an equation of the form (34) with the associated boundary condition:

$$\Phi_{K1,1}|_{\eta=0} = (-c_1 + \cos(\theta)) \frac{\partial T_{G0}}{\partial x_1} \quad (38)$$

$$\Phi_{K1,2}|_{\eta=0} = (-c_2 + \sin(\theta) \cos(\phi)) \frac{\partial T_{G0}}{\partial x_2} \quad (39)$$

$$\Phi_{K1,3}|_{\eta=0} = (-c_3 + \sin(\theta) \sin(\phi)) \frac{\partial T_{G0}}{\partial x_3} \quad (40)$$

Here x_2 and x_3 denote cartesian coordinates in the plane of the boundary, which along with x_1 form a right-handed set. The constants c_1, c_2, c_3 are uniquely determined by the condition that $\Phi_{K1,1}, \Phi_{K1,2}$ and $\Phi_{K1,3}$ individually tend to zero for $\eta \rightarrow \infty$. We also note that $c_1 + c_2 + c_3 = T_{G1}$.

Under the above conditions, $\Phi_{K1,2}$ and $\Phi_{K1,3}$ and the associated constants c_2 and c_3 can be found analytically. One can easily verify that $c_2 = c_3 = 0$, with

$$\Phi_{K1,2} = \begin{cases} \sin(\theta) \cos(\phi) \frac{\partial T_{G0}}{\partial x_2} \exp\left(\frac{-\eta}{\cos(\theta)}\right), & \text{for } \cos(\theta) > 0 \\ 0, & \text{for } \cos(\theta) < 0 \end{cases} \quad (41)$$

and

$$\Phi_{K1,3} = \begin{cases} \sin(\theta) \sin(\phi) \frac{\partial T_{G0}}{\partial x_3} \exp\left(\frac{-\eta}{\cos(\theta)}\right) & \text{for } \cos(\theta) > 0 \\ 0 & \text{for } \cos(\theta) < 0 \end{cases} \quad (42)$$

are solutions to (34) with boundary conditions (39), respectively, and (40). The temperature field associated with these functions is zero.

The problem for $\Phi_{K1,1}$ can be solved numerically [10] yielding $c_1 \approx 0.7104$. The temperature field per unit temperature gradient in the bulk solution associated with $\Phi_{K1,1}$, namely $\tau_{K1,1} \equiv T_{K1,1}/(\partial T_{G0}/\partial x_1)$ is plotted in Figure 1. We therefore showed that the boundary condition for the order 1 bulk temperature field is

$$T_{G1}(x_1 = 0) = c_1 \frac{\partial T_{G0}}{\partial x_1} \Big|_{x_1=0} \quad (43)$$

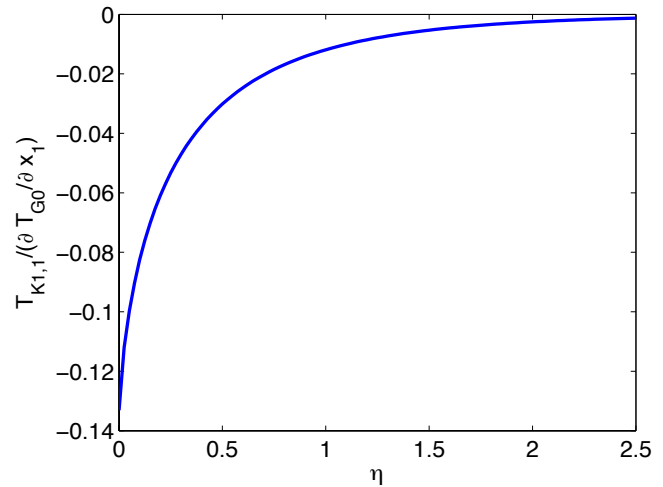


Figure 1. Temperature profile associated with $\tau_{K1,1} \equiv T_{K1,1}/(\partial T_{G0}/\partial x_1)$.

or more generally

$$T_{G1}|_{x_b} = c_1 \frac{\partial T_{G0}}{\partial \mathbf{n}} \Big|_{x_b} \quad (44)$$

where we use \mathbf{n} to denote the wall normal pointing into the material and \mathbf{x}_b the boundary location. In other words, the boundary condition is of the jump type and the associated temperature jump is proportional to the derivative of the 0th order solution in the direction normal to the boundary.

The amplitude of the corrective boundary layer that is added near the wall is also proportional to the normal derivative:

$$T_{K1} = \tau_{K1,1} \frac{\partial T_{G0}}{\partial \mathbf{n}} \Big|_{x_b} \quad (45)$$

Note that although a non-zero temperature field is associated with $\Phi_{K1,1}$, the corresponding heat flux is zero. This is explained by the fact that $\Phi_{K1,1}$, by construction, tends to 0 at infinity. Since the boundary layer problem is one-dimensional in space, by energy conservation, the heat flux has to be constant in x_1 and is therefore zero everywhere.

Boundary conditions for a diffuse adiabatic boundary

The case of diffuse adiabatic boundaries can be treated through a similar approach where the mismatch between the bulk asymptotic solution and the boundary condition is analyzed and corrected. The boundary condition in the single mean free path

case is [13]

$$\Phi(\mathbf{x}_b, 0 \leq \theta < \pi/2) = -\frac{1}{\pi} \int_{\theta > \pi/2, \phi} \Phi(\mathbf{x}_b, \theta, \phi) \Omega \cdot \mathbf{n} d^2\Omega \quad (46)$$

where θ is the angle between Ω and \mathbf{n} . A major difference from the prescribed temperature boundary is that applying this condition to the 0th order bulk solution gives no information, because Φ_{G0} satisfies (46) regardless of its value at the wall. The boundary condition for T_{G0} is obtained by analyzing the order 1 mismatch. The analysis yields

$$\left. \frac{\partial T_{G0}}{\partial \mathbf{n}} \right|_{\mathbf{x}_b} = 0, \quad (47)$$

which is compatible with the Neumann boundary conditions associated with adiabatic boundaries.

Condition (47) comes with an order 1 boundary layer, which is the manifestation of the mismatch between the anisotropic bulk terms and the imposed boundary condition (46). More details can be found in [10].

VALIDATION

In this section we validate our solution but also take the opportunity to demonstrate how the asymptotic solution can be used to construct solutions for the temperature field that are **rigorously** consistent with the Boltzmann equation by considering a simple 1D problem and comparing our results with precise Monte Carlo solutions of the Boltzmann equation using a variant of the method described in [6]. We consider a silicon slab of thickness L confined between two walls at different prescribed temperatures. Using dimensionless coordinates, the walls are located at $x_1 = 0$ and $x_1 = 1$ and have deviational temperatures T_L and T_R , respectively.

We recall that under the asymptotic analysis, the temperature field is given by

$$T(x_1) = T_{G0}(x_1) + \text{Kn}T_1(x_1) + O(\text{Kn}^2) \quad (48)$$

$$= T_{G0}(x_1) + \text{Kn}(T_{G1}(x_1) + T_{K1}(x_1)) + O(\text{Kn}^2) \quad (49)$$

The order 0 solution straightforwardly reads

$$T_{G0}(x_1) = T_L + (T_R - T_L)x_1 \quad (50)$$

since it is the solution of the heat conduction equation subject to no-jump boundary conditions. Therefore, the boundary condi-

tions for the order 1 field are

$$T_{G1}(x_1 = 0) = c_1 \frac{\partial T_{G0}}{\partial x_1} = c_1(T_R - T_L) \quad (51)$$

$$T_{G1}(x_1 = 1) = -c_1 \frac{\partial T_{G0}}{\partial x_1} = c_1(T_L - T_R) \quad (52)$$

which results in

$$T_{G1}(x_1) = c_1(T_R - T_L)(1 - 2x_1) \quad (53)$$

The boundary layer $T_{K1}(x_1) = (T_R - T_L)\tau_{K1,1}(x_1)$ contributes to the solution near the wall at $x_1 = 0$, while the function $(T_L - T_R)\tau_{K1,1}(1 - x_1)$ contributes close to the wall at $x_1 = 1$. The resulting solution correct to order 1 (eq (49)) is plotted in figure 2 for $\text{Kn} = 0.1$ and compared to our benchmark (adjoint Monte Carlo [12]) result. The agreement is excellent; we note in particular that even though the boundary layer correction is small at this Knudsen number, the temperature jumps are considerable and are accurately captured by the asymptotic solution.

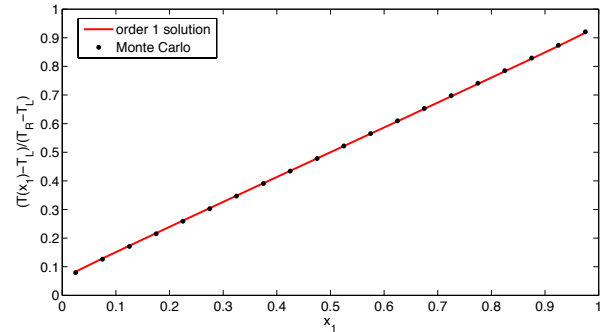


Figure 2. Order 1 solution (plain line) compared to the solution computed by highly resolved Monte Carlo simulation at $\text{Kn} = 0.1$.

Note on the treatment of the validation problem to higher order

If desired, calculation of $T(x_1)$ to second order in Kn proceeds by solving the heat conduction equation for T_{G2} subject to the appropriate boundary conditions, which will, in general, involve second derivatives of T_{G0} , as well as first derivatives of T_{G1} . Although not presented here, these boundary conditions have been determined for various types of boundaries and will be presented in a future publication [10].

Here, however, we note that due to the simplicity of the validation problem considered above, the second-order solution can

be calculated without knowledge of second-order boundary conditions because the second derivative of T_{G0} is 0. In this case, the bulk second order solution (eq. (24)) can be written as

$$\Phi_{G2} = T_{G2} - \Omega_1 \frac{\partial T_{G1}}{\partial x_1} \quad (54)$$

The analysis previously presented for order 1 can be applied identically to the second order, starting from

$$\Phi_{K2}|_{\eta=0} + \Phi_{G2}|_{\eta=0} = 0, \quad (55)$$

and using (54). It yields

$$T_{G2}(x_1 = 0) = c_1 \frac{\partial T_{G1}}{\partial x_1}(x_1 = 0) = -2c_1^2(T_R - T_L) \quad (56)$$

$$T_{G2}(x_1 = 1) = -c_1 \frac{\partial T_{G1}}{\partial x_1}(x_1 = 1) = 2c_1^2(T_R - T_L) \quad (57)$$

with the solution

$$T_{G2}(x_1) = -2c_1^2(T_R - T_L)(1 - 2x_1) \quad (58)$$

In fact, in this particular case where only first derivatives are non zero, this process can be repeated for all orders without knowledge of the higher order jump coefficients, leading to an asymptotic solution that is, in principle, correct to all orders. In other words, for $n \geq 1$:

$$T_{Gn}(x_1) = (-2)^{n-1} c_1^n (T_R - T_L)(1 - 2x_1) \quad (59)$$

Summing all orders (provided $2\text{Kn}c_1 < 1$), we obtain:

$$\frac{T_G(x_1) - T_L}{T_R - T_L} = x_1 + \frac{\text{Kn}c_1}{1 + 2\text{Kn}c_1}(1 - 2x_1) \quad (60)$$

The boundary layer corrections of all orders can also be obtained (and summed) using the same process. For example, for the boundary at $x_1 = 0$, we obtain

$$\frac{T_K(x_1)}{T_R - T_L} = \frac{\text{Kn}}{1 + 2\text{Kn}c_1} \tau_{K1}(x_1). \quad (61)$$

The second boundary layer (at $x_1 = 1$) is obtained analogously. This solution is asymptotically accurate to all orders; for a discussion on the error associated with the asymptotic expansion see [14].

Figure 3, compares the order 1, infinite order and “exact” (Monte Carlo) solution for $\text{Kn} = 0.5$. The infinite order solution is in very good agreement with the exact solution, while the order 1 solution is clearly inadequate at this Knudsen number.

Note on an alternative form for the jump boundary conditions

In the last section we derived a solution that is “asymptotically accurate to infinite order” by summing all terms in the power series in Kn under the assumption that it converges. This solution could also be obtained by directly solving the heat conduction equation subject to the boundary condition

$$T_G|_{x_b} - T_b = c_1 \text{Kn} \left. \frac{\partial T_G}{\partial \mathbf{n}} \right|_{x_b}, \quad (62)$$

a form that is very common in the rarefied gas literature [16].

One can show that this “implicit” form is equivalent to the staggered prescription derived above (eqs (33) and (44)) to order Kn . Specifically, expanding

$$T_G|_{x_b} = (T_{G0} + \text{Kn}T_{G1} + \text{Kn}^2T_{G2} + \dots)|_{x_b} \quad (63)$$

and similarly for $\partial T / \partial \mathbf{n}|_{x_b}$ at the boundary location and substituting into (62), one obtains $T_{G0}|_{x_b} = T_b$ to order Kn^0 and

$$T_{G1}|_{x_b} = c_1 \left. \frac{\partial T_{G0}}{\partial \mathbf{n}} \right|_{x_b} \quad (64)$$

to $O(\text{Kn})$, which are identical to eqs (33) and (44), respectively.

As will be shown in [10], at order Kn^2 and higher, additional terms involving higher derivatives appear in (56) and (57) and their higher order counterparts, requiring (62) to be modified if it is to be equivalent to the former to higher order than Kn . It is only in the special case of the validation problem discussed here, where all derivatives higher than order 1 are zero and therefore $T_{Gn+1} = c_1 \partial T_{Gn} / \partial \mathbf{n}$ at the boundary for any n , that (62) yields results that are correct to all orders.

CONCLUSION

We have presented an asymptotic solution method for solving the Boltzmann equation in the limit $\text{Kn} \leq 1$ for steady problems. The resulting solution provides governing equations and boundary conditions that determine the continuum temperature and heat flux fields in arbitrary three-dimensional geometries. Our results show that the equation governing the temperature field is the steady heat equation. Although this can be shown by the usual kinetic theory analysis [1,9] (expanding the distribution function about the *local* equilibrium and giving no consideration to boundaries), the novel contribution of the present work is the derivation of boundary conditions that complement this equation so that the resulting solutions of this system are *rigorously* consistent with solutions of the Boltzmann equation and explain the

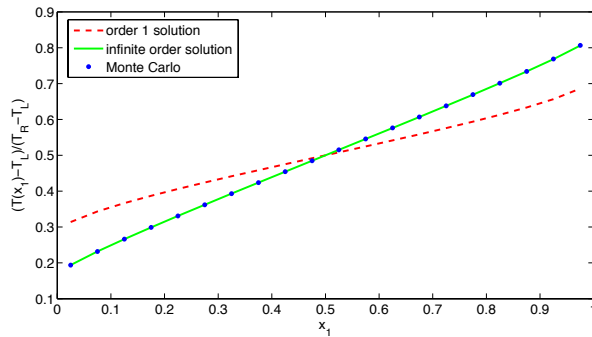


Figure 3. Order 1 solution (dashed line) and "infinite order" solution (solid line) compared to the solution computed by a finely resolved Monte Carlo simulation for $Kn = 0.5$. At this Knudsen number the boundary layer contribution is clearly visible (the solution is no longer a straight line).

temperature jumps at the boundaries previously observed and remarked upon [15].

The emergence of the heat equation as the governing equation is a manifestation of the fact that, in the $Kn \ll 1$ limit, the bulk description remains unperturbed and kinetic effects only appear at the boundaries. Specifically, one can show that, to first order in Kn , the heat flux in the bulk

$$\mathbf{J}_{G1} = \frac{1}{3} \int_{\omega,p} \Xi V_g^2 \tau d\omega \nabla_{\mathbf{x}} T_{G0} \quad (65)$$

is given by the same constitutive law derived by standard kinetic theory [1, 9]. Kinetic effects near boundaries can be captured by solution of the heat equation subject to jump boundary conditions at order 1 in Kn and higher, as well as the addition of boundary layer functions to the temperature field and the heat flux.

Additional results [10], not shown here, reveal that the physical picture described above remains unmodified when the mean free path depends on the frequency and polarization, with the latter only affecting the numerical details of the jump coefficients and boundary layers. In this sense, studying the single mean free path case is very useful.

Although the agreement of the first-order result at $Kn = 0.1$ with simulations was excellent, this may have been a result of the simplicity of the problem considered here. The asymptotic procedure outlined here can be extended to higher order in Kn to obtain, in principle, an even more accurate asymptotic description. Studies in rarefied gas dynamics [16] show that second-order asymptotic formulations are reliable to engineering accuracy up to $Kn \approx 0.4$ and in some cases beyond. An asymptotic theory to second order in Kn and extensive investigation of the limits of its validity will be presented in a future publication [10].

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REFERENCES

- [1] J. M. Ziman. *Electrons and Phonons*. Clarendon Press, Oxford, UK, 1960.
- [2] J. Y. Murthy and S. R. Mathur. Computation of Sub-Micron Thermal Transport Using an Unstructured Finite Volume Method, *J. Heat Transfer* 124(6), 1176-1181, 2002.
- [3] J. M. Loy, J. Y. Murthy, and D. Singh. A fast Hybrid Fourier Boltzmann Transport Equation Solver for Nongray Phonon Transport, *J. Heat Transfer* 135(1), 011008, 2012.
- [4] Q. Hao, G. Chen, and M. S. Jeng. Frequency-dependent Monte Carlo simulation of phonon transport in two-dimensional porous silicon with aligned pores. *J. Appl. Phys.* 106(11):114321, 2009.
- [5] J.-P. M. Péraud and N. G. Hadjiconstantinou. Efficient simulation of multidimensional phonon transport using energy-based variance-reduced Monte Carlo formulations. *Phys. Rev. B* 84:205331, 2011.
- [6] J.-P. M. Péraud and N. G. Hadjiconstantinou. An alternative approach to efficient simulation of micro/nanoscale phonon transport. *Appl. Phys. Lett.* 101:153114, 2012.
- [7] Y. Sone. "Asymptotic theory of flow of rarefied gas over a smooth boundary I", in *Proceedings of the Sixth International Symposium on Rarefied Gas Dynamics* (Academic, New York, 1969), Vol. 1, pp. 243-253.
- [8] Y. Sone and K. Aoki. Slightly rarefied gas flow over a specularly reflecting body. *Phys. Fluids* 20, 571-576, 1977.
- [9] G. Chen. *Nanoscale energy transport and conversion*, Oxford University Press, 2005.
- [10] J.-P. M. Péraud and N. G. Hadjiconstantinou, in preparation
- [11] H. Grad, Asymptotic theory of the Boltzmann equation, *Phys. Fluids* 6, 147-181, 1963.
- [12] J.-P. M. Péraud, C. D. Landon and N. G. Hadjiconstantinou. Monte Carlo Methods for Solving the Boltzmann Transport Equation. *Ann. Rev. Heat Transfer*, 2014.
- [13] S. Mazumder and A. Majumdar. Monte Carlo Study of Phonon Transport in Solid Thin Films Including Dispersion and Polarization. *J. Heat Transfer* 123(4), 749-759, 2001.
- [14] Y. Sone. *Kinetic Theory and Fluid Dynamics*. Birkhäuser Boston, 2002.
- [15] R. Yang, G. Chen, M. Laroche, and Y. Taur. Simulation of Nanoscale Multidimensional Transient Heat Conduction Problems Using Ballistic-Diffusive Equations and Phonon Boltzmann Equation. *J. Heat Transfer* 127(3), 298-306, 2005.
- [16] N. G. Hadjiconstantinou, The Limits of Navier-Stokes The-

ory and Kinetic Extensions for Describing Small Scale
Gaseous Hydrodynamics. *Phys. Fluids* 18, 111301, 2006