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Note

Gradient-dependent heat conductivity from the Grad solution of the Boltzmann equation

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Abstract

Using Grad's approximation for the solution of the Boltzmann equation, we obtained the dependence of the heat conductivity on the temperature gradient for a stationary gas at rest. This dependence is non-analytical.

INTRODUCTION

The Fourier law of heat transport

$$\boldsymbol{q} = -\lambda_0(T)\,\nabla T$$

both in the kinetic theory of gases (Ferziger and Kaper [1]) and in non-equilibrium statistical thermodynamics (Zubarev [2]) is the result of the first approximation in the expansion of the distribution function in gradients of thermodynamical parameters. Several attempts have been made to generalize the Fourier law using either the phenomenological approach or the Boltzmann equation and its models.

Khonkin [3] has derived a small correction to the Chapman–Enskog value of the heat conductivity under the assumption of a constant temperature gradient. Santos et al. [4] and Brey et al. [5] used the one-dimensional Bhatnagar–Gross–Krook model kinetic equation, and for constant pressure found no temperature gradient-dependent corrections to the heat flux. Computer simulation was also used to check this law [6] and has demonstrated its linearity in the one-dimensional case (also for $p = \text{const}$).

This note is an attempt to obtain a generalized Fourier law with non-linear dependence of the heat flux on the temperature gradient in the frame of Grad's transport equations. Grad [7] derived these equations from the Boltzmann equation using a thirteen-moment approximation of the distribution function.

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THIRTEEN MOMENT EQUATIONS

Consider the stationary gas at rest, $\partial/\partial t = 0$, $\boldsymbol{u} = 0$, so that the Burnett correction to the heat flux is zero. The equation of continuity is an identity, and the equations of moment and energy transport are

$$\partial p/\partial x_i = -\partial\sigma_{ij}/\partial x_j \tag{1}$$

$$\partial q_i/\partial x_i = 0 \tag{2}$$

The Grad relations for the viscous stress and the heat flux are

$$\sigma_{ij} = -(8\lambda_0/75pR)(\partial q_i/\partial x_j + \partial q_j/\partial x_i) \tag{3}$$

$$q_i = -\lambda_0 \partial T/\partial x_i - (7\lambda_0\sigma_{ij}/5p)\,\partial T/\partial x_j - (2\lambda_0 T/5p)\,\partial\sigma_{ij}/\partial x_j \tag{4}$$

Here R is the gas constant and $\lambda_0 = \lambda_0(T)$ is the Chapman–Enskog value of the heat conductivity.

NON-LINEAR HEAT CONDUCTIVITY

In order to obtain explicit analytical relationships we consider further the simple case of d-dimensional symmetry. From eqn. (2) we have in this case

$$r^{1-d}(\mathrm{d}/\mathrm{d}r)(r^{d-1}q) = 0$$

so that

$$q = q_0(r/r_0)^{1-d} \tag{5}$$

Inserting eqn. (5) into eqn. (3), we can define σ. After using these expressions for q and σ in eqns. (1) and (4) we obtain the following relations

$$\mathrm{d}(\ln\tau)/\mathrm{d}(\ln\xi) = [2s/5 - \kappa(1-s)]/[1 + 2(n+1)s/5 - 7s^2/5] \tag{6}$$

$$\mathrm{d}(\ln\pi)/\mathrm{d}(\ln\xi) = s(1 + n\kappa + 7s/5)/[1 + 2(n+1)s/5 - 7s^2/5] \tag{7}$$

Here we have introduced the dimensionless quantities

$$\tau = T/T_0,\ \pi = p/p_0,\ \xi = r/r_0,\ a = \mathrm{sign}(q_0)$$

$$s = \sigma/p = a(d-1)\tau^n\xi^{-d}\pi^{-2},\ \kappa = qr/\lambda_0 T = a\xi^{2-d}\tau^{-n-1} \tag{8}$$

and T_0, p_0 are chosen so that

$$16\,|q_0|\,\lambda_0(T_0) = 75p_0^2 r_0 R,\ \lambda_0(T_0)T_0 = |q_0|\,r_0$$

n is the exponent in the Chapman–Enskog dependence $\lambda_0(T) = \lambda_0(T_0)(T/T_0)^n$, which is true for power-like intermolecular potentials. For more realistic potentials, such as Lennard–Jones, one should use the inherent parameter: $T_0 = \epsilon/k$, so that $\lambda_0(T)$ is again a function of T/T_0.

In order to define pressure and temperature fields one should solve eqns. (6) and (7) with appropriate boundary conditions. However, to obtain the dependence of the effective heat conductivity λ properly defined

$$q = -\lambda \, \mathrm{d}T/\mathrm{d}r$$

on a dimensionless temperature gradient $\gamma = \mathrm{d}\tau/\mathrm{d}\xi$ is a matter of simple algebraic manipulation of eqns. (5)–(7)

$$l = \lambda/\lambda_0 = \kappa\left[1 + 2(n+1)s/5 - 7s^2/5\right]/\left[2s/5 - \kappa(1-s)\right] \tag{9}$$

where

$$s = -(d-1)\pi^{-2}\tau^{n(2d-1)/(d-1)}\,|l\gamma|^{1/(d-1)}l\gamma \tag{10}$$

$$\kappa = -\tau^{(1-d-n)/(d-1)}\,|l\gamma|^{-1/(d-1)}l\gamma \tag{11}$$

RESULTS AND DISCUSSION

For small γ we can derive from eqns. (9)–(11) the first correction to the Fourier law $l \equiv 1$

$$l = 1 + (2/5)\pi^{-2}\Big[2\tau^{(2nd+d-1)/(d-1)}\,|\gamma|^{2/(d-1)} - (n+7/2)\tau^{n(2d-1)/(d-1)}\,|\gamma|^{1/(d-1)}\gamma\Big]$$

This depends not only on the absolute value of the temperature gradient, but on its sign as well. The dependence on the gradient is moreover non-analytical in contrast to that derived by Khonkin [3]. The reason seems to be that we did not assume the temperature gradient to be constant.

Generally, eqns. (9)–(11) give the implicit relationship between l and γ for fixed τ and π. Figure 1 shows the dependence $l(\gamma)$ for $d = 3$, $n = 1$ (Maxwell molecules), $\pi = \tau = 1$. The dependence is multi-valued, so Fig. 1

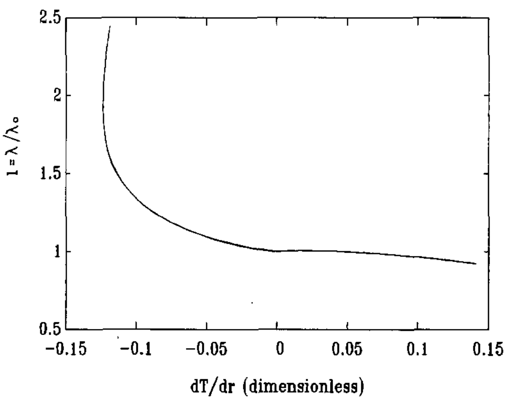

Fig. 1. Heat conductivity versus temperature gradient (eqns. (9)–(11)).

depicts only a physically correct branch that passes through $\gamma = 0$, $l = 1$. This branch begins at the turnover point ($\gamma \cong -0.124$, $l \cong 1.939$ for this specific case) and ends at $\gamma = +\infty$, $l = +0$.

Note that for $d = 2$ eqns. (9)–(11) define $\gamma(l)$ explicitly.

For the unidimensional case ($d = 1$) the first eqn. (8) immediately gives $s = 0$ and from eqn. (9) we see that $l \equiv 1$. This is why all one-dimensional attempts to obtain a non-linear Fourier law, either numerically or analytically (e.g., Tenenbaum et al. [6], Santos et al. [4] and Brey et al. [5]) give no result.

REFERENCES

1 J.H. Ferziger and H.G. Kaper, Mathematical Theory of Transport Processes in Gases, North-Holland, Amsterdam, 1972.
2 D.N. Zubarev, Nonequilibrium Statistical Thermodynamics, Plenum Press, New York, 1974.
3 A.D. Khonkin, Numerical methods in continuum mechanics (Chislennye Metody Mekh. Sploshnoi Sredy), 13 (1982) 130 (in Russian).
4 A. Santos, J.J. Brey and V. Garzó, Phys. Rev. A 34 (1986) 5047.
5 J.J. Brey, A. Santos and J.W. Dufty, Phys. Rev. A 36 (1987) 2842.
6 A. Tenenbaum, G. Ciccotti and R. Gallico, Phys. Rev. A 25 (1982) 2778.
7 H. Grad, Commun. Pure Appl. Math. 2 (1949) 331.