Divergence of the nonlinear thermal conductivity in the homogeneous heat flow

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The moment equations of the BGK kinetic equation are solved for a steady homogeneous heat flow generated by a nonconservative external force. It is shown that the presence of the external force leads to a divergence of the "thermal conductivity" for any finite value of the field strength.

In the past years, several techniques have been used in molecular dynamics simulations to produce fluxes in homogeneous systems. These techniques rely on the introduction of homogeneous, velocity-dependent external forces. Since these forces do work on the system, a drag force is usually added to keep the temperature constant. Nonequilibrium states generated in this way include uniform shear flow [1,2], heat flow, [3,4] and color diffusion [5]. Although these methods are quite efficient from the computer point of view, the relationship between the resulting states and those driven by realistic boundary conditions is not completely clear.

Here, we shall be concerned with the Evans method [3] to simulate heat flow by means of a homogeneous external force. As pointed out by Evans [3,6], no physical meaning outside the linear regime is known for the nonlinear transport coefficient $\lambda(\epsilon)$, ϵ being the external force parameter that mimics the effect of a thermal gradient $\nabla T/T$. Very recently, Loose [7] has studied this problem in dilute gases by using simulation as well as kinetic theory. Loose's kinetic theory study led him to conclude that the Evans method is useful in the linear regime, but the nonlinear "thermal conductivity" $\lambda(\epsilon)$ diverges for ϵ greater than a certain threshold value $\epsilon_{th}>0$. The latter conclusion is drawn from a qualitative analysis based on terms apparently dominant in the moment hierarchy of the Boltzmann equation, and also, at a quantitative level, from a finite-moment approximation to the Boltzmann equation. The first analysis indicates that all the coefficients $\lambda^{(r)}$ in the series expansion,

$$\lambda(\epsilon)=\sum_{r=0}^{\infty}\lambda^{(r)}\epsilon^{2r}, \tag{1}$$

are positive [7]. Although not explicitly stated, the spirit of the analysis is consistent with the expectation that the coefficients $\lambda^{(r)}$ do not tend to zero as r increases. In that case, the series (1) would diverge to infinity for any finite value of ϵ, i.e. $\epsilon_{th}=0$.

The purpose of this paper is to evaluate explicitly the coefficients $\lambda^{(r)}$ from the exact moment equations. The price to be paid is the use of the Bhatnagar–Gross–Krook (BGK) kinetic equation [8] as a model of the Boltzmann equation. In this model, the Boltzmann collision term is replaced by a single-time relaxation towards the local equilibrium distribution. It has been shown that the moment solutions to the BGK [9] and the Boltzmann [10] equations for the steady inhomogeneous heat flow have a great similarity. In other nonequilibrium situations, the first few moments of the BGK equation may exhibit a good quantitative agreement with those of the Boltzmann equation [11].

Let us consider a monatomic dilute gas in a steady homogeneous state in presence of the external force,

$$\boldsymbol{F}=-(\tfrac{1}{2}mv^2-\tfrac{3}{2}k_B T)\boldsymbol{\epsilon}-\alpha(\epsilon)\boldsymbol{v}, \tag{2}$$

where $\boldsymbol{v}$ is the velocity, m is the particle mass, k_B is the Boltzmann constant, T is the temperature, $\boldsymbol{\epsilon}=\epsilon\hat{\boldsymbol{x}}$ is a constant vector along the x axis, and $\alpha(\epsilon)$ is a parameter adjusted to keep the temperature constant. As stated above, the constant ϵ plays the role of a thermal gradient $\nabla T/T$, so that the force (2) induces a heat flux in the system. The BGK equation for this state reads

$$\frac{\partial}{\partial \boldsymbol{v}}\cdot\left(\frac{\boldsymbol{F}}{m}f(\boldsymbol{v})\right)=-\nu[f(\boldsymbol{v})-f^{(0)}(\boldsymbol{v})]\,, \qquad (3)$$

where $f(\boldsymbol{v})$ is the velocity distribution function, ν is the collision frequency, and

$$f^{(0)}(\boldsymbol{v})=n\left(\frac{m}{2\pi k_B T}\right)^{3/2}\exp\left(-\frac{mv^2}{2k_B T}\right) \qquad (4)$$

is the equilibrium distribution function, n being the number density. Because of the symmetry of the problem, the (dimensionless) relevant moments can be defined as

$$M_{kl}=\frac{1}{n}\left(\frac{m}{2k_B T}\right)^{k+l/2}\int \mathrm{d}\boldsymbol{v}\, v^{2k}v_x^l f(\boldsymbol{v})\,. \qquad (5)$$

Taking moments in eq. (3), one gets

$$[(2kM_{k,l+1}+lM_{k+1,l-1})-\tfrac{3}{2}(2kM_{k-1,l+1}+lM_{k,l-1})]$$
$$\times\tfrac{1}{2}\epsilon^*+\frac{\alpha}{m\nu}(2k+l)M_{kl}=-M_{kl}+M_{kl}^{(0)}\,. \qquad (6)$$

where

$$\epsilon^*=(2k_B T/m)^{1/2}\epsilon/\nu \qquad (7)$$

is a dimensionless nonequilibrium parameter, and

$$M_{kl}^{(0)}=\frac{(2k+l+1)!}{(l+1)2^{2k+l}(k+l/2)!}\,,\quad l\ \text{even}\,,$$
$$=0\,,\qquad l\ \text{odd}\,, \qquad (8)$$

are the equilibrium moments. The hierarchy of eq. (6) must be compatible with the consistency conditions $M_{00}=1$, $M_{01}=0$, and $M_{10}=3/2$. As a consequence, the parameter α is coupled to the heat flux

$$\frac{\alpha}{m\nu}=-\tfrac{1}{3}\epsilon^* M_{11}\,. \qquad (9)$$

This coupling renders eq. (6) nonlinear.

In order to get the moments M_{kl} as functions of ϵ^*, it is convenient to use the series representation,

$$M_{kl}=\sum_{r=0}^{\infty}\mu_{kl}^{(r)}\epsilon^{*r}\,, \qquad (10)$$

where $\mu_{kl}^{(r)}=0$ if $r+l=$odd. We shall call r the order and $2k+l$ the degree of the numerical coefficient $\mu_{kl}^{(r)}$. Eqs. (6) and (9) give rise to the following equations for $\mu_{kl}^{(r)}$:

$$\mu_{kl}^{(0)}=M_{kl}^{(0)}\,, \qquad (11)$$

$$\mu_{kl}^{(r)}=-\tfrac{1}{2}[(2k\mu_{k,l+1}^{(r-1)}+l\mu_{k+1,l-1}^{(r-1)})$$
$$-\tfrac{3}{2}(2k\mu_{k-1,l+1}^{(r-1)}+l\mu_{k,l-1}^{(r-1)})]$$
$$+\frac{2k+l}{3}\sum_{s=2}^{r}\mu_{11}^{(s-1)}\mu_{kl}^{(r-s)}\,,\quad r\geqslant 1\,. \qquad (12)$$

The summation term in eq. (12) appears only if $r\geqslant 2$. It is worth noting that the Boltzmann equation for Maxwell molecules would also generate eq. (12), except that a quadratic term involving coefficients of order less than or equal to r and degree less than $2k+l$ should be included. In both cases, the coefficients $\mu_{kl}^{(r)}$ can be obtained in a recursive way. The advantage of the BGK model is that it allows one to get those coefficients quite easily. In particular, table 1 shows the numerical values of the first coefficients $\lambda^{(r)}$ defined through the relation,

$$\lambda(\epsilon^*)=-\frac{4}{5}\frac{M_{11}}{\epsilon^*}=\sum_{r=0}^{\infty}\lambda^{(r)}\epsilon^{*2r}\,,$$
$$\lambda^{(r)}=-\tfrac{4}{5}\mu_{11}^{(2r+1)}\,, \qquad (13)$$

Table 1

First coefficients $\lambda^{(r)}$ in the expansion of the dimensionless analogue of the thermal conductivity λ in powers of ϵ^*, and their corresponding "smooth" coefficients $\bar{\lambda}^{(r)}$

r	$\lambda^{(r)}$	$\bar{\lambda}^{(r)}$
0	1.0000	1.0000
1	8.8833	0.5076
2	3.0330×10^{2}	0.3668
3	2.7514×10^{4}	0.3361
4	4.4285×10^{6}	0.3026
5	1.1744×10^{9}	0.2744
6	4.7656×10^{11}	0.2495
7	2.8140×10^{14}	0.2281
8	2.3224×10^{17}	0.2097
9	2.5925×10^{20}	0.1938
10	3.8094×10^{23}	0.1801

where $\lambda(\epsilon^*)$ is the dimensionless analogue of the thermal conductivity. In the limit $\epsilon^*\to 0$, $\lambda=\lambda^{(0)}=1$, which is consistent with the Navier–Stokes thermal conductivity. On the other hand, it is evident from table 1 that the coefficients $\lambda^{(r)}$ are all positive and grow very rapidly with r. Consequently, the series (1) diverges for any finite value of ϵ^*. Notice that the positiveness of the coefficients $\lambda^{(r)}$ excludes the interpretation of the series (13) as an asymptotic expansion. In fact, $\lambda(\epsilon^*)$ has clearly a lower bound in the series

$$\sum_{r=0}^{\infty} r!\,\epsilon^{*2r}=\int_0^{\infty} \mathrm{d}t \exp(-t)/(1-t\epsilon^{*2}) ,$$

which diverges for any nonzero real value of ϵ^*. A dominant-term analysis of eq. (12) shows that $\mu_{kl}^{(r)}$ essentially behaves for large r as

$$(-1)^l\mu_{kl}^{(r)} \sim \frac{(2k+l+r+1)!\,(2k+l+r-1)!}{2^{2k+l+2r}\frac{1}{2}(2k+l+r)!\,(2k+l-1)!} . \tag{14}$$

This suggests that one defines "smooth" coefficients $\bar{\lambda}^{(r)}$ through the relation,

$$\lambda^{(r)}=\frac{1}{360}\frac{(2r+5)!\,(2r+3)!}{2^{4r}(r+2)!}\bar{\lambda}^{(r)} . \tag{15}$$

These coefficients are plotted in fig. 1. Table 1 and fig. 1 show that the variation of $\bar{\lambda}^{(r)}$ is much slower than that of $\lambda^{(r)}$.

The divergence of the transport coefficient $\lambda(\epsilon^*)$ contrasts with the results obtained in ref. [7] from a seven-moment approximation of the Boltzmann equation. According to the latter, $\lambda(\epsilon^*)$ rapidly grows with ϵ^* but is otherwise finite for a certain range of field strengths. We think that the above discrepancy is due to inadequacies of the finite-moment approach rather than to failure of the BGK equation to account for the main qualitative features of the Boltzmann equation. In order to clarify this point, it is instructive to consider, for the sake of simplicity, the one-dimensional version of eq. (3)

$$-\frac{\partial}{\partial v_x}\left[\left(\tfrac{1}{2}v_x^2-\frac{1}{2}\frac{k_\mathrm{B}T}{m}\right)\epsilon+\frac{\alpha}{m}v_x\right]f(v_x)$$

$$=-\nu[f(v_x)-f^{(0)}(v_x)] . \tag{16}$$

Let us expand the distribution function in Hermite polynomials

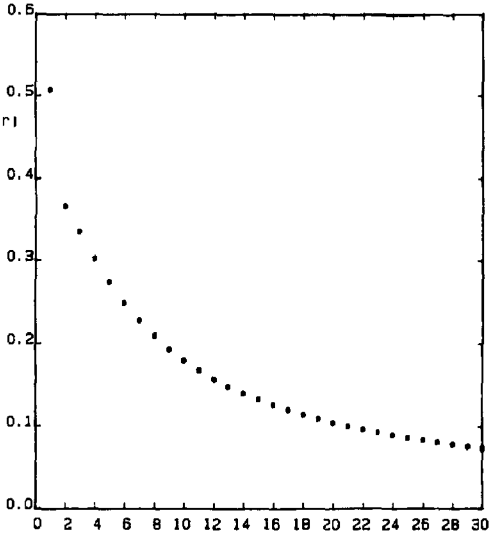

Fig. 1. Plot of the "smooth" coefficients $\bar{\lambda}^{(r)}$, eq. (14), of the thermal conductivity $\lambda(\epsilon^*)$.

$$f(v_x)=f^{(0)}(v_x)\sum_{k=0}^{\infty}\mathcal{M}_k H_k[(m/2k_\mathrm{B}T)^{1/2}v_x] . \tag{17}$$

Insertion into eq. (16) yields the following hierarchy for the (orthogonal) moments $\mathcal{M}_k$

$$[k(k+1)\mathcal{M}_{k+1}+(k-1)\mathcal{M}_{k-1}+\tfrac{1}{4}\mathcal{M}_{k-3}]\tfrac{1}{2}\epsilon^*$$

$$+(k\mathcal{M}_k+\tfrac{1}{2}\mathcal{M}_{k-2})\frac{\alpha}{m\nu}=-\mathcal{M}_k ,\quad k\geqslant 3 , \tag{18}$$

where $\mathcal{M}_0=1$, $\mathcal{M}_1=\mathcal{M}_2=0$, and $\alpha/m\nu=-6\epsilon^*\mathcal{M}_3$.

As in the case of eq. (6), eq. (18) represents a nonlinear infinite hierarchy. Inspection of eq. (18) shows that $\mathcal{M}_k$ is of order $\epsilon^{*2[(k+4)/6]}$ if k is even and of order $\epsilon^{*1+2[(k+1)/6]}$ if k is odd, respectively, where [ ] denotes the integer part. This seems to support a finite-moment approximation by introducing the closure $\mathcal{M}_{k'}=0$ for a chosen value of k' and getting $\mathcal{M}_k$ as a function of ϵ^* for $k\leqslant k'-1$. In that way, a closed equation for $\mathcal{M}_3$ or, equivalently, for the thermal conductivity $\lambda=-8\mathcal{M}_3/\epsilon^*$, can be obtained. In particular, the closures $\mathcal{M}_4=0$, $\mathcal{M}_5=0$, and $\mathcal{M}_7=0$ yield, respectively,

$$\epsilon^{*2}\lambda^2+\tfrac{4}{9}\lambda-\tfrac{4}{9}=0 , \tag{19}$$

$$\epsilon^{*4}\lambda^3+\tfrac{7}{9}\epsilon^{*2}\lambda^2+\tfrac{4}{27}(1-12\epsilon^{*2})\lambda-\tfrac{4}{27}=0 , \tag{20}$$

$$\epsilon^{*8}\lambda^5+\tfrac{19}{15}\epsilon^{*6}\lambda^4+\tfrac{238}{405}\epsilon^{*4}(1-\tfrac{45}{7}\epsilon^{*2})\lambda^3+\tfrac{16}{135}\epsilon^{*2}$$
$$\times(1-\tfrac{82}{3}\epsilon^{*2})\lambda^2+\tfrac{32}{3645}(1-\tfrac{311}{4}\epsilon^{*2}+\tfrac{1485}{4}\epsilon^{*4})\lambda$$
$$-\tfrac{32}{3645}(1-\tfrac{115}{2}\epsilon^{*2})=0\,. \tag{21}$$

Eqs. (19)–(21) are exact up to orders ϵ^{*0}, ϵ^{*2}, and ϵ^{*4}, respectively. In general, the closure $\mathcal{M}_{k'}=0$ allows one to get an equation of degree $k'-2$ for λ, which is exact up to order $\epsilon^{*2[(2k'-7)/3]}$. Thus, the finite-moment approximation is equivalent to retaining exactly the first few terms in the expansion of λ in powers of ϵ^* and replacing the remainder by an approximant. If the exact $\lambda(\epsilon^*)$ were regular at $\epsilon^*=0$, one might expect the approximate functions generated by finite-moment approximations to be rather insensitive to the number of moments retained, at least for a certain region of ϵ^*. In that case, Loose's seven-moment approximation, which plays the same role as our closure $\mathcal{M}_5=0$, eq. (20), could be viewed as relevant.

The (physical) solutions of eqs. (20) and (21) are plotted in fig. 2. It is evident that both solutions only agree at quite small values of ϵ^*. In fact, eq. (20) gives $\lambda=1+\frac{27}{4}\epsilon^{*2}+\frac{27}{8}\epsilon^{*4}+\ldots$, whereas eq. (21) gives the exact first three terms: $\lambda=1+\frac{27}{4}\epsilon^{*2}+\frac{2187}{8}\epsilon^{*4}+\ldots$. Further finite-moment approximations would retain more exact expansion coefficients (which grow very rapidly) and would overlap for values of ϵ^* tending to shrink towards $\epsilon^*\to 0$. In this respect, the qualitative agreement shown in fig. 1 of ref. [7] between the seven-moment solution and molecular dynamics results can be seen as fortuitous. A larger number of moments would probably produce important deviations for the range of field strengths considered.

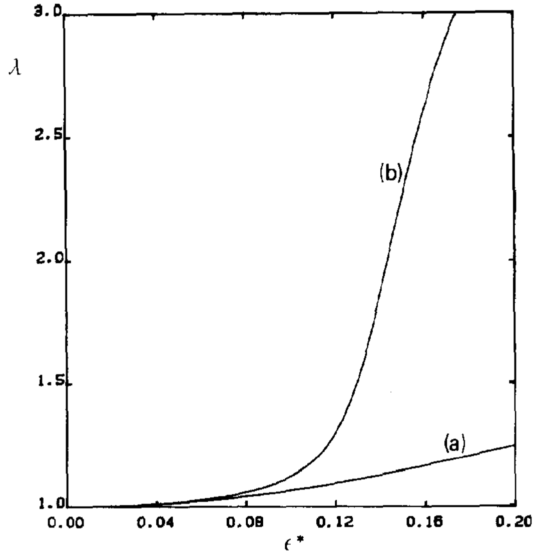

Fig. 2. Thermal conductivity as a function of the field strength in the one-dimensional case as obtained from the moment hierarchy by imposing the closures (a) $\mathcal{M}_5=0$ and (b) $\mathcal{M}_7=0$.

In summary, we have solved the moment equations obtained from the BGK equation model for a steady homogeneous heat flow induced in a dilute gas by a nonconservative external force. The results indicate divergence of the quantity measuring the nonlinear response of the system to the external perturbation. It is worth emphasizing that the BGK model is a one-relaxation-time approximation to the Boltzmann equation. In this respect, the possible extrapolation of our conclusions to the Boltzmann equation would require careful work. Nevertheless, the fact that the BGK equation accounts for the main qualitative features of the Boltzmann equation leads one to conclude that the usefulness of the Evans method can be restricted to situations asymptotically close to equilibrium. In the nonlinear regime, the velocity distribution function $f(v)$ possesses diverging moments of degree greater than 2. Alternatively, it is also possible that a strict steady state does not exist. In fact, recent simulation results in a two-dimensional fluid show the existence of an instability for large systems when ϵ exceeds a certain critical value [6]. Beyond that value, heat is conducted by means of a solitary shock wave and the apparent thermal conductivity abruptly increases with ϵ. Evans and Hanley [6] conjecture that the critical value of ϵ goes to zero in the thermodynamic limit. Notice that the simulations in ref. [7] were carried out far from that limit (128 particles). A similar instability has also been observed in the external-force-driving self-diffusion problem [5].

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