# Kinetic model for steady heat flow

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We construct a consistent solution of the Bhatnagar-Gross-Krook (BGK) model kinetic equation describing a system in a steady state with constant pressure and nonuniform temperature. The thermal profile is not linear and depends on the interaction potential. All the moments of the distribution function are given as polynomials in the local thermal gradient. In particular, the heat flux always obeys the (linear) Fourier law.

## I. INTRODUCTION

One of the main problems in statistical mechanics is in solving the kinetic equations in order to get information about the transport properties of a system. The most extensively studied case corresponds to a dilute gas described by the Boltzmann equation[1] (BE). The standard method of solving it is the Chapman-Enskog series expansion in the gradients of the thermodynamic fields. However, this approach is not very useful when dealing with highly nonlinear situations. It is then very important to know exact solutions of the BE for particular physical situations. The simplest cases correspond to steady flows. Even then, the structure of the BE is so complex that solving it is a difficult task. The only solution we are aware of corresponds to a system of Maxwell molecules under uniform shear flow, for which the generalized shear viscosity has been obtained.[2] Thus, one has to resort to simplified model kinetic equations.

A few years ago, Zwanzig[3] considered the uniform shear problem by using the Bhatnagar-Gross-Krook (BGK) model equation. He was able to get a closed equation for the pressure tensor, valid for $r^{-\mu}$ potentials. This equation has been used to analyze the convergence of the Chapman-Enskog expansion.[4]

In this paper we use the BGK model to study a system with a steady nonuniform distribution of temperature. One could think that the simplest possibility should correspond to a linear profile, but it seems that there is no consistent solution of the BGK equation describing such state. Our results show that a stationary solution with a constant pressure and a nonuniform temperature exists, but the temperature profile strongly depends on the interaction law. Once the distribution function is known, we are able to evaluate all its moments, and, in particular, the heat flux. Quite surprisingly, it always obeys the (linear) Fourier law, i.e., at each point of the system the heat flux is proportional to the local temperature gradient. The transport coefficient is given by the Navier-Stokes expression.

## II. MODEL AND ITS SOLUTION

We consider the BGK model kinetic equation for the one-particle distribution function $f(\mathbf{r},\mathbf{v},t)$,

$$\left[\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla\right]f=-\zeta(f-f_0) , \tag{1}$$

where $\zeta(\mathbf{r},t)$ is the collision frequency and $f_0(\mathbf{r},\mathbf{v},t)$ is the local equilibrium distribution function defined as

$$f_0=n\left[\frac{m}{2\pi k_B T}\right]^{3/2}\exp[-m(\mathbf{v}-\mathbf{u})^2/2k_B T] . \tag{2}$$

Here, $k_B$ is the Boltzmann constant, $m$ is the mass of a particle, and $n(\mathbf{r},t)$, $\mathbf{u}(\mathbf{r},t)$, and $T(\mathbf{r},t)$ are the local density, velocity, and temperature, respectively. In terms of the distribution function, they are given by

$$n(\mathbf{r},t)=\int d\mathbf{v}\,f(\mathbf{r},\mathbf{v},t) , \tag{3}$$

$$n(\mathbf{r},t)\mathbf{u}(\mathbf{r},t)=\int d\mathbf{v}\,\mathbf{v}f(\mathbf{r},\mathbf{v},t) , \tag{4}$$

$$\tfrac{3}{2}n(\mathbf{r},t)k_B T(\mathbf{r},t)=\frac{m}{2}\int d\mathbf{v}[\mathbf{v}-\mathbf{u}(\mathbf{r},t)]^2 f(\mathbf{r},\mathbf{v},t) . \tag{5}$$

All the details of the interaction potential are modeled through the dependence of the collision frequency upon the temperature, since for a dilute gas $\zeta$ is always proportional to the density. For instance, for a repulsive potential of the form $r^{-\mu}$, it is

$$\zeta \propto nT^\alpha \tag{6}$$

with $\alpha=\tfrac{1}{2}-2/\mu$.

Equation (1) is a model for the BE in which collisions are treated in a statistical way. Along with the BE, it has five collision invariants (mass, momentum, and energy) and verifies an $H$ theorem. One expects the most relevant features of the BE to be reasonably well mimicked by the BGK equation.[5]

We want to study a system in a steady state with a temperature gradient along the $x$ direction. In principle, this

requires the introduction of appropriate boundary conditions.[5] Nevertheless, we are interested here in transport properties in the bulk of the system far away from the boundaries. In this case, one can expect to obtain the correct answer by looking for a consistent solution to Eq. (1), regardless of the details of the boundary conditions. For a steady state with gradients along the $x$ direction only, Eq. (1) becomes

$$v_x \frac{\partial}{\partial x} f(x, \mathbf{v}) = -\zeta(x)[f(x, \mathbf{v}) - f_0(x, \mathbf{v})] , \qquad (7)$$

that can be rewritten as

$$f(x, \mathbf{v}) = \left[ 1 + \frac{v_x}{\zeta(x)} \frac{\partial}{\partial x} \right]^{-1} f_0(x, \mathbf{v}) . \qquad (8)$$

Of course, this expression is in general only formal, as both the collision frequency and the local distribution are highly nonlinear functionals of the actual distribution $f(x, \mathbf{v})$. Moreover, the functional form of $\zeta$ depends on the interaction model under consideration. Nevertheless, this influence of the interaction can be scaled out by introducing a new variable $s$ through the relation

$$ds = \zeta(x)dx . \qquad (9)$$

The idea is to use $s$ rather than $x$ as a space variable. In terms of this variable, Eq. (8) becomes

$$f(\mathbf{v}) = \left[ 1 + v_x \frac{\partial}{\partial s} \right]^{-1} f_0(\mathbf{v}) , \qquad (10)$$

where the spatial argument has been omitted. Therefore, the distribution $f(\mathbf{v})$, as a function of the variable $s$, is universal, i.e., does not depend on the interaction law. It is important to stress that this universality is possible because we are dealing with a steady state. Otherwise, the collision frequency depends both on space and time, and a relation such as (9) is senseless.

As said before, we are interested in studying a gas with a steady temperature gradient. Since boundary conditions will not be imposed explicitly, we will proceed in an heuristic way. A particular solution of Eq. (10) results when one proposes self-consistent expressions for the local hydrodynamic quantities. Here, we assume (to be confirmed in Sec. III) that a fully consistent solution of the BGK equation exists with a vanishing local velocity, a uniform pressure, and a temperature linear in $s$, i.e.,

$$\mathbf{u} = 0 , \qquad (11)$$

$$p = n(x)k_B T(x) = \text{const} , \qquad (12)$$

$$\frac{dT}{ds} = \frac{1}{\zeta} \frac{dT}{dx} = \epsilon = \text{const} . \qquad (13)$$

Equation (13) deserves some comments. It reads that regardless of the interaction considered, the temperature profile is linear when using $s$ instead of $x$ as space variable, no matter how large $\epsilon$ is. As $s$ is a nonlinear, nonuniversal function of $x$, Eq. (13) implies that the temperature gradient with respect to $x$ is not constant, but it depends on space in a way given by the interaction law. In order to get the $x$-dependent temperature, Eq. (13) has

to be supplemented with the relationship, such as Eq. (6), between the collision frequency and the temperature for a given interaction potential.

By taking into account Eq. (12), we see that all the spatial dependence of $f_0$ occurs through the temperature, and then Eq. (10) takes the form

$$f(\mathbf{v}) = \left[ 1 + \epsilon v_x \frac{\partial}{\partial T} \right]^{-1} f_0(\mathbf{v})$$

$$= \sum_{r=0}^{\infty} (-\epsilon v_x)^r \left[ \frac{\partial}{\partial T} \right]^r f_0(\mathbf{v}) . \qquad (14)$$

This expression provides an expansion of the distribution function in terms of well-known quantities. Notice that this is an expansion in powers of the gradients in the auxiliary variable $s$. Of course, one can use Eq. (13) and go back to the actual position variable $x$. An important feature of the resulting expansion is that only the first-order derivative of the temperature appears.

## III. HEAT FLUX AND FOURIER LAW

It still remains to be seen that Eq. (14) is self-consistent, i.e., Eqs. (3)—(5) are identically satisfied when Eq. (14) is inserted on the right-hand sides. We define the moments $M_{kl}$ as

$$M_{kl} = \int d\mathbf{v} \, v^{2k} v_x^l f(\mathbf{v}), \quad k, l \geq 0 . \qquad (15)$$

Because of the symmetry of the problem, these are the moments containing all the relevant information. From Eq. (14) one easily obtains

$$M_{kl} = \frac{p}{k_B} \sum_{\substack{r=0 \\ (l+r) \text{ even}}} (-\epsilon)^r \left[ \frac{k_B}{m} \right]^{k+(l+r)/2}$$

$$\times \frac{(2k+l+r+1)!!}{l+r+1} \left[ \frac{\partial}{\partial T} \right]^r$$

$$\times T^{k-1+(l+r)/2} . \qquad (16)$$

Although this expression looks like an infinite series, it actually has a finite number of terms, since the order of the derivative increases faster than the power of $T$. In particular, we have

$$M_{00} = \frac{p}{k_B T} = n , \qquad (17)$$

$$M_{01} = 0 , \qquad (18)$$

$$M_{10} = \frac{3p}{m} = \frac{3}{m} n k_B T , \qquad (19)$$

that proves the consistency of our solution. For $l + 2(k - 1) \geq 0$, Eq. (16) can be rewritten as

$$M_{kl} = (-1)^l n \left[ \frac{k_B T}{2m} \right]^{k+l/2} \sum_{\substack{r=0 \\ (l+r)\,\text{even}}}^{l+2(k-1)} \frac{(2k+l+r+1)!}{\left[ k-1+\frac{l-r}{2} \right]! \left[ k+\frac{l+r}{2} \right] (l+r+1)} \left[ \left[ \frac{k_B}{2mT} \right]^{1/2} \epsilon \right]^r . \tag{20}$$

We now proceed to calculate the transport of heat across the system. From the BGK equation, one easily derives the balance equation

$$\frac{3}{2} n k_B \frac{\partial T}{\partial t} = -\nabla \cdot \mathbf{J} , \tag{21}$$

where the heat flux $\mathbf{J}$ is given by

$$\mathbf{J} = \frac{m}{2} \int d\mathbf{v}\, v^2 \mathbf{v} f . \tag{22}$$

Upon writing these equations, we have used the fact that in our case $\mathbf{u} = 0$. Due to the symmetry of the distribution function, the only nonvanishing component is

$$J_x = \frac{m}{2} M_{11} . \tag{23}$$

Equation (20) yields

$$J_x = -\frac{5}{2} \frac{n k_B^2 T}{m} \epsilon , \tag{24}$$

i.e.,

$$J_x = -\lambda(x) \frac{\partial T}{\partial x} \tag{25}$$

with

$$\lambda(x) = \frac{5}{2} \frac{n(x) k_B^2 T(x)}{m \zeta(x)} . \tag{26}$$

Equation (25) is the Fourier law for the heat conduction, while Eq. (26) provides a microscopic expression for the thermal conductivity. Of course, as we are dealing with a nonuniform system, both expressions are local, i.e., they refer to a given point of the system. We see that the heat flux always obeys a linear law, in spite of the fact that the temperature profile, defined by Eq. (13), is in general highly nonlinear. Moreover, the transport coefficient $\lambda$ is given by the Navier-Stokes expression.

The $x$ dependence of $T$ varies with the interaction law through the collision frequency. As an illustration, let us consider repulsive potentials for which Eq. (6) applies. Thus, Eqs. (12) and (13) yield

$$T^{2-\alpha} = T_0^{2-\alpha} \left[ 1 + (2-\alpha) \frac{\zeta_0}{T_0} \epsilon x \right] , \tag{27}$$

$T_0$ and $\zeta_0$ being constants representing the temperature and the collision frequency at an arbitrary origin. Equation (27) can also be written in the form

$$T(x) = \zeta(x) \left[ \frac{T_0}{\zeta_0} + (2-\alpha)\epsilon x \right] , \tag{28}$$

where the influence of the local collision frequency is evident. In the vicinity of the point chosen as the origin, Eq. (27) can be approximated by the linear relation

$$T(x) \simeq T_0 + \epsilon \zeta_0 x . \tag{29}$$

Of course, this is not the temperature distribution in the whole bulk of the system. It only holds, in general, over a short-distance scale. Nevertheless, there is a case for which the temperature profile is exactly linear for all values of $x$. It corresponds to $\alpha = 1$, i.e., a collision frequency proportional just to the (constant) pressure. Although the value $\alpha = 1$ is not associated to any physical interaction potential, it can be viewed as representing the so-called very-hard-particle interaction.[6]

## IV. CONCLUDING REMARKS

We have solved the BGK model equation for a system in a steady state with a uniform pressure and a nonuniform temperature distribution along the $x$ direction. The main result is that the temperature profile is in general nonlinear, but the system always obeys the linear Fourier law. To put these results in proper context, the following comments seem appropriate.

(1) The fact that in the steady state the temperature gradient at each point is proportional to the local collision frequency is easy to understand physically. The molecular collisions are the mechanisms responsible for the energy transfer and it is sensible to think that the local variation of temperature depends on the rate at which collisions take place. As the functional form of the effective collision frequency depends on the interaction law, so does the shape of the temperature profile.

(2) The question arises of whether the macroscopic state we have assumed really corresponds to the bulk limit of a solution of Eq. (7) with some physical boundary conditions. The stationary BGK equation has been numerically solved for a system enclosed between two parallel plates at different temperatures. The plates are represented by diffuse boundary conditions of complete accommodation.[1,5] The results[7] are consistent with the profile defined by Eq. (13) in the bulk of the system. Obviously, the size of the effective bulk region increases as the Knudsen number decreases.

(3) For a system under uniform shear flow a nonequilibrium molecular dynamics method has been developed that allows to reproduce the bulk state having the desired velocity field.[8] There is no boundary layer in this computer simulation. One may wonder whether it is possible to introduce, in a similar way, virtual boundary conditions to simulate a bulk state for the heat conduction problem. Shear flow has a rather mechanical character and, then, a linear velocity profile is consistent with statistical mechanics.[9] On the other hand, heat flow is a pure thermal phenomenon and, in general, the resulting profile depends on the details of the interaction.[10]

(4) Although the results presented in this paper have been derived from the BGK model, it seems plausible to expect most of the qualitative features to be quite general. This conjecture is supported by some results. The problem of a dense Lennard-Jones fluid with a thermal gradient has been studied by means of molecular dynamics using diffuse boundary conditions.[11] The main conclusion is that the Fourier law applies over wide ranges of density and thermal gradient.

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