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Inconsistencies in moment methods

R. M. Velasco, F. J. Uribe, and L. S. García-Colín
Departamento de Física, Universidad Autónoma Metropolitana–Iztapalapa, 09340 México Distrito Federal, Mexico

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In this work we show that moment methods devised to solve the Boltzmann kinetic equation for a simple gas exhibit some inconsistencies. This puzzle, which also appears for the Chapman-Enskog method, is solved resorting to a perturbative expansion in the Knudsen number, thus allowing for a clear way to arrive at a closure condition.

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The classical moment problem, namely, the determination of a positive-density $f(x)$ from its moments

$$\int_a^b f(x)x^n dx, \quad n=0,1,2, \ldots, \tag{1}$$

has been of great use in a variety of situations both in equilibrium and nonequilibrium phenomena. Sufficient and necessary conditions for this to happen [1,2], as well as examples in which the distribution function is not determined from its moments, are available [3]. In the latter case, the corresponding function $f(x,t)$ is usually governed by nonlinear differential or integro-differential equations whose exact solution is not known. This implies the necessity of constructing suitable methods to find approximate solutions. Typical examples are the Fokker-Planck equation [4], the nonlinear Schrödinger equations [5], the kinetic theory of dense gases [6,7] and the Boltzmann equation where the moments method, or its variants, has been widely used with some success [8–32]. In this paper we would like to concentrate ourselves in the so-called Grad's moment method developed some fifty years ago [8–10] to solve the Boltzmann nonlinear integro-differential equation appearing in the kinetic theory of inert dilute gases taken as rigid spheres.

All moment methods developed to solve the Boltzmann kinetic equation share the hypothesis that the single-particle distribution function can be expanded in a complete set of orthonormal polynomials containing their molecular velocity dependence. Such an expansion, which in principle is an infinite series, must be approximated in order to obtain a finite summation of several terms. This means that we choose a finite set of relevant moments to study the behavior of the system [9]. As a result of this procedure we obtain the single-particle distribution function written in terms of some coefficients together with velocity polynomials. The coefficients are functions of the spatial coordinates and time, so they describe the macroscopic behavior of the system. To obtain the macroscopic equations for all relevant variables, we take the Boltzmann equation and construct the general Maxwell-Enskog (ME) transport equation [33]. Although the ME equation was written even before the Boltzmann equation, it has been somewhat ignored by its users that it allows for the construction of an infinite set of equations for all the functions of molecular velocity one is interested in. The question that obviously arises is if all such equations are independent and consistent among themselves.

The main result in this paper clearly exhibits this problem for a rather specific situation, and further shows that this scheme is inconsistent when we do not have an expansion parameter to properly classify the different terms occurring in the approximation. A solution is proposed by appealing to a power series expansion in terms of the Knudsen number.

Let us start with the Boltzmann equation for a simple monatomic gas consisting of rigid spheres without an external force,

$$\partial f/\partial t+\mathbf{c}\cdot\boldsymbol{\nabla}_{\mathbf{r}}f=J(f,f), \tag{2}$$

where $f(\mathbf{c},\mathbf{r},t)$ is the single-particle distribution function, $\mathbf{c}$ the molecular velocity, and $J(f,f)$ is the Boltzmann collision kernel [34]. The number density $n(\mathbf{r},t)$, the hydrodynamic velocity $\mathbf{u}(\mathbf{r},t)$, and the temperature $T(\mathbf{r},t)$ are defined as usual,

$$\begin{pmatrix} n(\mathbf{r},t) \\ \mathbf{u}(\mathbf{r},t) \\ \frac{3}{2}nk_BT(\mathbf{r},t) \end{pmatrix} = \int \begin{pmatrix} 1 \\ m\mathbf{c} \\ \frac{1}{2}m\mathbf{C}^2 \end{pmatrix} f(\mathbf{c},\mathbf{r},t)d\mathbf{c}. \tag{3}$$

The peculiar velocity is given by $\mathbf{C}=\mathbf{c}-\mathbf{u}$ and k_B is the Boltzmann constant. Now we consider a function $\psi(\mathbf{c},\mathbf{r},t)$, multiply Eq. (2) by ψ, and integrate over the molecular velocity to obtain

$$\frac{\partial n\langle\psi\rangle}{\partial t}+\boldsymbol{\nabla}_r\cdot(n\mathbf{u}\langle\psi\rangle+n\langle\mathbf{C}\psi\rangle)-n\left(\left\langle\frac{\partial\psi}{\partial t}\right\rangle+\langle\mathbf{c}\cdot\boldsymbol{\nabla}_r\psi\rangle\right)=\Sigma_\psi, \tag{4}$$

where

$$n\langle\psi\rangle=\int \psi(\mathbf{C},\mathbf{r},t)f(\mathbf{c},\mathbf{r},t)d\mathbf{c}, \tag{5}$$

and

$$\Sigma_\psi=\int \psi(\mathbf{C},\mathbf{r},t)J(f,f)d\mathbf{c} \tag{6}$$

is the source of the quantity ψ. Also $n(\mathbf{r},t)$ has been abbreviated by n. It is well known that when we choose any of the collisional invariants written in Eq. (3) as the functions ψ, the corresponding source vanishes and the ME equation re-

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produces the conservation equations. Also, the heat flux $\mathbf{q}(\mathbf{r},t)$ and the pressure tensor $\mathbf{P}(\mathbf{r},t)$ are defined as moments of the distribution function,

$$\mathbf{q}(\mathbf{r},t)=\int \frac{1}{2}m\mathbf{C}^2\mathbf{C} \;\; f(\mathbf{c},\mathbf{r},t)d\mathbf{c}, \tag{7}$$

$$\mathbf{P}(\mathbf{r},t)=\int m\mathbf{C}\mathbf{C} \;\; f(\mathbf{c},\mathbf{r},t)d\mathbf{c}, \tag{8}$$

and they will become important in the following discussion. Notice that the ME equation as written in Eq. (4) is exact, provided that f is an exact solution of the Boltzmann equation.

Due to the lack of such an exact solution of the Boltzmann equation, to illustrate our point we will first take the Grad's 13-moment approximation [8] for the distribution function,

$$\begin{aligned} f=f^{(0)}\bigg[&1+\mu_{xx}\left(\mathbf{C}_x^2-\frac{k_BT}{m}\right)+\mu_{xy}\mathbf{C}_x\mathbf{c}_y+\mu_{xz}\mathbf{C}_x\mathbf{c}_z+\mu_{yz}\mathbf{c}_y\mathbf{c}_z \\ &+\mu_{yy}\left(\mathbf{c}_y^2-\frac{k_BT}{m}\right)+\mu_{zz}\left(\mathbf{c}_z^2-\frac{k_BT}{m}\right)+\theta_x\mathbf{C}_x\left(\frac{m\mathbf{C}^2}{k_BT}-5\right) \\ &+\theta_y\mathbf{c}_y\left(\frac{m\mathbf{C}^2}{k_BT}-5\right)+\theta_z\mathbf{c}_z\left(\frac{m\mathbf{C}^2}{k_BT}-5\right)\bigg], \end{aligned} \tag{9}$$

where

$$f^{(0)}(\mathbf{c},\mathbf{r},t)=n\left(\frac{m}{2\pi k_BT}\right)^{3/2}\exp\left(-\frac{m\mathbf{C}^2}{2k_BT}\right) \tag{10}$$

is the usual local Maxwellian distribution function, and all other quantities are defined as follows:

$$\begin{gathered} \mu_{xx}=\frac{m}{2k_BT}\left(\frac{\mathbf{P}_{xx}}{nk_BT}-1\right), \quad \mu_{yy}=\frac{m}{2k_BT}\left(\frac{\mathbf{P}_{yy}}{nk_BT}-1\right), \\ \mu_{zz}=\frac{m}{2k_BT}\left(\frac{\mathbf{P}_{zz}}{nk_BT}-1\right), \quad \mu_{xy}=\frac{m}{k_B^2T^2n^2}\mathbf{P}_{xy}, \\ \mu_{yz}=\frac{m}{k_B^2T^2n^2}\mathbf{P}_{yz}, \quad \theta_x=\frac{m}{5k_B^2T^2n}\mathbf{q}_x, \quad \theta_y=\frac{m}{5k_B^2T^2n}\mathbf{q}_y. \end{gathered} \tag{11}$$

To simplify the calculations we consider a longitudinal and stationary flow such that $\mathbf{u}(\mathbf{r},t)=u(x)\hat{\mathbf{i}}$, and all other quantities only depend on the x coordinate. Also we consider that $\mathbf{P}_{xy}=\mathbf{P}_{xz}=\mathbf{P}_{yz}=0$, $\mathbf{q}_y=\mathbf{q}_z=0$, and $\mathbf{P}_{yy}=\mathbf{P}_{zz}$, as it is done in Ref. [10]. Further, the viscous tensor is given by $\mathbf{p}_{xx}^0=\mathbf{P}_{xx}-p$, where $p(x)$ is the hydrostatic pressure. We introduce the dimensionless components of the velocity as $v_x=\sqrt{m/k_BT}C_x$, $v_y=\sqrt{m/k_BT}c_y$, and $v_z=\sqrt{m/k_BT}c_z$. In this case the 13-moment distribution function given in Eq. (9) reduces to the form

$$\begin{aligned} f^G=n\left(\frac{m}{2\pi k_BT}\right)^{3/2}\exp\left(-\frac{\mathbf{v}^2}{2}\right)\bigg[&1+\frac{\mathbf{p}_{xx}^0}{4p}(2v_x^2-v_y^2-v_z^2) \\ &+\frac{1}{5p}\sqrt{\frac{m}{k_BT}}\;\mathbf{q}_xv_x(\mathbf{v}^2-5)\bigg]. \end{aligned} \tag{12}$$

Now, it is well known that the Grad's distribution function as given in Eq. (12) when used in the ME equation for the collisional invariants reproduces the conservation equations for the number density, the momentum density, and the energy. Moreover, in the Grad's method, the following step is given in order to obtain the transport equation for the pressure tensor and the heat flux. Let us concentrate in the equation for the heat flux and take, as usual, the function $\psi(\mathbf{C},\mathbf{r},t)=m\mathbf{C}^2\mathbf{C}_x$. Accordingly, we obtain the evolution equation for $\mathbf{q}_x$ in which we have the drift term that is nonlinear, and keeping only the linearized collision kernel we have

$$\begin{aligned} &\frac{\partial(2u\mathbf{q}_x)}{\partial x}+\frac{22}{5}\mathbf{q}_x\frac{\partial u}{\partial x}+2\frac{k_BT}{m}\frac{\partial\mathbf{p}_{xx}^0}{\partial x}+7\mathbf{p}_{xx}^0\frac{\partial}{\partial x}\left(\frac{k_BT}{m}\right) \\ &\qquad-\frac{2\mathbf{p}_{xx}^0}{\rho}\frac{\partial(p+\mathbf{p}_{xx}^0)}{\partial x}+5p\frac{\partial}{\partial x}\left(\frac{k_BT}{m}\right)+\frac{4}{3}\beta\rho\mathbf{q}_x=0, \end{aligned} \tag{13}$$

where β, which appears in the the collision kernel, is defined by $\rho\beta=p/\mu$ and μ is the shear viscosity of the fluid. Equation (13) with the equation for the pressure tensor were used by Grad to study the shock wave structure [10]. In fact, the usual variables, such as the number density, the hydrodynamic velocity, the temperature together with the viscous tensor, and the heat flux correspond to the most natural selection of relevant variables to describe the system. They have been used to study simple systems beyond the local equilibrium regime.

Further, the ME equation can be also used for other functions of the molecular velocity; particularly when we take $\psi=mC_x^3$, we obtain an equation for $n\langle\psi\rangle=n\langle mC_x^3\rangle=\mathbf{Q}_x$. The remarkable point is that one finds by direct calculation that $\mathbf{Q}_x=\frac{3}{5}\mathbf{q}_x$, so that in principle, the evolution equation for $\mathbf{Q}_x$ should be proportional to Eq. (13). However, a direct calculation shows that

$$\begin{aligned} &\frac{6}{5}u\frac{\partial\mathbf{q}_x}{\partial x}-3\frac{k^2T^2}{m}\frac{\partial n}{\partial x}+6\frac{kT}{m}\frac{\partial\mathbf{P}_{xx}}{\partial x}+3u\mathbf{P}_{xx}\frac{\partial u}{\partial x}+\frac{24}{5}\mathbf{q}_x\frac{\partial u}{\partial x} \\ &\qquad+6\frac{k\mathbf{P}_{xx}}{m}\frac{\partial T}{\partial x}-6\frac{nk^2T}{m}\frac{\partial T}{\partial x}=-\frac{4}{5}\rho\beta\mathbf{q}_x. \end{aligned} \tag{14}$$

A careful comparison between Eqs. (13) and (14) shows that they are different and independent, though they should be proportional to each other. It follows at once that this poses a serious problem since now we have two different equations for the same physical quantity $\mathbf{q}_x$, implying that their solution may be different.

On the other hand, we ask ourselves if this inconsistency is specific of the Grad's moment method, or if it arises when we use other approximate method. To illustrate this point we will take the distribution function arising from the Chapman-

Enskog solution to the Boltzmann equation. Consider first the same longitudinal stationary flow and introduce the same dimensionless components of the molecular velocity, so that the Chapman-Enskog distribution function up to first order in the Knudsen number can be written as follows:

$$f^{CE}=n\left(\frac{m}{2\pi k_BT}\right)^{3/2}\exp\left(-\frac{\mathbf{v}^2}{2}\right)\left[1-\frac{\mu}{3p}\left(\frac{\partial u}{\partial x}\right)(2v_x^2-v_y^2-v_z^2)\right.$$
$$\left.-\frac{3\mu}{4pT}\sqrt{\frac{k_BT}{m}}\left(\frac{\partial T}{\partial x}\right)v_x(\mathbf{v}^2-5)\right]. \qquad (15)$$

We notice that the Chapman-Enskog (CE) distribution function has the same structure in the molecular velocity as the Grad's function in Eq. (12). Moreover, it is consistent with the Navier-Newton-Fourier constitutive laws that are written as [34]

$$\mathbf{p}_{xx}^{CE}=-\frac{4\mu}{3}\left(\frac{\partial u}{\partial x}\right),\quad \mathbf{q}_x^{CE}=-\frac{15}{4}\frac{k_B\mu}{m}\left(\frac{\partial T}{\partial x}\right). \qquad (16)$$

Using Eqs. (15) and (16), f^{CE} can be brought into a form similar to that of Eq. (12), from where it follows that the evolution equations constructed from the ME equation will become the same as Eqs. (13) and (14). This rather relevant argument shows that the CE method will have the same inconsistency as that arising from the Grad's equations.

Here we have illustrated the inconsistency in the simplest way for two quantities that, being proportional to one another, lead to a different set of equations which in principle should be equivalent.

Although both Grad's and Chapman-Enskog's distribution functions exhibit the same inconsistency, we recall that the last one can be written in terms of the Knudsen number $\epsilon=l/L$, where $l=(4\mu/3p)\sqrt{k_BT/m}$ is the mean free path and L the typical macroscopic length, so that

$$\frac{\mathbf{p}_{xx}^0}{p}=-\frac{3}{2}\epsilon\frac{\partial u^*}{\partial x^*}, \qquad (17)$$

$$\frac{\mathbf{q}_x}{p}\sqrt{\frac{m}{k_BT}}=-\frac{45}{16}\epsilon\frac{\partial T^*}{\partial x^*}, \qquad (18)$$

where the asterisked variables are dimensionless. Direct substitution of Eqs. (17) and (18) in the drift term of Eq. (13) shows that

$$\frac{\partial}{\partial x^*}\left(-\frac{45pk_BT}{m}\frac{\epsilon}{L}u^*\frac{\partial T^*}{\partial x^*}\right)-\frac{21}{2}p\frac{\epsilon}{L}\left(\frac{\partial u^*}{\partial x^*}\right)\left(\frac{\partial}{\partial x^*}\frac{k_BT}{m}\right)$$
$$-\frac{99}{8}\frac{pk_BT}{mL}\epsilon\left(\frac{\partial T^*}{\partial x^*}\right)\left(\frac{\partial u^*}{\partial x^*}\right)-3\frac{k_BT}{m}\frac{\partial}{\partial x^*}\left(\frac{\epsilon p}{L}\right)\left(\frac{\partial u^*}{\partial x^*}\right)$$
$$+\frac{3k_BT}{m}\frac{\epsilon}{L}\left(\frac{\partial u^*}{\partial x^*}\right)\left[\frac{\partial}{\partial x^*}p\left(1-\frac{3}{2}\epsilon\frac{\partial u^*}{\partial x^*}\right)\right]$$
$$+\frac{5p}{L}\left(\frac{\partial}{\partial x^*}\frac{k_BT}{m}\right)=-\frac{16}{9l}\sqrt{\frac{k_BT}{m}}\ \mathbf{q}_x^{CE}, \qquad (19)$$

where we have also subtituted the value for the collision integral in terms of the x component of the heat flux in the Chapman-Enskog approximation, such that $-\frac{4}{3}\rho\beta\mathbf{q}_x=-16/9l\sqrt{k_BT/m}\mathbf{q}_x^{CE}$. The terms in Eq. (19) can now be separated according to their order in the Knudsen number. In fact, the heat flux can be written as follows:

$$q_x^{CE}=-\frac{45}{16}p\epsilon\sqrt{\frac{m}{k_BT}}\left(\frac{\partial}{\partial x^*}\frac{k_BT}{m}\right)+\epsilon^2\frac{9}{16}\sqrt{\frac{m}{k_BT}}\left[\frac{\partial}{\partial x^*}\right.$$
$$\times\left(-\frac{45pk_BT}{m}u^*\frac{\partial T^*}{\partial x^*}\right)-\frac{21}{2}p\left(\frac{\partial u^*}{\partial x^*}\right)\frac{\partial}{\partial x^*}\frac{k_BT}{m}$$
$$-\frac{99}{8}p\frac{k_BT}{m}\left(\frac{\partial T^*}{\partial x^*}\right)\left(\frac{\partial u^*}{\partial x^*}\right)-3\frac{k_BT}{m}\frac{\partial}{\partial x^*}p\left(\frac{\partial u^*}{\partial x^*}\right)$$
$$\left.+3\frac{k_BT}{m}\left(\frac{\partial u^*}{\partial x^*}\right)\left(\frac{\partial p}{\partial x^*}\right)\right]$$
$$-\epsilon^3\frac{9}{16}\sqrt{\frac{m}{k_BT}}\left[\frac{9k_BT}{2m}\left(\frac{\partial u^*}{\partial x^*}\right)\frac{\partial}{\partial x^*}p\left(\frac{\partial u^*}{\partial x^*}\right)\right]. \qquad (20)$$

According to the Chapman-Enskog method, it is just the first term in Eq. (20) which we can take as a result, because the single-particle distribution function used corresponds to an expansion up to first order in ϵ. On the other hand we could write the collision integral in terms of the temperature gradient. It means that $-(4/3)\rho\beta\mathbf{q}_x=(5k_BT/lm)p\epsilon(\partial T^*/\partial x^*)$ in such a way that its direct substitution in the second member of Eq. (20) shows how the terms in the first order in ϵ cancel, and therefore, all others must add to zero. Taking into account that this expansion is valid only up to first order in ϵ, the second and higher-order terms are negligible, so instead of an additional condition we simply have to neglect them.

On the other hand, we have Eq. (14) that is also valid for the heat flux, so that the same procedure can be carried out. It means that we substitute the Navier-Stokes-Fourier constitutive equations expressed in terms of the Knudsen number and arrange each term accordingly; so

$$-\frac{27}{8}\sqrt{\frac{k_BT}{m}}u^*\frac{\partial}{\partial x^*}\left(\sqrt{\frac{k_BT}{m}}\ p\epsilon^2\frac{\partial T^*}{\partial x^*}\right)$$
$$-9\frac{k_BT}{m}\left(\frac{\partial}{\partial x^*}p\epsilon^2\frac{\partial u^*}{\partial x^*}\right)$$
$$-\frac{9}{2}\sqrt{\frac{k_BT}{m}}p\epsilon^2\left(\frac{\partial}{\partial x^*}\sqrt{\frac{k_BT}{m}}\ u^*\right)\left[u^*\left(\frac{\partial u^*}{\partial x^*}\right)\right.$$
$$\left.+3\left(\frac{\partial T^*}{\partial x^*}\right)\right]-9\frac{k_Bp}{m}\epsilon^2\left(\frac{\partial u^*}{\partial x^*}\right)\left(\frac{\partial T^*}{\partial x^*}\right)+3\frac{k_Bp}{m}\epsilon\frac{\partial T}{\partial x^*}$$
$$=-\frac{16}{15}\sqrt{\frac{k_BT}{m}}q_x^{CE}. \qquad (21)$$

Equations (19) and (21) show that to lowest order in the Knudsen number, both are equivalent and consistent with the Fourier's law. The remaining terms are of higher order in ϵ, and therefore we do not have the right to impose that the equations must be satisfied, since we are using a distribution function valid only up to first order in ϵ. It is obvious that the higher-order conditions cannot be satisfied, and in general, they are not the same for any arbitrary ψ function we choose to describe the behavior of the system. The same argument can be extended to classify terms of order ϵ^n, $n \geqslant 2$.

To summarize, the lack of an exact solution to the Boltzmann equation drives us to take some approximation to solve it. Several methods have been developed in the literature to account for such a task. In particular, the Grad's 13-moment approximation has been used to study problems like the shock wave structure and others [35]. However, we assert here that the set of equations for the moments chosen to be relevant can be evaluated along several lines. In fact, the ME equation gives us the procedure to construct an arbitrary number of equations related to the chosen moments. Of course, one would expect that all those equations should be equivalent. What we have shown in this work is a surprising result, in which the ME equation gives us two or more different evolution equations for the same quantity. Also, the first-order Chapman-Enskog distribution function leads to the same difficulty. It means that the averages of ψ functions calculated with this distribution function yields equations that are not equivalent, for the same dynamical quantities.

The important and subtle point to understand is how can we obtain consistent results, a fact deeply buried in the structure of the nonlinearity in the Boltzmann equation. The drift terms in the Boltzmann equation, which are nonlinear, lead to different results according to the specific approximation performed in the distribution function. On the other hand, the Grad's method does not have any small parameter to follow the order of the approximation, so we have to impose on the solution an arbitrary number of additional conditions coming from the ME equation. In contrast, the Chapman-Enskog solution contains the Knudsen number as a small parameter and being a first-order approximation we do not have to require the solution to satisfy such conditions. As we have shown, the Chapman-Enskog solution is completely consistent up to first order in the Knudsen number, as it should be. In the case of the Grad's distribution function, we do not have any reason to eliminate the conditions imposed by the ME equation, because the existence of a perturbative approach in terms of a small parameter is not guaranteed. The only way to use the Grad's approximate solution is through an additional expansion that takes into account an iterative solution in powers of the Knudsen number to order the terms. Obviously, this fact makes the Grad's method somewhat useless in practice. We expect that the deficiency reported here for the Grad's moments method is also present in other applications of the moments method, the details will be published later on.

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