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Abstract

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ON THE METHOD OF MAXIMIZING ENTROPY IN THE THEORY OF RAREFIED GASES

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To truncate the chain of Maxwell moment equations, Grad ([1]) used a statistical hypothesis according to which the distribution of molecules $f(\mathbf{x}, \mathbf{v}, t)$ is represented by a finite segment of a series in the orthogonal Hermite functions. Grad' s method has certain shortcomings. Being tied to a definite orthogonal system of functions, it requires modification in the case of a gas with internal degrees of freedom of the molecules or of a degenerate gas. In addition, the entropy of an isolated gas, calculated from Grad' s distribution, does not increase by virtue of Grad' s equations.

The purpose of the present note is to discuss a statistical hypothesis free of these shortcomings. This hypothesis consists in using, among all distributions with the same values of the selected moments, the distribution of maximum entropy ([2]).

1°. Let us consider the case of 10 moments, corresponding to Grad' s second approximation, characteristic of a system in which only viscous processes are essential. The maximum of the entropy of a unit volume

$$\rho S = -k \int f \ln f \, dv \tag{1}$$

under the supplementary conditions

$$\int mf \, dv = \rho, \qquad \int mv_i f \, dv = \rho u_i, \qquad \int m(v_i - u_i)(v_k - u_k) f \, dv = p_{ik}, \tag{2}$$

where m is the molecular mass, ρ the density, u_i the velocity, and $p_{ik} = p\delta_{ik} + \sigma_{ik}$ the gas pressure tensor, is attained at the function

$$f = \frac{\rho}{m(2\pi)^{3/2}} \sqrt{\frac{\rho^3}{\det \|p_{ik}\|}} \exp\left\{-\frac{\rho}{2} p^{ik}(v_i - u_i)(v_k - u_k)\right\}. \tag{3}$$

Here p^{ik} is the matrix inverse to p_{ik}. Truncation of the Maxwellian chain of equations with the aid of (3) leads to Grad' s second approximation,

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0, \qquad \frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_i u_k + p_{ik})}{\partial x_n} = 0, \tag{4}$$

$$\frac{\partial (p_{ik} + \rho u_i u_k)}{\partial t} + \frac{\partial [p_{ik} u_l + p_{il} u_k + p_{kl} u_i + \rho u_i u_k u_l]}{\partial x_l} + \frac{p}{\mu} \sigma_{ik} = 0,$$

where μ is the viscosity coefficient. In (4) the moment of the collision integral is calculated with accuracy up to first order in the stresses σ_{ik} (analogously to ([1])). Using (3), one can obtain slip boundary conditions for (4),

$$\sigma_{1i} + \frac{2(1-\alpha)}{1+\alpha} u_i \sqrt{\frac{\rho(p + \sigma_{11})}{2\pi}} = 0 \qquad (i = 2, 3). \tag{5}$$

In (5), α is the fraction of specularly reflected molecules; the remaining ones are reflected diffusely. The Grad distribution of the second approximation coincides with the dis–

expansion (3) to first order in σ_{ik}. This expansion is used in ([5]) for deriving the boundary conditions that follow from (5), if the root is expanded to first order in σ_{11}.

The entropy (1) for (3) has the form

$$S = -\frac{5}{2} R \ln \rho + \frac{1}{2} R \ln \det \|p_{ik}\|, \tag{6}$$

where $R = k/m$ is the gas constant. In view of (5), the entropy balance is

$$\frac{\partial \rho S}{\partial t} + \frac{\partial \rho S u_i}{\partial x_i} = \frac{R}{2} \frac{\rho p}{\mu} \left[\frac{1}{3} p_{kk} p^{ll} - 3\right]. \tag{7}$$

The right-hand side is nonnegative and is equal to zero only when $\sigma_{ik} = 0$. Expansion of (6) in σ_{ik} to second order gives

$$S = -\frac{5}{2} R \ln \rho + \frac{3}{2} R \ln p - \frac{R}{4} \frac{\sigma_{ik} \sigma_{ik}}{p^2}. \tag{8}$$

Grad obtained the coefficient $-R/2$ in the last term of (8). For small deviations from equilibrium, the production of entropy per unit volume in view of (7) is equal to $\sigma_{ik}\sigma_{ik}/2\mu T$, and the energy dissipation is $\sigma_{ik}\sigma_{ik}/2\mu$.

As an exact consequence of the system of equations for small perturbations, obtained from (4) by linearization, the second-order energy balance is valid:

$$\frac{\partial}{\partial t}\left(\rho\frac{u^2}{2}+\frac{5}{6}\frac{p_0}{\rho_0^2}\rho^2+\frac{\sigma_{ik}\sigma_{ik}}{4p_0}\right)+\frac{\partial(p\delta_{ik}+\sigma_{ik})u_i}{\partial x_k}+\frac{\sigma_{ik}\sigma_{ik}}{2\mu}=0, \tag{9}$$

where p_0 and ρ_0 are the unperturbed pressure and density.

The expression under the time derivative in (9) is the mechanical energy of the perturbation of a unit volume of gas.

For the case of Grad's 13-moment equations ([1]), by expanding the corresponding maximum-entropy distribution with accuracy to third order in σ_{ik} and the heat flux Q_i, the entropy can be calculated with accuracy to third order:

$$S=-\frac{5}{2}R\ln\rho+\frac{3}{2}R\ln p-\frac{R}{4}\frac{\sigma_{ik}\sigma_{ik}}{p^2}-\frac{R}{5}\frac{\rho Q_{iQ}i}{p^3}+\frac{R}{6}\frac{\sigma_{ik}\sigma_{kl}\sigma_{li}}{p^3}+$$

$$+\frac{9}{25}R\frac{\sigma_{ik}Q_{iQ}k}{p^4}. \tag{10}$$

In view of the 13-moment equations, for S the following entropy balance is valid with accuracy to second order:

$$\frac{\partial\rho S}{\partial t}+\frac{\partial\rho S u_i}{\partial x_i}+\frac{\partial[Q_i/T-{}^2/_5\,\sigma_{il}Q_i/pT]}{\partial x_l}=\frac{\sigma_{ik}\sigma_{ik}}{2\mu T}+\frac{Q_{iQ}i}{\varkappa T^2}. \tag{11}$$

Here $\varkappa$ is the coefficient of thermal conductivity. The balance of the mechanical energy of the perturbation as an exact consequence of the linearized 13-moment equations has the form

$$\frac{\partial}{\partial t}\left\{\frac{\rho_0 u^2}{2}+\frac{5}{6}\frac{p_0}{\rho_0^2}\rho^2+\frac{3}{4p_0}\left(p-\frac{5}{3}\frac{p_0}{\rho_0}\rho\right)\left(p-\frac{1}{3}\frac{p_0}{\rho_0}\rho\right)+\frac{1}{4p_0}\sigma_{ij}\sigma_{ij}+\right. \tag{12}$$

$$\left.+\frac{\rho_0}{5p_0^2}Q_{iQ}i\right\}+\frac{\partial}{\partial x_j}\left\{u_i(p\delta_{ij}+\sigma_{ij})+\frac{2}{5p_0}\sigma_{ij}Q_i+\frac{T}{T_0}Q_j\right\}+\frac{\sigma_{ij}\sigma_{ij}}{2\mu}+\frac{Q_{iQ}i}{\varkappa T_0}=0.$$

2°. The method under discussion is also easily applied to the case of a gas consisting of molecules with internal degrees of freedom. If the determining

process is relaxation between translational and some kind of internal energy, then the entropy should be maximized at constant values of ρ, ρu_i, the internal energy E and its translational part Π. The entropy maximum is attained for a function in which different temperatures correspond to the translational and internal degrees of freedom ([4]). For example–

for example, for the molecular model of rough spheres

$$\rho = \int mf(\mathbf{x}, \mathbf{v}, \mathbf{w}, t)\, d\mathbf{v}\, d\mathbf{w}, \qquad \rho u_i = \int mv_i f\, d\mathbf{v}\, d\mathbf{w},$$

$$\rho E = \int \left[\frac{m(\mathbf{v}-\mathbf{u})^2}{2} + \frac{I\mathbf{w}^2}{2}\right] f\, d\mathbf{v}\, d\mathbf{w}, \qquad \rho\Pi = \int \frac{m(\mathbf{v}-\mathbf{u})^2}{2} f\, d\mathbf{v}\, d\mathbf{w}, \quad (13)$$

where $\mathbf{w}$ is the angular velocity of the molecule, and I is its moment of inertia. The maximum of the entropy under the conditions (13) is attained on the function

$$f = \frac{\rho}{(2\pi)^3} m^{1/2} (I\alpha\beta)^{3/2} \exp\left\{-\frac{m\alpha}{2}(\mathbf{v}-\mathbf{u})^2 - \frac{I\beta}{2}\mathbf{w}^2\right\}. \quad (14)$$

Here $\alpha = 3/2m\Pi$, $\beta = 3/2m(E-\Pi)$. For a general molecular model, truncation of the corresponding chain of equations by means of the maximum-entropy function leads to the equations of relaxation gas dynamics

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0,$$

$$\rho\frac{\partial u_i}{\partial t} + \rho u_k \frac{\partial u_i}{\partial x_k} + \frac{\partial p}{\partial x_i} + \frac{\partial \varepsilon}{\partial x_i} = 0,$$

$$\frac{\partial p}{\partial t} + \frac{\partial p u_i}{\partial x_i} + (\gamma - 1)(p+\varepsilon)\frac{\partial u_i}{\partial x_i} = 0, \quad (15)$$

$$\frac{\partial \varepsilon}{\partial t} + \frac{\partial \varepsilon u_i}{\partial x_i} + \left(\frac{5}{3} - \gamma\right)(p+\varepsilon)\frac{\partial u_i}{\partial x_i} + \frac{\varepsilon}{\tau} = 0.$$

In (15) $\gamma = c_p/c_v$ is the ratio of heat capacities, and as independent parameters, instead of E and Π, the equilibrium pressure $p = (\gamma-1)\rho E$ and the kinetic addition to it $\varepsilon = \rho[{}^2/_3\Pi - (\gamma-1)E]$ have been chosen.

For the case of rough spheres the relaxation time is computed exactly:

$$\frac{1}{\tau} = \frac{32}{3}\frac{\sigma^2\sqrt{\pi}}{m}\frac{K}{(K+1)^2}\sqrt{\rho(p+\varepsilon)}, \tag{16}$$

where σ is the diameter of the molecule, $K = I/m\sigma^2$.

For other models τ must be taken into account phenomenologically. For small ε it may be regarded as depending only on ρ and p, and then it is related to the coefficient of second viscosity ξ by the relation [5]

$$\xi = \left(\frac{5}{3} - \gamma\right) p\tau. \tag{17}$$

The entropy has the form

$$S = \frac{3}{2}R\ln(p+\varepsilon) + \frac{5-3\gamma}{2(\gamma-1)}R\ln\left[p - \frac{3(\gamma-1)}{5-3\gamma}\varepsilon\right] - \frac{\gamma}{\gamma-1}R\ln\rho. \tag{18}$$

By virtue of (15), the entropy balance holds:

$$\frac{\partial\rho S}{\partial t} + \frac{\partial\rho S u_i}{\partial x_i} = \frac{R\rho\varepsilon^2}{\tau\left(\frac{5}{3}-\gamma\right)(p+\varepsilon)\left[p - \frac{3(\gamma-1)}{5-3\gamma}\varepsilon\right]} \geqslant 0. \tag{19}$$

To accuracy up to second order in ε, the production of entropy from (19) is equal to $\varepsilon^2/\xi T$, and the dissipation of energy per unit volume is ε^2/ξ. As a consequence of the system obtained from (15) by linearization, we have the balance of the mechanical energy of the perturbation

$$\frac{\partial}{\partial t}\left[\frac{\rho_0\mathbf{u}^2}{2} + \frac{\gamma p_0}{2\rho_0^2}\rho^2 + \frac{\varepsilon^2}{2\left(\frac{5}{3}-\gamma\right)p_0}\right] + \frac{\partial(p+\varepsilon)u_i}{\partial x_i} + \frac{\varepsilon^2}{\xi} = 0. \tag{20}$$

3°. We can simultaneously take into account the processes of first and second viscosity. For this purpose, in (13), instead of $\rho\Pi$ we must choose p_{ik}, analogously to how this was done in (2). With the aid of the maximum-entropy distribution for the chosen moments one can obtain the system of equations

$$\frac{\partial\rho}{\partial t} + \frac{\partial\rho u_i}{\partial x_i} = 0,$$

$$\rho\frac{\partial u_i}{\partial t} + \rho u_k\frac{\partial u_i}{\partial x_k} + \frac{\partial(\rho\delta_{ik} + \varepsilon\delta_{ik} + \sigma_{ik})}{\partial x_k} = 0, \tag{21}$$

$$\frac{\partial p}{\partial t} + \frac{\partial p u_i}{\partial x_i} + (\gamma-1)[(p+\varepsilon)\delta_{ik} + \sigma_{ik}]\frac{\partial u_i}{\partial x_k} = 0,$$

$$\frac{\partial \sigma_{ik}}{\partial t} + \frac{\partial \sigma_{ik} u_l}{\partial x_l} + \sigma_{kl}\frac{\partial u_i}{\partial x_l} + \sigma_{il}\frac{\partial u_k}{\partial x_l} - \frac{2}{3}\delta_{ik}\sigma_{rs}\frac{\partial u_r}{\partial x_s} + \\ + (p+\varepsilon)\left[\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} - \frac{2}{3}\delta_{ik}\frac{\partial u_l}{\partial x_l}\right] + \frac{p}{\mu}\sigma_{ik} = 0, \tag{21}$$

$$\frac{\partial \varepsilon}{\partial t} + \frac{\partial \varepsilon u_l}{\partial x_l} + \left(\frac{5}{3} - \gamma\right)\left[(p+\varepsilon)\delta_{ik} + \sigma_{ik}\right]\frac{\partial u_i}{\partial x_k} + \frac{\left(\frac{5}{3} - \gamma\right)p}{\xi}\varepsilon = 0.$$

In (21), the moments with respect to the collision integral are taken into account up to first order in ε and σ_{ik}. If (21) is linearized, then, as a consequence of the system obtained, there is a balance of the mechanical energy of the disturbance

$$\frac{\partial}{\partial t}\left\{\frac{\rho_0 u^2}{2} + \frac{\gamma p_0}{2p_0^2}\rho^2 + \frac{\sigma_{ik}\sigma_{ik}}{4p_0} + \frac{\varepsilon^2}{2\left(\frac{5}{3} - \gamma\right)p_0}\right\} + \\ + \frac{\partial (p\delta_{ik} + \varepsilon\delta_{ik} + \sigma_{ik})u_i}{\partial x_k} + \frac{\sigma_{ik}\sigma_{ik}}{2\mu} - \frac{\varepsilon^2}{\xi} = 0. \tag{22}$$

As an example of the degenerate case, let us consider heat conduction of a simple lattice of a dielectric at low temperature. It is natural to choose as the defining quantities the energy E and the heat flux Q_i

$$E(\mathbf{x}) = \sum_{l,k} n_l(\mathbf{x}, \mathbf{k})\, h\omega_l(\mathbf{k}),$$

$$Q_i(\mathbf{x}) = \sum_{l,k} n_l(\mathbf{x}, \mathbf{k})\, h\omega_l(\mathbf{k})\, \frac{\partial \omega_l(\mathbf{k})}{\partial k_i}. \tag{23}$$

In (23), $\omega_l(\mathbf{k})$ is the dispersion relation for a phonon of polarization l; $n_l(\mathbf{x}, \mathbf{k})$ is the mean number of phonons, h is Planck' s constant ([6]). The maximum of entropy under the conditions (23), taking symmetric statistics into account, is attained in the case where

$$n_l(\mathbf{x}, \mathbf{k}) = \frac{1}{\exp\left[\beta h\omega_l + \sum_i \alpha_i h\omega_l \frac{\partial \omega_l}{\partial k_i}\right] - 1}, \tag{24}$$

where α_i and β are found from (23). Truncating the chain of equations following from the kinetic equation for n_l ([6]), with the help of (24), leads in the linear approximation to the equations

$$\frac{\partial E}{\partial t} + \operatorname{div} \mathbf{Q} = 0, \qquad \frac{\partial \mathbf{Q}}{\partial t} + A\ \operatorname{grad} E + c_v A \Lambda^{-1} \mathbf{Q} = 0. \tag{25}$$

In (25), the thermal-conductivity tensor Λ is taken into account phenomenologically. The tensor A is determined by the form of $\omega_l(k)$. The entropy, to accuracy of second order, has the form

$$S = S_0(E) - \frac{1}{2c_{vT}^2} A^{ij} Q_{iQ} j. \tag{26}$$

Here $S_0(E)$ is the equilibrium entropy, A^{ij} is the tensor inverse to A.

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Note: Figure translations are in progress. See original paper for figures.