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Exact Solution of Boltzmann Equations for Multicomponent Systems*

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Exact solutions of similarity type are obtained for Boltzmann equations describing the temporal relaxation to equilibrium of an N-component gas with elastic collision cross sections of special form.

In an earlier communication,[1] we presented certain exact solutions of the nonlinear Boltzmann equation for the temporal relaxation to equilibrium of a one-component gas. In many cases of interest (e.g., gas-phase reactions, D-T fusion), it is necessary to consider relaxation in multicomponent systems. The purpose of this Letter is to indicate how exact solutions can be obtained for an N-component gas with $N \geq 2$. The generalization from one to N components is nontrivial; in the latter case, such exact solutions exist only when the parameters that describe the system satisfy certain conditions.

Consider an infinite, spatially homogeneous, and isotropic gas composed of N species of molecules which interact only through binary elastic collisions. The state at time t is specified by N distribution functions $n_a f_a(v, t)$ $(a = 1, \ldots, N)$ where $\vec{v}$ is a velocity variable, $v = |\vec{v}|$, and n_a is the constant number density of a molecules. We consider models in which the cross section for collision of a molecules with b molecules has the form

$$\sigma_{ba}(b, \chi) = \kappa_{ba}\varphi_{ba}(\chi)/g, \quad a, b = 1, \ldots, N, \tag{1}$$

where g is the relative speed, the $\kappa_{ba} = \kappa_{ab}$ are constants, and the $\varphi_{ba} = \varphi_{ab}$ are general functions of the center-of-mass scattering angle χ. For conciseness, attention will here be confined to isotropic scattering, i.e., $\varphi_{ba} \equiv 1$, and to the case $N = 2$.

For the single-component case, the exact solution has the form[1]

$$f(v, \tau) = \Phi(v; \alpha(\tau))\,[P(\tau) + Q(\tau)v^2], \tag{2}$$

where τ is a dimensionless time variable, α, P, and Q are certain functions, and

$$\Phi(v; \alpha) \equiv (2\pi\alpha)^{-3/2}\exp(-v^2/2\alpha). \tag{3}$$

In this solution, the high-energy tail is initially highly depleted (because of the factor Φ), and subsequently builds up gradually to the appropriate Maxwellian value. The process is slow because two particles of relatively high energy have to collide in a special way to give one of them appreciably higher energy.

In the case of N components, we again seek solutions of the form

$$f_a(v, \tau) = \Phi(v; \alpha_a(\tau))\,[P_a(\tau) + Q_a(\tau)v^2], \quad a = 1, \ldots, N. \tag{4}$$

If the "mean" kinetic energies (KE) of the various components, as represented by the factor $\Phi(v; \alpha_a(\tau))$, were initially different, the components with lower KE would rapidly increase their KE by collisions with components of higher mean KE. Their high-energy Maxwellian tails would then build up in a way completely different from the case of a single component. We therefore expect the mean KE of all the components to be the

same:

$$m_1\alpha_1(\tau)=m_2\alpha_2(\tau)=\ldots=m_N\alpha_N(\tau)\equiv\zeta(\tau), \tag{5}$$

say, where m_a is the mass of an a molecule. This is a rather strong constraint. Thus the exact solutions have a more special character in the multicomponent than in the single-component case. As will appear later, such solutions are possible only if parameters describing the system satisfy certain conditions.

The elastic collisions of a molecules with b molecules can be represented symbolically by

$$(m_a,\vec{v})+(m_b,\vec{w})\xrightarrow{\chi,\epsilon}(a,\vec{v}')+(b,\vec{w}') \qquad (a,b=1,2), \tag{6}$$

where, with the notation

$$\vec{G}\equiv\frac{m_a\vec{v}+m_b\vec{w}}{m_a+m_b},\quad \vec{g}\equiv\vec{v}-\vec{w},\quad \vec{g}'=\vec{v}'-\vec{w}'. \tag{7}$$

ϵ is the angle between the plane of $\vec{g}$, $\vec{G}$ and the plane of $\vec{g}$, $\vec{g}'$. It is easily established that

$$v'^2=v^2+\frac{2m_b}{m_a+m_b}S,\quad w'^2=w^2-\frac{2m_a}{m_a+m_b}S, \tag{8}$$

where

$$S=(\vec{G}\cdot\vec{g})(\cos\chi-1)+|\vec{G}\times\vec{g}|\sin\chi\cos\epsilon. \tag{9}$$

Let $\bar{\kappa}$ be some mean value of the κ_{ba}, and (for $N=2$) set

$$\lambda_{ba}\equiv n_b\kappa_{ba}/(n_1+n_2)\bar{\kappa}\quad (a,b=1,2). \tag{10}$$

Then, in terms of the dimensionless time variable $\tau\equiv4\pi(n_1+n_2)\bar{\kappa}t$, the Boltzmann equations for the system assume the form

$$\frac{\partial f_a(v,\tau)}{\partial\tau}=\sum_{b=1}^{2}\frac{\lambda_{ba}}{4\pi}\iint\{-f_a(v,\tau)f_b(w,\tau)+f_a(v',\tau)f_b(w',\tau)\}\,d\Omega\,d\vec{w} \tag{11}$$

(for $a=1,2$), where $d\Omega\equiv\sin\chi\,d\chi d\epsilon$.

We now seek solutions of the form (4) subject to the constraints (5). It is convenient to set $R_a(\tau)\equiv Q_a(\tau)\alpha_a(\tau)$ $(a=1,2)$. Conservation of particles and of energy then implies that

$$P_a+3R_a\equiv1\quad(a=1,2), \tag{12}$$

$$\zeta\sum_{a=1}^{2}n_a(P_a+5R_a)=(n_1+n_2)\kappa_B T, \tag{13}$$

where κ_B is Boltzmann's constant and T is the constant kinetic temperature of the system.

It is convenient to define parameters μ, p_1, and p_2 as follows:

$$\mu\equiv4m_1m_2/(m_1+m_2)^2,$$

$$p_1\equiv\lambda_{22}-\lambda_{21}\mu(3-2\mu), \tag{14}$$

$$p_2\equiv\lambda_{11}-\lambda_{12}\mu(3-2\mu).$$

When Eqs. (4), (5), (8), and (9) are substituted into the Boltzmann equations (11), all integrations can be performed explicitly. We thus obtain two equations, each representing equality of a pair of expressions quadratic in v^2. Equation of coefficients then leads to a system of six nonlinear differential equations for the five functions $\zeta(\tau)$, $P_a(\tau)$, and $R_a(\tau)$ $(a=1,2)$.

Accordingly, it is possible to find solutions provided that one condition is satisfied for all τ. It turns out, fortunately, that this condition is actually independent of τ, and is

$$(p_1-p_2)\left[2\mu^2\left(\frac{\lambda_{21}}{p_1}-\frac{\lambda_{12}}{p_2}\right)-1\right]=0.$$

Therefore explicit exact solutions can be found when *either* (i)

$$p_1=p_2, \tag{15a}$$

or (ii)

$$2\mu^2(\lambda_{21}/p_1-\lambda_{12}/p_2)=1. \tag{15b}$$

In either case, the solution can be expressed in terms of a function

$$R(\tau)\equiv\{A\exp[A(\tau-\tau_0)]-B\}^{-1}A, \tag{16}$$

where

$$A\equiv\tfrac{1}{6}\{\lambda_{11}+\lambda_{21}\mu(3-2\mu p_2/p_1)\}, \tag{17}$$

$$B\equiv\tfrac{1}{3}\{\lambda_{11}p_1+\lambda_{21}\mu(3-2\mu)p_2\}, \tag{18}$$

and the constant τ_0 corresponds to the arbitrary choice of a time origin. Then

$$R_a(\tau)=p_aR(\tau)\quad(a=1,2) \tag{19}$$

and

$$\zeta(\tau)=\frac{(n_1+n_2)}{(n_1+n_2)+2(n_1p_1+n_2p_2)R(\tau)}. \tag{20}$$

The determination of α_1, α_2 and P_1, P_2 from Eqs. (5) and (12) is straightforward. This completes the solution.

The two conditions (15) are of rather different nature physically. Given as masses and cross sections, it is often possible to find a relative density n_1/n_2 such that the first condition is satisfied. On the other hand, the densities do not appear in the second condition. In other words, if the second condition is satisfied, exact solutions can be written down for all values of n_1/n_2.

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[1]M. Krook and T. T. Wu, Phys. Rev. Lett. 36, 1107 (1976).

Exactly Solvable Model for the Roughening Transition of a Crystal Surface

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An exactly solvable model of the crystal-vacuum interface is constructed which exhibits a roughening transition. The model is obtained as a special limit of a ferromagnetic Ising model and it is isomorphic to the symmetric six-vertex model. Some of the thermodynamic properties of the system are discussed.

The concept of interface roughening was introduced in the theory of crystal growth by Burton and co-workers[1,2] on the basis of a comparison between a crystal surface and the quadratic Ising model. From a different point of view Gallavotti conjectured[3] that the cubic Ising model might show a roughening transition for an interface between phases of opposite magnetization. His conjecture was supported by Weeks, Gilmer, and Leamy,[4] who used low-temperature expansions to estimate the roughening temperature T_R of the isotropic cubic Ising model and the solid-on-solid (SOS) model, which is obtained from the cubic Ising model by letting the vertical coupling constant go to infinity while keeping the horizontal coupling constants fixed (an interface is maintained by imposing appropriate boundary conditions). Their estimates of T_R are well below the bulk critical temperature in either case. Further evidence for the existence of a roughening transition comes from computer simulations of the interface in the SOS model and the discrete Gaussian (DG) model.[5-8] A rigorous proof for the existence of such a transition, however, to our knowledge has not been given before.

Here I discuss an exactly solvable model which does show a roughening transition. We start from a body-centered-cubic Ising model of $2N\times 2N\times 2N$ sites with ferromagnetic nearest-neighbor coupling J_0 (between particles in the center and on a corner of an elementary cube) and next-nearest-neighbor couplings J_x, J_y, and J_z in the three main lattice directions. The spins in the two bottom layers are kept positive, those in the two top layers negative, and free boundary conditions are imposed on the side walls (in the crystal interpretation positive spins correspond to occupied lattice sites and negative spins to empty ones). The body-centered solid-on-solid (BCSOS) model is obtained by letting J_0 approach infinity, keeping J_x, J_y, and J_z constant. In this limit the so-called SOS condition is satisfied (this means that in no column of the lattice is a negative spin to be found below a positive one). In Fig. 1 some spin configurations are sketched on a "ladder" of two neighboring columns of spins on a lattice of height 8. Because of the imposed boundary conditions such a ladder always contains at least one $(+-)$ bond of strength $+J_0$ [e.g., bond 2 in Fig. 1(a)], but in the limit as $J_0\to\infty$ configurations in which any ladder contains more than one $(+-)$ bond such as in Fig. 1(b) are strictly forbidden. From this the SOS condition follows di-

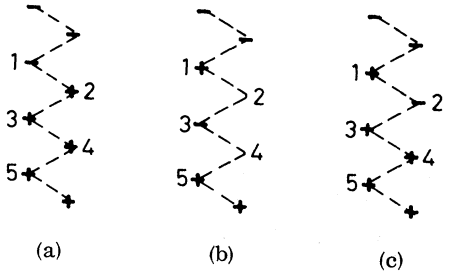

FIG. 1. Some spin configurations on a ladder of two neighboring columns.