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Dynamical aspects of one-dimensional Maxwellian relaxation

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Subtle features of the relaxation of one-dimensional binary mixtures of elastic particles are explored for two extreme mass ratios, corresponding to the minimum as well as a very large relaxation time of the velocity distribution functions of the system. An interpretation of the relaxation time is also given in the context of thermodynamics. [S1063-651X(98)00402-4]

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Recently, we reported the results of investigations on the relaxation of one-dimensional binary mixtures of elastically colliding particles by solving the nonlinear Boltzmann equation and computer simulations [1]. The results confirmed some of those obtained by other investigators [2–4] and revealed some different interesting features of the system. In this Brief Report we explain some of the subtleties of the evolution of such systems towards equilibrium.

When the mass ratio in a one-dimensional binary mixture of elastic particles is either unity or infinity, the system is nonergodic and the initial velocity distribution is conserved. At all other mass ratios, the velocity distribution for each type of particle oscillates between unimodal and bimodal Gaussian-like forms, which eventually evolves into a single Gaussian, with a minimum relaxation time at the mass ratio of $3+2\sqrt{2}$.

We will show that the unimodal and bimodal distributions observed during the relaxation of the system are actually systems of a large number of spikes with binomial envelopes. As time increases, these peaks approach each other, the number of spikes in each envelope increases, and each envelope evolves into a Gaussian. The shorter the relaxation time, the faster these evolutions. At the mass ratio of $3+2\sqrt{2}$, when the relaxation time is a minimum, the distribution function is always unimodal with a binomial envelope, which relaxes into a Gaussian in a minimum time. We also give an interpretation of the minimum relaxation time, as defined previously [1], in the context of the principle of equipartition of energy.

In a binary mixture of elastic particles in one dimension, consisting of equal numbers of mass unity and mass m particles $(m>1)$, and the initial conditions

$$f(v,0)=\tfrac{1}{2}[\delta(v-v_0)+\delta(v+v_0)],\quad g(u,0)=\delta(u),\quad (1)$$

the velocity distribution function of the mass-1 particles in Fourier space at even time steps is given by [1,5]

$$F(k,t)=\prod_{m=0}^{t/2}\cos^{\binom{t}{2m}}[\alpha^{t-2m}(\beta\gamma)^{m}k].\quad (2)$$

In this equation the exponent of each cosine function is a binomial coefficient

$$\binom{t}{2m}=\frac{t!}{(2m)!(t-2m)!},\quad (3)$$

the parameters α, β, and γ are defined by

$$\alpha\equiv\frac{1-m}{1+m},\quad \beta\equiv\frac{2}{1+m},\quad \gamma\equiv\frac{2m}{1+m},\quad (4)$$

and the units are chosen so that $v_0=1$.

We consider a small mass difference between the two particles as the mathematics is amenable. Let $m=1+\epsilon$, where $\epsilon\ll 1$. Then $\alpha\approx-\epsilon/2$, $\beta\approx 1-\epsilon/2$, and $\gamma\approx 1+\epsilon/2$. The low-$v$ behavior of the distribution function will be dominated by the highest-frequency term in $F(k,t)$, which will be (in order of descending frequency)

$$\begin{aligned}F(k,t)&=\cos[(\beta\gamma)^{t/2}k]\cos^{\binom{t-2}{t}}[\alpha^2(\beta\gamma)^{t/2-1}k]\times\cdots\\&\approx\cos\left[\left(\frac{4(1+\epsilon)}{(2+\epsilon)^2}\right)^{t/2}k\right]\cos^{\binom{t-2}{t}}\left[\left(\frac{\epsilon}{2}\right)^2k\right]\times\cdots\\&\approx\frac{1}{2^{\binom{t}{t-2}+1}}\sum_{n=0}^{\binom{t}{t-2}}\left(\begin{matrix}\binom{t}{t-2}\\ n\end{matrix}\right)\\&\quad\times\left(\exp\left\{i\,\frac{\epsilon^2k}{4}\left[2n-\binom{t}{t-2}\right]+i\left(\frac{4(1+\epsilon)}{(2+\epsilon)^2}\right)^{t/2}k\right\}\right.\\&\quad\left.+\exp\left\{i\,\frac{\epsilon^2k}{4}\left[2n-\binom{t}{t-2}\right]-i\left(\frac{4(1+\epsilon)}{(2+\epsilon)^2}\right)^{t/2}k\right\}\right),\end{aligned}\quad (5)$$

which results in

$$\begin{aligned}f(v,t)\approx&\frac{1}{2^{\binom{t-2}{t}+1}}\sum_{n=0}^{\binom{t}{t-2}}\left(\begin{matrix}\binom{t}{t-2}\\ n\end{matrix}\right)\\&\times\left[\delta\left(v-\frac{\epsilon^2}{4}\left[2n-\binom{t}{t-2}\right]-\left(\frac{4(1+\epsilon)}{(2+\epsilon)^2}\right)^{t/2}\right)\right.\\&\left.+\delta\left(v-\frac{\epsilon^2}{4}\left[2n-\binom{t}{t-2}\right]+\left(\frac{4(1+\epsilon)}{(2+\epsilon)^2}\right)^{t/2}\right)\right]\end{aligned}\quad (6)$$

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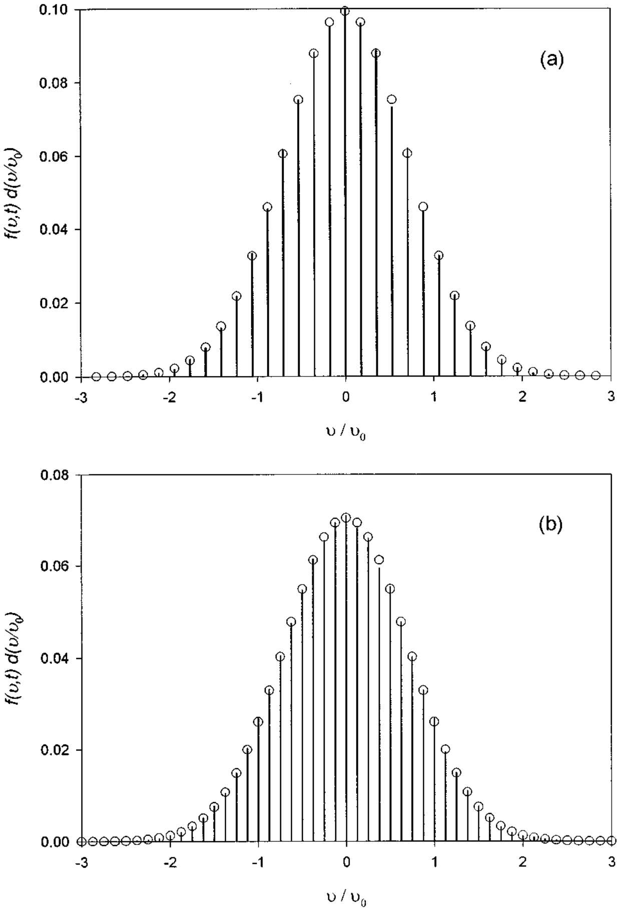

FIG. 1. Velocity distribution function of the mass-1 particles in a binary mixture with a mass ratio of $3+2\sqrt{2}$ after (a) 7 time steps and (b) 8 time steps. The vertical lines are computer simulation results and the circles are from the theory.

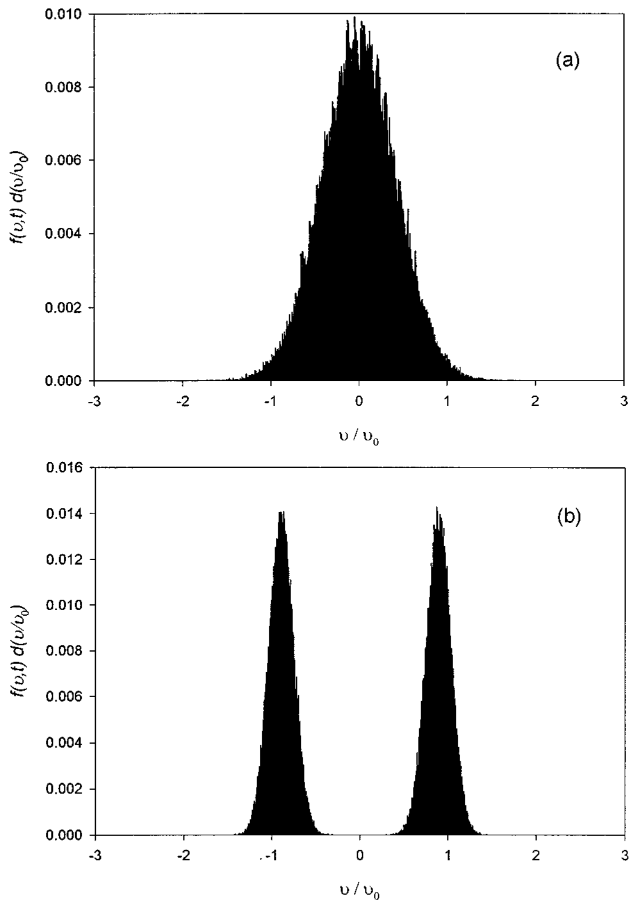

FIG. 2. Computer simulation results for the velocity distribution function of the mass-1 particles in a binary mixture with a mass ratio of 1.1 after (a) 99 time steps and (b) 100 time steps. Each dark region is developed by the congestion of a very large number of spikes.

representing two families of discrete peaks with binomial envelopes centered at

$$v=\pm\left(\frac{4(1+\epsilon)}{(2+\epsilon)^2}\right)^{t/2} \tag{7}$$

that converge on Gaussian envelopes while approaching each other as time evolves. Clearly, for $\epsilon=0$ the distribution remains forever a pair of spikes at $v=\pm 1$. For $\epsilon\neq 0$, on the other hand, the spikes in the binomial envelopes move towards each other with a rate that increases with ϵ, ultimately merging into a single Gaussian distribution centered at $v=0$.

In the special case $m=3+2\sqrt{2}$, the distribution function in Fourier space reduces to a simple closed form [1], from which the velocity distribution can be obtained exactly,

$$f(v,t)=\left(\frac{1}{2}\right)^{2^{t-1}} \sum_{n=0}^{2^{t-1}} \binom{2^{t-1}}{n} \delta\left(v-\left(\frac{2^{t-1}-2n}{2^{t/2}}\right)\right). \tag{8}$$

Equation (8) shows that for this mass ratio the velocity distribution function is unimodal at all times, consisting of a family of spikes with a binomial envelope, which converges on a Gaussian as $t\rightarrow\infty$.

Figure 1 shows the velocity distribution function for the mass-1 particles after $t=7$ and 8 time steps, when the mass ratio in the system is $3+2\sqrt{2}$. These results are obtained by Monte Carlo computer simulations, using the algorithm described in Ref. [1]. The theoretical results, which are in excellent agreement with the simulations, are also given for comparison. Note that according to Eq. (8), the spikes are equally spaced and are located at the positions given by

$$v_n=\frac{2^{t-1}-2n}{2^{t/2}}, \quad n=0,1,2,3,\ldots,2^{t-1}. \tag{9}$$

Figure 2 shows the same results for the mass ratio of $m=1.1$ after $t=99$ and 100 time steps, in which the switching behavior of the distribution function between unimodal and bimodal is obvious. It should be noted that for any mass ratio other than $3+2\sqrt{2}$, the spikes within the binomial envelopes are not equally spaced. Finally, Fig. 3 shows the theoretical and simulational results for the approaching rate of the binomial peaks in the bimodal distribution of the mass-1 particles when the mass ratio is 1.1.

We will now give an interpretation of the relaxation time for the system [1],

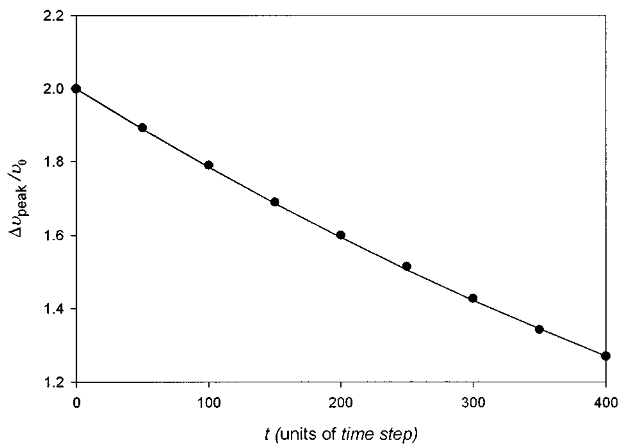

FIG. 3. Peak-to-peak distance in the bimodal velocity distribution function of the mass-1 particles as a function of time, when the mass ratio is 1.1. The continuous curve is from Eq. (7) and the markers are the computer simulation results.

$$\tau \equiv -\frac{1}{\ln|\xi|}, \tag{10}$$

where ξ is defined by

$$\xi \equiv \alpha^2 - \beta\gamma = \frac{1-6m+m^2}{(1+m)^2}. \tag{11}$$

Since the root of ξ is at $3+2\sqrt{2}$ (for $m>1$), the relaxation time is zero at this mass ratio. We consider the difference in the kinetic energies of a mass-1 and a mass-m particle after a binary collision $\Delta_1 T$ in terms of their velocities before the collision. Using the usual equations for energy and momentum conservation, we get

$$\Delta_1 T \equiv \frac{1}{2}mu'^2 - \frac{1}{2}v'^2 = \frac{1-6m+m^2}{(1+m)^2}\left(\frac{1}{2}mu^2 - \frac{1}{2}v^2\right) - \frac{4m(1-m)}{(1+m)^2}uv = \xi\Delta_0 T - \frac{4m(1-m)}{(1+m)^2}uv, \tag{12}$$

where $\Delta_0 T$ is the difference in the kinetic energies before the collision. We see that for the mass ratio of $3+2\sqrt{2}$, when $\xi=0$ and the relaxation time is a minimum (zero), the elastic collision equally divides the energy between the two particles only if one of the particles is initially at rest. However, even in this case, the second collision breaks the energies apart. Therefore, the problem of minimum relaxation time cannot be related to the individual binary collisions between the two types of particles.

We now consider the average of $\Delta_1 T$ over all colliding pairs in the binary system of particles, with respect to the pair distribution function. Assuming molecular chaos, the quantity $\langle uv\rangle = 0$ and Eq. (12) reduces to

$$\langle \Delta_1 T\rangle \equiv = \xi\langle \Delta_0 T\rangle. \tag{13}$$

Similarly, the average difference in the kinetic energies after the second time step $\Delta_2 T$ is given by

$$\langle \Delta_2 T\rangle = \xi\langle \Delta_1 T\rangle = \xi^2\langle \Delta_0 T\rangle \tag{14}$$

and so on. Therefore, after t time steps we have

$$\langle \Delta_t T\rangle = \xi^t\langle \Delta_0 T\rangle. \tag{15}$$

Equation (15) describes the evolution of the system into the equipartitioned state. The smaller the ξ the faster the energy divides itself equally (on the average) among the particles of the system. For the mass ratio of $3+2\sqrt{2}$ when $\xi=0$, this happens after the first collision.

In summary, we see that even though in these systems the tail of the distribution function for each type of particle, determined by the small-k behavior of its Fourier transform, relaxes to the expected Gaussian form in a minimal time for the mass ratio of $3+2\sqrt{2}$ [1], other portions of the distribution, namely, the low-velocity region, evolves much more slowly. The relaxation of the distribution around $v=0$ therefore sets the limit for overall relaxation rate of the distribution, requiring a reinterpretation of what precisely is meant by the relaxation time of the system. Evolution towards the equipartition of energy occurs at the same pace as the evolution of the tail of the velocity distribution in this model, which is obvious from the fact that

$$\langle v^2(t)\rangle = \int v^2 f(v,t)dv \tag{16}$$

contains no contributions from the portion of the distribution that is evolving the slowest, namely, the $v=0$ region, and weights the high-v portion (the tail) most heavily.

Since the system is assumed to be at constant volume and uniform density, the only thermodynamic variable is the temperature T. This means that since all thermodynamic potentials are obtained from the derivatives of the partition function with respect to T and that the Hamiltonian is quadratic in v, all thermodynamic potentials will relax with the tail of the velocity distributions, which are the most rapidly evolving parts of the distributions.

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[5] As in Ref. [1], a *time step* is defined to be the time in which, on the average, every particle undergoes exactly one binary collision.