Relaxation of one-dimensional binary mixtures

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(Received 26 December 1996; revised manuscript received 13 February 1997)

Temporal evolution of one-dimensional binary mixtures of small-diameter elastic particles is studied from different theoretical and simulational perspectives. The nonlinear Boltzmann equation for the system is solved exactly in the Fourier space. The simulational algorithm used is extremely fast and produces results that are in perfect agreement with the theory, even with a fairly small number of particles involved. Both theoretical and simulational results show that the relaxation time of a non-Maxwellian mixture is a minimum for the mass ratio of $3+2\sqrt{2}$, consistent with earlier investigations, and that for this choice of mass ratio, the distribution functions reduce to simple closed forms. The evolving distribution oscillates between a bimodal and unimodal form. [S1063-651X(97)00206-7]

PACS number(s): 51.10.+y, 02.70.Lq, 05.20.−y, 05.20.Dd

I. INTRODUCTION

One-dimensional gas systems have been of interest for quite some time both from mathematical and statistical mechanical points of view [1–3]. One of the unique properties of the one-dimensional system is that elastic collision between particles of equal mass results in a complete exchange of momentum and energy. Consequently, these particles can be regarded as being transparent to one another as long as they are indistinguishable. A one-dimensional gas of equal-mass elastic particles, therefore, conserves its initial velocity distribution. This is in contrast to the two- or three-dimensional case, where partial exchange of energy and momentum causes relaxation of the initial distributions into a Maxwellian form.

In a molecular-dynamics simulation, Masoliver and Marro [4] showed that a one-dimensional binary mixture of impenetrable (hard core) particles with different masses, when half of the particles are randomly assigned an initial velocity of $+v_0$ and the other half $-v_0$, evolve toward a Maxwellian velocity distribution, unlike the corresponding nonergodic system with equal masses. Later, using similar computer simulations, they showed that the relaxation time for the temporal evolution of a binary mixture of hard rods in a ring toward the Maxwellian distribution was a function of the mass ratio of the particles in the mixture [5]. More specifically, they observed that the relaxation time diverges as the mass ratio approaches unity and again increases, although not so rapidly, as the mass ratio tends to infinity. Clearly, the divergence of the relaxation time at mass ratios of unity and infinity are expected. Consequently, the relaxation time must be a minimum somewhere between these two limits. Marro and Masoliver found this minimum to be around the mass ratio of 5.

In a theoretical treatment of the dynamics of a one-dimensional two-component gas of ''soft'' Maxwellian point particles, Dickman [6] obtained the eigenvalue spectrum of the linearized collision operator. He found that the highest nonzero eigenvalue, which controls the long-time relaxation of the velocity distribution function, vanishes for the mass ratios of unity and infinity. Furthermore, his calculations show that this eigenvalue has a maximum value at a mass ratio of $3+2\sqrt{2}\approx 5.8284$, corresponding to a minimum relaxation time, in qualitative agreement with the computer simulations of Masoliver and Marro. The exact solution of the kinetic and ergodic properties of a one-dimensional binary system, however, is still lacking [4].

This work is based on an entirely different theoretical treatment of a binary mixture of small-diameter elastic particles, in which the nonlinear Boltzmann's transport equation is solved exactly in the Fourier space. The problem is further attacked by a very simple, yet extremely accurate computer simulation technique. The algorithm is not molecular dynamical in nature and, hence, does not keep track of the phase-space trajectories of the particles. Consequently, it is very fast. The computer simulation and the theoretical results are compared with each other, and are found to be in perfect agreement. These results are used to resolve some of the subtle points in the temporal evolution of this type of system toward equilibrium that have been overlooked by previous investigators.

II. THEORETICAL ANALYSIS

Consider a spatially homogeneous one-dimensional binary mixture of gases, consisting of equal number of mass-unity and mass-a particles. The Boltzmann equation for temporal evolution of the velocity distribution $f(v,t)$ of the unit mass particles due to elastic collisions is given by [7]

$$\frac{\partial f(v,t)}{\partial t}=\int du\, dv' du' [\sigma(u',v';u,v)F^{(2)}(u',v';t) - \sigma(u,v;u',v')F^{(2)}(u,v;t)], \quad (1)$$

in which $F^{(2)}(u,v;t)$ is the pair distribution, and $\sigma(u,v;u',v')$ is the probability that a binary collision changes the velocity of mass 1 and mass-a particles from

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v,u to v',u', respectively. Invoking the assumption of molecular chaos and using conservation of energy and momentum with

$$\sigma(u',v';u,v)=\sigma(u,v;u',v')$$
$$=\delta(v+au-v'-au')\delta(\tfrac{1}{2}v^2+\tfrac{1}{2}au^2-\tfrac{1}{2}v'^2-\tfrac{1}{2}au'^2), \quad (2)$$

we find that for discrete times

$$\frac{\partial f(v,t)}{\partial t}+f(v,t)=f(v,t+1)=\int du\ f(\gamma u+\alpha v,t)\times g(\beta v-\alpha u,t), \quad (3)$$

in which

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

Similarly, for velocity distribution of the mass-a particles, $g(u,t)$, we find

$$g(u,t+1)=\int dv\ f(\gamma u+\alpha v,t)g(\beta v-\alpha u,t). \quad (5)$$

Fourier transforming,

$$F(k,t)\equiv\int e^{ikv}f(v,t)dv, \quad (6)$$

and changing variables to

$$q\equiv\alpha v+\gamma u,\quad w\equiv-\alpha u+\beta v, \quad (7)$$

we arrive at the equations

$$F(k,t)=F(\alpha k,t-1)G(-\gamma k,t-1),$$
$$G(k,t)=G(\alpha k,t-1)F(\beta k,t-1). \quad (8)$$

A simple case to analyze both in simulation and in theory is one in which initially one type of particle is at rest and the other type has velocity $\pm v_0$, with no net center-of-mass motion. Taking these to be mass-a and mass-1 particles, respectively, we demonstrate in Appendix A that for even times, namely, $t=2j$, where $j=1,2,3,\ldots$,

$$F(x,2j)=\prod_{m=0}^{j}\cos^{P(j,m)}[\alpha^{2j-2m}C(j,m)x] \quad (9)$$

and

$$G(x,2j)=\prod_{m=0}^{j-1}\cos^{Q(j,m)}[\alpha^{2j-2m}D(j,m)x], \quad (10)$$

in which $x\equiv kv_0$ is a dimensionless quantity, $C(j,m)=(\beta\gamma)^m=(\alpha/\beta)D(j,m)$, and

$$P(j,m)=\frac{(2j)!}{(2m)!(2j-2m)!},$$
$$Q(j,m)=\frac{(2j)!}{(2m+1)!(2j-2m-1)!}. \quad (11)$$

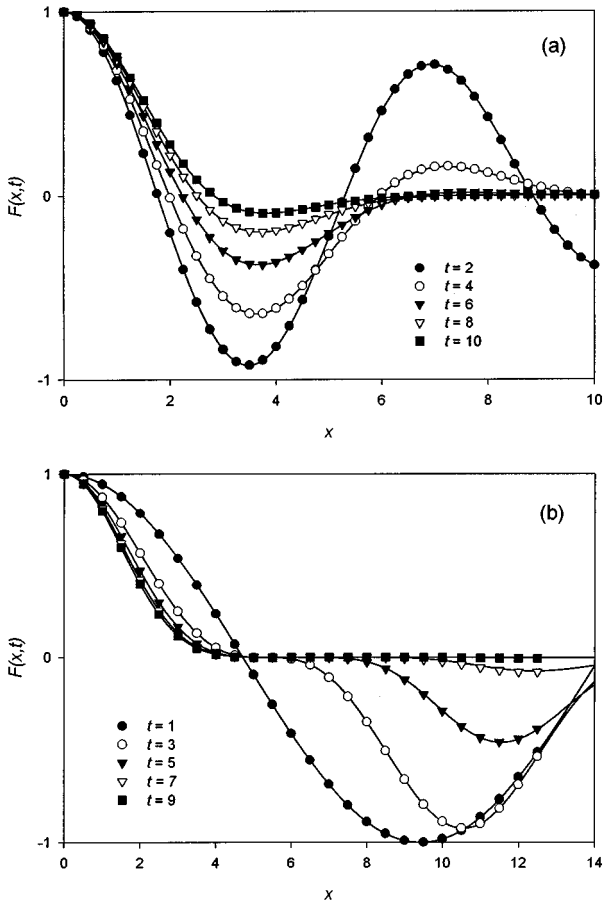

FIG. 1. Temporal evolution of the Fourier transform of normalized velocity distribution of mass-1 particles in a binary mixture with a mass ratio of 2. Continuous curves are from the theory and markers are from Monte Carlo simulations. Note the switching behavior of the distribution between unimodal and bimodal as time goes through even and odd values, respectively. All quantities are dimensionless.

Figure 1(a) shows $F(x,t)$ as a function of x for various (even) t values. We mention in passing that the derivation for odd times proceeds in a similar fashion, and the results are shown in Fig. 1(b).

For each particle type, the analytical solution approaches a Maxwellian form for large time (j) values. The approximation

$$\cos^{2j}(x)\approx e^{-x^2j} \quad (12)$$

becomes increasingly accurate around the maxima of the cosine function as j increases. This function becomes a series of Gaussian peaks centered at the points $x=n\pi$, and for large j the peaks are narrow and do not overlap. This causes the product solutions above to become expressible as a product of periodic Gaussian functions with different frequencies, suppressing one another except near $x=0$, where all share a maximum. We find that near this maximum

$$\ln F(x,2j)\approx\sum_{m=0}^{j}\left[-\frac{x^2}{2}\,\alpha^{4j}\binom{2j}{2m}\left(\frac{\beta\gamma}{\alpha^2}\right)^{2m}\right]$$
$$=-\frac{x^2}{4}[1+(\alpha^2-\beta\gamma)^{2j}] \quad (13)$$

and

$$\ln G(x,2j) \approx \sum_{m=0}^{j-1} \left[-\frac{\beta^2 x^2}{2} \alpha^{4j-2} \binom{2j}{2m+1} \left(\frac{\beta\gamma}{\alpha^2}\right)^{2m} \right] = -\frac{\beta x^2}{4\gamma} [1-(\alpha^2-\beta\gamma)^{2j}], \quad (14)$$

where we have used $\alpha^2+\beta\gamma=1$. For sufficiently large j, we obtain

$$F(x,2j)=e^{-(x^2/4)(1+\xi^{2j})}, \quad G(x,2j)=e^{-(\beta x^2/4\gamma)(1-\xi^{2j})}, \quad (15)$$

where

$$\xi \equiv \alpha^2-\beta\gamma=\frac{1-6a+a^2}{1+2a+a^2}. \quad (16)$$

Note that ξ is bounded by ± 1, and has roots at $a=3\pm 2\sqrt{2}$, which are reciprocals of each other. Inverse Fourier transforming, we find that the long-time velocity distributions are Maxwellian with time-dependent variances given by

$$\sigma_1^2=\frac{1+\xi^t}{2}$$

and

$$\sigma_a^2=\frac{1-\xi^t}{2a}, \quad (17)$$

in which t is arbitrarily even or odd; the computations for $t=2j+1$ are straightforward and give the same result.

Since for any even distribution function, $f(x)$, and its Fourier transform, $F(k)$, we have

$$\sigma^2=\langle x^2\rangle=-\frac{d^2}{dk^2} F(k)|_{k=0}, \quad (18)$$

our results for $\sigma^2(t)$ obtained by small-x expansion are, in fact, the exact variances for all times.

III. COMPUTER SIMULATIONS

Our computer simulation model consists of 100 mass-1 and mass-a particles each, on a straight line. Half of the former are randomly assigned an initial velocity of $+v_0$, and the other half an initial velocity of $-v_0$. Mass-a particles are all initially at rest. All velocities are measured in units of v_0. We do not keep track of the position of the particles. We perform an ensemble Monte Carlo simulation in which particles of different mass undergo a large number of collisions. During one time step (unit of time) each particle of mass 1 randomly chooses a partner from the collection of mass-a particles and elastically collides with it. No particle undergoes more than one collision per time step. This task is accomplished by shuffling the ordered set of mass-a particles, and then allowing particle number n ($n=1,2,3,\ldots$) from the set of mass-1 particles to collide with particle number n from the set of mass-a particles. After each time step, the new velocities of the particles in each set are calculated, and the step is repeated. Collisions between like particles are neglected as these particles are transparent to one another. All the data are collected over ensembles of 1000 such systems.

Figure 1 compares the computer simulation and the theoretical distribution functions in Fourier space at various times, both even and odd. As can be seen, the agreement between the simulation results and the theory is perfect, despite the fact that the theoretical results are solely based on the Boltzmann transport equation and are completely independent of the model or algorithm used in the simulations. Furthermore, these graphs reveal that the shapes of the distribution functions are quite different at even and odd times, alternating between essentially unimodal and bimodal forms, respectively.

Figure 2 shows computer simulation results for the temporal evolution of the distribution function $f(v,t)$, for a mass ratio of 2, after eight, nine, and ten time steps. It is interesting that the molecular dynamics results of Masoliver and Marro [4], which is based on an algorithm originally developed by Adler and Wainwright [8], shows that the initial distribution function degenerates into two Gaussians centered symmetrically on the two sides of the origin that finally evolve into a single Gaussian centered at the origin. Both our simulation and our theoretical results, however, show that this is not the case. In fact, the distribution function oscillates between a one Gaussian-like and a two separate Gaussian-like functions at odd and even times, respectively, all of which merge into a single Gaussian in perfect agreement with our theoretical results, as the system evolves toward equilibrium. This is further evidenced in Fig. 1, where the Fourier transform of the distribution function $F(k,t)$ shows completely different functional behavior for even and odd times. The evolution of the distribution function of mass-a particles also shows this switching behavior but in reverse order. One may suspect that this discrepancy is caused by the difference in the initial conditions used in our simulations and those by the aforementioned investigators. Nevertheless, when we simulated the system with the symmetric initial conditions used by Masoliver and Marro, namely, ± 1 for both types of particles, we still obtained the switching behavior between the unimodal and bimodal Gaussian-like distribution functions. We believe that this discrepancy is caused by the fact that the details of the evolution of the distribution function were obscured in Masoliver and Marro's simulations as they used time steps that corresponded to only even number of collisions per particle of each type.

In order to simulate the relaxation time of the standard deviations of the distribution functions, we first note that since t is either an even or an odd integer, and that ξ can be either positive or negative, therefore, the quantity ξ^t is either positive or negative. We define a relaxation time τ by

$$\exp(-t/\tau)\equiv|\xi|^t$$

or

$$\tau \equiv -\frac{1}{\ln|\xi|}. \quad (19)$$

Therefore, the standard deviations reduce to

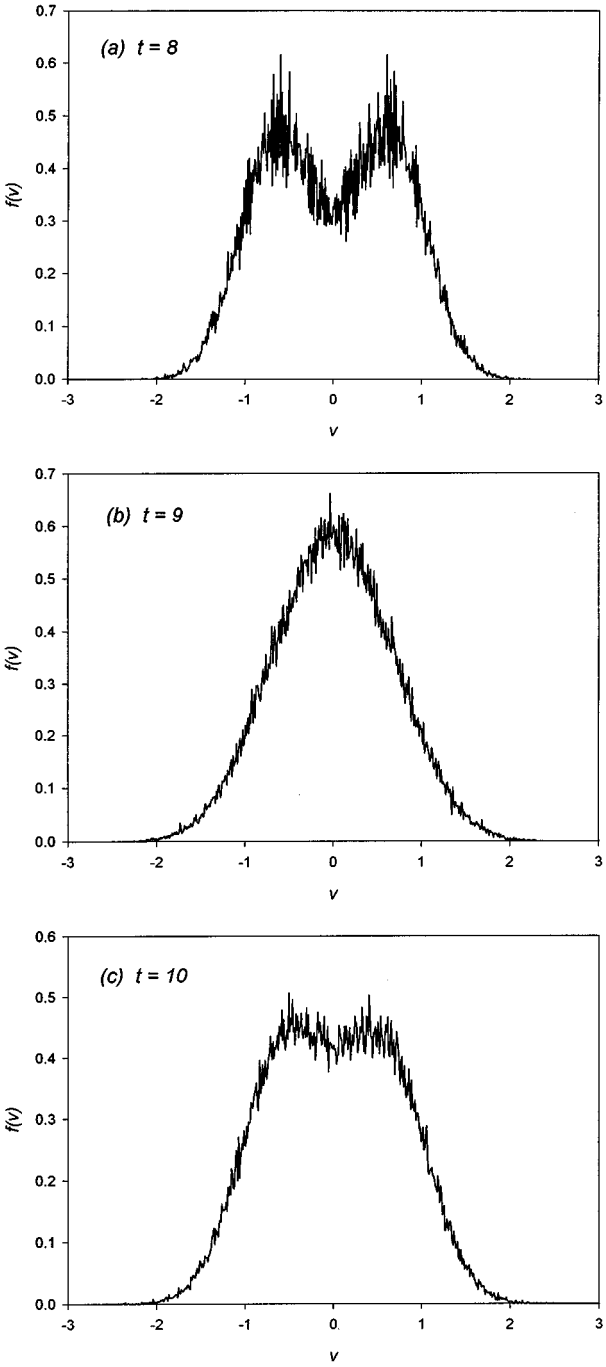

FIG. 2. Normalized velocity distribution of mass-1 particles in a binary mixture with a mass ratio of 2 at three different times. The unimodal-bimodal switching behavior described in Fig. 1 is again evident here. All quantities are dimensionless.

$$\sigma_1=\left(\frac{1\pm e^{-t/\tau}}{2}\right)^{1/2},\quad \sigma_a=\left(\frac{1\mp e^{-t/\tau}}{2a}\right)^{1/2}, \tag{20}$$

where the upper or the lower signs should be used when ξ^t is positive or negative, respectively.

Figure 3 shows computer simulation results for standard deviation of the mass-1 particles as a function of time with $a=2$. Note that according to Eqs. (20) two branches of data should be generated for each type of particles. For example, for mass-1 particles and after an even number of collisions, the standard deviation is given by the first of Eqs. (20) with

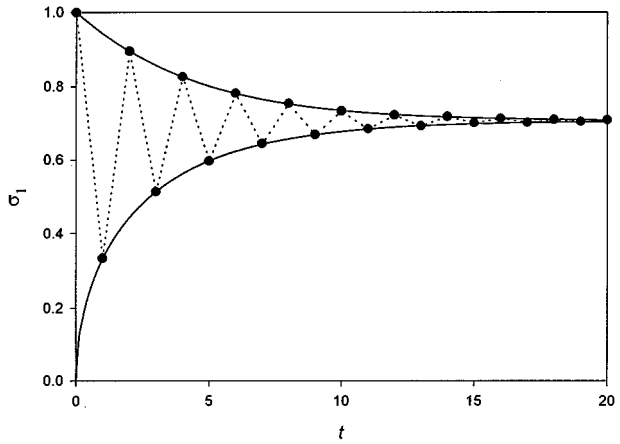

FIG. 3. Standard deviation of velocity distribution of mass-1 particles as a function of time in a binary mixture with a mass ratio of 2. Solid markers are computer simulation data. Continuous curves are from a least-squares fit of the relaxation time τ to the data at even times (upper branch). The same relaxation time (in this case $\tau=3.9824$) also generates curves that perfectly match both branches of data for the mass-a particles (not shown). All quantities are dimensionless.

the upper sign chosen, whereas for an odd number of collisions the lower sign should be used since for $a=2$, ξ is negative. However, when we fitted the relaxation time τ by a nonlinear least-square method to the even-time data for the mass-1 particles, it generated curves according to Eqs. (20) that perfectly matched the odd-time branch of the data for these particles as well as both branches of data for the mass-a particles. For all values of a that we examined, Eqs. (20) were in perfect agreement with the simulation results.

Figure 4 shows the dependence of relaxation time of the standard deviations of the distribution functions on the mass ratio. The simulational data are obtained by the method described above, whereas the theoretical results are from Eqs. (16) and (19). Again, the two are in perfect agreement. It may seem that including data in the region $a<1$ is redundant. However, we have included this region as we are using nonsymmetrical initial conditions for the two types of particles. As can be seen from this figure, the computer simulation data in the vicinity of $a=3+2\sqrt{2}$ become scattered and, in fact, impossible to obtain as this mass ratio is approached. This is due to the fact that the relaxation time for the standard deviations, but not the distributions themselves, becomes so small in this region that even after one collision the standard deviation has essentially completely relaxed. Consequently, in the vicinity of this mass ratio, collection of data with any reliability becomes literally impossible. The same difficulty is encountered near the other root, $a=3-2\sqrt{2}$. It is, however, interesting to note that for these values of the mass ratio, the distribution functions in Fourier space can be reduced to a simple closed form for all discrete values of $t>0$, as we have shown in Appendix B.

IV. CONCLUDING REMARKS

Perfect agreement between theory and computer simulation results in all cases and the coherency between them is indicative of the correctness and self-consistency in both ap-

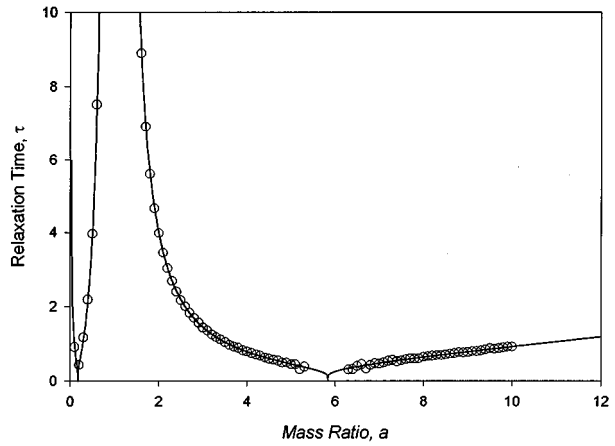

FIG. 4. Relaxation time (dimensionless) of the standard deviations of the velocity distributions in a binary mixture as a function of the mass ratio. Circles are the computer simulation data and the continuous curve is from the theory.

proaches and techniques. The simulation algorithm, not being molecular dynamical in nature and, therefore, not keeping track of the trajectories of the individual particles in the phase space, is extremely fast, accurate, and efficient. Only 100 particles of each type have produced results that are in perfect agreement with the theory, which is algorithm independent.

The molecular dynamic curve of Marro and Masoliver [5] for the relaxation time of the velocity distributions of the particles toward equilibrium is very broad and only suggests that the minimum of the relaxation time occurs roughly somewhere around the mass ratio of 5, as they have indicated. Furthermore, theoretical treatment of a system of one-dimensional two-component gas of ''soft'' (Maxwellian) point particles by Dickman [6] shows that the highest nonzero eigenvalue of the linearized collision operator indicates a minimum relaxation time at a mass ratio of $3+2\sqrt{2}\approx 5.8284$.

It is true that the relaxation time for the standard deviations is not necessarily the relaxation time of the distribution function toward a Gaussian, as there are infinitely many distribution functions with the same standard deviation as that of a Gaussian. In fact, Eqs. (16) and (19) show that for $a=3+2\sqrt{2}\approx 5.8284$ and $a=3-2\sqrt{2}\approx 0.1716$, the relaxation time of the standard deviation is zero. This means that for these choices of the mass ratio, the initial standard deviation of the distribution function is conserved. The relaxation of the actual distribution function of each type of particle toward a Gaussian, however, is finite and proceeds in a fashion similar to that depicted in Fig. 2. Nevertheless, since for all values of a different from the roots, $3\pm 2\sqrt{2}$, the distribution function as well as its standard deviation relaxes into a Maxwellian, therefore, by a limiting argument we can conclude that the relaxation time of the actual distribution function is, in fact, a minimum at these roots.

APPENDIX A

Taking the initial distributions for mass-1 and mass-a particles to be

$$f(v,0)=\tfrac{1}{2}[\delta(v-v_0)+\delta(v+v_0)], \quad g(v,0)=\delta(v), \tag{A1}$$

for which

$$F(k,0)=\cos(kv_0), \quad G(k,0)=1, \tag{A2}$$

it is clear that solutions will be products of cosines. From the double iterates

$$F(x,2j)=F(\alpha^2 x,2j-2)G^2(\alpha\gamma x,2j-2)F(\beta\gamma x,2j-2) \tag{A3}$$

and

$$G(x,2j)=G(\alpha^2 x,2j-2)F^2(\alpha\gamma x,2j-2)G(\beta\gamma x,2j-2), \tag{A4}$$

and assuming product solutions of the forms (9) and (10), and that $C(j,m)$ is independent of α, we obtain

$$\begin{aligned}\prod_{m=0}^{j} &\cos^{P(j,m)}[\alpha^{2j-2m}C(j,m)x]\\ &=\cos^{P(j-1,m)}[\alpha^{2j-2m-2}\alpha^2 C(j-1,m)x]\\ &\quad\times\prod_{m=0}^{j-2}\cos^{2Q(j-1,m)}[\alpha^{2j-2m-2}\alpha\gamma D(j-1,m)x]\\ &\quad\times\prod_{m=0}^{j-l}\cos^{P(j-1,m)}[\alpha^{2j-2m-2}\beta\gamma C(j-1,m)x].\end{aligned} \tag{A5}$$

Matching the exponents of the terms of frequency α^{2j} and α^{2j-2} on both sides, we find that

$$P(j,0)=1$$

and

$$C(j-1,1)=\beta\gamma C(j-1,0), \tag{A6}$$

from which we establish that

$$C(j,m)=(\beta\gamma)^m. \tag{A7}$$

Furthermore,

$$\alpha^{2j-2}C(j-1,1)=\alpha^{2j}\,\frac{\beta\gamma}{\alpha^2}=\alpha^{2j}\,\frac{\beta}{\alpha}\,D(j-1,0), \tag{A8}$$

and so,

$$D(j-1,0)=\frac{\beta}{\alpha}, \quad D(j,m)=\frac{\beta}{\alpha}\,(\beta\gamma)^m. \tag{A9}$$

By matching the exponents of the terms of frequency $\alpha^{2j-2p}(\beta\gamma)^p$ on both sides of Eq. (A5), as well as the analogous equation for the G distribution, we obtain

$$P(j,p)=P(j-1,p)+2Q(j-1,p-1)+P(j-1,p-1) \tag{A10}$$

and

$$Q(j,p)=Q(j-1,p)+2P(j-1,p-1)+Q(j-1,p-1), \tag{A11}$$

which can be iterated from their initial values at $j=0$, to the forms given by Eqs. (11).

APPENDIX B

For the special case of $a=3\pm2\sqrt{2}$ and the initial conditions given by Eqs. (A1), the exact solutions of $F(x,t)$,

$$F(x,2j)=\prod_{m=0}^{j}\cos^{\binom{2j}{2m}}[\alpha^{2j-2m}(\beta\gamma)^m x], \tag{B1}$$

simplify dramatically since for these values of a, we have $\beta\gamma=\alpha^2=\frac{1}{2}$, and the transformed distribution reduces to

$$\begin{aligned}F(x,2j)&=\prod_{m=0}^{j}\cos^{\binom{2j}{2m}}\left[\left(\frac{1}{2}\right)^{j-m}\left(\frac{1}{2}\right)^m x\right]\\&=\prod_{m=0}^{j}\cos^{\binom{2j}{2m}}\left(\frac{x}{2^j}\right)\\&=\cos^{\sum_{m=0}^{j}\binom{2j}{2m}}\frac{x}{2^j}=\left[\cos\left(\frac{x}{2^j}\right)\right]^{2^{2j-1}}.\end{aligned} \tag{B2}$$

For odd times, we have

$$F(x,2j+1)=F(\alpha x,2j)G(\gamma x,2j), \tag{B3}$$

and since $\alpha=1/\sqrt{2}$ and $\beta\gamma/\alpha=1/\sqrt{2}$, we find

$$F(x,2j+1)=\left[\cos\left(\frac{x}{\sqrt{2}^{2j+1}}\right)\right]^{2^{2j}}. \tag{B4}$$

Therefore, for generic $t>0$ (even or odd), we have

$$F(x,t)=\left[\cos\left(\frac{x}{\sqrt{2}^t}\right)\right]^{2^{t-1}},\quad G(x,t)=\left[\cos\left(\frac{x}{a\sqrt{2}^t}\right)\right]^{2^{t-1}}. \tag{B5}$$

Therefore, for the mass ratios $a=3\pm2\sqrt{2}$, corresponding to a minimum relaxation time, the distribution functions in Fourier space reduce to simple closed forms.

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