Homogeneous cooling and heating states of dilute soft-core gases under nonlinear drag

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Abstract. The temperature evolution of dilute soft inertial gas-solid suspensions is theoretically analyzed when the gas particles are influenced by a nonlinear drag force from a background fluid. The kinetic theory is extended to this system, and the time evolutions of the temperature and the kurtosis of the velocity distribution are derived. Molecular dynamics simulations are also performed to check the validity of the theory, and they show good agreement with the theoretical predictions.

1 Introduction

Anomalous relaxation processes have recently received much attention from physicists. The Mpemba effect [1], which is an example of this, is known as a process where an initially hotter liquid can be frozen faster than a colder liquid. Similar processes are widely observed in many situations. In particular, the recent theoretical studies on granular gases [2, 3] clarified that the appearance of the Mpemba effect in these systems relates to the non-Gaussianity of the velocity distribution function (VDF), which exists when the restitution coefficient is smaller than unity. Recently, Santos and Prados [4] considered the system where molecular particles are suspended by a background fluid, where the temperature determined from the kinetic energy of the molecules converges to the environmental temperature, which is determined from the background fluid. They reported that the Mpemba effect appears even in this elastic system when there exists a nonlinear effect of the drag from the background fluid. Their analysis shows that the VDF deviates from the Gaussian in the transient regime, and the magnitude of this deviation determines whether the Mpemba effect appears. However, the comparison of the theory with the simulation is not given in their paper, which means that the applicability of the theory should be clarified.

To this end, we consider the system where soft particles are suspended by the nonlinear background fluid. Recently, the steady-state rheology of this system under shear is theoretically analyzed in terms of the kinetic theory [5], where the softness of particles affects the rheological properties when the shear plays a dominant role with respect to the softness. In this paper, we consider the time evolution of this system under no external forces. We try to extend the theory for the hard-core system to this system, and derive a set of equations that describes the system.

The organization of this paper is as follows: In the next section, we briefly explain our model. Using this information, we extend the kinetic theory to this system in Sec. 3. The time evolutions of the temperature and the kurtosis of the VDF are derived from the kinetic theory. We solve the time evolution of them from the theory and the simulations in Secs. 4 and 5, respectively. In the last section, we discuss and conclude our results.

2 Model

The model of this study is explained in this section. We consider monodisperse particles in the three-dimensional system, where the mass and diameter are $m$ and $\sigma$, respectively. The interaction between particles is given by the harmonic potential [5]

$$U(r) = \frac{k}{2} \left( \sigma - r \right)^2 \Theta(\sigma - r),$$

where $r$ is the distance between particles, $k$ relates to the magnitude of the repulsive force, and $\Theta(x)$ is the step function. The scattering process for this potential is needed in the following calculation. The scattering angle $\chi$ is, in general, written by a function of the impact parameter $b$ and the relative speed $v$ between particles. The explicit form of this angle is presented in Ref. [5], which is also used in this paper.

These particles are distributed in the background fluid. If we assume that the effect from the background fluid is simply written by the random force and the kick back interaction, the equation of motion of the particles is described by the Langevin equation

$$m \frac{d\mathbf{v}_i}{dt} = \mathbf{F}_i - \zeta \mathbf{v}_i + \mathbf{\xi}_i,$$
We note that this model is a kind of idealized gas-solid suspension model [4–8]. Here, we should determine the form of the drag coefficient ζ. Let us consider a situation where the particles move in a collection of smaller particles (solvent) with the mass $m_b$, the diameter $\sigma_b$, and the density $n_b$ [4, 9]. The expression of ζ is derived when we choose a collision model between them. For simplicity, when the collisions between them are assumed to occur via hard-core, the following velocity dependence of ζ is obtained by solving a scattering problem (see Refs. [4, 9, 10]):

$$\zeta(v) = \frac{2}{3} n_b (\sigma + \sigma_b)^3 \frac{\sqrt{2\pi} m_b k_B T_{\text{env}}}{m + m_b} \left(1 + \frac{m_b}{10m} \frac{m v^2}{k_B T_{\text{env}}} \right).$$

(3)

where $T_{\text{env}}$ is the environmental temperature of the smaller particles. Of course, more complicated velocity dependences appear for dense systems. In this paper, however, we consider the system that the nonlinearity appears via the quadratic dependence as above, and for simplicity, we put the form of ζ given by Eq. (3) as [4, 10]

$$\zeta(v) = \zeta_0 \left(1 + \gamma \frac{m v^2}{k_B T_{\text{env}}} \right),$$

(4)

where $\zeta_0 \propto T_{\text{env}}^{1/2}$, and $\gamma \geq 0$ is assumed to be sufficiently smaller than unity. Therefore, ξ, is the random force which satisfies the following relations [11]:

\[
\langle \xi(t) \rangle = 0, \tag{5a}
\]

\[
\langle \xi_t(t) \xi_j(t') \rangle = 2m \zeta_0 \left[1 + \gamma \frac{m v^2}{k_B T_{\text{env}}} \right] T_{\text{env}} \delta_{ij} \delta_{tt}(t-t'), \tag{5b}
\]

where the bracket $\langle \rangle$ represents the ensemble average. Here, we introduce the dimensionless parameter $\xi_{\text{env}}$ which characterizes the magnitude of the drag as

$$\xi_{\text{env}} = \sqrt{\frac{k_B T_{\text{env}}}{m} \frac{1}{\zeta_0}}.$$  \hspace{1cm} (6)

The cooling (heating) process is observed when the initial temperature of the system is higher (lower) than the environmental temperature. In the next section, we derive the equations for the time evolution of the temperature and the non-Gaussianity in terms of the kinetic theory.

3 Kinetic theory

Using the above information, we extend the kinetic theory to this system. The Boltzmann equation corresponding to the Langevin equation (2) is given by

$$\frac{\partial}{\partial t} f(v) - \frac{\partial}{\partial v} \left[\zeta(v) \left( v + \frac{k_B T_{\text{env}}}{m} \right) f(v) \right] = J[v|f, f], \tag{7}
$$

where $f(v)$ is the VDF and $J[v|f, f]$ is the collision integral given by [6–8, 12]

$$J[v_1|f, f] = \int dv_2 \int dk \Theta(\sigma - |v_2 - k|) \times \left[ \sigma_v(\chi, v_{12}) f(v_1') f(v_2') - \sigma_v(\chi, v_{12}) f(v_1) f(v_2) \right], \tag{8}
$$

where $v_{12} = v_1 - v_2$ is the relative velocity, $\sigma_v$ is the scattering cross section which is determined from the scattering angle $\chi$, and $(v_1', v_2')$ are the post-collisional velocities satisfying

$$v_1' = v_1 - (v_{12} \cdot \hat{k}) \hat{k}, \hspace{0.5cm} v_2' = v_2 + (v_{12} \cdot \hat{k}) \hat{k}. \tag{9}
$$

We note that the softness of the particles appears in the integral (8).

By considering the second moment of Eq. (7) with respect to the velocity, the temperature evolution is given by [4]

$$\frac{dT}{dt} = -2\zeta_0 (T - T_{\text{env}}) \left(1 + 5 \frac{T}{T_{\text{env}}} \right) - 10 \zeta_0 \frac{T^2}{T_{\text{env}}} a_2. \tag{10}
$$

Here, we have introduced the kurtosis of the VDF as

$$a_2 = 3 \frac{\langle v^4 \rangle}{\langle v^2 \rangle^2} - 1. \tag{11}
$$

This is because the VDF deviates from the Gaussian when the temperature evolves [4].

Let us expand the dimensionless VDF $\tilde{f} \equiv (v^2 / m) f(v)$ in terms of the Sonine polynomials [4]

$$\tilde{f}(e) = \pi^{-3/2} \exp(-\frac{e^2}{2}) \left[1 + a_2 \left(\frac{e^2}{2} - \frac{5}{2} e^2 + 15 \pi \right)\right], \tag{12}
$$

with the thermal velocity $v_T = \sqrt{2T/m}$ and the dimensionless velocity $e \equiv v / v_T$, where we only consider the lowest order of $a_2$ in Eq. (12). It is noted that this coefficient $a_2$ is consistent with Eq. (11). We assume that the coefficient $a_2$ is sufficiently small with respect to unity, which will be checked later.

Using the dimensionless form of the VDF and the Sonine expansion (12), Eq. (7) can be rewritten as

$$\frac{\partial}{\partial t} \tilde{f}(e) - \frac{\partial}{\partial e} \left[ \frac{1}{2T} \frac{\partial T}{\partial e} \tilde{f} + \zeta_0 \left(1 + \frac{2T}{T_{\text{env}}} \right) \right] \times \left(\tilde{e} + \frac{T_{\text{env}}}{2T} \frac{\partial T}{\partial e} \right) \tilde{f}(e) = \nu_{\text{env}} \sqrt{\frac{T_{\text{env}}}{T}} J[e|\tilde{f}, \tilde{f}], \tag{13}
$$

with the collision frequency

$$\nu_{\text{env}} = n \sigma^2 \sqrt{\frac{2k_B T_{\text{env}}}{m}}. \tag{14}
$$

Here, $n$ is the number density of the system.

For further calculation, let us introduce the fourth moment of the collision integral $\mu_4$ [13]:

$$\mu_4 = \frac{\sqrt{\pi}}{4} a_2 \int_0^\infty dc \int_0^\infty db^* b^* c^3 \sin^2 \chi \exp \left( \frac{-c^2}{2} \right), \tag{15}
$$

with $b^* \equiv b / \sqrt{\sigma}$. We note that the fourth collisional moment $\mu_4$ relates to the Omega integral [5, 12]

$$\Omega_{4,\beta}(T) = \sqrt{\frac{k_B T}{\pi m}} \int_0^\infty dy \exp(-y^2) \mathcal{Q}(2y \sqrt{\frac{k_B T}{m}}), \tag{16}
$$

as

$$\mu_4(T') = 4 \sqrt{\frac{\pi a_2}{\Omega_{2,2}(T')}} \equiv 4 \sqrt{\frac{\pi a_2 \Omega_{2,2}(T')}{\Omega_{2,2}(T')}}, \tag{17}
$$

\]
where \( Q(v) \) is defined by

\[
Q(v) = 2\pi \int_0^\infty db \, b \left[ 1 - \cos(kv) \right].
\]

Here, \( T^* = k_B T/(kr^2) \) is the dimensionless temperature, and \( \Omega^{(ini)}_2(T) = 2\pi^2/(k_B T/m)^{1/2} \) is the hard-core limit of \( \Omega_2(T) \). We note that \( \Omega^{(ini)}_2(T^*) \) behaves as \( 1 - \Omega^{(ini)}_2(T^*) \propto T^{-1/2} \) for \( \Omega^{(ini)}_2(T) \approx 1 \) and \( \Omega^{(init)}_2(T^*) \approx T^{-1} \) in the low temperature regime.

\( T^{-1/2} \) and \( \Omega^{(ini)}_2(T^*) \) at high temperature regimes, respectively, as shown in Fig. 1 (see also Fig. 5 of Ref. [5]). For practical calculations, we prepare a numerical table of \( \Omega^{(ini)}_2(T^*) \) for \( k_B T/(kr^2) = 10^{10} \) (\( n \) is an integer) in the range \( 10^{-10} \leq k_B T/(kr^2) \leq 10^6 \) and interpolate the value for any \( T \).

### 4 Homogeneous cooling and heating states

**Figure 1.** Temperature dependence of the dimensionless Omega integral \( \Omega^{(ini)}_2(T^*) \), where we have introduced \( T^* = k_B T/(kr^2) \) and \( \Omega^{(ini)}_2(T^*) = \Omega^{(ini)}_2(T)/\Omega^{(ini)}_2(T^*) \). The triangle represents the slope of \( 1 - \Omega^{(ini)}_2(T^*) \) in the low temperature regime.

In this section, let us solve the time evolution of the system. So far, we assume that the environmental temperature is fixed. However, we can control the value of the environmental temperature at \( t = 0 \) as shown in Fig. 2. We introduce two environmental temperatures \( T_{\text{env}}^{(ini)} \) and \( T_{\text{env}}^{(t)} \), which correspond to \( t < 0 \) and \( t \geq 0 \), respectively. Here, the system is in equilibrium with the initial parameter \( \xi^{(ini)}_{\text{env}} = (k_B T^{(ini)}_{\text{env}}/(m)^{1/2}/(k_B T^{(ini)}_{\text{env}}/(m)^{1/2}/(\sigma\xi_0)) \) for \( t < 0 \), and we discontinuously change the value of \( \xi_{\text{env}} \) to \( \xi_{\text{env}}^{(t)} = (k_B T^{(t)}_{\text{env}}/(m)^{1/2}/(\sigma\xi_0)) \) at \( t = 0 \). Here, we choose the values of the softness as \( k^* \equiv k/(m\xi_0^2) = 10^4, 10^6, \) and \( 10^{-2} \). In this paper, we fix \( \xi^{(ini)}_{\text{env}} = 1.0 \) and \( \gamma = 0.1 \) for simplicity.

To describe the dynamics of the system, let us introduce the following dimensionless parameters:

\[
\theta = \frac{T_{\text{env}}^{(ini)}}{T_{\text{env}}^{(t)}}, \quad \theta_0 = \frac{T_{\text{env}}^{(ini)}}{T_{\text{env}}^{(t)}}, \quad \gamma = \gamma_0 t.
\]

From Eqs. (10) and (13), we obtain a set of equations as

\[
\frac{d\xi}{d\tau} = -2(\theta - 1)(1 + 5\theta + 10\theta^2)\xi,
\]

\[
\frac{d\gamma}{d\tau} = -8\gamma(\theta - 1) - \frac{4}{\theta} - 8\gamma + 44\gamma\theta + \frac{64}{5\sqrt{\pi}}\phi_0 \sqrt{T_{\text{env}}^{(ini)}} \frac{1}{(k_B T)^{1/2}} \xi^2.
\]

This set of equations is equivalent to that reported in Ref. [4] when we consider the hard-core limit. We note that the expression of the time evolution of the temperature \( (20a) \) is the same with that for hard-core gases, which is because the symmetric property of the second moment of the collision integral is unchanged even when we consider the soft-core gases. This means that the softness affects the system only via the evolution of the non-Gaussianity \( \alpha_2 \) (20b). If we can ignore \( \alpha_2 \) in Eq. (20a), the time evolution of the dimensionless temperature is explicitly given by

\[
\theta_{\alpha_2 = 0}(t) = 1 + \frac{(1 + 5\gamma)(\theta_0 - 1)}{(1 + 5\gamma)(\phi_0)^2 + 5\gamma(\theta_0 - 1)}.
\]

It should be noted that, as explained in the above, this expression is independent of the potential (1).

**Figure 2.** Schematic of the protocol. The environmental temperature is set as \( T_{\text{env}} = T_{\text{env}}^{(ini)} \) for \( t < 0 \), and is changed to \( T_{\text{env}} = T_{\text{env}}^{(t)} \) at \( t = 0 \). Here, the case for \( T_{\text{env}}^{(ini)} > T_{\text{env}}^{(t)} \) is shown.

**Figure 3.** Time evolutions of the dimensionless temperature from the theory (20a) for \( \theta_0 = 2 \) (solid line) and 0.5 (dashed line) when we choose the softness of the particles as \( k^* \equiv k/(m\xi_0^2) = 10^4, 10^6, \) and \( 10^{-2} \). Here, the difference between lines is almost invisible. The symbols represent the simulation results. We note that the error bars are smaller than the symbols.

Let us solve the set of equations (20) with the initial condition \( \theta(0) = \theta_0 \). It should be noted that \( \alpha_2(0) = 0 \) is satisfied because the system is in equilibrium for \( t < 0 \). Figures 3 and 4 show the time evolutions of \( \theta \) and \( \alpha_2 \) with \( \theta_0 = 2 \) and 0.5, respectively. We find that the time evolutions are almost independent of the softness of the particles. We also find that the transient process of the temperature is monotonic, independent of cooling and heating processes. Here, the magnitude of \( \alpha_2 \) is always smaller than
the temperature (20a) is the same as that for the hard-core
explained previously, the equation for the time evolution of
whose interparticle interaction is given by Eq. (1). As ex-
examined in terms of the definition (11).

5 Molecular dynamics simulations

In this section, let us check the validity of the theory by per-
We prepare \( N = 10^3 \) particles in the cubic box, where
the linear length of the system is fixed as \( L = 37.1\sigma \).
Here, the correspondingly packing fraction becomes \( \varphi = (\pi/6)N\sigma^3/L^3 = 1.0 \times 10^{-2} \). We also adopt the periodic
boundary condition in all directions. We numerically solve the
equation of motion (2) for each particle with the di-

development model of the system is the soft particles
ensemble average of the results. Here, the kurtosis is evalu-
expressed in terms of the definition (11).

As shown in Figs. 3 and 4, the simulation results well
reproduce the theoretical prediction of the time evolutions of
the dimensionless temperature and the kurtosis of the
VDF. Even in the simulations, the measured value of \( \alpha_2 \)
is much smaller than unity, which suggests the validity of
the assumption used to derive the set of equations. We also
note that the dependence of the evolutions on the softness
is small in the simulations.

6 Discussion and Conclusion

In this paper, the system consists of the soft particles
whose interparticle interaction is given by Eq. (1). As ex-
plained previously, the equation for the time evolution of
the temperature (20a) is the same as that for the hard-core
system reported in Ref. [4]. The difference between hard
and soft-core systems appears only from \( \alpha_2 \), but this effect
is sufficiently small because the magnitude of \( \alpha_2 \) is smaller
than unity as shown in Fig. 4.

The Mpemba effect is observed when one controls the
initial non-Gaussianity \( \alpha_2 \) in the hard-core limit [4]. To
check the realization of this in our model is important, but
this is our future work. There, we should consider how
we control the initial non-Gaussianity \( \alpha_2 \) is not simple in
experiments or simulations.

In this paper, we have investigated the time evolution
of the temperature when molecular gases are influenced by
the nonlinear drag. We have derived the evolutions of the
temperature and the non-Gaussianity of the velocity distri-
bution function from the kinetic theory. We have also per-
formed the molecular dynamics simulations, and we have
confirmed that the numerical results are well reproduced
by those from the kinetic theory for the wide range of the
softness of the particles.

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