Intermediate Regimes in Granular Brownian Motion:
Superdiffusion and Subdiffusion

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Brownian motion in a granular gas in a homogeneous cooling state is studied theoretically and by means of molecular dynamics. We use the simplest first-principles model for the impact-velocity dependent restitution coefficient, as it follows for the model of viscoelastic spheres. We reveal that for a wide range of initial conditions the ratio of granular temperatures of Brownian and bath particles demonstrates complicated nonmonotonic behavior, which results in a transition between different regimes of Brownian dynamics: It starts from the ballistic motion, switches later to a superballistic one, and turns at still later times into subdiffusion; eventually normal diffusion is achieved. Our theory agrees very well with the molecular dynamics results, although extreme computational costs prevented us from detecting the final diffusion regime. Qualitatively, the reported intermediate diffusion regimes are generic for granular gases with any realistic dependence of the restitution coefficient on the impact velocity.

Introduction.—Brownian motion is a fundamental process in nature which takes place on very different time and length scales [1]. In its classical formulation it implies a random motion of a big (Brownian) particle driven by thermal motion of much smaller bath particles. The mean-square displacement of Brownian particles grows with time as $\langle R_B^2 \rangle \sim t^\beta$, with $\beta = 1$ for normal diffusion. Anomalous diffusion with $\beta > 1$ (superdiffusion) and $\beta < 1$ (subdiffusion) has been found in a variety of systems [2] ranging from supercooled and glass forming liquids, e.g., [3], to surfaces [4], biological [5] and granular [6] systems; usually a few diffusion regimes with a crossover between them are observed. Mechanisms of anomalous diffusion are seemingly very different— macromolecular crowding in solutions and cells [5], caging in glassy liquids [3], trapping in a random potential [4], etc. Nevertheless, one can possibly infer an important common feature—anomalous diffusion always arises due to interplay of different basic dynamics in a system: For instance, a (fast) hopping dynamics in glass forming liquids interferes with a (slow) dynamics of structural rearrangements, resulting in subdiffusion. Moreover, anomalous diffusion in most of the systems manifests as an intermediate regime, which transforms asymptotically into normal diffusion, e.g., Refs. [2–4].

In the present Letter we report intermediate anomalous diffusion in granular systems, where particles interact with dissipative forces. Although the microscopic mechanism of this phenomenon is novel and related to inelastic collisions, it again results, as it is shown below, from the interplay of different dynamics represented by evolution of two granular temperatures.

Granular Brownian motion demonstrates a large variety of new surprising phenomena, among which is the violation of energy equipartition in a mixture of massive and light particles [7–9]: Both granular temperatures of Brownian (T_B) and bath (T) particles decrease in a force-free granular gas, while their ratio rapidly relaxes to a steady-state value $(T_B/T)_{s.s.} > 1$. Moreover, $(T_B/T)_{s.s.}$ increases with increasing inelasticity and the mass ratio m_B/m of Brownian (m_B) and bath (m) particles [7,8]. It has been also shown that Brownian motion in these systems may change qualitatively—from diffusive to a ballistic one, depending on the steady state value of $\varphi = (T_B m)/(T m_B)$ [10]. Surprisingly, one can treat this phenomena as a *phase transition* with the *order parameter* φ [10], which, however, is not observed as a real process, since the steady state φ is constant.

To date, most theoretical studies of Brownian motion are done with the assumption of a constant restitution coefficient $\varepsilon = g'/g$ [7], where g and g' are, respectively, the normal components of the relative interparticle velocities before and after a collision. The simplifying hypothesis of constant ε, however, contradicts experimental results, which indicate that ε does depend on g and that $\varepsilon(g)$ is a decreasing function of the impact velocity [11]; it is not also consistent with a rigorous theoretical analysis [7]. The impact-velocity dependence of the restitution coefficient may, however, crucially change the behavior of a granular system, e.g., Ref. [12]. In particular, it has been shown that in a gas of viscoelastic particles, where the impact-velocity dependence of ε stems from the simplest first-principles model [13], clusters and vortices manifest as transient phenomena [14], in sharp contrast with the case of a constant ε [15]. Furthermore, in a mixture of massive and light particles, the temperature ratio T_B/T, as well as φ, evolve with time in a homogeneous cooling state (HCS) [16], again in a contrast with the case of $\varepsilon = $ const. Therefore, one can expect that in a granular gas of viscoelastic particles, where

φ varies with time, the phase transition between different regimes of Brownian motion may occur during the gas evolution as a real physical process.

We analyze granular Brownian motion in a gas of visco-elastic particles in a HCS—the basic state of a force-free granular gas by means of molecular dynamics (MD), and theoretically. We have revealed a sequence of new diffusive regimes for a Brownian particle—superballistic motion (superdiffusion), which follows after the ballistic one and transforms then to subdiffusion. Eventually, normal diffusion is observed.

MD simulations.—We perform event-driven simulations [17] for a force-free system, using $N = 64\,000$ bath particles of mass m and diameter σ and one Brownian particle of mass $m_B \gg m$ and diameter σ_B (for simplicity we take $\sigma_B = \sigma$) in a cube of length $L = 130\sigma$ with periodic boundary conditions. The number density of the bath particles was $n = N\pi\sigma^3/(6L^3) \simeq 0.015$. The reported results correspond to averages over 20 or 50 independent runs, depending on the initial conditions.

In our simulations we use the restitution coefficient, as it follows for the model of viscoelastic particles [13,18]:

$$\varepsilon = 1 + \sum_{k=1}^{\infty} C_k \delta^{k/2} (2u)^{k/20} w^{k/10}. \tag{1}$$

Here, C_k's are numerical coefficients, which have been computed up to $k = 20$ [18] and δ quantifies the dissipative interactions. Equation (1) describes both types of collisions—between the Brownian particle and a bath particle and between the bath particles themselves. In the former case, $w = |(\vec{c}_{Bi} \cdot \vec{e})|$, where $\vec{c}_{Bi} = \vec{v}_{Bi}/v_T$, with $\vec{v}_{Bi} = \vec{v}_B - \vec{v}_i$ being the relative velocity of the Brownian ($\vec{v}_B$) and the ith bath ($\vec{v}_i$) particle, $v_T = \sqrt{2T/m}$ is the thermal velocity of the bath particles, and $\vec{e}$ is the unit vector, joining the particles' centers at the collision instant. In the latter case $w = |(\vec{c}_{ij} \cdot \vec{e})|$, where $\vec{c}_{ij} = \vec{v}_{ij}/v_T$, with $\vec{v}_{ij} = \vec{v}_i - \vec{v}_j$ being the relative velocity of the colliding ith and jth bath particles. For both types of collisions we use for simplicity the same $\delta = 0.1$. The quantity $u(t) = T(t)/T(0)$ is the dimensionless temperature of the bath at time t, and granular temperatures are defined as usual, $3T/2 = \langle m\vec{v}^2/2 \rangle$ and $3T_B/2 = \langle m_B \vec{v}_B^2/2 \rangle$. The results of the MD simulation are presented in Fig. 1.

Theory.—Since the concentration of Brownian particles is much smaller than that of the bath particles, we assume that Brownian particles do not affect evolution of the bath [7]: In a force-free gas T gradually decreases, due to dissipative collisions, with the cooling coefficient $\xi(t) = -(dT/dt)/T(t)$. As temperature T tends to zero, ε tends to unity, and all collisions tend to be elastic [7].

The evolution of Brownian particles may be described using the Boltzmann equation, $\dot{f}_B(\vec{v}_B, t) = I(f_B, f)$, for the velocity distribution function, $f_B(\vec{v}_B, t)$, e.g., Ref. [7]; the
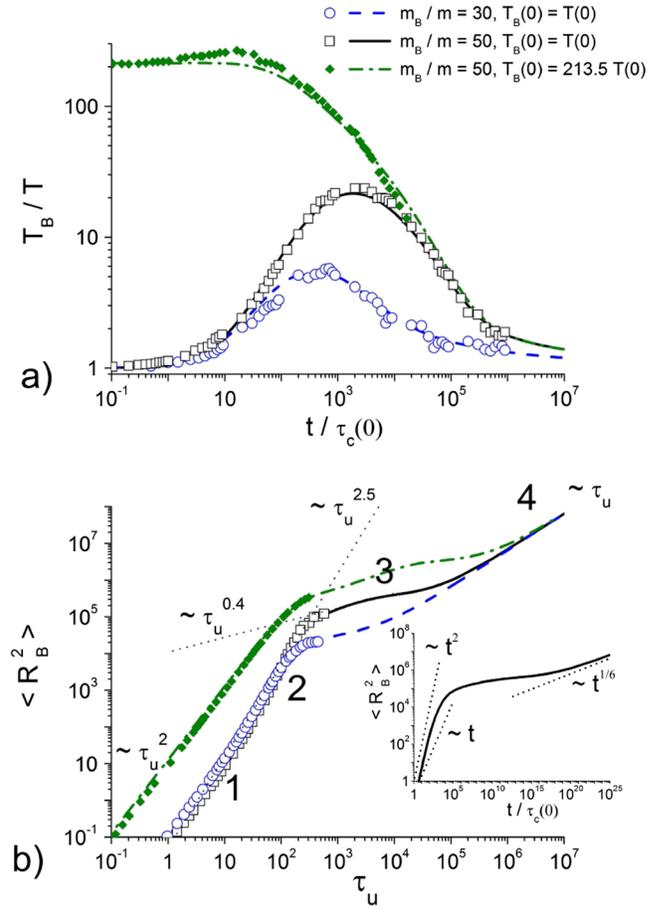
FIG. 1 (color online).   (a) Time dependence of the temperature ratio of Brownian (T_B) and bath (T) particles. (b) The mean-square displacement of Brownian particles $\langle R_B^2 \rangle$ as the function of the re-scaled time τ_u and the laboratory time t (inset). Lines—theory, symbols—MD data. Numbers indicate different regimes: 1—ballistic motion, $\langle R_B^2 \rangle \sim \tau_u^2$; 2—superballistic regime (superdiffusion), $\langle R_B^2 \rangle \sim \tau_u^\beta$ with $\beta > 2$; 3—subdiffusion, $\langle R_B^2 \rangle \sim \tau_u^\beta$ with $\beta < 1$; 4—normal diffusion $\langle R_B^2 \rangle \sim \tau_u$.

collision integral $I(f_B, f)$ accounts for the alteration of $f_B(\vec{v}_B, t)$ in pairwise collisions with the collision rule,

$$\vec{v}_B' = \vec{v}_B - (1 + \varepsilon)\mu(\vec{v}_{Bi} \cdot \vec{e})\vec{e}. \tag{2}$$

Here, $\vec{v}_B'$ is the velocity of a Brownian particle after a collision and $\mu \equiv \frac{m}{m_B + m}$. Solving the Boltzmann equation with the standard technique, e.g., Ref. [7], one obtains the distribution function f_B. Brownian dynamics may be described with very compact notations if the pseudo-Liouville operator $\hat{L}$ is used [7]:

$$\dot{\vec{v}}_B = \hat{L}\vec{v}_B = \hat{L}_0\vec{v}_B + \sum_i \hat{T}_{Bi}\vec{v}_B, \tag{3}$$

where $\hat{L}_0 = \vec{v}_B \cdot \vec{\nabla}_{\vec{r}_B}$ describes the free streaming and

$$\hat{T}_{Bi} = \sigma_0^2 \int d\vec{e}\, \Theta(-(\vec{v}_{Bi} \cdot \vec{e}))|\vec{v}_{Bi} \cdot \vec{e}|\delta(\vec{r}_{Bi} - \vec{e}\sigma_0)(\hat{b}_{Bi} - 1)$$

the binary collisions of particles. The radius vector $\vec{r}_{Bi}$ in the above equation joins centers of Brownian and bath particle, $\sigma_0 = (\sigma_B + \sigma)/2$ and the operator $\hat{b}_{Bi}$ acts on the velocities, as $\hat{b}_{Bi}\vec{v}_B = \vec{v}'_B$ with the collision rule (2).

Taking into account that $\vec{R}_B(t) = \int_0^t \vec{v}_B(t_1)dt_1$, the mean-square displacement of Brownian particles reads in terms of the velocity autocorrelation function: $\langle R_B^2(t) \rangle = \int_0^t dt_1 \int_0^t dt_2 \langle \vec{v}_B(t_1)\vec{v}_B(t_2) \rangle$. We introduce the reduced time τ_B, defined as $d\tau_B = dt\sqrt{T_B(t)/T_B(0)}/\tau_c(0)$, where $\tau_c^{-1}(t) = 4\sqrt{\pi}\sigma^2 g_2(\sigma)n\sqrt{T(t)/m}$ is the mean collision time of bath particles, with $g_2(\sigma)$ being the contact value of the pair correlation function [7]. In this time scale one deals with the reduced velocities, $\vec{c}_B = \vec{v}_B/\sqrt{2T_B/m_B}$, and the granular temperature of the Brownian particles remains constant. Hence, the decay of the (reduced) velocity correlation function occurs similarly, as in equilibrium gases: A particle loses memory of its initial velocity in random collisions; in dilute gases the velocity correlation function is exponential [19]; therefore, we approximate

$$\langle \vec{c}_B[\tau_B(t_1)]\vec{c}_B[\tau_B(t_2)] \rangle = \langle c_B^2 \rangle \exp\left[-\frac{\tau_B(t_2) - \tau_B(t_1)}{\hat{\tau}_{vB}(t_1)} \right],$$
(4)

where $\langle c_B^2 \rangle = 3/2$ and $\hat{\tau}_{vB}$ is the (reduced) velocity relaxation time. Exploiting the above form of the correlation function, we obtain the mean-square displacement

$$\langle R_B^2(t) \rangle = 6 \int_0^t dt_1 D_B(t_1)\left[1 - \exp\left(-\frac{\tau_B(t) - \tau_B(t_1)}{\hat{\tau}_{vB}(t_1)} \right) \right].$$

Here, $D_B = T_B(t)\tau_{vB}(t)/m_B$ is the time-dependent diffusion coefficient of a Brownian particle, expressed in terms of $\tau_{vB}(t) = \hat{\tau}_{vB}(t)\tau_c(0)/\sqrt{T_B(t)/T_B(0)}$—the velocity relaxation time in laboratory time units. The reduced relaxation time $\hat{\tau}_{vB}(t)$ in the exponential function in Eq. (4) may be easily found from its time derivative at $t_1 \to t_2$, yielding [7,20]

$$\tau_{vB}^{-1} = -(N-1)\frac{\langle \vec{v}_b \hat{T}_{Bi}\vec{v}_b \rangle}{\langle \vec{v}_b^2 \rangle} - \frac{1}{2}\xi_B,$$
(5)

with the cooling coefficient of Brownian particles

$$\xi_B = -\frac{1}{T_B}\frac{dT_B}{dt} = -(N-1)\frac{\langle \hat{T}_{Bi}v_B^2 \rangle}{\langle v_B^2 \rangle}.$$
(6)

Performing the averaging in Eqs. (5) and (6), we ignore, for simplicity, deviations of the velocity distribution function from the Maxwellian [12]; it may be, however, shown that their impact on the calculated quantities is negligible. Hence, we obtain the velocity relaxation time

$$\frac{\tau_{vB}^{-1}(t)}{\tau_c^{-1}(0)} = \sqrt{\frac{8u}{9}}\frac{\mu^2(1+\varphi)^{3/2}}{\varphi}\frac{\sigma_0^2 g_2(\sigma_0)}{\sigma^2 g_2(\sigma)}\left[1 + \frac{1}{2}\sum_{i=2}^{\infty} A_i B_i \right]$$

and the cooling coefficient of Brownian particles:

$$\xi_B(t) = 2\tau_c^{-1}(0)\sqrt{\frac{8u}{9}}(1+\varphi)^{1/2}\mu\frac{\sigma_0^2 g_2(\sigma_0)}{\sigma^2 g_2(\sigma)}$$
$$\times \left[1 - \mu\frac{1+\varphi}{\varphi} + \sum_{i=2}^{\infty} B_i\left(C_i - \frac{1}{2}\mu\frac{1+\varphi}{\varphi}A_i \right) \right],$$

where $A_i = 4C_i + \sum_{j+k=i} C_j C_k$ are pure numbers and

$$B_i(t) = \delta^{i/2}[2u(t)]^{i/20}[1 + \varphi(t)]^{i/20}\left(\frac{20i+i^2}{800} \right)\Gamma\left(\frac{i}{20} \right)$$

with $\Gamma(x)$ being the Gamma function.

The temperature of the Brownian particles T_B can be found from the equation $dT_B(t)/dt = -\xi_B(t)T_B(t)$, while the temperature $T(t)$ and the mean-squared displacement $\langle R^2(t) \rangle$ of the bath particles—from the above results using the substitute $m_B \to m$ and $\sigma_B \to \sigma$.

Results and discussion.—The theoretical predictions are compared with the simulation data in Fig. 1. First we consider the case of the initial energy equipartition, $T_B(0) = T(0) = 400/3$. The time dependence of the ratio T_B/T demonstrates here a complicated nonmonotonic behavior: It initially increases, reaches a maximum, and then decreases, tending eventually to unity, Fig. 1(a). This is in sharp contrast with the case of a constant ε, where T_B/T rapidly relaxes to a steady-state value. One can explain this effect as follows. From the collision rules [see, e.g., Eq. (2)], the ratio of energy losses of Brownian (ΔE_B) and bath (ΔE) particles at a collision scales as $\Delta E_B/\Delta E \sim v_B/v_i \sim \sqrt{(T_Bm)/(Tm_B)}$. Initially, $\Delta E_B \ll \Delta E$, since $T_B = T$ and $m_B \gg m$; therefore Brownian particles cool down significantly slower than the bath particles and the temperature ratio T_B/T increases. One can call this effect as a *retarded cooling*, which may be also understood as a tendency of a system to reach the ratio of $T_B/T > 1$, corresponding to the steady-state value $(T_B/T)_{s.s.} > 1$ of a gas with the respective constant ε. The larger the mass ratio the more pronounced the effect [Fig. 1(a)]. In the course of time the temperature ratio T_B/T gets so large that ΔE_B and ΔE become comparable; the granular temperatures start then to equilibrate. At this stage T_B/T decreases—Brownian particles cool faster than the bath particles and one can call this regime as *accelerated cooling*. Again, this effect may be understood, noticing that the ratio of $(T_B/T)_{s.s.} > 1$ is smaller for larger ε and that the effective restitution coefficient grows as the gas cools down; see Eq. (1). For very large times ε tends to unity, the system becomes elastic and the energy equipartition is achieved. This complicated temperature dependence results in transition between different diffusion regimes, which may be most clearly seen using the rescaled time τ_u, defined as $d\tau_u = dt\sqrt{u(t)}/\tau_c(0)$. In this time scale the average velocity of the bath particles is constant and they move, as in an equilibrium molecular gas, that is, ballistically, $\langle R^2 \rangle \sim \tau_u^2$, for $\tau_u \sim 1$ and diffusively, $\langle R^2 \rangle \sim \tau_u$, for $\tau_u \gg 1$ [7,20]. Brownian motion demonstrates, however, four different regimes—ballistic [regime 1 in Fig. 1(b)],

superballistic motion or superdiffusion (regime 2), subdiffusion (regime 3), and normal diffusion (regime 4). Physically, the superballistic motion, which starts after a short ballistic regime corresponds to the retarded cooling, while the subsequent subdiffusion—to the accelerated cooling. In the former case Brownian particles get hotter and hotter with respect to the surrounding gas and $\langle R_B^2 \rangle$ grows with time faster than for normal diffusion; in the latter case, Brownian particles cool more rapidly than the gas, so that $\langle R_B^2 \rangle$ grows with time slower. The duration of the subdiffusion regime increases with the mass ratio m_B/m and may be very long. Asymptotically, at $\tau_u \to \infty$, the system returns to the equipartition, demonstrating the normal diffusion, $\langle R_B^2 \rangle \sim \tau_u$.

The respective transition between diffusion regimes is also seen for the laboratory time t [Fig. 1(b), inset], where the normal diffusion is described by $\langle R_B^2 \rangle \sim t^{1/6}$, as it follows for the gas of viscoelastic particles [7,20]. If we consider the time scale τ_B, where T_B keeps constant, the superballistic motion does not appear; all three other diffusion regimes are, nevertheless, present.

Since superballistic motion is caused by the retarded cooling, it is not observed if T_B/T does not increase. This happens for initial conditions, when the ratio T_B/T is already large, or more precisely, when T_B/T exceeds some threshold, estimated as the ratio $(T_B/T)_{s.s.}$ for a gas with a constant ε, equal to the effective restitution coefficient ε_{eff} for a gas of viscoelastic particles at $t = 0$. In our case, Eq. (1) with $u(0) = 1$ and $\langle w \rangle = 4/\sqrt{2\pi}$ yields $\varepsilon_{\text{eff}}(0) = 0.876$ and $T_B(0)/T(0) = (T_B/T)_{s.s.} = 213.5$. Hence, this initial temperature ratio delimits two incipient diffusion regimes: For $T_B(0)/T(0) < 213.5$ the ballistic and then superballistic motion takes place, while otherwise only ballistic regime is observed, Fig. 1(b). Interestingly, the ballistic motion in the latter case lasts for significantly longer time, than for normal diffusion; this follows from the fact that trajectories of heavy Brownian particles are almost not affected by the much colder bath of light particles. The subsequent subdiffusion and normal diffusion persist independently on initial conditions; see Fig. 1(b). This is the universal feature of Brownian motion in a gas of viscoelastic particles. As it follows from Fig. 1, a very good agreement between our theory and simulation data are observed for evolution of temperature and mean-square displacement for intermediate ballistic, superballistic, and the onset of subdiffusive regimes; due to extreme computational costs we failed to detect numerically the final regime of normal diffusion.

Conclusion.—We have studied Brownian motion in a force-free granular gas, composed of particles interacting with an impact-velocity dependent restitution coefficient $\varepsilon(g)$, as it follows from the model of viscoelastic spheres. We have revealed that for a wide range of initial conditions the ratio of granular temperatures of massive and light particles T_B/T demonstrates complicated nonmonotonic dependence on time as the system evolves in the HCS.

Somewhat similar to other systems with anomalous diffusion, this interplay of different dynamics of Brownian and bath particles, quantified by their temperatures, gives rise to a sequence of intermediate diffusive regimes in granular Brownian motion: At early times the ballistic motion is observed, which alters then to the superballistic one (for nonmonotonic evolution of T_B/T). At still later times the opposite regime of subdiffusion—motion, slower than normal diffusion, always takes place; it lasts for a relatively long time and tends asymptotically to normal diffusion. Qualitatively, these features of granular Brownian motion are not specific to a particular model of $\varepsilon(g)$, but generic for granular systems with any realistic restitution coefficient that increases with decreasing impact velocity.

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