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Quantifying non-ergodic dynamics of force-free granular gases

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Brownian motion is ergodic in the Boltzmann–Khinchin sense that long time averages of physical observables such as the mean squared displacement provide the same information as the corresponding ensemble average, even at out-of-equilibrium conditions. This property is the fundamental prerequisite for single particle tracking and its analysis in simple liquids. We study analytically and by event-driven molecular dynamics simulations the dynamics of force-free cooling granular gases and reveal a violation of ergodicity in this Boltzmann–Khinchin sense as well as distinct ageing of the system. Such granular gases comprise materials such as dilute gases of stones, sand, various types of powders, or large molecules, and their mixtures are ubiquitous in Nature and technology, in particular in Space. We treat—depending on the physical-chemical properties of the inter-particle interaction upon their pair collisions—both a constant and a velocity-dependent (viscoelastic) restitution coefficient ε . Moreover we compare the granular gas dynamics with an effective single particle stochastic model based on an underdamped Langevin equation with time dependent diffusivity. We find that both models share the same behaviour of the ensemble mean squared displacement (MSD) and the velocity correlations in the limit of weak dissipation. Qualitatively, the reported non-ergodic behaviour is generic for granular gases with any realistic dependence of ε on the impact velocity of particles.

1. Introduction

Granular materials such as sand or different types of powders are ubiquitous in Nature and technology, for instance, in the cosmetic, food, and building industries.¹ Rarefied granular systems, in which the distance between particles exceeds their size, are called granular gases.^{2–4} Such granular gases represent a fundamental physical system in statistical mechanics, extending

the ideal gas model to include dissipation on particle collisions. Within granular matter physics granular gases represent a reference model system.⁵ On Earth, granular gases may be realised by placing granular matter into a container with vibrating⁶ or rotating⁷ walls, applying electrostatic⁸ or magnetic⁹ forces, *etc.* Granular gases are common in Space, occurring in protoplanetary discs, interstellar clouds, and planetary rings (*e.g.* of Saturn).¹⁰

Ergodicity is a fundamental concept of statistical mechanics. Starting with Boltzmann, the ergodic hypothesis states that long time averages $\overline{\mathcal{O}}$ of a physical observable \mathcal{O} are identical to their ensemble averages $\langle \mathcal{O} \rangle$.^{11,12} In this sense, Brownian motion is ergodic even at out-of-equilibrium conditions, while a range of anomalous diffusion processes exhibit a distinct disparity $\langle \mathcal{O} \rangle \neq \overline{\mathcal{O}}$: for instance, for sufficiently long observation times the time averaged mean squared displacement (MSD) of a Brownian particle converges to the corresponding ensemble average $\langle R^2(t) \rangle$,^{13,14} calling for generalisation of the classical ergodic theories.¹² In fact, similar concepts were already discussed in the context of glassy systems.¹⁵ In the wake of modern microscopic techniques, such as single particle tracking,¹⁶ in which individual trajectories of single molecules or submicron tracers are routinely measured, knowledge of the ergodic properties of the system is again pressing. While the time averages are measured in single particle assays or massive computer simulations, generally ensemble averages are more accessible theoretically. How measured time averages can be interpreted in terms of ensemble approaches and diffusion models is thus an imminent topic.^{13,14}

Here we quantify in detail from analytical derivations and extensive simulations how exactly the ergodicity is violated in simple mechanical systems such as force-free granular gases. Our results for generic granular gases are relevant both from a fundamental statistical mechanical point of view and for the practical analysis of time series of granular gas particles from observations and computer simulations. Specifically, (i) we here derive the time and ensemble averaged MSDs and show that for both constant and viscoelastic restitution coefficients the time averaged MSD is fundamentally different from the corresponding ensemble MSD. (ii) Moreover, the amplitude of the time averaged

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MSD is shown to be a decaying function of the length of the measured trajectory (ageing). (iii) We study an effective single particle mean field approach to the granular gas dynamics. This underdamped scaled Brownian motion (SBM) demonstrates how non-ergodicity and ageing emerge from the non-stationarity invoked by the time dependence of the granular temperature, which translates into the power-law time dependence of the diffusion coefficient of SBM. We note that systems with time dependent diffusion coefficients are in fact common in nature, ranging from mobility of proteins in cell membranes,¹⁷ motion of molecules in porous environments,¹⁸ water diffusion in brain as measured by magnetic resonance imaging,¹⁹ to snow-melt dynamics.^{20,21}

II. Collisions in granular gases

Granular gas particles collide inelastically and a fraction of their kinetic energy is transformed into heat stored in internal degrees of freedom. The dissipative nature of granular gases effects many interesting physical properties.² In absence of external forces the gas gradually cools down. During the first stage of its evolution, the granular gas is in the homogeneous cooling state characterised by uniform density and absence of macroscopic fluxes,² realised *e.g.* in microgravity environments.²² Eventually instabilities occur and vertexes develop in the system.^{2,23} Hereafter, we focus on spatially uniform granular systems.

The energy dissipation in a pair-wise collision event of granular particles is quantified by the restitution coefficient

$$\varepsilon = \left| \frac{(\mathbf{v}_{12}' \cdot \mathbf{e})}{(\mathbf{v}_{12} \cdot \mathbf{e})} \right|, \quad (1)$$

where $\mathbf{v}_{12}' = \mathbf{v}_2' - \mathbf{v}_1'$ and $\mathbf{v}_{12} = \mathbf{v}_2 - \mathbf{v}_1$ are the relative velocities of two particles after and before the collision, respectively, and \mathbf{e} is a unit vector connecting their centres at the collision instant. The post-collision velocities are related to the pre-collision velocities \mathbf{v}_1 and \mathbf{v}_2 as²

$$\mathbf{v}_{1/2}' = \mathbf{v}_{1/2} \mp \frac{1 + \varepsilon}{2} (\mathbf{v}_{12} \cdot \mathbf{e}) \mathbf{e}. \quad (2)$$

The case $\varepsilon = 1$ denotes perfectly elastic collisions, while $\varepsilon = 0$ reflects the perfectly inelastic case. In oblique collisions negative values of the restitution coefficient may be observed.²⁴ For $0 < \varepsilon < 1$ the granular temperature

$$T(t) = m \langle \mathbf{v}^2 \rangle / 2 \quad (3)$$

given by the mean kinetic energy of particles with mass m continuously decreases according to Haff's law for granular gases,²⁵

$$T(t) = T_0 / (1 + t/\tau_0)^2. \quad (4)$$

Here $\tau_0^{-1} = \frac{1}{6}(1 - \varepsilon^2)\tau_c^{-1}(0)$ is the inverse characteristic time of the granular temperature decay, involving the initial value of the inverse mean collision time scaling as $\tau_c^{-1}(t) \propto \sqrt{T(t)/m}$. Weak dissipation ($\varepsilon \simeq 1$) thus implies $\tau_0 \gg \tau_c$. Due to the

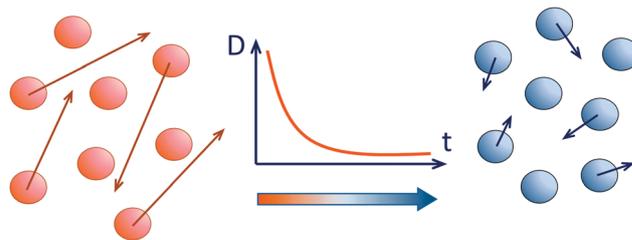


Fig. 1 Collisions in a free granular gas with a restitution coefficient $\varepsilon < 1$ lead to its cooling with time. Along with the reduced kinetic energy of the gas particles, the diffusion coefficient in a free cooling granular gas decreases with time.

temperature decrease the self-diffusion coefficient $D(t)$ of the gas is time dependent,^{2,26–29}

$$D(t) = T(t)\tau_v(t)/m = D_0/(1 + t/\tau_0), \quad (5)$$

where $\tau_v(t)$ is the velocity correlation time, $D_0 = T_0\tau_v(0)/m$ (see Fig. 1). For $\varepsilon = 1$ we recover normal diffusion with the constant diffusivity.

Most studies of granular gases assume that ε is constant. Different approaches consider the dependence of ε on the relative collision speed of the form^{30,31}

$$\varepsilon(v_{12}) \simeq 1 - C_1 A \kappa^{-2/5} (\mathbf{v}_{12} \cdot \mathbf{e})^{1/5} + C_2 A^2 \kappa^{4/5} (\mathbf{v}_{12} \cdot \mathbf{e})^{2/5}. \quad (6)$$

Here the numerical constants are $C_1 = 1.15$ and $C_2 = 0.798$, where A quantifies the specific viscous material properties of particles, $\kappa = (3/2)^{3/2} Y \sigma^{1/2} / [m(1 - \nu^2)]$ is the elastic constant, Y is Young's modulus, ν is the Poisson ratio, and σ is the diameter of the particles. The granular temperature of the viscoelastic gas scales as $T(t) \sim t^{-5/3}$ ^{33,34} implying²⁶

$$D(t) \sim t^{-5/6}, \quad (7)$$

which leads to crossover from super- to subdiffusion in granular Brownian motion.³⁵ We note that there exist more elaborate models for the viscoelastic restitution coefficient.³¹ However, as the continuous decay of temperature is common to all these models, the properties of non-ergodicity and ageing obtained in this work are also generic to these more elaborate models.

III. Computer simulations and observables

We perform event-driven Molecular Dynamics (MD) simulations of a gas of hard-sphere granular particles of unit mass and radius, colliding with constant (see Fig. 2) and viscoelastic (Fig. 3) restitution coefficients. Our simulations code is based on the algorithm suggested in ref. 36. The particles move freely between pairwise collisions, while during the collisions the particle velocities are updated according to eqn (2). The duration time of collision is equal to zero, that is, the velocities of particles are updated instantaneously. We simulate $N = 1000$ particles in a three dimensional cubic box with edge length $L = 40$ and periodic boundary conditions. The box size is

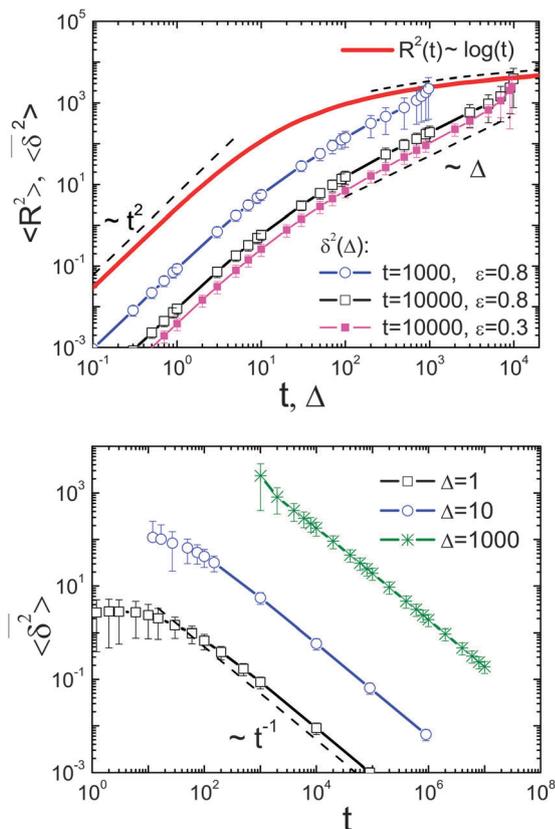


Fig. 2 Ensemble $\langle R^2(t) \rangle$ and time averaged $\langle \delta^2(\Delta) \rangle$ MSDs versus (lag) time (upper graph) and $\langle \delta^2(\Delta) \rangle$ versus length t of the time series (lower graph), from event-driven MD simulations of a granular gas with two different values of the restitution coefficient, $\varepsilon = 0.3$ and 0.8 . While the ensemble MSD crosses over from ballistic motion $\langle R^2(t) \rangle \sim t^2$ for $t \ll \tau_0$ to the logarithmic law $\langle R^2(t) \rangle \sim \log(t)$ for $t \gg \tau_0$, the time averaged MSD starts ballistically and crosses over to the scaling $\langle \delta^2(\Delta) \rangle \sim \Delta/t$ given by eqn (A10).

expressed in terms of the particle radius. The particle volume density is $\phi \approx 0.065$ and the initial granular temperature in the system is $T_0 = 1$.

We evaluate the gas dynamics in terms of the standard ensemble MSD $\langle R^2(t) \rangle$, obtained from averaging over all gas particles at time t , as well as the time averaged MSD

$$\langle \delta^2(\Delta) \rangle = \frac{1}{t - \Delta} \int_0^{t-\Delta} \langle [\mathbf{R}(t' + \Delta) - \mathbf{R}(t')]^2 \rangle dt' \quad (8)$$

for a time series $\mathbf{R}(t)$ of length t as function of the lag time Δ . Eqn (8) is a standard definition to evaluate time series in experiments and simulations.^{13,14,37,38} Here the angular brackets denote the average

$$\langle \delta^2(\Delta) \rangle = \frac{1}{N} \sum_{i=1}^N \overline{\delta_i^2(\Delta)} \quad (9)$$

over all N particle traces. For an ergodic system, such as an ideal gas with unit restitution coefficient corresponding to normal particle diffusion, the ensemble and time averaged MSDs are equivalent at any time, $\langle R^2(\Delta) \rangle = \langle \delta^2(\Delta) \rangle$.^{13,14} In contrast,

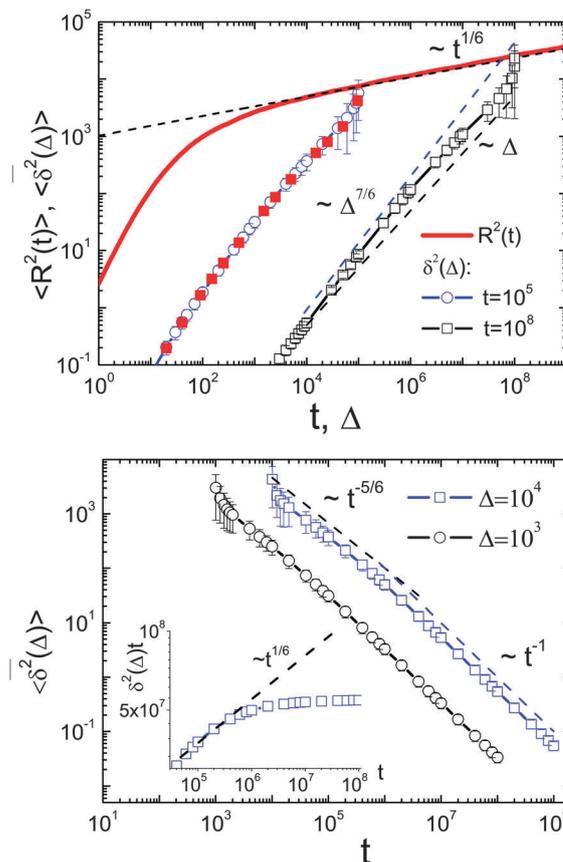


Fig. 3 MSDs $\langle R^2(t) \rangle$ and $\langle \delta^2(\Delta) \rangle$ as function of (lag) time (top) and $\langle \delta^2(\Delta) \rangle$ versus the measurement time t (bottom) from MD simulations (symbols) of a granular gas with viscoelastic $\varepsilon(v_{12})$. We observe the scaling $\langle R^2(t) \rangle \sim t^{1/6}$ in the limit $t \gg \tau_0$. The scaling of the time averaged MSD slowly changes between the indicated slopes (dashed lines). The continuous change of slope of $\langle \delta^2(\Delta) \rangle$ as function of the length t of time traces from slope $-5/6$ to -1 is seen in the inset of the bottom graph. The results for the time averaged MSD with the restitution coefficient computed according to the Padé approximation³² (see text for details) are shown as the red filled squares in the top panel.

several systems characterised by anomalous diffusion with power-law MSD $\langle R^2(t) \rangle \simeq t^\alpha$ ($\alpha \neq 1$) or a corresponding logarithmic growth of the MSD, are non-ergodic and display the disparity $\langle R^2(\Delta) \rangle \neq \langle \delta^2(\Delta) \rangle$.^{13–15,38–41}

Fig. 2 shows the results of our computer simulations of a granular gas with constant $\varepsilon = 0.8$ and 0.3 . The ensemble MSD shows initial ballistic particle motion, $\langle R^2(t) \rangle \sim t^2$. Eventually, the particles start to collide and gradually lose kinetic energy. The ensemble MSD of the gas in this regime follows the logarithmic law $\langle R^2(t) \rangle \sim \log(t)$ (the red line in Fig. 2, top panel).² The time averaged MSD at short lag times Δ preserves the ballistic law $\langle \delta^2(\Delta) \rangle \sim \Delta^2$. At longer lag times, we observe the linear growth $\langle \delta^2(\Delta) \rangle \sim \Delta$ (black symbols in Fig. 2, top). In addition to this non-ergodic behaviour, the time averaged MSD decreases with increasing length t of the recorded trajectory, $\langle \delta^2 \rangle \sim 1/t$. This highly non-stationary behaviour is also

referred to as ageing, the dependence of the system dynamics on its time of evolution.⁴¹ The dependence on the trace length we observe in the bottom panel of Fig. 2 implies that the system is becoming progressively slower. We observe the convergence $\lim_{\Delta \rightarrow t} \langle \overline{\delta^2(\Delta)} \rangle \rightarrow \langle R^2(t) \rangle$.

Fig. 3 depicts the results of MD simulations for a granular gas with viscoelastic restitution coefficient (6) with $A\kappa^{2/5} = 0.2$. In this case the ensemble MSD scales as

$$\langle R^2(t) \rangle \sim t^{1/6} \quad (10)$$

for the time scale $t \gg \tau_0$. The time averaged MSD does not seem to follow a universal scaling law but appears to transiently change from the power-law

$$\langle \overline{\delta^2(\Delta)} \rangle \sim \Delta^{7/6} \quad (11)$$

at intermediate lag times to $\langle \overline{\delta^2(\Delta)} \rangle \sim \Delta$ at longer Δ . As function of the length t of particle traces, we observe the crossover from $\langle \overline{\delta^2} \rangle \sim t^{-5/6}$ to $\langle \overline{\delta^2} \rangle \sim 1/t$, see the bottom panel in Fig. 3.

IV. Granular gas with constant ε

Let us explore this behaviour in more detail. The dynamics of a granular gas can be mapped to that of a molecular gas by a rescaling of time from t to τ as $d\tau = \sqrt{T(t)/T(0)}dt$.^{2,28,42} Using Haff's law (4), it follows that

$$\tau = \tau_0 \log(1 + t/\tau_0). \quad (12)$$

The correlation function for the dimensionless velocity $\mathbf{c}(t) = \mathbf{v}(t)/\sqrt{2T(t)/m}$ of granular particles decays exponentially in this time scale,²

$$\langle \mathbf{c}(\tau_1)\mathbf{c}(\tau_2) \rangle = (3/2)\exp(-|\tau_2 - \tau_1|/\tau_v(0)). \quad (13)$$

In the real time t we find ($t_2 \geq t_1$)

$$\langle \mathbf{v}(t_1)\mathbf{v}(t_2) \rangle = \frac{3T_0}{m}(1 + t_1/\tau_0)^{\beta-1}(1 + t_2/\tau_0)^{-\beta-1} \quad (14)$$

for the velocity correlator; here

$$\beta = \tau_0/\tau_v(0).$$

The MSD is

$$\langle R^2(t) \rangle = 6D_0 \left[\tau_0 \log(1 + t/\tau_0) + \tau_v(0) \left[(1 + t/\tau_0)^{-\beta} - 1 \right] \right]. \quad (15)$$

At short times the particles move ballistically, $\langle R^2(t) \rangle \sim 3D_0 t^2/\tau_v(0)$, crossing over to the logarithmic growth $\langle R^2(t) \rangle \sim 6D_0 \tau_0 \times \log(t/\tau_0)$, as seen in the top panel of Fig. 2.

From the autocorrelation function (14) we obtain the time averaged MSD (see Appendix A)

$$\langle \overline{\delta^2(\Delta)} \rangle \simeq 6D_0 \tau_0 \Delta / t \quad (16)$$

valid in the range $\tau_0 \ll \Delta \ll t$, where τ_0 is the characteristic temperature decay time in eqn (4). This result indeed explains the behaviour observed in Fig. 2: the time averaged MSD scales

linearly with the lag time and inverse-proportionally with the trace length t . Comparison of eqn (15) and (16) demonstrates the non-ergodicity and ageing properties of the system of granular gas particles.

V. Viscoelastic granular gas

For a velocity-dependent restitution coefficient $\varepsilon(v_{12})$ the temperature decays like $T(t) \simeq T_0(t/\tau_0)^{-5/3}$, and the time transformation reads $\tau = 6\tau_0^{5/6}t^{1/6}$. The MSD in this case exhibits the long time scaling

$$\langle R^2(t) \rangle \sim 36D_0 \tau_0^{5/6} t^{1/6},$$

seen in the top panel of Fig. 3. For the time averaged MSD we analytically obtain the bounds

$$\langle \overline{\delta^2(\Delta)} \rangle \sim \Delta^{7/6} / t$$

and

$$\langle \overline{\delta^2(\Delta)} \rangle \sim \Delta / t^{5/6},$$

compare the details in Appendix A. These bounds are given by the dashed lines in the top panel of Fig. 3. Concurrent to this change of slopes as a function of the lag time, the bottom panel of Fig. 3 shows the change of slope of $\langle \overline{\delta^2(\Delta)} \rangle$ as function of the trajectory length t from the slope $-5/6$ to -1 at a fixed lag time Δ .

We note that a more explicit expression for the viscoelastic restitution coefficient can be obtained in terms of the Padé approximant $[3/6]_v$, as derived in ref. 32. In Fig. 3 we demonstrate, however, that for the range of parameters used in our simulations—corresponding to relatively slow collision velocities of granular particles (scaled thermal velocity $v^* < 0.3$)—we obtain nearly the same results for the time averaged MSD as our previous simulations with the restitution coefficient (6), see the red filled squares in Fig. 3.

VI. Scaled Brownian motion

For the unit restitution coefficient individual gas particles at long times perform Brownian motion at a fixed temperature defined by the initial velocity distribution of the particles. For the dissipative granular gases considered herein, the granular temperature scales like $T(t) \simeq 1/t^2$ and $\simeq 1/t^{5/3}$, respectively. Single particle stochastic processes with power-law time-varying temperature or, equivalently, time dependent diffusivity $D(t)$, are well known. Such SBM is described in terms of the overdamped Langevin equation (neglecting the inertia term) with the diffusivity

$$D(t) \sim t^{\alpha-1} \quad (17)$$

for $0 < \alpha < 2$.^{43,44} SBM is a highly non-stationary process and is known to be non-ergodic and ageing.^{14,44-46} Recently, the case of $\alpha = 0$ corresponding to ultraslow SBM was considered.⁴⁷

To study whether SBM provides an effective single particle description of diffusion in dissipative granular gases we extend

SBM to the underdamped case. We thus take the inertial term explicitly into account when considering the dynamics,

$$d\mathbf{v}/dt + \mathbf{v}/[\tau_v(t)] = \sqrt{2D(t)}/\tau_v(t) \times \boldsymbol{\xi}(t), \quad (18)$$

driven by white Gaussian noise $\boldsymbol{\xi}(t)$ with correlation function $\langle \xi_i(t_1)\xi_j(t_2) \rangle = \delta_{ij}\delta(t_1 - t_2)$ for the components.

For $\alpha = 0$ the velocity correlation may be derived from the Langevin eqn (18), namely

$$\langle \mathbf{v}(t_1)\mathbf{v}(t_2) \rangle = \frac{3T(0)\tau_0}{m\tau_v(0)(\beta - 1)} \frac{(1 + t_1/\tau_0)^{\beta-2}}{(1 + t_2/\tau_0)^\beta}. \quad (19)$$

This result for the ultraslow SBM in the underdamped limit (see ref. 47) formally coincides with the velocity correlation function (14) for granular gases in the limit $\beta \gg 1$, in which the velocity correlation time $\tau_v(0)$ is much shorter than the characteristic decay time τ_0 of the granular temperature. This is achieved for sufficiently weak dissipation in the system ($\varepsilon \lesssim 1$).

VII. Conclusions

The occurrence of non-ergodicity in the form of the disparity between long time and ensemble averages of physical observables and ageing, is not surprising in strongly disordered systems described by the prominent class of continuous time random walk models involving divergent time scales of the dynamics.^{13–15,39} Examples include diffusive motion in amorphous semiconductors, structured disordered environments, or living biological cells.¹⁴

Here, we demonstrated how non-ergodicity arises in a simple mechanistic systems such as force-free granular gases. Physically, it stems from a strong non-stationary character of this process brought about by the continuous decay of the gas temperature. Therefore, the ergodicity breaking is expected independent of the particular model of the restitution coefficient ε , while the precise behaviour of the MSD and time averaged MSD clearly depends on the specific law for ε .

For a constant restitution coefficient, the MSD of gas particles $\langle R^2(t) \rangle$ grows logarithmically, while the time averaged MSD $\langle \overline{\delta^2(\Delta)} \rangle$ is linear in the lag time and decays inverse proportionally with the trace length (ageing). We derived the observed non-ergodicity and the ageing behaviour of granular gases from the velocity autocorrelation functions. We note that ageing in the homogeneous cooling state of granular gases was reported previously,⁴⁸ however, it was not put in context with the diffusive dynamics of gas particles.

The decaying temperature of the dissipative force-free granular gas corresponds to an increase of the time span between successive collisions of gas particles, a feature directly built into the SBM model.⁴⁴ As we showed here, SBM and its ultraslow extension with the logarithmic growth of the MSD indeed captures certain features of the observed motion and may serve as an effective single particle model for the granular gas. It is particularly useful when more complex situations are considered, such as the presence of external force fields. Our results shed new light on the physics of granular gases with respect to

their violation of ergodicity in the Boltzmann sense. They are important for a better understanding of dissipation in free gases as well as the analysis of experimental observations and MD studies of granular gases.

It will be interesting to compare the results obtained herein—based on the two standard assumptions for the restitution coefficient—with experimental observations of granular gas systems. Similarly, it might be of interest to see to what extent the present scenario pertains to dilute gases of complex molecules with a large number of internal degrees of freedom ready to absorb a part of the collision energies.^{2–4}

Appendix A: constant restitution coefficient

In this section and the next we present details of the derivation of the results from the main text of the manuscript as well as an additional figure.

The time averaged MSD of the granular gas with constant restitution coefficient, eqn (8) in the main text, may be written as

$$\langle \overline{\delta^2(\Delta)} \rangle = \frac{1}{t - \Delta} \int_0^{t-\Delta} (\langle R^2(t' + \Delta) \rangle - \langle R^2(t') \rangle - 2A(t', \Delta)) dt', \quad (A1)$$

where the MSD $\langle R^2(t) \rangle$ is defined by eqn (15) and

$$\begin{aligned} A(t, \Delta) &= 3 \int_0^t dt_1 \int_t^{t+\Delta} dt_2 \langle v_x(t_1)v_x(t_2) \rangle \\ &= \frac{3T_0\tau_v^2(0)}{m} \left[1 - \left(1 + \frac{t}{\tau_0}\right)^{-\beta} \right. \\ &\quad \left. - \left(1 + \frac{\Delta}{\tau_0 + t}\right)^{-\beta} + \left(1 + \frac{t + \Delta}{\tau_0}\right)^{-\beta} \right]. \end{aligned} \quad (A2)$$

This term accounts for the position correlations at different time instants t and $t + \Delta$. In the present consideration, this term is non-zero. It arises due to the fact that the normal component of the relative velocity of the colliding particles decreases while the tangential component remains unchanged in the course of collisions. Introducing eqn (A2) and (15) into eqn (A1), we obtain the time averaged MSD in the form

$$\langle \overline{\delta^2(\Delta)} \rangle = \langle \overline{\delta_0^2(\Delta)} \rangle + \Xi(\Delta). \quad (A3)$$

The first term is the time averaged MSD for overdamped SBM,

$$\begin{aligned} \langle \overline{\delta_0^2(\Delta)} \rangle &= \frac{6D_0\tau_0}{t - \Delta} \int_0^{t-\Delta} \log\left(\frac{\tau_0 + t' + \Delta}{t' + \tau_0}\right) dt' \\ &= \frac{6D_0\tau_0}{t - \Delta} [(t + \tau_0) \log(t + \tau_0) \\ &\quad - (\Delta + \tau_0) \log(\Delta + \tau_0) \\ &\quad - (t - \Delta + \tau_0) \log(t - \Delta + \tau_0) \\ &\quad + \tau_0 \log \tau_0]. \end{aligned} \quad (A4)$$

For $\tau_0 \ll \Delta \ll t$

$$\langle \overline{\delta_0^2(\Delta)} \rangle \sim \frac{6D_0\tau_0\Delta}{t} \left[\log\left(\frac{t}{\Delta}\right) + 1 \right]. \quad (\text{A5})$$

The second term in eqn (A3) has the form

$$\Xi(\Delta) = \frac{6D_0\tau_v(0)}{t-\Delta} \int_0^{t-\Delta} dt' \left[\left(1 + \frac{\Delta}{t'+\tau_0}\right)^{-\beta} - 1 \right] < 0,$$

where $\beta = \tau_0/\tau_v(0)$, see the main text. Introducing the new variable $y = \Delta/t'$ we get in the limit $\tau_0 \ll \Delta$ that

$$\Xi(\Delta) \sim -6D_0\tau_v(0) \left(1 - \frac{\Delta}{t-\Delta} I(t, \Delta)\right), \quad (\text{A6})$$

where

$$I(t, \Delta) = \int_{\Delta/(t-\Delta)}^{\infty} \frac{dy}{y^2(1+y)^\beta}. \quad (\text{A7})$$

This integral can be taken by parts

$$I(t, \Delta) = \frac{t-\Delta}{\Delta} \left(1 - \frac{\Delta}{t}\right)^\beta + \beta \log\left(\frac{\Delta}{t-\Delta}\right) \left(1 - \frac{\Delta}{t}\right)^{\beta+1} + \beta C(\beta), \quad (\text{A8})$$

where

$$C(\beta) = -(\beta+1) \int_{\Delta/(t-\Delta)}^{\infty} dy \frac{\log y}{(1+y)^{\beta+2}} \sim \gamma + \frac{1}{\beta} + \psi(\beta), \quad (\text{A9})$$

$\gamma = 0.5772\dots$ is the Euler's constant, and $\psi(z) = d \log \Gamma(z)/dz$ is the digamma function. Finally we find in the limit $t \gg \Delta$ that

$$\langle \overline{\delta^2(\Delta)} \rangle \sim 6D_0\tau_0 C(\beta) \frac{\Delta}{t} \simeq \Delta. \quad (\text{A10})$$

This confirms the linear scaling of the time averaged MSD.

Appendix B: velocity-dependent restitution coefficient

Similarly, for the viscoelastic granular gas with $\varepsilon = \varepsilon(v_{12})$ the time averaged MSD may be presented as the sum of two parts, see eqn (A3). The first term corresponds to the time averaged MSD of the SBM process, described by the overdamped Langevin equation to yield

$$\begin{aligned} \langle \overline{\delta_0^2(\Delta)} \rangle &= \frac{36D_0\tau_0^{5/6}}{t-\Delta} \int_0^{t-\Delta} dt' \left[(t'+\Delta)^{1/6} - t'^{1/6} \right] \\ &= \frac{216D_0\tau_0^{5/6}}{7(t-\Delta)} \left[t^{7/6} - \Delta^{7/6} - (t-\Delta)^{7/6} \right]. \end{aligned} \quad (\text{B1})$$

The second term becomes

$$\begin{aligned} \Xi(\Delta) &= \frac{6D_0\tau_v(0)}{t-\Delta} \int_0^{t-\Delta} dt' \\ &\times \left[\exp\left(-\frac{6\tau_0^{5/6}}{\tau_v(0)} \left[(t'+\Delta)^{1/6} - t'^{1/6} \right] \right) - 1 \right]. \end{aligned} \quad (\text{B2})$$

This integral can be presented as a sum of three parts

$$\begin{aligned} &\int_0^{t-\Delta} dt' \left[\exp\left(-\frac{6\tau_0^{5/6}}{\tau_v(0)} \left[(t'+\Delta)^{1/6} - t'^{1/6} \right] \right) - 1 \right] \\ &= \int_0^{k_1\Delta} [\dots] dt' + \int_{k_1\Delta}^{k_2\Delta} [\dots] dt' + \int_{k_2\Delta}^{t-\Delta} [\dots] dt'. \end{aligned} \quad (\text{B3})$$

We choose the coefficients $k_{1,2}$ in the following ranges

$$1 \ll k_1 \ll \tau_0\Delta^{1/5}/\tau_v^{6/5}(0)$$

and

$$\tau_0\Delta^{1/5}/\tau_v^{6/5}(0) \ll k_2 \ll t/\Delta.$$

This enables us to evaluate the first integral in eqn (B3) as follows

$$\int_0^{k_1\Delta} dt' \left[\exp\left(-\frac{6\tau_0^{5/6}}{\tau_v(0)} \left[(t'+\Delta)^{1/6} - t'^{1/6} \right] \right) - 1 \right] \sim -k_1\Delta. \quad (\text{B4})$$

The third term in eqn (B3) can be evaluated as

$$\begin{aligned} &\int_{k_2\Delta}^{t-\Delta} dt' \left[\exp\left(-\frac{6\tau_0^{5/6}}{\tau_v(0)} \left[(t'+\Delta)^{1/6} - t'^{1/6} \right] \right) - 1 \right] \\ &\sim \int_{k_2\Delta}^{t-\Delta} dt' \left(-\frac{6\tau_0^{5/6}}{\tau_v(0)} \left[(t'+\Delta)^{1/6} - t'^{1/6} \right] \right) \\ &= \frac{36\tau_0^{5/6}}{7\tau_v(0)} \left[-t^{7/6} + (t-\Delta)^{7/6} + \left((k_2+1)^{7/6} - k_2^{7/6} \right) \Delta^{7/6} \right]. \end{aligned} \quad (\text{B5})$$

For the chosen range of parameters $k_{1,2}$ the contribution (B4) can be neglected. Finally, assuming that the second term in eqn (B3) is small enough compared to eqn (B5) we get to leading order

$$\langle \overline{\delta^2(\Delta)} \rangle \sim 36k_2^{1/6} D_0\tau_0^{5/6} \frac{\Delta^{7/6}}{t}. \quad (\text{B6})$$

For longer lag times Δ , in the range $\tau_v(0)t^{5/6}/\tau_0^{5/6} \ll \Delta \ll t$ that is opposite to the condition for k_2 above, we have the upper estimate for the correction $\Xi(\Delta)$ to the time averaged MSD of the SBM process, namely

$$|\Xi(\Delta)| \leq 6D_0\tau_v(0) \ll \langle \overline{\delta_0^2(\Delta)} \rangle. \quad (\text{B7})$$

Then we get in the limit $\Delta \ll t$ that

$$\langle \overline{\delta^2(\Delta)} \rangle \sim \langle \overline{\delta_0^2(\Delta)} \rangle \simeq \frac{D_0\tau_0^{5/6}\Delta}{t^{5/6}}. \quad (\text{B8})$$

In addition to these analytical estimates, we computed numerically the full expression (A3). It agrees well with our MD simulation data, compare the curves in Fig. 4 where we explicitly plot $\langle \overline{\delta^2} \rangle / \Delta$. It shows that in the range of parameters τ_0 , τ_v and D_0 consistent with the results of simulations presented in the main text, the transient scaling behaviour $\langle \overline{\delta^2(\Delta)} \rangle \sim \Delta^{7/6}$ is realised in a limited range of Δ . Note also that in this range the linear SBM scaling for $\langle \overline{\delta^2(\Delta)} \rangle$ as prescribed by eqn (B8) is no longer valid.

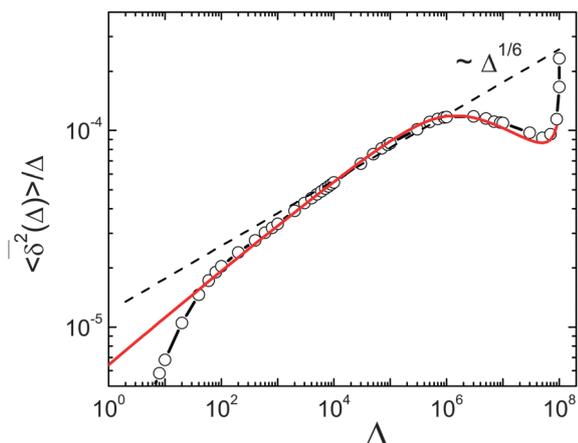


Fig. 4 Time averaged MSD $\langle \delta^2(\Delta) \rangle$ divided by lag time Δ as function of Δ from MD simulations (symbols) of a granular gas with velocity-dependent restitution coefficient. The lines connecting the symbols guide the eye. Red line corresponds to numerical calculation of $\langle \delta^2(\Delta) \rangle$ in eqn (A3) for $\tau_0 = 25$, $\tau_v = 2$, $D_0 = 2$. These values ensure the closest agreement and are consistent with the parameters of the granular gas as used in MD simulations apart from very short lag times. Dashed line shows the asymptotic $\langle \delta^2(\Delta) \rangle / \Delta \sim \Delta^{1/6}$ behaviour according to eqn (B8).

The reason is that for large values of Δ , when $\Delta \rightarrow t$ for any length of the trajectory, in eqn (B2) the evolution of the time averaged MSD with the lag time Δ becomes inherently nonlinear.

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