# Energy Decay in Three-Dimensional Freely Cooling Granular Gas

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The kinetic energy of a freely cooling granular gas decreases as a power law $t^{-\theta}$ at large times $t$. Two theoretical conjectures exist for the exponent $\theta$. One based on ballistic aggregation of compact spherical aggregates predicts $\theta = 2d/(d+2)$ in $d$ dimensions. The other based on Burgers equation describing anisotropic, extended clusters predicts $\theta = d/2$ when $2 \le d \le 4$. We do extensive simulations in three dimensions to find that while $\theta$ is as predicted by ballistic aggregation, the cluster statistics and velocity distribution differ from it. Thus, the freely cooling granular gas fits to neither the ballistic aggregation or a Burgers equation description.

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The freely cooling granular gas, a collection of ballistically moving inelastic particles with no external source of energy, has been used to describe dynamics of granular materials [1–3], large scale structure formation in the universe [4], and geophysical flows [5]. It is also of interest as a system far from equilibrium, limiting cases being amenable to exact analysis [6,7], has close connection to the well studied Burgers equation [6,8–11], and is an example of an ordering system showing nontrivial coarsening behavior [12–15]. Of primary interest is clustering of particles due to inelastic collisions and the temporal evolution of the kinetic energy $E(t)$ at large times.

At initial times, particles remain homogeneously distributed and kinetic theory predicts that $E(t)$ decreases as $(1 + t/t_0)^{-2}$ (Haff's law), where the time scale $t_0 \propto (1 - r^2)^{-1}$ for constant coefficient of restitution $r$ [16]. At later times, this regime is destabilized by long wavelength fluctuations into an inhomogeneous cooling regime dominated by clustering of particles [17–19]. In this latter regime, $E(t)$ no longer obeys Haff's law but decreases as a power law $t^{-\theta}$, where $\theta$ depends only on dimension $d$ [20,21]. Direct experiments on inelastic particles under levitation [22] or in microgravity [23,24] confirm Haff's law. However, being limited by a small number of particles and short times, they do not probe the inhomogeneous regime, giving no information about $\theta$.

Different theories predict different values of $\theta$. The extension of kinetic theory into the inhomogeneous cooling regime using mode coupling methods leads to $E(\tau) \sim \tau^{-d/2}$, where the relation between the average number of collisions per particle $\tau$ and time $t$ is unclear [25]. This result agrees with simulations for near-elastic ($r \approx 1$) gases, but fails for large times and strongly inelastic ($r \ll 1$) gases [25]. Any theory involving perturbing about the elastic limit $r = 1$ is unlikely to succeed since extensive simulations in one [20] and two [21] dimensions show that for any $r < 1$, the system is akin to a *sticky gas* ($r \to 0$), such that colliding particles stick and form aggregates.

If it is assumed that the aggregates are compact spherical objects, then the sticky limit corresponds to the well studied ballistic aggregation model (BA) (see Ref. [26] for a review). For BA in the dilute limit and the mean field assumption of uncorrelated aggregate velocities, scaling arguments lead to $\theta_{\rm BA}^{mf} = 2d/(d+2)$ and the presence of a growing length scale $\mathcal{L}_t \sim t^{1/z_{\rm BA}^{mf}}$ with $z_{\rm BA}^{mf} = (d+2)/2$ [27]. In one dimension, BA is exactly solvable and $\theta_{\rm BA} = \theta_{\rm BA}^{mf}$ [6,8]. However, in two dimensions and for dilute systems, it has been shown that $\theta_{\rm BA}^{mf}$ is smaller than the numerically obtained $\theta_{\rm BA}$ by 17% because of strong velocity correlations between colliding aggregates [28,29].

The sticky limit has also been conjectured [20,21] to be describable by a Burgers-like equation (BE) [30]. This mapping is exact in one dimension [10] and heuristic in two and higher dimensions [21], and leads to $\theta_{\rm BE} = 2/3$ in $d = 1$, $\theta_{\rm BE} = d/2$ for $2 \le d \le 4$, and $\theta_{\rm BE} = 2$ for $d > 4$ [4,31,32].

The exponents $\theta_{\rm BA}^{mf}$ and $\theta_{\rm BE}$ coincide with each other in one and two dimensions and also with numerical estimates of $\theta$ for the freely cooling granular gas in these dimensions [20,21]. In three dimensions, they differ with $\theta_{\rm BA}^{mf} = 6/5$ and $\theta_{\rm BE} = 3/2$. However, simulations that measure $\theta$ in three dimensions have been inconclusive, being limited by small system sizes and times, and the measured value of $\theta$ ranges from $\theta = 1.35 - 1.6$ [33] to $\theta \sim 1$ [34,35]. Thus, it remains an open question as to which of the theories, if either, is correct.

In this Letter, we study the freely cooling granular gas in three dimensions using event-driven molecular dynamics simulations and conclude that $\theta \approx \theta_{\rm BA}^{mf}$, conclusively ruling out $\theta_{\rm BE}$ as a possible solution. Comparing with the results of three dimensional BA, we find that $\theta_{\rm BA}^{mf}$ describes the energy decay in BA only when densities are high and multiparticle

 

collisions are dominant. We also find that the cluster size and the velocity distributions of the particles in the granular gas and BA are strikingly different from each other.

Consider $N$ identical hard-sphere particles distributed uniformly within a periodic three-dimensional box of linear length $L$ and with initial velocities chosen from a normal distribution. The mass and diameter of the particles are set equal to one. All lengths, masses, and times are measured in units of particle diameter, particle mass, and initial mean collision time. The system evolves in time without any external input of energy. All particles move ballistically until they undergo momentum conserving, deterministic collisions with other particles: if the velocities before and after collision are $\mathbf{u}_1$, $\mathbf{u}_2$, and $\mathbf{v}_1$, $\mathbf{v}_2$, respectively, then

$$\mathbf{v}_{1,2} = \mathbf{u}_{1,2} - \frac{1+r}{2}[\mathbf{n} \bullet (\mathbf{u}_{1,2} - \mathbf{u}_{2,1})]\mathbf{n}, \qquad (1)$$

where $0 < r < 1$ is the coefficient of restitution and $\mathbf{n}$ is the unit vector directed from the center of particle 1 to the center of particle 2. The tangential component of the relative velocity is unchanged and the longitudinal component is reduced by a factor $r$.

The above system is studied using large scale event-driven molecular dynamics simulations [36,37] for system sizes up to $N = 8 \times 10^6$. For constant coefficient of restitution, infinite collisions occur in finite time [38]. An efficient scheme of avoiding this computational difficulty is to make the collisions elastic ($r = 1$) when the relative velocity is less than a cutoff velocity $\delta$, and $r = r_0 < 1$ otherwise [20].

We first present results for the decrease of kinetic energy with time. We find that for $r_0 = 0.10$ and volume fraction $\phi = 0.208$, the homogeneous regime is very short-lived and the inhomogeneous regime is reached at early times. However, the energy decay deviates from the universal power law $t^{-\theta}$ for times larger than a crossover time that increases with system size $L$. We assume that $E(t)$ obeys the finite size scaling form

$$E(t) \simeq L^{-z\theta} f\left(\frac{t}{L^z}\right), t, L \to \infty, \qquad (2)$$

where $z$ is the dynamical exponent, and the scaling function $f(x) \sim x^{-\theta}$ for $x = tL^{-z} \ll 1$. The simulation data for different $L$ collapse onto a single curve (see Fig. 1) when $E(t)$ and $t$ are scaled as in Eq. (2) with $\theta = \theta_{\mathrm{BA}}^{mf} = 6/5$ and $z = z_{\mathrm{BA}}^{mf} = 5/2$. The power law $x^{-6/5}$ extends over nearly five decades, confirming that the energy decay in the freely cooling granular gas in three dimensions has the exponents that are numerically indistinguishable from the mean-field BA. The data conclusively rule out $\theta_{\mathrm{BE}} = 3/2$ as being the correct exponent. From Fig. 1, we see that $f(x) \sim x^{-\eta}$ for $x \gg 1$ with $\eta \approx 1.83$, such that at large times $t \gg L^z$, $E(t) \sim L^{1.58} t^{-1.83}$.

We now show that $\theta$ measured from the data in Fig. 1 is independent of the volume fraction $\phi$, $r_0$, and $\delta$. With increasing $\phi$, we find that the crossover from homogeneous

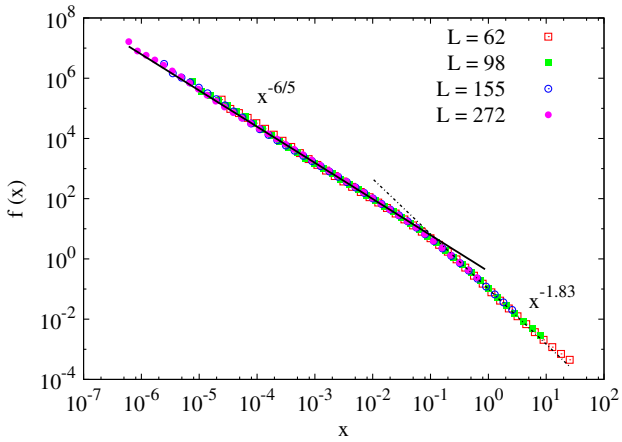


FIG. 1 (color online). The data for kinetic energy $E(t)$ for different system sizes $L$ collapse onto a single curve when $t$ and $E(t)$ are scaled as in Eq. (2) with $\theta = \theta_{\mathrm{BA}}^{mf} = 6/5$ and $z = z_{\mathrm{BA}}^{mf} = 5/2$. The power law fits are shown by straight lines. The data are for $\phi = 0.208$, $r_0 = 0.1$, and $\delta = 10^{-4}$.

$[E(t) \sim t^{-2}]$ to inhomogeneous regime $[E(t) \sim t^{-6/5}]$ occurs at earlier times [see Fig. 2(a)]. In the inhomogeneous regime, the curves are indistinguishable from each other. Thus, we see that the exponent $\theta = 6/5$ holds even in the limit $\phi \to 0$. Similarly, with increasing $r_0$, though the inhomogeneous regime sets in at later times, it nevertheless exists with the same power law $t^{-\theta}$ [see Fig. 2(b)]. Similar behavior has been observed in one and two dimensions [20,21]. We also find no discernible dependence of the data on the parameter $\delta$ [see Fig. 2(c)]. However, we note that at much larger times ($\sim\delta^{-2/\theta}$), collisions become mostly elastic and $E(t)$ stops decreasing with time [20,39]. A nonzero $\delta$ also results in nontrivial coarsening [13]. Finally, we check that using a more realistic velocity dependent coefficient of restitution does not change the value of the exponent $\theta$ (see the Supplemental Material [40]).

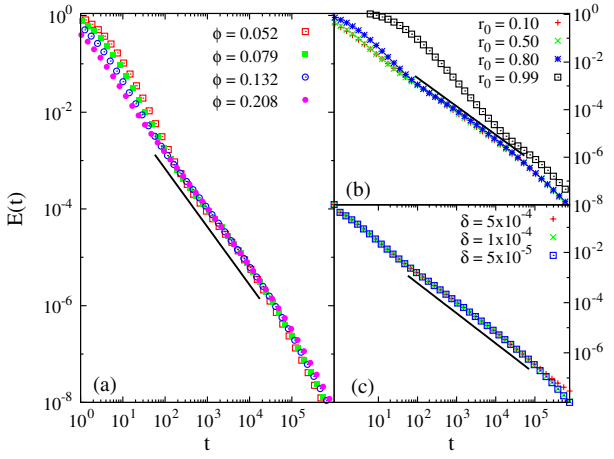


FIG. 2 (color online). The dependence of kinetic energy $E(t)$ on (a)volume fraction $\phi$, (b) $r_0$, and (c) $\delta$. The solid lines are power laws $t^{-6/5}$. The data are for $\phi = 0.208$, $r_0 = 0.10$, $\delta = 10^{-4}$ unless it is the varying parameter.

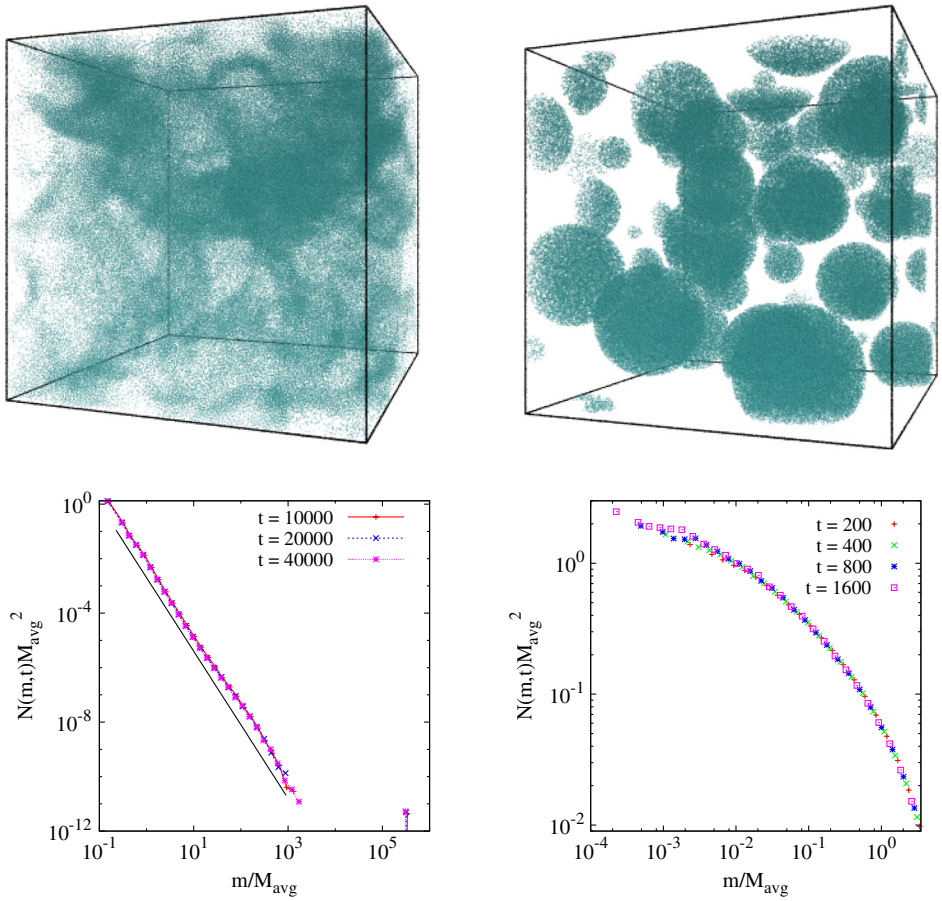


FIG. 3 (color online). Snapshots of granular gas (upper left) and BA (upper right) in the inhomogeneous regime. The lower panel shows the scaled mass distribution for the granular gas (left) and BA (right). $M_{\rm avg}$ is the mean cluster size. The solid line is a power law $m^{-2.7}$. The data are for $\phi = 0.208$, $r_0 = 0.10$.

We note that $\theta_{\rm BA}^{mf}$ need not be equal to the actual BA exponent $\theta_{\rm BA}$ [28,29]. We study this discrepancy in three dimensions by simulating BA directly. Two colliding particles are replaced with a single particle whose volume is the sum of the volumes of the colliding particles. The newly formed aggregate may overlap with other particles leading to a chain of aggregation events. These multiparticle collisions result in the exponent $\theta_{\rm BA}$ being dependent on the volume fraction $\phi$. We find that as $\phi$ increases from 0.005 to 0.208, $\theta_{\rm BA}$ decreases from $1.283 \pm 0.005$ to $1.206 \pm 0.005$ and appears to converge to the $\theta_{\rm BA}^{mf} = 1.2$ with increasing $\phi$. Thus, it is remarkable that the mean field result describes well only the systems with $\phi \gtrsim 0.2$, while its derivation [27] assumes the limit $\phi \to 0$.

The energy decay in granular gas and BA at higher densities being similar, how do other statistical properties compare? We first study clusters of particles in the inhomogeneous regime. Snapshots of granular gas and BA (see Fig. 3) show that clusters in granular gas are extended as opposed to compact spherical clusters (by construction) in BA. The spatial distribution of particles is partially quantified by measuring the cluster size distribution $N(m,t)$. For the granular gas, the simulation box is divided into boxes of a side equal to the diameter of a particle. A box is said to be occupied if it contains the center of a particle. Two occupied boxes belong to the same cluster if connected by nearest neighbor occupied boxes. The cluster size distribution is then measured using the Hoshen-Kopelman algorithm [41]. $N(m,t)$ for the granular gas and BA, shown in the lower panel of Fig. 3, are significantly different from one another. For the granular gas, $N(m,t)$ consists of two parts: a power law ($\sim m^{-2.7}$) and a peak at large cluster sizes. The power law describes all clusters other than the largest cluster that accounts for the peak. The largest cluster contains about 75% of the particles. For BA, $N(m,t)$ is a power law for small cluster sizes ($\sim m^{-0.2}$) and exponential for cluster sizes larger than the mean cluster size. Both of these distributions are different from the mean field result for $N(m,t)$ obtained from the Smoluchowski equation describing the temporal evolution of $N(m,t)$:

$$\dot{N}(m,t) = \sum_{m_1=1}^{m-1} N(m_1,t)N(m-m_1,t)K(m_1,m-m_1) - 2\sum_{m_1=1}^{\infty} N(m_1,t)N(m,t)K(m_1,m)\ \ m = 1,2,\ldots, \tag{3}$$

where

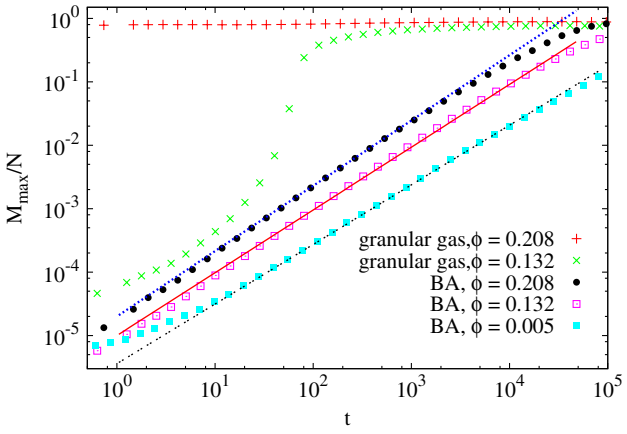


FIG. 4 (color online). The largest mass $M_{\max}$ as a function of time. For the granular gas, $r_0 = 0.10$, $\delta = 10^{-4}$. Straight lines are power laws $t^{0.94}$, $t^{0.99}$, $t^{1.03}$ (bottom to top).

$$K(m_1, m_2) \propto (m_1^{-1/2} + m_2^{-1/2})(m_1^{1/3} + m_2^{1/3})^2 \quad (4)$$

is the collision kernel [26,42]. For this kernel, it is known that that $N(m,t) \sim \exp(-\text{const} \times m^{-1/2})$ for small $m$ and $N(m,t) \sim \exp(-\text{const} \times m)$ for large $m$ [26]. While the simulation results for BA matches for large $m$, it is different (being a power law) for small $m$.

Also, for the kernel in Eq. (4), it is expected that the largest cluster size $M_{\max}$ increases with time $t$ as a power law $t^{6/5}$ [26,42], the mean field answer. We compare this prediction with the simulations for the granular gas and BA. For the granular gas, rather than a power law growth as in one and two dimensions and in mean field, there is a rapid increase in $M_{\max}$ (see upper two curves of Fig. 4) at a time that coincides with the onset of the inhomogeneous cooling regime. This rapid growth is similar to the gelation transition where a gel containing a fraction of the total number of particles is formed in finite time. However, the kernel for BA is nongelling with mass dimension $1/6$, whereas the gelation transition requires mass dimension to be larger than one [26,42]. For BA, $M_{\max}$ increases as a power law (see bottom three curves of Fig. 4), with an exponent that increases with $\phi$, and possibly converges to the mean field value $6/5$. Similar behavior is seen for the growth of the average cluster size of BA which grows as a power law with an exponent ranging from 1.06 for $\phi = 0.005$ to 1.19 for $\phi = 0.313$.

We further compare the velocity distributions $P(v,t)$, where $v$ is any velocity component, of the granular gas with that of BA. $P(v,t)$ has the scaling form $P(v,t) = v_{\text{rms}}^{-1}\Phi(v/v_{\text{rms}})$, where $v_{\text{rms}}$ is the time dependent root mean square velocity. The scaling function $\Phi(y)$ is shown in Fig. 5 for different times. We note that $\Phi(y)$ does not depend on $r_0$ or the initial velocity distribution, having checked for Gaussian, uniform, and exponential distributions. For the granular gas, at short times when the system is homogeneous ($t = 5$, 10 in Fig. 5), $\Phi(y)$ is an exponential $e^{-\alpha y}$ as predicted by kinetic theory. We find

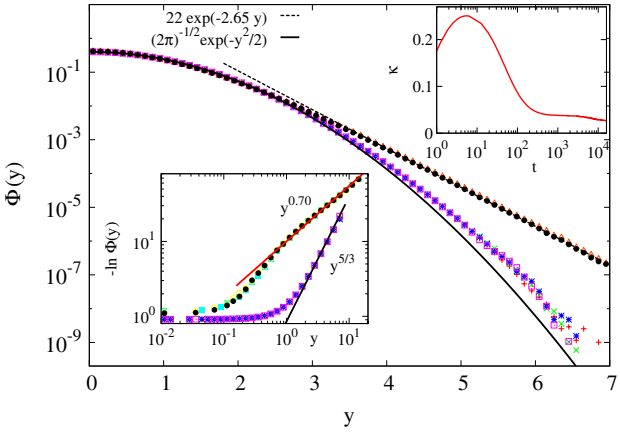


FIG. 5 (color online). The scaled velocity distribution function $\Phi(y)$ for the granular gas at times $t = 5$, 10 (upper collapsed data) and $t = 2000$, 4000, 6000, 8000 (lower collapsed data). The solid curve is a Gaussian. The data are for $\phi = 0.208$, $r_0 = 0.10$. Upper inset: The kurtosis $\kappa$ as a function of time $t$. Lower inset: $-\ln \Phi(y)$ as a function of $y$ for the granular gas (lower data) and BA (upper data). For BA, the times are $t = 400$, 800, 1600, and $\phi = 0.208$.

$\alpha = 2.65$, in good agreement with the kinetic theory value 2.60 [43]. For larger times ($t = 2000$–$8000$ in Fig. 5), $\Phi(y)$ is clearly non-Gaussian (see comparison with Gaussian in Fig. 5). A quantitative measure of the deviation from the Gaussian is the kurtosis, $\kappa = \langle v^4 \rangle / \langle v^2 \rangle^2 - 5/3$, shown in the upper inset of Fig. 5. The kurtosis after an initial increase, decreases, and saturates to a nonzero value. The large $y$ behavior of $\Phi(y)$ is shown in the bottom inset of Fig. 5. It has been argued that the probability that a particle never undergoes a collision up to time $t$ is an exponential in $t$, resulting in $-\ln[\Phi(y)] \sim y^{2/\theta}$, $y \gg 1$ [21]. For the granular gas, we find that $-\ln[\Phi(y)] \sim y^{5/3}$, consistent with $\theta = 6/5$. However, for BA, we find $-\ln[\Phi(y)] \sim y^{0.70}$. The deviation of BA is surprising, but may be rationalized. The argument for the exponential form of survival probability implicitly assumes that the number of clusters reach a time independent distribution resulting in a constant rate of collision. That this is true for the granular gas and not for BA can be seen from the lower panels of Fig. 3, where $M_{\max}$ and hence, $M_{\text{avg}}$ (mean cluster size) is nearly a constant for the granular gas and time dependent for BA (see Fig. 4) at large times.

Thus, in spite of having the same form of energy decay, the local environment that a particle in a granular gas sees around itself, is distinct from those in BA. In BA, two colliding clusters rearrange their masses to form a new spherical cluster at every step. Due to the lack of such dynamic cluster rearrangements, the granular gas remains locally structurally anisotropic and disordered.

To summarize, we showed that the energy $E(t)$ of a three dimensional freely cooling granular gas decreases as $t^{-\theta}$, with $\theta \approx 6/5$, indistinguishable from the mean field result for dilute ballistic aggregation. This rules out Burgers-like equations as a

description of the granular gas at large times. We also showed that the relation to ballistic aggregation appears coincidental with the energy of the dilute ballistic gas decaying with a different exponent. In addition, the cluster size distribution as well as the velocity distribution of ballistic aggregation are strikingly different from that of the granular gas. We hope that this Letter will prompt research into finding the correct continuum equations for the granular gas as well as in the design of experiments to probe the inhomogeneous cooling regime, microgravity [23,24,44,45] being a promising candidate. While frictionless freely cooling experiments have been limited to the homogeneous regime, inhomogeneous clustering has been observed in experiments where only one particle or location is excited [46–48]. For these systems, scaling arguments based on the sticky gas explain the experimental results [49–51]. Multiple localized excitations may result in a crossover to the freely cooling system, making such experiments suitable to probing the inhomogeneous regime.

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