Mpemba effect in an anisotropically driven granular gas

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Abstract – The Mpemba effect refers to the counterintuitive relaxation wherein a hotter system equilibrates faster than a cooler system when quenched to a cold temperature. Even though the effect has been illustrated for isotropically driven granular gases, a prototypical system far from equilibrium, its existence requires non-stationary initial states, limiting experimental realisation. In this paper, we demonstrate the existence of the Mpemba effect in anisotropically driven granular gases, even when quenched from initial states that are stationary. Our theoretical predictions, based on kinetic theory, for the regular, inverse and strong Mpemba effects agree well with results of event-driven molecular dynamics simulations of hard discs.

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When two identical physical systems, initially at two different temperatures, are quenched to the same lower temperature, one would intuitively expect that the hotter system takes a longer time to equilibrate. However, there exists a counterintuitive observation that hotter water may freeze faster than colder water, as documented centuries ago by Aristotle [1,2], and is referred to as the Mpemba effect after Mpemba and Osborne [3] who quantified the phenomenon. Although the exact mechanism for such anomalous behaviour found in water is not known, several candidates have been proposed: evaporation [4], convection [5], supercooling [6], dissolved gases [7], hydrogen bonding [8–10] and non-equipartition of energy among the different degrees of freedom [11]. The Mpemba effect has also been demonstrated in other physical systems such as clathrate hydrates [12], magnetic alloys [13], polylactides [14] and more recently in colloidal systems [15].

Theoretical analysis has focused on model spin systems [16,17], molecular gases [18,19] and three state Markov systems [20–22]. In the third case, the exact condition for the existence of the Mpemba effect could be derived by tracking the distance between probability distributions during the relaxation process. Moreover, such a framework also suggests the existence of an inverse Mpemba effect [20], where an initially colder system can heat up faster than an initially hotter system, the strong Mpemba effect [21], where an initial state results in an exponentially faster cooling, and optimal heating protocols [16] for such systems. However, these systems are mostly for equilibrium systems and while single particle experimental realisation is possible [15], the same is not true for many particle systems.

An area where a strong interplay between experiments and analytical calculations is possible, promoting a deeper understanding on the Mpemba effect, is driven granular systems, a prototypical far from equilibrium system where the external driving compensates for the loss of kinetic energy in inelastic collisions. The Mpemba effect has been demonstrated for homogeneous and isotropically driven smooth as well as rough gases, which requires the initial states to be non-stationary [23–26]. The results from an exact analysis of the driven, inelastic Maxwell gas where the rate of collision is taken to be independent of the relative velocity of the colliding particles, is consistent with the above results for the mono-dispersed gas [26]. However, the lack of stationarity of the initial conditions makes it difficult for experimental realisation because while stationary states are easy to achieve due to them being attractive, non-stationary states require careful preparation of the initial state. The Mpemba effect has been demonstrated, starting from steady-state initial conditions, in sheared inertial suspensions [27] of inelastic hard spheres provided one of the system is prepared in a quasi-equilibrium (unsheared) state while the other system is prepared in a non-equilibrium sheared state.

In this paper, we present an analysis of an anisotropically driven, mono-dispersed granular gas in two
dimensions, and show the existence of the Mpemba effect for two identical systems starting from initial conditions that are stationary. In addition, we derive the conditions for the inverse and the strong Mpemba effect in this system. The analysis is exact for stationary states that are close to the final stationary state. For generic initial stationary states, we verify our theoretical predictions with detailed event-driven molecular dynamics simulations of hard discs. We propose that this set-up of anisotropically driven granular gases is ideal for studying the Mpemba effect, and later for possibly more practical applications.

Consider a two-dimensional granular gas composed of identical, smooth, inelastic hard particles. The velocities of these particles change in time through momentum-conserving binary collisions. When two particles \( i \) and \( j \) with velocities \( v_i \) and \( v_j \) collide, the new velocities \( v'_{i} \) and \( v'_{j} \) are given by

\[
\begin{align*}
    v'_{i} &= v_i - \frac{1 + r}{2} [(v_i - v_j) \cdot \hat{e}] \hat{e}, \\
v'_{j} &= v_j + \frac{1 + r}{2} [(v_i - v_j) \cdot \hat{e}] \hat{e},
\end{align*}
\]  

where \( r \) is the coefficient of restitution and \( \hat{e} \) is the unit vector along the line joining the centres of the particles at contact. The particles are anisotropically driven at a constant rate. At long times, the system goes into a stationary state.

The velocity distribution function \( f(v, t) \), defined as the number density of particles having velocity \( v \) at time \( t \), obeys the Enskog-Boltzmann equation [28]

\[
\frac{\partial}{\partial t} f(v, t) = \chi I(f, f) + \left( \frac{\xi_{xx}^2}{2} \frac{\partial^2}{\partial v_x^2} + \frac{\xi_{yy}^2}{2} \frac{\partial^2}{\partial v_y^2} \right) f(v, t),
\]  

where \( \chi \) [29] is the pair correlation function, \( I(f, f) \) is the collision integral which accounts for the rate of collision of two particles being proportional to their relative velocity (see eq. (S2) of the Supplemental Material Supplementarymaterial.pdf (SM)), and \( \xi_{xx}^2 \) and \( \xi_{yy}^2 \) are the variances or strengths of the white noise along the \( x \)- and \( y \)-directions, respectively.

Note that in eq. (2), we have introduced different driving strengths along the two directions, and we will refer to such driving as anisotropic driving. The Enskog-Boltzmann equation can be used to describe a spatial system but here we consider a spatially homogeneous system such that the spatial degrees of freedom are ignored. Moreover, as usually assumed in kinetic theory for dilute gases, we apply the molecular chaos hypothesis to use product measure for the joint velocity distribution function in the collision integral \( I(f, f) \) (see SM).

The anisotropic driving implies that, though the system remains homogeneous with \( \langle v \rangle = 0 \), the mean kinetic energies per particle (granular temperature) along the two directions are different. The granular temperatures are defined as \( T_i(t) = \frac{2}{3n} \int dv_i v_i^2 f(v, t) \), where \( n = \int dv f(v, t) \) is the number density, \( m \) is the mass of the particles, and \( i = x, y \). We note that granular systems are far from equilibrium and there is no notion of temperature as in equilibrium systems. However, in the literature on driven granular systems, temperature has been used to denote the mean kinetic energy, and we continue to do the same. We introduce two quantities \( T_{tot} \) and \( T_{dif} \) which are the total and the difference of the temperatures in the two directions:

\[
\begin{align*}
    T_{tot}(t) &= T_x(t) + T_y(t), \\
    T_{dif}(t) &= T_x(t) - T_y(t).
\end{align*}
\]  

Within kinetic theory, the velocity distribution of a driven granular gas, \( f(v, t) \), is expanded about the Gaussian in terms of Sonine polynomials [28,29]. For the sake of simplicity, we restrict ourselves to the first term in the expansion, namely a Gaussian. Adding more terms will not change the qualitative results obtained in the paper. Thus, we write

\[
f(v, t) = \frac{mn}{2\pi \sqrt{T_{tot}(t)}} \exp \left[ -\frac{mv_x^2}{2T_x(t)} - \frac{mv_y^2}{2T_y(t)} \right].
\]  

Substituting eq. (4) into eq. (2), we find that the equations governing the temporal evolution of \( T_{tot} \) and \( T_{dif} \) form a closed set of coupled non-linear differential equations, and is given by

\[
\begin{align*}
    \frac{\partial}{\partial t} T_{tot}(t^*) &= F(T_{tot}, T_{dif}), \\
    \frac{\partial}{\partial t} T_{dif}(t^*) &= G(T_{tot}, T_{dif}).
\end{align*}
\]  

Here, we have defined the dimensionless variable for time, \( t^* \) in terms of mean collision time as

\[
t^* = \frac{\sigma \sqrt{2(T_{tot} + T_{dif})}}{\pi n} E\left( \frac{2T_{dif}}{T_{tot} + T_{dif}} \right) t,
\]  

where \( E(x) \) is the elliptic integral of second kind and \( \sigma \) is the diameter of the particles. The details of the derivation and the functional forms for \( F(T_{tot}, T_{dif}) \) and \( G(T_{tot}, T_{dif}) \) are given in the SM.

We define the Mpemba effect as follows. Consider two systems with different initial \( T_{tot} \). Both systems are quenched to the same final stationary state whose temperature is lower. If the system that is initially hotter reaches the final stationary state faster, then we say that the system shows the Mpemba effect. Likewise, if the initial systems are heated to a higher temperature and the cooler system equilibrates faster, we will say that the system shows the inverse Mpemba effect. Finally, for both effects, we will say that the system shows strong Mpemba effect, if the hotter system relaxes exponentially faster than the cooler system for the Mpemba effect and vice versa for the inverse Mpemba effect. We will demonstrate the existence of all these four features for the anisotropically driven granular gas, both analytically using a linearised theory as well as through event-driven molecular dynamics simulations.
We first analytically demonstrate the Mpemba effect by considering only those initial stationary states that are close to the final stationary state, allowing for linearisation of the system thus making it tractable. This method of linearisation closely follows that of ref. [23]. We denote the parameters of the final stationary state by $T^\text{tot}_{\text{st}}$ and $T^\text{dif}_{\text{st}}$. The analysis for the variation of stationary temperatures, $T^\text{tot}_{\text{dif}}$ and $T^\text{dif}_{\text{tot}}$, as a function of system parameters is given in the SM. In the stationary state, the time derivatives in eq. (5) can be set to zero and hence $F(T^\text{tot}_{\text{tot}}, T^\text{dif}_{\text{dif}}) = 0$ and $G(T^\text{tot}_{\text{tot}}, T^\text{dif}_{\text{tot}}) = 0$. Let $\delta T^\text{tot}(t^*) = T^\text{tot}_\text{tot}(t^*) - T^\text{tot}_{\text{tot}}$ and $\delta T^\text{dif}(t^*) = T^\text{dif}_\text{tot}(t^*) - T^\text{dif}_{\text{tot}}$ denote the time-dependent deviation from the stationary state values. For small deviations, the non-linear differential equations in eq. (5) can be linearised about the stationary state values to give

$$\frac{d}{dt^*} \delta T^\text{tot}(t^*) = -R \left[ \delta T^\text{tot}(t^*) \right],$$

where $R$ is a 2 x 2 matrix with constant entries $R_{ij}$ as given in eqs. (S13) of the SM. $\delta T^\text{tot}(t^*)$ and $\delta T^\text{dif}(t^*)$ then relax in time to zero as

$$\delta T^\text{tot}(t^*) = K_+ e^{\lambda_t - t^*} + K_- e^{-\lambda_t - t^*},$$

$$\delta T^\text{dif}(t^*) = L_+ e^{\lambda_{\text{dif}} - t^*} + L_- e^{-\lambda_{\text{dif}} - t^*},$$

where the coefficients $K_+, K_-, L_+$ and $L_-$ are as given in eqs. (S15) of the SM, $\lambda_{\pm}$ are the eigenvalues of $R$ and $\gamma = \lambda_t - \lambda_{\text{dif}}$.

We now derive the condition for the Mpemba effect to be present in the linearised regime, based on the analysis of eq. (8). Consider two systems $P$ and $Q$ whose stationary state parameters are denoted as $[T^\text{tot}_{\text{tot}}, T^\text{dif}_{\text{tot}}]$ and $[T^\text{tot}_{Q}, T^\text{dif}_{Q}]$, respectively. We will assume that $P$ is hotter than $Q$, i.e., $T^\text{tot}_P > T^\text{tot}_Q$. On quenching to $T^\text{tot}_{\text{tot}}$, the Mpemba effect will be present when there exists a finite time $\tau$ such that $T^\text{tot}_P(t^*) < T^\text{tot}_Q(t^*)$ for $t^* > \tau$. To characterise the difference between the two systems, we introduce the quantities $\Delta T^\text{tot} = T^\text{tot}_P(0) - T^\text{tot}_Q(0)$ and $\Delta T^\text{dif} = T^\text{dif}_P(0) - T^\text{dif}_Q(0)$. From eq. (8), written for both $P$ and $Q$, the time $\tau$ at which the two relaxation curves cross, corresponding to $T^\text{tot}_P(\tau) = T^\text{tot}_Q(\tau)$, is given by

$$\tau = \frac{1}{\gamma} \ln \left[ \frac{R_{12} \Delta T^\text{dif} - (\lambda_+ - R_{11}) \Delta T^\text{tot}}{R_{12} \Delta T^\text{tot} - (\lambda_+ - R_{11}) \Delta T^\text{dif}} \right].$$

For the Mpemba effect to be present, we require that $\tau > 0$, or equivalently (since $\gamma > 0$), the argument of the logarithm in eq. (9) should be greater than one. We immediately obtain the criterion for the crossing of the two trajectories as

$$R_{12} \Delta T^\text{dif} > (\lambda_+ - R_{11}) \Delta T^\text{tot}.$$  (10)

In fig. 1(a), we choose initial conditions $P$ and $Q$ such that eq. (10) is satisfied. The trajectories cross at the point as predicted by eq. (9). For initial stationary states that are close to the final state, there is little difference between the linearised (dotted lines) and the full numerical solutions (solid lines).

In fig. 2, we identify the region of phase space (initial conditions) where the Mpemba effect is observable for varying coefficient of restitution $r$, based on eq. (10). The initial conditions in the region below the line in the phase diagram show the Mpemba effect whereas the other region does not show the effect. The phase diagram is for a generic final stationary state with parameters $T^\text{tot}_{\text{tot}} = 1.0$ and $T^\text{dif}_{\text{tot}} = 0.15$. As $r$ approaches unity, the gas becomes more isotropic, and the the key feature responsible for the presence of the Mpemba effect, i.e., anisotropy of temperatures, is lost and hence the Mpemba effect is not observed.

It can be shown that an inverse Mpemba effect also exists wherein the system is heated instead of being cooled. The condition for the inverse Mpemba effect to be present turns out to be the same as in eq. (10). An example is illustrated in fig. 1(b). Initially $Q$ is at a lower temperature. On being heated to a common higher temperature, it can be seen that $Q$ equilibrates faster. Again, the difference between the exact linearised solution and the full numerical solution of the non-linear equation is negligible.

We also explore the possibility of the strong Mpemba effect in which the system at higher temperature cools exponentially faster. The linear evolution equation in eq. (8) allows a certain set of initial conditions to relax to the final stationary state exponentially faster compared to other initial states. The effect may be realised when the coefficient associated with the slower relaxation rate in the time evolution of total temperature, $T^\text{tot}(t^*)$, vanishes. Setting the coefficient (K) associated with the slower relaxation
The critical line does not show the Mpemba effect. Line show the Mpemba effect whereas the region on the other side of the critical line does not show the Mpemba effect.

Fig. 2: The $\Delta T_{tot}/\Delta T_{diff}$-r phase diagram showing regions where the Mpemba effect is observed and $r$ is the coefficient of restitution. All other parameters are kept constant. Here, both the systems are quenched to the final stationary state given by $T_{tot} = 1.0$ and $T_{diff}/T_{tot} = 0.15$. The region below the critical line show the Mpemba effect whereas the region on the other side of the critical line does not show the Mpemba effect.

Fig. 3: Time evolution of $T_{tot}(t^*)$ with $t^*$ for two identical systems $P$ and $Q$ with initial conditions $T_{tot}^{P(0)}/T_{tot} = 1.026$, $T_{diff}^{P(0)}/T_{tot} = 0.456$ ($\xi_{0y}/\xi_{0x} = 0.08$), $T_{tot}^{Q(0)}/T_{tot} = 1.014$ and $T_{diff}^{Q(0)}/T_{tot} = 0.2$ ($\xi_{0y}/\xi_{0x} = 0.438$) which are chosen close to the final stationary state values of $T_{tot} = 1.0$ and $T_{diff}/T_{tot} = 0.1$ ($\xi_{0y}/\xi_{0x} = 0.667$). $P$ cools exponentially faster than $Q$ though it has higher initial temperature and thus exhibits the strong Mpemba effect. The other parameters used for the systems are $m = 1$, $n\sigma^2 = 0.02$ and $r = 0.2$.

Fig. 4: (a) The time evolution of $T_{tot}(t^*)$ with time $t^*$ for two systems $P$ and $Q$, with initial conditions $T_{tot}^{P(0)}/T_{tot} = 1.051$, $T_{diff}^{P(0)}/T_{tot} = 0.294$ ($\xi_{0y}/\xi_{0x} = 3.64 \times 10^{-3}$), $T_{tot}^{Q(0)}/T_{tot} = 1.046$ and $T_{diff}^{Q(0)}/T_{tot} = -0.172$ ($\xi_{0y}/\xi_{0x} = 3.87$), show the Mpemba effect when quenched to the final stationary state values of $T_{tot} = 1.0$ and $T_{diff}/T_{tot} = 0.279$ ($\xi_{0y}/\xi_{0x} = 3.89 \times 10^{-3}$). (b) The initial conditions $T_{tot}^{P(0)}/T_{tot} = 0.953$, $T_{diff}^{P(0)}/T_{tot} = 0.267$ ($\xi_{0y}/\xi_{0x} = 3.59 \times 10^{-3}$), $T_{tot}^{Q(0)}/T_{tot} = 0.948$ and $T_{diff}^{Q(0)}/T_{tot} = -0.156$ ($\xi_{0y}/\xi_{0x} = 3.89$) show the inverse Mpemba effect when heated to the final stationary state values of $T_{tot} = 1.0$ and $T_{diff}/T_{tot} = 0.279$ ($\xi_{0y}/\xi_{0x} = 3.89 \times 10^{-3}$). The solid lines represent the exact time evolution of $T_{tot}$ and the points represent the results from simulation. The other parameters used for the systems are $m = 1$, $n\sigma^2 = 0.02$ and $r = 0.65$.

Fig. 4 shows the time evolution of the total temperature, $T_{tot}$, with time, $t^*$, when the two systems, $P$ and $Q$ are driven from their different stationary state initial conditions to a same final state. In order to compare between the theory and simulation results, we plot the ratio of $T_{tot}/T_{tot}^{\ast}$ obtained from the respective theoretical and simulation results. The solid lines represent the theoretical predictions as obtained by solving the full non-linear equation (5) by assuming Gaussian distribution for the velocity distribution function whereas the points denote the results obtained from the MD simulations. Clearly, there is a good agreement between the theoretical predictions and the results from the MD simulations for both the Mpemba effect (see fig. 4(a)) and its inverse (see fig. 4(b)).
For much larger initial temperatures (twice as large), the comparison between simulation and the numerical solution of eq. (5) is shown in fig. 2 of the SM. While there is a small quantitative difference, the qualitative features of the Mpemba effect persist.

To summarise, we showed the existence of the Mpemba effect, the inverse Mpemba effect and the strong Mpemba effect in an anisotropically driven granular gas. The key feature is that the initial states are stationary states unlike earlier analysis of the Mpemba effect in isotropically driven granular systems which required the initial states to be non-stationary. Our analysis also shows that anisotropy in the velocity distribution of particles is a key ingredient for the existence of such anomalous behaviour, and the Mpemba effect vanishes when the collisions become elastic. It also demonstrates that the Mpemba effect, though usually studied in detailed balanced systems, is more general and is applicable to systems far from equilibrium. The time taken to relax to the steady state could depend anomalously on the distance of the steady state from which it is quenched. Though the exact results were based on a linearised theory for a spatially homogeneous system, MD simulations of hard discs in two dimensions show that the results are true for a spatially extended system also. Achieving anisotropic driving in experiments is not difficult as the amplitude and frequency of shaking can be chosen to be different in different directions, and should therefore allow for an experimental realisation, which has been hitherto lacking, of the Mpemba effect in granular systems.

Data availability statement: The data that support the findings of this study are available upon reasonable request from the authors.

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