Traces of Integrability in Relaxation of One-Dimensional Two-Mass Mixtures

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Abstract We study relaxation in a one-dimensional two-mass mixture of hard-core particles. A heavy-light-heavy triplet of three neighboring particles can form a little known unequal mass generalization of Newton’s cradle at particular light-to-heavy mass ratios. An anomalous slow-down in the relaxation of the whole system is expected due to the presence of these triplets, and we provide numerical evidence to support this prediction. The expected experimental realization of our model involves mixtures of two internal states in optical lattices, where the ratio between effective masses can be controlled at will.

Keywords Newton’s cradle · hard-core particles · mass mixture · integrability · thermalization · ergodicity · root systems · kaleidoscopes

1 Introduction

A large finite collection of equal mass, hard-core, point particles undergoing elastic collisions in one dimension with periodic boundary conditions is a strictly non-ergodic system [1]. Ergodicity is expected to emerge however, should the masses be made unequal [2]. Yet while such a system of unequal mass particles may be ergodic as a whole—any observable of the whole system is expected to relax towards its ensemble average—collisions between

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particles within a subset of the system may not always contribute to the overall relaxation of the whole system. This of course is trivially true for subsets that only consist of equal mass particles, but we will demonstrate that it is also true for certain subsets of three unequal mass particles that form a generalized Newton’s cradle.

2 A Generalization of Newton’s Cradle with Three Particles

Newton’s cradle is usually encountered as a simple device used to demonstrate the conservation of energy and momentum. The typical cradle consists of a line of identical pendulums. When a pendulum on one end is lifted and released, it will fall and strike the other stationary pendulums with some velocity. After a cascade of two-body collisions, the pendulum on the other end will be ejected with that same velocity, while all other pendulums are now stationary. There are numerous variations to this basic process, such as imparting multiple pendulums with an initial velocity before the cascade. Although there are many subtleties underlying the operation of the physical Newton’s cradle [3], we will overlook these and only focus on one particular phenomenon: if equal mass particles are indistinguishable, then the set of mass-velocity pairs before and after a cascade of collisions should be identical in a Newton’s cradle. Taking this as a defining characteristic, we will generalize Newton’s cradle to include unequal masses, while still conserving the mass-velocity pairs over cascades of collisions.

Consider a system of three hard-core particles on an open line. Let their masses be $m_1$, $m_2$, $m_3$ with positions $x_1$, $x_2$, $x_3$. The Lagrangian of this system may be written as

$$L = \frac{1}{2} \sum_{i=1}^{3} m_i \dot{x}_i^2 + V(x_1, x_2, x_3).$$  \hspace{1cm} (1)

Without loss of generality, we may choose $x_1 \leq x_2 \leq x_3$, which will fix the potential as

$$V(x_1, x_2, x_3) = \begin{cases} 0 & \text{if } x_1 \leq x_2 \leq x_3, \\ \infty & \text{otherwise} \end{cases}.$$  \hspace{1cm} (2)

Using the Jacobi coordinates (see for example [4])

$$x = \sqrt{\frac{m_1 m_2}{m_1 + m_2}} (x_1 - x_2),$$  \hspace{1cm} (3)

$$y = \sqrt{\frac{m_3 (m_1 + m_2)}{m_1 + m_2 + m_3}} \left( \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2} - x_3 \right),$$  \hspace{1cm} (4)

$$z = \frac{1}{\sqrt{m_1 + m_2 + m_3}} (m_1 x_1 + m_2 x_2 + m_3 x_3),$$  \hspace{1cm} (5)

the Lagrangian can be transformed into

$$L = \frac{1}{2} (\dot{x}^2 + y^2 + z^2) + V(x, y, z),$$  \hspace{1cm} (6)
Fig. 1 The $x$ and $y$ Jacobi coordinates for the relative motion in a three particle system. The system is confined to the $x_1 \leq x_2 \leq x_3$ shaded region by choice. There are six wedged regions that correspond to the possible permutations of three particles on a line. In this figure, we have set $m_1 = m_3 = M$ and $m_2 = m$ with $m/M = \sqrt{5} - 2$. The angle between the $x_1 = x_2$ and $x_2 = x_3$ line here is $\pi/5$.

with a potential of

$$V(x, y, z) = \begin{cases} 
0 & \text{if } x \leq 0 \text{ and } y \leq \left( \frac{m_1 m_3}{m_2 (m_1 + m_2 + m_3)} \right)^{1/2} x \\
\infty & \text{otherwise}
\end{cases}$$

(7)

The $z$ coordinate above is proportional to the center of mass coordinate of the three particles. Since the time evolution of the center of mass is decoupled from the collision dynamics of the particles, we may eliminate the $z$ coordinate from our analysis. The motion of three particles in one dimension can thus be mapped into the motion of one particle of unit mass in two dimensions as seen in Fig. 1.

On this two-dimensional plane, the relative positions of the three particles are encoded within the $x$ and $y$ coordinates. The trajectory of the three particles is represented by a ray, the orientation of which determines the relative velocities of the three particles up to a rescaling of time. As a consequence of choosing $x_1 \leq x_2 \leq x_3$, the single point that now represents the particles will be constrained to move within a wedged region bounded by two hard walls. The scalar mass of this point also obliges it to undergo specular reflection whenever it impacts the two hard walls. The overall setup here resembles that of a dynamical billiard, except for the open boundaries. A proper triangular billiard with closed boundaries would correspond to a system of two particles in one dimension bounded by two hard walls [5,6,7].

The presence of specular reflection allows our transformed system to be studied with the method of images as in Fig. 2. Consider the case where the
Applying the method of images when the light-to-heavy mass ratio is \( m/M = \sqrt{5} - 2 \) results in \( \theta = \pi/5 \). As this corresponds to an odd kaleidoscope, the angle between the outgoing ray and the wall opposite the “wall of first impact” is equal to the angle between the incoming ray and the “wall of first impact”. Unlike the even kaleidoscopes, the outgoing and incoming rays are generally not parallel. Shaded region is the \( x_1 \leq x_2 \leq x_3 \) domain as seen in Fig. 1.

\( x_1 = x_2 \) and \( x_2 = x_3 \) boundaries cross at an angle \( \theta \) such that \( n = \pi/\theta \) is an integer. This allows the wedged region in which the system is confined within to tile the \( x-y \) plane. This tiling is significant because it ensures that a given set of initial velocities \( v_1, v_2, v_3 \) for three particles will always produce a unique set of final velocities \( v'_1, v'_2, v'_3 \) regardless of the order of collisions between the particles. In terms of the rays that represent the trajectory of the system, tiling allows a set of parallel incoming rays to remain parallel with each other after they undergo a cascade of reflections, regardless of which wall the rays first connect with.

In the context of quantum mechanics, the tiling property will lead to scattering without diffraction [8] and signals the integrability of the system via Bethe-ansatz. For the particular system depicted in Fig. 2 with \( n = 5 \), and similar ones with \( n \geq 7 \), the integrability would formally originate from non-crystallographic generalized kaleidoscopes associated with the \( I_2 (n) \) root systems [9]. For historical reasons, these kaleidoscopes have not been the subject in traditional studies of particle systems [4,10,11].

For the two-mass mixture that is the subject of this study, we shall set \( m_1 = m_3 = M \) to be the heavy mass and \( m_2 = m \) to be the light mass. The mass ratio can then be related to the angle \( \theta = \pi/n \) as

\[
\frac{m}{M} = \frac{1 - \cos (\pi/n)}{\cos (\pi/n)}. \tag{8}
\]

If \( n \) is odd, a system point which has not experienced any previous collisions will undergo a cascade of \( n \) collisions with the walls. The angle between
the incoming ray and the first wall will also be equal to that between the outgoing ray and the last wall. In the center of mass frame, this results in the exchange of velocities between the left and right heavy particles while the middle light particle retains its velocity. The mass-velocity pairs will be conserved even if the center of mass velocity is not zero, and such a triplet will therefore constitute a generalized Newton’s cradle. The actual outcome of a cascade at odd $n$ is

$$\begin{align*}
\begin{bmatrix}
  v_1 \\
  v_2 \\
  v_3
\end{bmatrix} \xrightarrow{n \text{ collisions}} \begin{bmatrix}
  v_3 \\
  v_2 \\
  v_1
\end{bmatrix}.
\end{align*}$$

(9)

Imagine now that three particles with odd $n$ are embedded within a gas of some other particles. Most of the time, this triplet will not manifest the behavior of a Newton’s cradle, because the necessary cascade of $n$ two-body collisions are likely to be interrupted by collisions with neighboring particles of the host gas. With finite probability however, the three particles may find themselves in such close proximity that they can complete a cascade of $n$ two-body collisions uninterrupted. Given such a complete revival of the local velocity distribution, one would expect a slowdown in the relaxation rate of the many-body system as a whole. This effect will be our focus in the next section.

If $n$ is even, a system point which has not experienced any previous collisions will also undergo a cascade $n$ collisions with the walls, but the incoming and outgoing rays will now remain parallel to each other. In the center of mass frame, this corresponds to a complete reversal of all particle velocities after such a cascade of collisions. The resulting change in velocity distribution is

$$\begin{align*}
\begin{bmatrix}
  v_1 \\
  v_2 \\
  v_3
\end{bmatrix} \xrightarrow{n \text{ collisions}} \begin{bmatrix}
  V_{CM} - (v_1 - V_{CM}) \\
  V_{CM} - (v_2 - V_{CM}) \\
  V_{CM} - (v_3 - V_{CM})
\end{bmatrix},
\end{align*}$$

(10)

where $V_{CM}$ is the center of mass velocity. In principle, such a process is not expected to change the relaxation rate of the many-body system as a whole, although there exists conditions in which it will come into effect. These circumstances will be relevant in the next section.

3 Numerical Simulation of a Two-Mass Mixture

The slowdown in the relaxation rate for a large system due to the presence of heavy-light-heavy triplets that form a generalized Newton’s cradle is demonstrated by a numerical simulation with the results shown in Fig. 3. The initial condition consists of 100 light and 200 heavy particles randomly positioned within the $[0,1]$ interval. We set $M = 1$ and adjust $m$ to achieve different mass ratios. All light particles are initially stationary, while half the heavy particles are randomly chosen to have initial momentum +1, and the other
Fig. 3 Relaxation time of the observable $\chi \equiv \langle E^2 \rangle / \langle E \rangle^2$ (see main text for full definition) as a function of mass ratio. The vertical axis is the relaxation time in units of $(\rho_l v_h)^{-1}$, where $\rho_l$ is the number density of the light particles, and $v_h$ is the initial speed of the heavy particles. The $(\rho_l v_h)^{-1}$ parameter provides an order-of-magnitude estimate for the mean free time between collisions with light particles for a given heavy particle. Vertical dotted lines correspond to mass ratios where $\pi/\theta$ is an integer and peaks are expected to occur, starting from $\theta = \pi/10$ on the left and progressing to $\theta = \pi/4$ on the right. The $I_2(n)$ symbol denotes a root system that generates a two-mirror two-dimensional kaleidoscope with an angle of $\pi/n$ between the two mirrors [9].

half $-1$. To monitor the rate of relaxation, we chose the observable

$$\chi = \frac{\langle E^2 \rangle}{\langle E \rangle^2},$$

where the average kinetic energy and average of kinetic energy squared are taken over all particles. This observable has a value of 1.5 under our initial condition and is expected to rise to 3 if the system is fully thermalized into a Maxwell-Boltzmann distribution. Since equal mass collisions do not contribute to relaxation, the simulation is carried out over a fixed length of 10,000 light-heavy collisions. At each mass ratio, the simulation is repeated 5,000 times and the average value of $\chi$ as a function of the number of light-heavy collisions is fit to an exponential curve to extract a time constant.

Figure 3 demonstrates that there are clear peaks in the relaxation time at the expected mass ratios where $\pi/\theta$ is an integer. The background curve also exhibits two expected features. As $m/M \to 1$ on the right, the relaxation time should diverge as the system is approaching the exactly integrable equal mass configuration. When $m/M \to 0$ on the left, the relaxation time should also diverge since it will take infinitely many light-heavy collisions to change the velocity of the heavy particles.
Notice that the peaks are present at both odd and even values of $n$. As discussed in the previous section, peaks in relaxation time are expected around odd values of $n$ as a result of local triplets forming a generalized Newton’s cradle. For even values of $n$, a complete uninterrupted cascade of two-body collisions merely reverses all velocities in the center of mass frame, and there is no a priori expectation that this will result in a slowdown in the overall rate of relaxation for the many-body system as a whole. Two effects may contribute to these peaks at even $n$:

1. The tiling property for all kaleidoscopes guarantees that any set of initial velocities will always produce a unique set of final velocities after a complete cascade of collisions. The uncertainty in the final velocity distribution is therefore lower at these kaleidoscopic mass ratios when compared to a generic sequence of collisions, for both even and odd $n$.

2. With our initial velocity distribution, any heavy-light-heavy triplet that is ready to undergo a complete cascade will have zero center of mass velocity: the two heavy particles must be approaching the stationary light particle in between them. For this initial condition, the reflection of all velocities about the center of mass velocity after a complete cascade is equivalent to a revival of the initial velocity distribution. As the many-body system continues to relax however, memory of the initial distribution should also erode and weaken this effect.

Neither effects above have been quantified in detail, and a complete explanation for the increase in relaxation time at mass ratios with even $n$ is still required.

4 Conclusions and Outlook

Using simple geometric arguments, we showed that a triplet of heavy-light-heavy hard-core particles in one dimension can form a generalized Newton’s cradle at particular light-to-heavy mass ratios. This generalized Newton’s cradle will preserve the velocity distribution of the particles as they undergo a cascade of collisions: a series of two-body collisions that begins with the triplets not having any prior collisions, and ends with them moving away from each other and never colliding again. We provided numerical evidence that the presence of this generalized Newton’s cradle at the three-body level manifests itself in a larger many-body system as peaks in the relaxation time as a function of the mass ratio. The expected experimental realization of our model involves mixtures of two internal states in optical lattices, where the ratio between effective masses can be controlled at will [12].

There are several questions that remain open for study. Both the peak-to-background ratio and overall background curve require a quantitative theoretical foundation. A better explanation for the peaks in relaxation time at even $n$ is also needed. An interesting possibility for future research is provided by possible cases of integrability at the four-body level [13].

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