Incomplete thermalization from trap-induced integrability breaking: lessons from classical hard rods

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The familiar Newton’s cradle can be modeled as a one-dimensional gas of hard rods trapped in a harmonic potential, which breaks integrability of the hard-rod interaction in a non-uniform way. We explore the consequences of such broken integrability for the dynamics of a large number of particles and find three distinct regimes: initial, chaotic, and stationary. The initial regime is captured by an evolution equation for the phase-space distribution function. However, for any finite number of particles, this hydrodynamics breaks down due to a “complexity crisis” and the dynamics become chaotic after a characteristic time scale determined by the inter-particle distance and scattering length. At long times, the system fails to thermalize and the time-averaged ensemble of individual trajectories is not micro-canonical, but it is a stationary state of the hydrodynamic evolution. We close by discussing logical extensions of the results to similar systems of quantum particles.

Introduction. It has been known since the work of Poincaré that even the simplest mechanical systems can exhibit complex dynamics, with chaotic behavior as the norm and integrability as a somewhat special case. This distinction is only sharpened as the number of degrees of freedom increases. The time-evolution of a generic interacting many-body system is chaotic and ergodic: starting from any initial condition, trajectories of the system sample uniformly all configurations allowed by a few conservation laws, and are subject to the laws of statistical mechanics. The integrable many-body systems are exceptions to this rule, and are able to escape ergodicity and conventional thermalization thanks to the existence of an extensive number of conserved quantities.

In practice, exact integrability is fine-tuned and vulnerable to real-world imperfections, so that systems with broken integrability are more abundant than perfectly integrable ones. Moreover, broken integrability provides valuable insights into the general theory of dynamical systems. For example, in classical mechanics, the KAM theorem [1] states that for weak enough perturbations, integrability is preserved in some finite portion of the phase space. For a uniform perturbation of a many-body system, the integrability-preserving phase-space often becomes vanishingly small, and no such “gray zone” is allowed. Such a sharp distinction extends in general to quantum many-body systems [2], although thermalization can be parametrically slow with weak integrability breaking [3–5].

In this work, we examine the consequences of the non-uniform integrability breaking that results from placing an integrable many-body system in a trap. A famous experimental realization of this scenario is the “quantum Newton’s cradle”, which consists of a trapped, quasi one-dimensional Bose gas in a harmonic trap [6, 7]. In the absence of the trap, the system is integrable and does not thermalize; even with the trap, which destroys the higher conservation laws needed for integrability, it is found that the system fails to thermalize over experimentally accessible time-scales. Here, the trap plays a delicate role: it is needed to observe periodic motion, rather than a simple expansion of the trapped gas, but also liable to destroy it eventually due to its breaking integrability. This raises two natural questions: what is the time scale \( t_s \) induced by integrability breaking, defined as the advent of chaos, and does the system reach thermal equilibrium in the long-time limit?

In the present work, we address these questions starting from the classical Newton’s cradle, idealized as a one-dimensional gas of hard rods [8] in a harmonic trap, whose time evolution can be obtained exactly from molecular dynamics simulations. We propose the following simple scaling law for \( t_s \), in terms of the potential curvature \( V''(x) \), particle mass \( m \), the scattering length (rod length) \( a \) and the maximal gas density \( \rho_m \),

\[
\frac{1}{t_s} = C \rho_m a \omega, \quad \omega = \sqrt{V''(x)/m},
\]

where \( C \) is an order-unity dimensionless pre-factor. Our short answer to the second question is unexpectedly no: the system is chaotic but does not thermalize even on rather long time scales. The full answer is quite elaborate and related to the other theme of this work: the validity of classical and quantum hydrodynamical equations in systems whose integrability is destroyed by a trap [9].

We find that both an initial transient period and the long-time stationary ensemble of the classical Newton’s cradle are usefully captured by the kinetic theory of hard rods [10–12], albeit in different senses, while there is an intervening chaotic regime in which hydrodynamics fails. An area of recent progress is that kinetic equations of the same (dissipationless Boltzmann) type capture the large-scale dynamics of quantum integrable systems [13–22], with a self-consistent velocity functional drawn from the Bethe equations. In the presence of a trap, the range of validity of the minimal adaptation of the kinetic equation for Lieb-Liniger is not yet clear [15]. Here, we obtain
suggestive results about the range of validity by studying the analogous problem for the classical hard-rod gas, as it is straightforward to write down a trapped hard-rod equation (tHRE) in the presence of an external potential. By a direct comparison against microscopic simulations, we show that the tHRE is accurate in an initial regime $t < t_*$, but must eventually break down for any finite system-size, due to a “complexity crisis” that will be explained. Despite the onset of chaos, we find that the late-time non-thermal ensembles define stationary solutions to the tHRE.

**Trapped hard-rod gas.** The hard-rod gas in a harmonic trap is equivalent to \( N \) one-dimensional harmonic oscillators with hard-core repulsive interaction. The Hamiltonian reads

\[
H = \sum_{j=1}^{N} \left[ \frac{1}{2} p_j^2 + V(x_j) \right] + \sum_{j<k} U(x_j - x_k) \tag{2a}
\]

\[
V(x) = \frac{1}{2} \omega^2 x^2, \quad U(\delta x) = \begin{cases} 0 & |\delta x| > a \\ \infty & |\delta x| \leq a, \end{cases} \tag{2b}
\]

where \( a > 0 \) denotes the rod length, and \( x_j \) and \( p_j \) denote positions and momenta (we set \( m = 1 \)). Upon re-scaling time as \( t \to t \omega \), we may set \( \omega = 1 \) without loss of generality. Starting from a configuration such that \( x_{j+1} - x_j \geq a \), \( j = 1, \ldots, N - 1 \), the gas evolves as \( N \) decoupled oscillators, until the next collision (i.e., \( x_{j+1} - x_j = a \) for some \( j \)) in which the rods \( j \) and \( j + 1 \) exchange their velocities spontaneously. Such a dynamics can be efficiently and exactly simulated. There are two integrable limits. Upon removing the trap, one recovers the usual hard-rod gas. Its momentum distribution is conserved and its dynamics map to those of \( N \) independent particles. Meanwhile, in the limit of vanishing rod length \( a = 0 \), we obtain \( N \) decoupled harmonic oscillators. Yet, in the presence of both trap and interaction, we find no other conserved quantities besides the total energy and the center of mass energy \( H_m \), which we set to 0 [23].

To provide more convincing evidence of microscopic non-integrability, we studied the three-body problem. Its phase space, subject to the constraints \( H_m = 0 \) and \( H = \text{const} \), is three-dimensional and one can visualize the orbits of the Poincaré recurrence map, defined on a 2D sector of colliding configurations, as in Fig. 1. The fractal structure observed is inconsistent with the existence of any higher analytic integrals of motion. Yet, most trajectories do not cover the available phase space, so are not micro-canonical.

**Hydrodynamics.** The large-scale, coarse-grained dynamics of the hard-rod gas without the trap is described by a Boltzmann-type equation, which governs the single-particle phase space distribution \( \rho(x, p) = \frac{d^N x}{dx dp} \). Collisions conserve particles’ momenta but modify their effective velocities. The resulting kinetic equation,

\[
\partial_t \rho + \partial_x (vp) = 0, \quad v[p](p) = p + \frac{\int v' \rho(p') \rho(x, p')}{1 - \int v' \rho(x, p')}, \tag{3}
\]

was first obtained by Percus [10], and rigorously proven to define an Euler-scale hydrodynamics of the hard-rod gas in Ref. [11]. Recently, equations similar to eq. (3) were shown to capture a variety of large-scale dynamics in quantum integrable systems [13–22], in which context we call eq. (3) the Bethe-Boltzmann equation (BBE), since the analogue of \( v[p](p) \) is obtained from thermodynamic Bethe ansatz. A modification of BBE in an external potential was proposed in Ref. [15], which coincides with the standard Boltzmann correction for the Lieb-Liniger and quantum hard-rod models [24]. For classical hard-rods, the same correction can be obtained by different arguments [25], and yields

\[
\partial_t \rho + \partial_x (vp) - \partial_x V \partial_v \rho = 0. \tag{4}
\]

Since the trap breaks integrability of the microscopic dynamics, the validity of eq. (4) is so far a hypothesis to be tested.

Nevertheless, the tHRE is conceptually helpful as a guide to defining the thermodynamic \( (N \to \infty) \) limit. Indeed, eq. (4) has an emergent scale-invariance, \( (\rho, a) \to (\lambda \rho, a/\lambda) \) in any potential \( V \), which relates pairs of systems with different \( N \). Now, in a harmonic trap, we can further apply a spatial rescaling \( (x, a) \to (\lambda x, \lambda a) \), and define profiles of different \( N \) corresponding to a fixed hydrodynamic profile \( \bar{\rho} \), with \( a = 1 \) fixed:

\[
\rho(x, k) := \bar{\rho}(\tilde{x} = x/N, \tilde{p} = p/N) / N. \tag{5}
\]

Therefore, we will set \( a = 1 \) in what follows.
We consider initial conditions (ICs) with Gaussian profiles: $\hat{\rho}(\hat{x}, \hat{p}) = \exp\left( -\frac{\sigma_x^2}{2\pi^2} - \frac{\sigma_p^2}{2\pi^2} \right) / (2\pi\sigma_x\sigma_p)$. We can check that $\sigma = \sqrt{\sigma_x^2 + \sigma_p^2}$ and $N$ fixes the total energy. We also define a characteristic density:

$$\rho_m = 1/\sqrt{\pi\sigma}. \tag{6}$$

$\rho_m$ is proportional to the density of $\rho(x, p)$ at origin, with a pre-factor depending only on $\sigma/\sigma_x$, which describes how “squeezed” the IC is.

The results will be discussed in three consecutive time regimes: initial, chaotic and late-time.

**Initial regime and tHRE breakdown.** Using the protocols defined above, we can compare the exact microscopic dynamics against predictions from tHRE, which we expect to be valid at least at short times, when integrability remains unbroken. To this end, we adapt the scheme developed in Refs. [17, 18] to solve numerically the tHRE; the microscopic result is averaged over many ICs sampling the same initial hydrodynamic profile. An example comparison is illustrated in Fig. 2. A damped density oscillation is observed in the short-time dynamics, and is accurately captured by tHRE. Therefore, damping per se is not a signature of integrability breaking. To understand the nature of damping, we visualize the evolution of $\rho(x, p)$ in Fig. 3(a), choosing more squeezed ICs to accentuate damping. Recall that the absence of interaction ($a = 0$) would lead to a simple rotation of the IC with unique frequency $\omega = 1$. The interaction induces a dephasing, responsible for the damping. In the $x$-$p$ phase space, the dephasing generates a complex structure, reminiscent of a growing galaxy. Such galaxy formation is also observed in the numerical solution of the tHRE. Because the tHRE is dissipationless, we believe that the galaxy’s arms will grow forever. In other words, the tHRE solution has ever-increasing complexity, which any finite-$N$ system cannot reproduce exactly: then, tHRE must break down, due to a “complexity crisis”. Systems with larger $N$ have higher resolution and resist the complexity crisis better.

Now, the quantitative measure of the complexity crisis is nothing but entropy growth. Indeed, the dissipation-less tHRE conserves the entropy functional of the hard-rod gas,

$$S := \int_x \rho \ln \theta, \quad \text{where} \quad \theta(x, p) := \frac{\rho(x, p)}{1 - a \rho(x, p) \rho(x', p')} \tag{7}$$

Hence, measuring the time-evolution of $S$ from microscopic simulations is a stringent test of the validity of tHRE without solving it directly. The result, in Fig. 3 (b), shows a clear entropy growth after $t \sim 10$, invalidating tHRE. The growth is suppressed for larger $N$, as expected. Note that for the circular IC studied in Fig. 2, the entropy is almost constant, consistent with the observed success of tHRE.

**Advent of chaos.** Having studied in some detail the qualitative mechanism of tHRE breakdown, we now turn to its time scale, and present evidence for the scaling relation eq. (1). To this end, we measure chaos as it is defined: the exponential separation of $N$-body phase space trajectories [26]. We first consider circular ICs with varying $\rho_m a$, and small initial perturbations to the leftmost rod position $\delta x_1(0) = -10^{-4}$, and measure the average deviation induced particle positions $\delta x_i(t)$ after evolution [27]. The result, shown Fig. 4-a, displays a clear cross-over from the initial regime to a chaotic one, at a time $1/t_s = C\rho_m a$, eq. (1), where $C \approx 0.1$. This scaling relation is non-trivial: the period of short-time oscillation does not scale with $\rho_m a$, but its envelope evolution does so. The data collapse at the exponential chaos regime also implies the Lyapunov exponent scaling $\gamma \propto a \rho_m$. The proportionality constant above depends on other aspects of the IC, but is in general positively correlated with the amount of entropy growth, see Fig. (3). Now,
this reasonable sounding observation has the following unlikely consequence: chaos is suppressed in the thermodynamic $N \to \infty$ limit! In fact our data are consistent with the power law

$$\gamma \propto a \rho_m N^{-v}, \quad v \approx 0.25,$$

shown in Fig. (4)-b. Such a many-body suppression of chaos implies that the limits $t \to \infty$ and $N \to \infty$ do not commute. We expect this to be a general feature of “weak” integrability breaking in a trap. Although microscopic integrability is destroyed by a trap, infinitely many conserved quantities (including the entropy) of the HRE remain conserved for the tHRE [28], and are responsible for suppressing chaos and entropy growth in large systems.

Late time ensemble. The previous results all involve averaging over some initial configuration ensemble. From now on, we focus on single, long trajectories, and average only over time. In a generic thermalizing system, such a time-averaged ensemble converges swiftly to the microcanonical ensemble, even when the IC is highly atypical thermodynamically (consider filling only a half of a box with gas). Thermalization is usually associated with chaos, since exponential separation of nearby trajectories means that the initial condition is quickly forgotten. Therefore, one would expect that the trapped hard-rod gas thermalizes at late times $t \gg \tau_c$.

One can test for thermalization by studying the late-time velocity distribution, which is Gaussian in the canonical ensemble, and thus also in the microcanonical ensemble for large $N$ under equivalence of ensembles. In Fig. 5, we perform a standard Gaussian test for the velocity distribution of time-averaged ensembles obtained from evolving some squeezed IC with $\rho_m a = 1/2$ (to ensure fast advent of chaos), up to $\theta = 2 \times 10^4$. The result shows a clear deviation from Gaussianity, which persists in the stationary regime and moreover amplifies as $N$ increases, barring finite-size effects. In comparison, a modified dynamics which shuffles randomly the velocities every unit time thermalizes far more quickly. The observed failure to thermalize does not depend on the IC chosen. Indeed, even for thermally typical ICs, the time-averaged ensembles show visible (although smaller) deviation from Gaussianity [29]. Furthermore, the dependence on ICs is unpredictable, due to chaos.

Nevertheless, we propose a simple description of the late-time ensembles: their phase-space distribution is a stationary solution of the tHRE:

$$\partial_x (v \rho) - \partial_x V \partial_p \rho = 0. \quad (9)$$

The idea is quite simple: the late-time ensemble is by definition independent of time, and so should be void of macroscopic momentum flow on average, which the tHRE calculates to leading order (in a derivative expansion). Since late-time ensemble distributions are usually quite smooth and gently varying, it seems reasonable to hope that eq. (9) will perform well.

To test our proposal, we invoke the following fact: $\rho$ solves eq. (9) if and only if the corresponding Fermi factor $\theta$ [see eq. (7)] depends only on $\frac{1}{2} p^2 + \int_0^\infty \left( 1 - a \int_{p'} \rho(y, p') \right) y dy$. This makes it possible to reconstruct the velocity distribution of any solution $\rho$ from its density. We can apply this to the time-averaged density and compare with the true velocity distribution: our proposal holds if the true and reconstructed distributions coincide. We performed this test on numerous late-time ensembles, and show two examples in Fig. 5. The results are excellent almost everywhere, except that a small discrepancy is observed near sharp central peaks, possibly due to diffusive corrections [12]. Overall, the proposed description is remarkably successful given its simplicity, and suggests a tempting scenario of non-thermalization: the resurrection of tHRE implies that its conserved quantities become again microscopically conserved after time-averaging (for the entropy, this can be seen in Fig. 3), and prevents the late-time system from thermalizing further.
Conclusion. The idealized classical Newton’s cradle is a paradigm of integrability breaking by a trap, and displays dynamical features which defy commonly held beliefs regarding the behavior of many-body interacting systems. Chaos is suppressed in larger systems, and does not lead to thermalization. The relation with kinetic theory via tHRE is also intriguing: the latter is valid at short time and long time, and breaks down during the intermediate chaotic regime.

It would be very interesting to explore how far the above findings extend to quantum many-body systems, and it seems reasonable to expect that the three-regime scenario remains valid in regimes where the quantum-mechanical wavelength $\lambda$ is much smaller than $a$ and $1/p$. Otherwise, the eq. (1) is possibly a lower bound: $t_\ast \geq 1/(C a \rho \omega)$. Indeed, in the weakly interacting limit, $a \rightarrow \infty$ in 1D, but an infinitely fast advent of chaos is unphysical. At the same time, quantum coherence may make finite-$N$ systems more resilient to the complexity crisis [26]. Nevertheless, since the above arguments are general, we expect that the late-time ensemble of a trapped $\delta$ Bose gas still satisfies the corresponding kinetic equation, even in fully quantum regimes.

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