Nonergodicity and localization of invariant measure for two colliding masses

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We show evidence, based on extensive and carefully performed numerical experiments, that the system of two elastic hard-point masses in one dimension is not ergodic for a generic mass ratio and consequently does not follow the principle of energy equipartition. This system is equivalent to a right triangular billiard. Remarkably, following the time-dependent probability distribution in a suitably chosen velocity direction space, we find evidence of exponential localization of invariant measure. For nongeneric mass ratios which correspond to billiard angles which are rational, or weak irrational multiples of π, the system is ergodic, consistent with existing rigorous results.

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I. INTRODUCTION

The famous ergodic hypothesis formulated by Boltzmann in the second half of the nineteenth century is at the foundation of all of statistical physics, both classical and quantum [1]. A main result is the equivalence of time averages with phase averages, which, in particular, implies energy equipartition among different degrees of freedom. The problem of the foundations of statistical physics has a long and very rich history culminating in the celebrated work of Fermi, Pasta, and Ulam [2], which, contrary to general expectations, showed the lack of equipartition in a system of interacting particles. This discovery, which Fermi himself considered one of his most important contributions, gave birth to the field of nonlinear dynamics and chaos. On the rigorous side, the contributions from Poincaré [3] to Kolmogorov-Arnold-Moser (KAM) [4] have shown that generic Hamiltonian systems are not ergodic but display a phase space with a very complicated and intricate structure of stability islands embedded in a sea of chaotic trajectories.

It has to be remarked that, as shown independently in 1913 by Plancherel and Rosenthal [5], the original Boltzmann ergodic hypothesis, namely, that an orbit in the course of time passes through every point of a constant-energy surface in phase space, is not compatible with Newton's law. To overcome this difficulty P. Ehrenfest and T. Ehrenfest-Afanassjewa [6] proposed to substitute the ergodic hypothesis with the weaker "quasi-ergodic hypothesis," that is that the trajectory lies densely (i.e., passes arbitrarily close to every point) on the energy hypersurface. The quasiergodic hypothesis does not mathematically entail that time averages are equal to phase averages, but this has always been considered mainly as an abstract mathematical difficulty, whereas a common expectation was that physical quasiergodic systems are also ergodic. Essentially all known nonergodic systems belong to the usual KAM scenario of divided phase space with the presence of stable islands with positive measure [7].

In this paper we present an extremely simple physical model with no stability islands and for which the orbits are dense on the energy surface, yet the system is nonergodic and violates equipartition of energy. The reason for such a remarkable and surprising property is rooted in a "localization phenomenon" in the velocity space as described below, so that some regions of phase space are visited with exponentially small probability. Our conclusion is based on accurate numerical evidence, while a rigorous mathematical proof is likely to be extremely difficult.

We consider a bound system with two degrees of freedom, namely, two point particles in one dimension with masses m_1 and m_2 which collide elastically with each other and with the walls of a container placed at an arbitrary distance. The dynamics of the model can be reduced to a simple, elementary, map. Let x_1, x_2 and v_1, v_2 be the positions and velocities of the two particles. After the collision, the new velocities v'_1, v'_2 are given by

$$\begin{pmatrix} v'_1 \\ v'_2 \end{pmatrix} = \begin{pmatrix} \cos\alpha & 1 - \cos\alpha \\ 1 + \cos\alpha & -\cos\alpha \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \qquad (1)$$

where

$$\cos\alpha = \frac{m_1 - m_2}{m_1 + m_2}. \qquad (2)$$

To simplify the dynamical description it is convenient to introduce the rescaling $y_i = \sqrt{m_i}x_i$, $w_i = \sqrt{m_i}v_i$, $(i = 1,2)$. Then by letting $\tan\theta = w_2/w_1$, Eq. (1) can be written as $\tan(\theta') = \tan(\alpha - \theta)$. The collisions with the left and right boundary only imply inversion of a particle's velocity and are described by $\theta' = \pi - \theta$ or $\theta' = -\theta$, respectively. It is interesting to notice that our model is equivalent to a point particle with coordinate (y_1, y_2) and velocity (w_1, w_2) moving inside a right triangular billiard with one acute angle given by $\alpha/2$.

If we now denote by C the particles collision, L and R the collision with the left and right wall, respectively, it is easy to see that CR merely rotates the velocity vector $w = (w_1, w_2)$ by the angle α while RC performs the inverse rotation. Taking into account that $L = -R$, the overall dynamics in the velocity space can be described as a rotation by an angle $\pm\alpha$ where the sequence of left and right rotations is determined by the given orbit. In other words, for a given trajectory starting with the initial angle θ_0 of direction in the scaled velocity space, the final value θ, after a finite sequence, can be written as $\varphi + K\alpha$ with K being an integer and φ being one of the following four constant values: θ_0, $-\theta_0$, $\pi - \theta_0$, and $\theta_0 - \pi$ where the

four different values correspond to the four different signs in the velocity pair. In terms of the integer K, the dynamics merely reduces to the map $K' = -K + 1$ (particles collision) and $K' = -K$ (boundary collision).

This model has been extensively studied both analytically and numerically, and in spite of its seemingly simplicity, no definite conclusion has been reached so far concerning its dynamical properties even though the prevailing opinion is that, for α being an irrational multiple of π, the system should be ergodic and weakly mixing. Indeed, if α/π is rational, i.e., $\alpha = 2\pi p/q$ with coprime integers p and q, then there are precisely $4q$ distinct velocity pairs allowed which means that K can take only q different integer values. On the other hand, when α/π is irrational, the allowed θ values become uniformly dense in the interval $[0, 2\pi]$, and it is at least possible for the system to be ergodic in the velocity space. This latter possibility has actually been suggested long ago on the basis of the first numerical investigations of the model [8] even though the authors themselves pointed out the surprisingly large total number of collisions required to observe all the allowed q values of K. Subsequent numerical investigations [9] confirmed this original conclusion. In a more recent paper [10], the case of a generic triangular billiard with all angles irrational has been considered. (The dynamics of a point particle in this billiard is equivalent to the motion of three hard-core point particles on a ring [10,11]. Triangular billiards have also been studied in Ref. [12].) Here, while empirical evidence strongly demonstrates that irrational triangular billiards are mixing, it is pointed out that no definite conclusions can be made concerning the, qualitatively different, right-triangular billiards, a problem which still remains open.

On the analytical side, the problem has attracted a lot of interest in the mathematical community [13]. For a review we refer to Ref. [14]. In particular, in Ref. [15] the rational case is considered for which the orbits with fixed initial θ_0 lie on an invariant surface M_{θ_0} determined by the finite number of velocities. A theorem of Ref. [15] states that for almost every θ_0 the flow $f_t|M_{\theta_0}$ is uniquely ergodic. This result indicates that in the irrational case an orbit densely covers the energy surface. However, it does not allow us to conclude that the system in a generic irrational case is ergodic. Indeed, it is known that the quasiergodic hypothesis, namely, that an orbit comes arbitrarily close to every point on the energy surface, is not sufficient to guarantee ergodicity, namely, that time averages are equal to phase space averages. A more recent, interesting result in Ref. [16] proves that the system is ergodic for special, nongeneric irrational values of α/π, which are very quickly approximated by sequences of rational numbers. The interesting problem remains open of what happens for a typical (generic) irrational value of α/π.

It is the purpose of this work to examine this question with the help of a highly accurate numerical analysis unaccessible previously. The result turns out to be very surprising: numerical evidence strongly suggests that for a typical irrational value of α/π, the system is nonergodic with typical invariant measures being exponentially localized in the integer direction index K.

Without loss of generality, we fix the length of the box to be unity, the mass of the first particle to be unity, $m_1 = 1$, and the total energy of the system to be $E_1 + E_2 = 1/2$.

II. THE "STRONG" IRRATIONAL CASE

We consider a mass ratio corresponding to the most irrational case $\alpha = \alpha_g$ with $\alpha_g/\pi = (\sqrt{5} - 1)/2$. In order to investigate its dynamical properties we consider a sequence of principal convergents $\alpha/\pi = M/N$ in the continued fraction representation, namely, $M/N = [0, 1, 1, 1, 1, \ldots] = 1/2, 2/3, 3/5, 5/8, 8/13, \ldots, f_i/f_{i+1}, \ldots$, where $f_{i+1} = f_i + f_{i-1}$. The idea is that the dynamical behavior of each principal convergent might allow us perhaps to draw some conclusions for the limiting $N \to \infty$, golden mean case $\alpha = \alpha_g$.

A necessary condition for ergodicity is certainly equipartition of energy in velocity space. Therefore, for a given principal convergent, it is natural to evaluate the time required for an orbit to equally populate, in time average, all the allowed ($2N$ for odd M or N for even M) values of K. It turns out that this time is exceedingly long, and for a very low approximant it already goes beyond accessible computing resources.

We then inquire about a shorter, relevant time scale, denoted by τ_K and defined as the shortest time for a trajectory to visit all the allowed values of K. Since τ_K wildly fluctuates from a trajectory to another, we compute the average $\langle \tau_K \rangle$ over an ensemble of trajectories with different initial particle positions. (The initial velocities are fixed.) The results, presented in Fig. 1, show that $\langle \tau_K \rangle$ increases exponentially with N thus implying that for the golden mean case this time diverges to infinity astonishingly fast. One may argue that the question of ergodicity for such a system may be an abstract issue, physically irrelevant: even for a low convergent M/N with $N = 500$, if one assumes that there are 10^{10} collisions per second, the time required to visit all the allowed values of velocities would be much larger than the age of the universe. Nevertheless, abstract models are known to play an important role in the theory of dynamical systems. We introduce therefore a second, much shorter time scale τ^* which will allow us to approach much closer to the golden mean via the sequence of principal convergents.
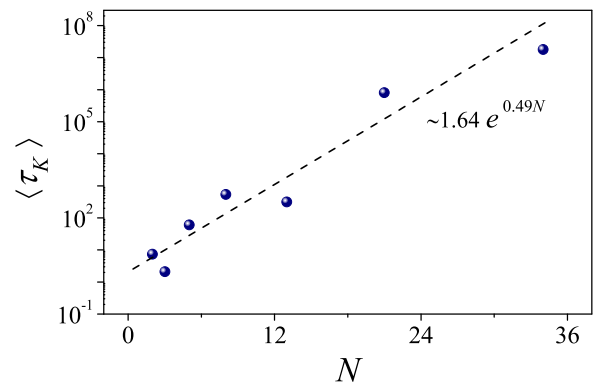

FIG. 1. (Color online) The ensemble-averaged τ_K for eight low-order rational approximants of $\alpha/\pi = (\sqrt{5} - 1)/2$. The ensemble consists of 10^4 trajectories with fixed $\theta_0 = e\pi$ but different particle positions randomly assigned. The error of each data point (not shown) is smaller than the symbol. The numerical results suggest that $\langle \tau_K \rangle$ has an exponential dependence on N. The dashed line indicates the result of the best linear fitting: $\langle \tau_K \rangle \sim e^{0.49N}$.
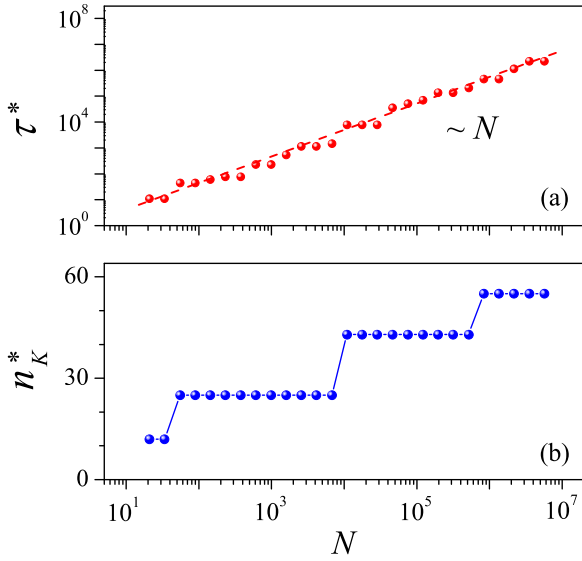
FIG. 2. (Color online) (a) The dependence of τ^* on N, in the continued fraction rational approximation M/N of $\alpha/\pi = (\sqrt{5}-1)/2$, for a given, fixed, initial condition of $\theta_0 = e\pi$ and randomly assigned particle positions. The dashed line $\sim N$ is plotted for reference. For each rational approximation, the number n_K^* of different K values visited by the trajectory up to time τ^* is shown in (b).

Let us consider two subsequent principal convergents M/N and M'/N' (with $N' > N$); the two trajectories obtained by evolving the same initial condition with $\alpha/\pi = M/N$ and M'/N', respectively, would follow the same symbolic collision sequence (of letters C, L, R) up to some time $\tau^*(N,N')$. This means that up to time $\tau^*(N,N')$, the sequence of collisions will be the same as for the limiting golden mean case. In Fig. 2(a) we plot $\tau^*(N,N')$ for a given fixed initial condition where $\theta_0/\pi = e$, and the particle positions are assigned randomly. Despite fluctuations, it can be seen that, fairly accurately, τ^* increases linearly with N. In Fig. 2(b) the number n_K^* of different K values visited by the trajectory up to time τ^* is shown. Surprisingly, we notice that while τ^* increases linearly with N, the number n_K^* of actually visited K values increases very slowly with N. Even though it is difficult to determine with sufficient accuracy the dependence on N due to the presence of sudden jumps and long plateaus, this dependence seems to be logarithmic $n_k^* \sim \ln(N)$. Therefore, for any approximant M/N of the golden mean case, the system visits only a small fraction of the allowed values of direction K up to time $\tau^* \sim N$.

We now turn to the direct consideration of the irrational case $\alpha = \alpha_g$. For this case we compute the probability density distribution function $P(K,t)$ obtained by evolving an ensemble of trajectories with the same initial particle velocities but with random initial positions in the interval $[0,1]$. In order to suppress fluctuations we make an additional, partial time average of $P(K,t)$ in the interval $[t, t + \delta t]$. The results are shown in Fig. 3, where we plot $P(K,t)$ at different times t, from 10^4 to 10^8. The main outcome is that the distribution $P(K,t)$ remains very narrow (of width ~ 100) even at very large times. As time increases the tails build up and one can observe an overall tendency to an exponential distribution.
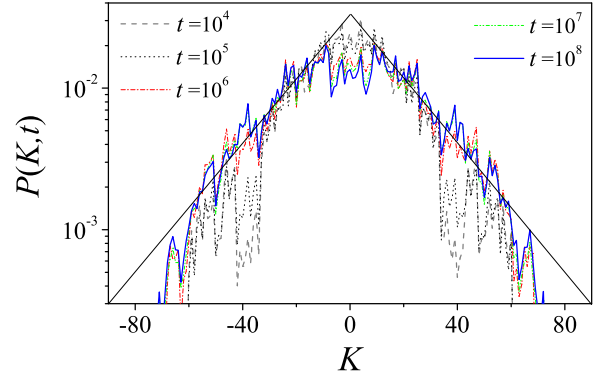

FIG. 3. (Color online) The probability density distribution function $P(K,t)$ computed at various times t for the strong irrational case with α/π being the golden mean. Starting from the lower tail, the curves are for $t = 10^4$ (dashed), 10^5 (dotted), 10^6 (dash-dotted), 10^7 (dash-dot-dotted), and 10^8 (solid), respectively. The thin black lines are drawn for reference. $\theta_0 = \pi/\sqrt{2}$, $\delta t = t/10$, and an average ensemble of 5200 trajectories is taken for evaluating $P(K,t)$ (see the text).

In Fig. 4 we plot the variance of $P(K,t)$. It is seen that the variance appears to saturate even though the convergence is very slow, probably due to the slow convergence of the tails to the exponential distribution seen in Fig. 3. The scenario which seems to emerge from Figs. 2–4 is that the system gradually "sees" the successive principal convergents of the golden mean limiting case. Correspondingly, the distribution slowly converges to an exponential shape. This implies the conjecture that for asymptotically long times $t \to \infty$, infinitely many directions K are visited. This in turn implies that typical orbit densely covers the entire phase space.

One should be very careful in drawing definite conclusions from numerical computations. However, the following results, namely, (1) the fraction of different K values visited by an orbit up to time τ^* is negligibly small, of order $\ln(N)/N$, while $\tau^* \sim N \to \infty$ in the golden mean limit, and (2) the probability distribution $P(K,t)$ has an exponential shape in the limit $t \to \infty$, strongly suggest that the golden mean case is nonergodic.
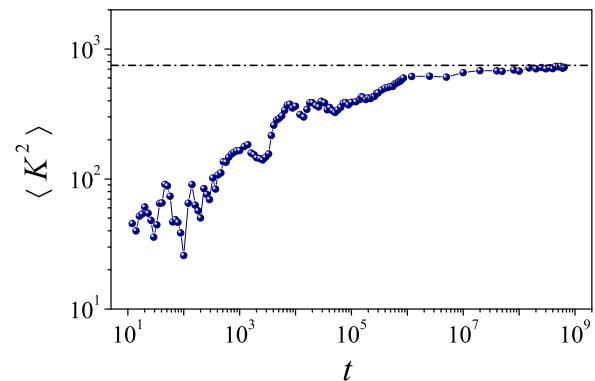

FIG. 4. (Color online) The time dependence of the variance of $P(K,t)$ for the data of Fig. 3 (bullets). The horizontal dash-dotted line is the expected saturation value corresponding to the exponential distribution in Fig. 3.

III. WEAK IRRATIONAL CASE

So far we have considered a particular mass ratio given by $\alpha = \alpha_g$. The natural question is how generic is the dynamical behavior displayed by this case. To this end we recall an important rigorous result by Vorobets [16], which states that the billiard flow in a right triangular with one acute angle $\alpha/2 = \pi(a_5^{-1} + a_{10}^{-1} + \cdots + a_{5n}^{-1} + \cdots)$, where the sequence a_n is given by $a_0 = 1$ and $a_{n+1} = 2^{a_n}$ $(n = 0,1,2,\ldots)$, is ergodic. Therefore, ergodicity takes place for an irrational α/π which is very close to rational numbers in the sense that the sequence of rational approximants has an impressively fast convergence. This result is in nice agreement with our numerical analysis. Indeed, given two subsequent principal convergents $M_i/N_i, M_{i+1}/N_{i+1}$ of an irrational α/π, in order to be ergodic it is at least necessary that the time $\tau^*(N_i,N_{i+1})$ is larger than the time $\tau_K(N_i)$ needed to visit all the allowed velocities at the ith rational approximant. Since, as we have seen, τ_K increases exponentially with N while τ^* increases only linearly, it follows that a necessary condition for ergodicity of the limiting irrational α is that $N_{i+1} \sim \exp(N_i)$. Therefore our numerical analysis not only is in agreement with the rigorous result [16] but also provides a hint for identifying the set of irrational α/π for which the system can be ergodic. These irrationals are inside the so-called set of Liouville numbers [17], which are known to have zero Lebesgue measure.

IV. DISCUSSION

It is interesting to remark that the predicted lack of ergodicity is not related to the usual picture of divided phase space with islands of stability and region of chaotic motion. Moreover, in our case, following the result of Ref. [15], a typical orbit is expected to densely cover the energy surface. Instead the nonergodic behavior derives from the exponential decay of the probability distribution $P(K,t)$ indicating exponential localization of invariant measures. This feature explains why previous numerical investigations failed to identify nonergodic behavior. The reason is not the larger computational power now available; instead it is the dynamical quantities that were investigated. To make a clear example, by the popular surface of section method it would be absolutely impossible to provide numerical evidence of nonergodic behavior in a system where the orbits are dense on the energy surface.

The behavior of our model is reminiscent of the dynamical localization phenomenon in the quantum kicked rotator [18] in which the relevant parameter is the kicking period τ. Indeed, it is known that for a typical irrational τ/π, exponential localization takes place, while it has been rigorously proven that there exist irrational values of period τ/π for which there is no localization. Actually, heuristic arguments [19] lead to the conclusion that such irrationals belong to the set of Liouville numbers. Quite clearly this analogy should be taken *cum grano salis* since the two systems belong to completely different domains. Yet they have in common that a key role is played by the randomness property of the sequence of digits of the irrational α/π or τ/π. This may open the way for a better understanding of the mechanism leading to the suppression of classical and quantum diffusion. In addition, one is confronted one more time with the fascinating richness of dynamical behavior of seemingly extremely simple systems.

[1] A. I. Khinchin, *Mathematical Foundations of Statistical Mechanics* (Dover, New York, 1949).

[2] E. Fermi, J. Pasta, and S. Ulam, Los Alamos report LA-1940 (1955); republished in *Collected Papers of Enrico Fermi*, edited by E. Segre (University of Chicago Press, Chicago, 1965).

[3] H. Poincaré, *Les Methodes Nouvelles de la Mecanique Celeste* (Gauthier-Villars et fils, Paris, 1892–1899). Translated, edited, and introduced by Daniel L. Goroff as *New Methods of Celestial Mechanics* (American Institute of Physics, Woodbury, NY, 1993).

[4] A. N. Kolmogorov, Dokl. Akad. Nauk SSSR **98**, 527 (1954); V. I. Arnold, Usp. Mat. Nauk. **18**, 13 (1963); J. Moser, Nachr. Akad. Wiss. Goettingen Math. Phys. Kl. II **1962**, 1 (1962).

[5] S. Brush, Transport Theory and Statistical Physics **1**, 287 (1971).

[6] P. Ehrenfest and T. Ehrenfest-Afanassjewa, *The Conceptual Foundations of the Statistical Approach in Mechanics* (Cornell University Press, Ithaca, NY, 1956).

[7] A. Lichtenberg and M. Lieberman, *Regular and Stochastic Motion* (Springer, Berlin, 1983).

[8] G. Casati and J. Ford, J. Comput. Phys. **20**, 97 (1976).

[9] R. Artuso, G. Casati, and I. Guarneri, Phys. Rev. E **55**, 6384 (1997).

[10] G. Casati and T. Prosen, Phys. Rev. Lett. **83**, 4729 (1999).

[11] S. L. Glashow and L. Mittag, J. Stat. Phys. **87**, 937 (1997).

[12] T. Araujo Lima, S. Rodriguez-Perez, and F. M. de Aguiar, Phys. Rev. E **87**, 062902 (2013).

[13] E. Gutkin, Physica D **19**, 311 (1986).

[14] E. Gutkin, J. Stat. Phys. **83**, 7 (1996).

[15] S. Kerckhoff, H. Masur, and J. Smillie, Ann. Math. **124**, 293 (1986).

[16] Ya. B. Vorobets, Russ. Mat. Surv. **51**, 756 (1996).

[17] The Liouville numbers are those numbers which are approximated by rationals M/N faster than any power of N.

[18] G. Casati, B. V. Chirikov, F. M. Izraelev, and J. Ford, *Lecture Notes in Physics* (Springer, New York, 1979), Vol. 93, p. 334.

[19] G. Casati and B. V. Chirikov, in *Quantum Chaos* (Cambridge University Press, Cambridge, 1995), p. 40.