

Non-ergodicity of Two Particles Interacting via a Smooth Potential

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We examine two point particles interacting via a smooth Lennard-Jones-type potential of finite range on a two-dimensional torus. We find situations under which this system contains a stable, elliptic periodic orbit and hence is not ergodic. This result is in contrast to the case of hard spheres interacting via inelastic collision, which are always ergodic for two particles, are conjectured to be ergodic for arbitrarily many particles, and can never contain elliptic periodic orbits.

KEY WORDS: Boltzmann ergodic hypothesis; non-ergodic; elliptic orbit; KAM theory; generalized Sinai billiard; Lennard-Jones potential.

1. INTRODUCTION

Do gas molecules interacting in a box behave ergodically? This question was originally raised by Boltzmann who asserted that the molecules should behave ergodically. This assertion, known as the Boltzmann ergodic hypothesis, has exerted an important influence in the development of dynamical systems and ergodic theory.⁽¹⁾ The most common mathematical interpretation of this problem is that the molecules are hard spheres that interact by inelastic collisions. This formulation has come to be called the Boltzmann–Sinai ergodic hypothesis and asserts that the motion of n such particles on a torus are ergodic for all $n \geq 2$.

The idea that hard sphere gases should be ergodic was first suggested by the work of Krylov⁽²⁾ and then proven by Sinai.⁽³⁾ The first case to be understood consisted of two disks (i.e., two-dimensional molecules) of equal mass moving on a two-dimensional torus. Sinai showed that this system can be reduced to the motion of a point particle moving on a torus

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that bounces off a circular scatterer, the celebrated Sinai billiard, and that the motion of this system was ergodic.⁽⁴⁾ Sinai and Chernov then showed that two balls on a three-dimensional torus were ergodic.⁽⁵⁾ For larger numbers of balls, the system again reduces to a billiard type system with a single particle moving in a high dimensional phase space but now bouncing off cylindrical shaped obstacles. Great progress has been achieved over the past decade in showing ergodicity of these systems under various conditions⁽⁶⁻¹⁰⁾ although at present the proof of ergodicity for an arbitrary number of three-dimensional balls has not been obtained.

From statistical mechanics,⁽¹¹⁾ one knows that under certain situations, such as high pressure and low temperature, the hard sphere model is a poor predictor of gas properties. A more accurate model is obtained by replacing the inelastic collision between particles by an interaction caused by a smooth potential field V . We examine the simplest possible case of such a system: two particles moving on a two-dimensional torus. We show that this system can contain a stable elliptic periodic orbit and hence be non-ergodic. A system of two hard spheres interacting by inelastic collision is always ergodic. Thus there is a fundamental difference in the dynamics governed by inelastic collisions as compared to smooth potentials. Although our results only apply to two-particle systems, they raise the possibility that systems with large numbers of particles interacting by smooth potentials could also be non-ergodic.

A potential that is often used in statistical mechanics is the Lennard-Jones 6-12 potential given by $V(r) = c_1 \{ (c_2/r)^{12} - (c_2/r)^6 \}$. This potential is strongly repelling at short distances and weakly attracting at larger distances (Fig. 1a). We will study the motion of two particles moving on a two-dimensional torus T^2 that interact under a potential of the same general shape as the Lennard-Jones potential (Fig. 1b), but the potential has finite range: for some R , $V(R) = 0$, $r \geq R$.

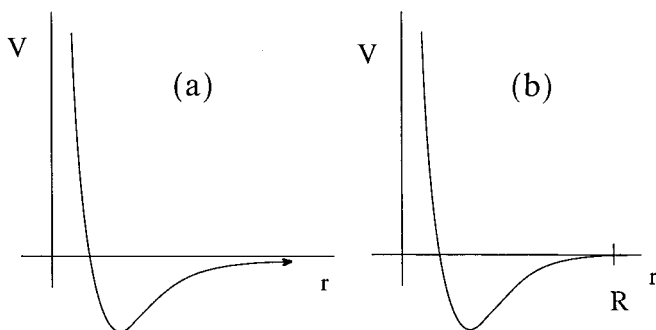


Fig. 1. (a) Lennard-Jones potential. (b) Finite range Lennard-Jones potential.

Definition 1.1. We call a smooth potential of finite range of type Lennard-Jones if

(1) $V^k(R) = 0, k = 0, 1, 2, \dots$

(2) The potential is attracting for large r : for all r sufficiently close to R ,

$$V'(r) > 0, \quad V''(r) < 0, \quad V'''(r) > 0$$

(3) The potential has a repelling core,

$$\lim_{r \rightarrow 0} V(r) = +\infty$$

The class of potentials covered by these conditions is very broad. For example, potentials that have an exponentially repelling force at short distances fit into this class.

Theorem 1.2. Given two point particles interacting under a Lennard-Jones potential of finite range, there exist tori T^2 on which the system is non-ergodic.

A precise statement of this result is given in Theorem 5.1.

Our work shows that for any fixed energy level (with high energy), there exist tori of certain sizes for which the system restricted to that energy level is non-ergodic. For tori of other sizes, it is possible that the system on this energy level is ergodic, although proving such a result looks to be very difficult problem. We conjecture that for most tori and for most energy levels, the system is non-ergodic.

Turaev and Rom-Kedar^(12, 30) have results that are similar in spirit to ours. They look at the problem of approximating scattering billiards by systems governed by smooth repelling potentials. These potentials are concentrated in a narrow strip around the boundary of the billiard and are strongly repelling. A point particle moving in a scattering billiard is ergodic.⁽⁴⁾ However, under appropriate conditions, the authors show that the smooth approximating systems can contain elliptic islands and hence be non-ergodic. Although it is not clear whether their conditions are satisfied in the two-particle systems we are studying (see Remark 3.3), the moral of our two papers is the same. When one takes an ergodic system governed by inelastic collision and replaces the inelastic collision by an interaction caused by a smooth potential, ergodicity can be destroyed.

Although our result only applies to the case of two particles in two dimensions, it raises the possibility that a system of n particles interacting under a potential field in three dimensions could also be non-ergodic and

suggests a mechanism (partial focusing) by which non-ergodicity could be produced for many-particle systems (see Remark 2.3). The non-ergodicity of our examples is caused by partial focusing (Section 2). In a partially focusing system, an infinitesimal family of nearby trajectories that starts out parallel will at a later time be converging very slowly. If one of these trajectories becomes periodic while the family is still converging (and hence before the family focuses), then the orbit will be elliptic and hence can destroy ergodicity. For higher dimensional systems, the notion of partial focusing and its relation to elliptic orbits is not yet well understood. However using a version of partial focusing, M. Wojtkowski⁽¹³⁾ has produced elliptic periodic orbits for billiards inside three-dimensional domains. Our hope is that by using a higher-dimensional version of partial focusing, one could find many-particle systems interacting under smooth potentials that are non-ergodic. Even if one could find such examples though, the measure of the set of trajectories constrained to lie near the elliptic periodic orbits is likely to be very small. Thus from a practical point of view, these systems may appear to be ergodic.

Hermann⁽¹⁴⁾ has recently found other situations in which interacting particle systems are non-ergodic. He examines particles interacting by inelastic collision but in boxes of roughly spherical shape rather than the traditional rectangular box and has constructed examples with arbitrarily many particles for which the system is non-ergodic.

Our approach to proving Theorem 1.2 is as follows. We reduce the two-particle system to a one-particle generalized Sinai billiard (Section 4) and then use our previous results about generalized Sinai billiards⁽¹⁵⁾ in which we created elliptic periodic orbits.

For two disc-like particles of equal mass (or rationally related masses) interacting by inelastic collision, Sinai [4, Section 8] showed that under a change of variables, the system was equivalent to a Cartesian product of two systems, one being a one-particle scattering billiard and the other being a linear motion on the torus. Having shown that the scattering billiard system was ergodic, he was able to conclude that the original two-particle system was also ergodic. Sinai's change of variables involved using the center of mass coordinates. However, because the motion takes place on a torus, rather than the plane, the center of mass is not well-defined when the ratio of the masses is irrational. To handle the case of irrationally related masses, Simanyi and Wojtkowski⁽¹⁷⁾ used a different change of variables and showed that the two-particle system contained a one-particle scattering billiard as a factor.

In reducing our two-particle system with interactions caused by a potential field to a one-particle system interacting with a finite range potential (i.e., a generalized Sinai billiard), we adapt these techniques used for

inelastic collisions. When the ratio of the masses is rational, we use the center of mass reduction (Section 4a) to show that the system is equivalent to a Cartesian product of two systems, one of which is a generalized Sinai billiard. For the case of general masses, we use the Simanyi-Wojtkowski reduction to show that the two-particle system has a factor consisting of a generalized Sinai billiard (Section 4b). In either case, when the one-particle generalized Sinai billiard is non-ergodic, then the original two-particle system is also non-ergodic (Section 5). For the special case of equal masses and total momentum zero, we present a geometrical reduction (Appendix), closely related to the Sinai reduction, which allows one to visualize the relationship between orbits for the generalized Sinai billiard and the corresponding orbits for the two-particle system.

The motion of a point particle on a torus being acted upon by a symmetric potential field of finite range gives rise to what is known as a generalized Sinai billiard (Section 2). In a generalized Sinai billiard, a point particle moves on a torus which contains a disk. When the particle is outside the disk, it moves in a straight line. When it reaches the disk, it undergoes a generalized reflection. Its angle of reflection equals its angle of incidence but in addition the particle is also rotated around the disk by an amount $\Delta\theta(\phi)$ which depends on the angle of incidence ϕ (Fig. 2). We call $\Delta\theta(\phi)$, which determines the net amount that the particle rotates around the disk, the rotation function. For a regular billiard, the rotation function $\Delta\theta(\phi)$ is identically zero. For our system, the particle is acted upon by a symmetric potential which allows us to explicitly solve the equations of motion and calculate the rotation function (Section 3).

Generalized Sinai billiards have been extensively studied^(3, 15, 18–26) and various conditions have been found under which such a system is ergodic. The most general sufficient conditions were given by Donnay and Liverani.⁽²⁵⁾ Donnay⁽¹⁵⁾ used the notion of partially focusing disks to show

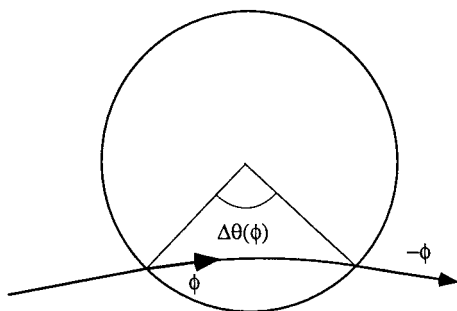


Fig. 2. Rotation function for generalized billiard.

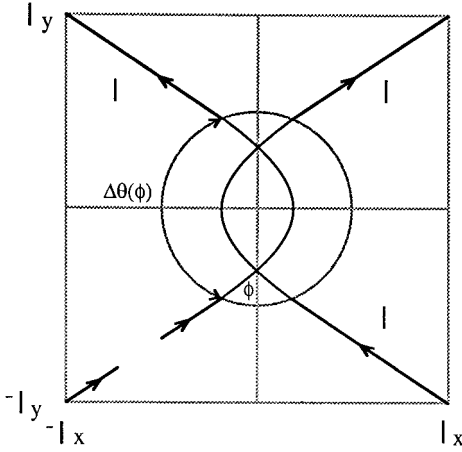


Fig. 3. Stable periodic orbit for partially focusing billiard arising from Lennard-Jones type potential.

that these sufficient conditions were also necessary conditions for ergodicity.

Definition 1.3. A rotation function is termed partially focusing if

- (1) there is an angle ϕ^* for which the rotation function satisfies $\Delta\theta'(\phi^*) = 2$,
- (2) in a neighborhood of ϕ^* , $\Delta\theta'$ is continuous and takes on values less than 2.

We call a disk partially focusing if its rotation function is partially focusing.

For a partially focusing disk, we will be able to construct a periodic orbit (Fig. 3) that is elliptic and stable in the sense of KAM theory. Thus such a system will be non-ergodic. In this construction, we take a trajectory that enters the disk with an angle ϕ_0 for which $\Delta\theta'(\phi_0) < 2$ but very close to 2. We arrange the size of the torus so that this trajectory is periodic. Providing that a technical condition

$$\Delta\theta(\phi^*) \neq 2\phi^* \pmod{\pi} \tag{1}$$

is satisfied, we can show that this orbit is elliptic and stable. This result is contained in the following theorem.

Theorem 1.4.⁽¹⁵⁾ Given a partially focusing disk that satisfies condition (1), one can place the disk on a torus in such a way that there

exists a stable, elliptic periodic orbit and hence the resulting generalized billiard system is not ergodic. The size of the torus can be made arbitrarily large in this construction.

We make use of partially focusing disks to study the motion of a point particle under a Lennard-Jones potential. For low energies, there are trajectories that start inside the range of the potential field and are not energetic enough to escape from the potential. For such energies, the one-particle system is clearly not ergodic. Thus in studying ergodicity, one first has to insure that the energy level is sufficiently high so that trajectories are not trapped by the potential inside the disk. For high energies, there is no apriori barrier to ergodicity.

A key property of Lennard-Jones potentials is

Theorem 1.5.⁽¹⁵⁾ For all sufficiently high energies, a Lennard-Jones potential of finite range generates a partially focusing rotation function $\Delta\theta_E$.

To prove our main result, Theorem 1.2, we reduce the two-particle system to a one-particle system with Lennard-Jones potential (Section 4). This one-particle system gives rise to a generalized billiard that is partially focusing for all sufficiently high energies. We fix one of these energy levels and, providing that condition (1) holds, we choose the size of the torus so there is an elliptic, stable orbit for the system (Section 2) restricted to this energy level and thereby produce non-ergodicity for the reduced system. This in turn implies that the original two-particle system is non-ergodic (Section 5).

The existence of elliptic islands is stable under small perturbations to the system. Thus once we have elliptic islands for our symmetric, finite range potential, the elliptic islands will persist for small (smooth) perturbations to the potential. In this way, we can create systems with non-finite range, non-symmetric potentials, that have elliptic islands and are non-ergodic. This issue is discussed in [15, Section 5].

Rather than using a Lennard-Jones type potential, we could consider a finite range potential that is strictly repelling, $V'(r) < 0$, $r \in (0, R]$, and that goes smoothly to zero as r approaches R . The corresponding rotation function would be partially focusing for all energy levels.⁽¹⁵⁾ However, the critical angle ϕ^* at which $\Delta\theta'(\phi^*) = 2$ is $\phi^* = 0$, and the technical condition (1) fails to hold since $\Delta\theta(\phi^*) = 0 = 2\phi^*$. We discuss this case further in Section 3. Our methods do not suffice to show that a system with a smooth, repelling potential is non-ergodic. However, because such a system is partially focusing, there are trajectories that if they were to become periodic at

certain times would be elliptic. We conjecture that typically such a system would have stable elliptic orbits and be non-ergodic.

The outline of the paper is as follows. We first discuss generalized Sinai billiards (Section 2) and then show that symmetric, finite range potentials give rise to such billiards (Section 3). We reduce the two-particle system to a one-particle system (Section 4) and discuss the connection between the one-particle system being non-ergodic and the two-particle system being non-ergodic (Section 5). For the case of equal masses and zero total momentum, we present a geometric reduction (Appendix).

2. GENERALIZED SINAI BILLIARD

A generalized Sinai billiard consists of a point particle moving on a torus $T^2 = (-l_x, l_x) \times (-l_y, l_y)$ that contains one or more disks. While outside the disks, the particle moves in a straight line at unit speed. When the particle reaches a disk, it undergoes a generalized billiard reflection: the angle of reflection equals angle of incidence but in addition the particle is now rotated around the boundary of the disk a certain amount that depends on the angle of incidence. In what follows, our torus will have only one disk. The disk will have radius R and be centered at the origin.

We give the boundary of the disk coordinates (ϕ, θ) where $\phi \in (0, \pi)$ is the angle of entering the disk, measured relative to the boundary of the disk, and $\theta \in [0, 2\pi)$ is the point of entry on the boundary. We set $\theta = 0$ to be the point $(R, 0)$ on the positive x axis. If the trajectory enters the disk at a point (ϕ, θ) , it will leave the disk at a point $(-\phi, \theta + \Delta\theta(\phi))$, where $\Delta\theta(\phi)$ is the rotation function.

Let the rotation function $\Delta\theta(\phi)$, $\phi \in [0, \pi]$ be piecewise C^4 smooth with $\Delta\theta(0) = 0$, $\Delta\theta'(0) = 2$, $\Delta\theta^{(k)}(0) = 0$, $k = 2, 3, 4$. These latter conditions are necessary to produce a smooth flow at $\phi = 0$.

When the rotation function is partially focusing (Definition 1.3), the resulting system can be made non-ergodic as the following theorem shows.

Theorem 2.1.⁽¹⁵⁾ Given a partially focusing disk for which $\Delta\theta(\phi^*) \neq 2\phi^* \bmod(\pi)$, one can choose lengths $\{l_x, l_y\}$ for the torus in such a way that the resulting generalized billiard system is not ergodic. The lengths $\{l_x, l_y\}$ can be made arbitrarily large in this construction.

For certain classes of rotations functions, the system becomes ergodic if the disks are placed far enough apart.⁽²⁵⁾ In this case, no matter how large the torus, and hence no matter how far apart the disks, the system remains non-ergodic.

Sketch of Proof of Theorem 2.1. We construct an elliptic periodic orbit for the system that is stable in the sense of KAM theory and hence prevents ergodicity.

First we show how to construct a periodic trajectory that enters the disk with angle ϕ , for any $\phi \in (0, \pi)$ (Fig. 3). We will require that $\Delta\theta(\phi) \neq 2\phi, \pmod{\pi}$. Under the additional assumption that $0 < \Delta\theta'(\phi) < 2\phi$, this trajectory will be elliptic and stable.

Choose ϕ . This choice determines the value $\Delta\theta(\phi)$. Denote by θ_{in} , the point at which the trajectory enters the disk, and by θ_{out} , the point at which the trajectory leaves the disk. We want these points to be symmetry with respect to the y axis. Since $\theta_{\text{out}} = \theta_{\text{in}} + \Delta\theta(\phi)$, this symmetry will be achieved by setting $\theta_{\text{in}} = 3\pi/2 - \Delta\theta(\phi)/2$.

We extend the trajectory that enters the disk at θ_{in} backwards a distance l from the disk. The point we arrive at is a ‘‘corner’’ of the torus; its coordinates are $(-l_x, -l_y)$. The length l is a free parameter in the construction; it can take on any value subject to the conditions $l_x, l_y > R$. This condition is necessary to insure that disk does not overlap itself on the torus. Thus as we vary the length l , we will generate tori of different sizes.

By symmetry, when we extend the trajectory that leaves the disk at θ_{out} forwards a distance l , it will also arrive at a corner of the torus. This corner has coordinates $(l_x, -l_y)$. We identify this corner of the torus with the corner $(-l_x, l_y)$ and extend the trajectory an additional distance l ; it enters the disk a second time, now with angle $\pi - \phi$. The points of entering and leaving the disk this second time are again symmetric with respect to the y axis. After leaving the disk and traveling a further distance l , it will reach the corner (l_x, l_y) . The resulting orbit is now periodic on the torus.

The following theorem⁽¹⁵⁾ gives conditions under which this periodic orbit is elliptic and stable.

Theorem 2.2. Let $\phi \in (0, \pi)$ and assume that

$$0 < \Delta\theta'(\phi) < 2$$

(1) The periodic orbit constructed above will be elliptic providing that the parameter l satisfies

$$l < \left(\frac{\Delta\theta'(\phi)}{2 - \Delta\theta'(\phi)} \right) \sin \phi$$

(2) Consider the periodic orbit as a function of the parameter l . Except for isolated values of l , the orbit will be stable in the sense of KAM theory.

To finish the proof of Theorem 2.1, we describe how to make a family of tori $T_n^2 = (-l_x^n, l_x^n) \times (-l_y^n, l_y^n)$ with the lengths l_x^n, l_y^n going to infinity on which the particle motion is non-ergodic.

We have an angle $\phi^* \in (0, \pi/2)$ for which $\Delta\theta'(\phi^*) = 2$ such that $\Delta\theta(\phi^*) \neq 2\phi^* \pmod{\pi}$. Choose a sequence of angles ϕ_n with $\phi_n \rightarrow \phi^*$, $\Delta\theta'(\phi_n) < 2$ and $\Delta\theta'(\phi_n) \rightarrow 2^-$.

For each ϕ_n , we construct a stable, elliptic periodic orbit as described above. The parameter l_n , determining the length of this orbit, must satisfy

$$l_n < \left(\frac{\Delta\theta'(\phi_n)}{2 - \Delta\theta'(\phi_n)} \right) \sin \phi_n$$

Thus as $\phi_n \rightarrow \phi^*$, we can choose the lengths $l_n \rightarrow \infty$. The corresponding lengths l_x^n, l_y^n of the tori will also approach infinity.

The requirement that $\Delta\theta(\phi^*) \neq 2\phi^* \pmod{\pi}$ is needed for the following reason. Suppose $\Delta\theta(\phi^*) = 2\phi^*$. Then for ϕ near ϕ^* , $\Delta\theta(\phi)$ is very close to 2ϕ . In the construction of the periodic orbit, the periodic trajectory entering the disk with angle ϕ and with $\Delta\theta(\phi)$ close to 2ϕ will be very nearly parallel to the x axis. Thus l will need to be very large to insure that $l_y > R$. Recall that this condition is necessary to insure that the disk does not have self-intersection on the torus. However, if

$$l > \left(\frac{\Delta\theta'(\phi)}{2 - \Delta\theta'(\phi)} \right) \sin \phi$$

then the periodic orbit is no longer elliptic. It becomes hyperbolic and no longer presents an obstacle to ergodicity. Thus such a system could conceivably be ergodic.

A calculation,⁽¹⁵⁾ shows that in general as $\phi_n \rightarrow \phi^*$ with $\Delta\theta(\phi^*) = 2\phi^*$, then the lengths l_n needed to insure $l_y^n > R$ grow to infinity so rapidly that

$$l_n > \left(\frac{\Delta\theta'(\phi_n)}{2 - \Delta\theta'(\phi_n)} \right) \sin \phi_n$$

and the periodic orbit constructed is no longer elliptic.

The results for the case $\Delta\theta(\phi^*) = 2\phi^* + \pi$ are similar. In this case, the periodic orbit entering with angle ϕ and $\Delta\theta(\phi)$ close to $2\phi + \pi$ will be nearly vertical. The length l will have to be very long to insure that $l_x > R$.

Remark 2.3. The intuition as to how partial focusing contributes to non-ergodicity is as follows. When $\Delta\theta' > 2$, an infinitesimal family of trajectories that is parallel when they enter the disk will start to diverge as

they pass through the disk and will then be diverging when they leave the disk (see Fig. 2 in ref. 15). Such a divergence of trajectories contributes to producing sensitive dependence on initial conditions, positive Lyapunov exponents and ergodicity. If $\Delta\theta' < 2$, then an infinitesimal family of trajectories that is parallel when they enter the disk will start to converge as they pass through the disk and be converging when they leave the disk. If the time before they return to the disk is sufficiently long, then the converging family will be able to focus, after which time it will again be diverging. This behavior of convergence followed by focusing and then by divergence is called defocusing. L. Bunimovich,⁽²⁷⁾ in his celebrated Stadium billiard, was the first to show that defocusing can also generate chaotic dynamics.

If however the trajectory were to close up and become periodic before the converging variation had time to focus, then the orbit would be elliptic. As $\Delta\theta'$ approaches 2 from below, the time to focusing goes to infinity. This follows by continuity since for $\Delta\theta' = 2$, the parallel family is again parallel when it leaves the disk and will never focus in the flat region.

Thus ergodicity can be destroyed by slowly converging trajectories that become periodic before focusing occurs. There will always be lots of slowly focusing trajectories in a partially focusing system but in general one does not know if these orbits will become periodic.

One could look for a similar mechanism of slow convergence for higher dimensional systems and try to use this mechanism to construct elliptic periodic orbits for particle systems with many particles. Using a version of slow focusing, Wojtkowski⁽¹³⁾ has produced elliptic periodic orbits for billiards inside three-dimensional domains.

3. SYMMETRIC POTENTIALS OF FINITE RANGE

We examine the motion of a point particle moving on a torus T^2 and being acted upon by a symmetric potential V of finite range R . We give the system coordinates so that the potential is centered at the origin. Then the finite range condition is expressed by the condition that $V(r) = 0$, $r \geq R$.

The total energy E of the system is conserved under the flow. Thus, a trajectory lies on a fixed energy surface. Let the particle have total energy E . While outside the range of the potential, the particle moves in a straight line.

Let $(r(t), \theta(t))$ be the coordinates of the particle as it passes through the disk. Let the particle have angular momentum l . Then using the conservation of angular momentum, one finds⁽²⁸⁾ that

$$\frac{d\theta}{dr} = \frac{l^2}{r^2 \sqrt{2(E - V_{\text{eff}}(r))}}$$

where $V_{\text{eff}}(r) = V(r) + l^2/2r^2$ is called the effective potential. The $r(t)$ coordinate evolves as if a point particle was moving in one dimension under the influence of the potential $V_{\text{eff}}(r)$.

For a particle that enters the disk with angle $\phi \in [0, \pi/2]$, has angular momentum $l = \sqrt{2E} R \cos \phi$ and total energy E , the total rotation is

$$\Delta\theta_E(\phi) = 2 \int_{\hat{r}}^R \frac{l^2}{r^2 \sqrt{2(E - V_{\text{eff}}(r))}} dr \quad (2)$$

where \hat{r} is the minimum radius that the particle reaches in the disk. This minimum radius is the value of r closest to R for which $V_{\text{eff}}(r) = E$.

There is a symmetry in the rotation function between angles ϕ and $\pi - \phi$: a trajectory that enters the disk with angle $\pi - \phi$, $\phi \in [0, \pi/2]$, will rotate clockwise by the same amount that that a trajectory entering with angle ϕ rotates counterclockwise.

Hence we see that a point particle with fixed energy E moving under the influence of a symmetric potential $V(R)$ of finite range gives rise to a generalized Sinai billiard with rotation function $\Delta\theta_E(\phi)$ given by (2).

For a symmetric potential of finite range of Lennard-Jones type (see Definition 1.3), the flow on the energy surface is clearly non-ergodic for low energies. There are trajectories that start inside the disk and never leave: they are trapped in a potential well. Since there is a set of positive measure of such trajectories, ergodicity fails.

As the energy level increases, these trapped trajectories will cease to exist and all trajectories that start in or enter the disk will leave the disk. Apriori, for such energy levels, the system could be ergodic.

Theorem 3.1.⁽¹⁵⁾ Let $V(r)$ be a Lennard-Jones potential of finite range. Then for all sufficiently high energies E :

1. Every trajectory that starts inside the disk, or enters the disk, will leave the disk.
2. The potential generates a partially focusing rotation function $\Delta\theta_E$.
3. If the partially focusing rotation function satisfies $\Delta\theta_E(\phi^*) \neq 2\phi^* \pmod{\pi}$, we can construct tori $T^2 = (-l_x, l_x) \times (-l_y, l_y)$, with l_x, l_y arbitrarily large, for which the particle system is non-ergodic.

If the potential were identically zero, then a simple calculation shows that $\Delta\theta_E(\phi) \equiv 2\phi$ so that $\Delta\theta'_E(\phi) \equiv 2$. In our case, since the potential goes smoothly to zero at the edge of the disk, we have that $\Delta\theta_E(0) = 0$ and that $\Delta\theta'_E(0) = 2$. For small ϕ , the attracting nature of the potential implies $\Delta\theta'(\phi) > 2$. For large ϕ , the particle feels the repelling core of the potential which implies that $\Delta\theta_E(\pi/2) = 0$ (Fig. 4). We conclude that $\Delta\theta'_E(\phi)$ must

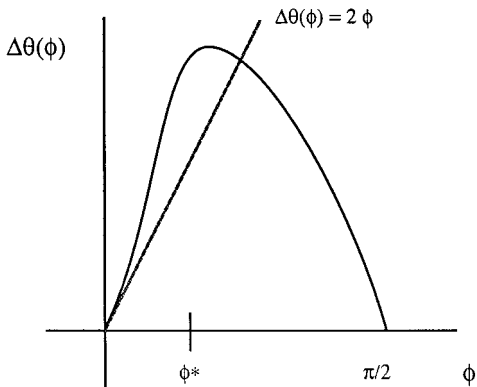


Fig. 4. Rotation function for Lennard-Jones potential.

pass from above two to below two and so there is an angle ϕ^* for which $\Delta\theta'_E(\phi^*) = 2$.

We choose a sufficiently high energy level E_0 so that the rotation function $\Delta\theta_{E_0}$ is partially focusing. Then providing that $\Delta\theta_{E_0}(\phi^*) \neq 2\phi^* \pmod{\pi}$, we use the method described in Section 2 to create a fixed torus T^2 with sides l_{x_0}, l_{y_0} that contains an elliptic, stable periodic orbit. Thus the particle system restricted to the energy level E_0 is non-ergodic. Under small perturbations to the system, the periodic orbit will persist, by the Implicit Function Theorem, and it will also remain stable. Thus we can show for an open set of energy levels and open set of tori, the particle system is non-ergodic.

Corollary 3.2. For a system satisfying the assumptions of Theorem 3.1, there exists an energy level E_0 and torus lengths l_{x_0}, l_{y_0} such that for some $\varepsilon > 0$, the particle system on the torus $T^2 = (-l_x, l_x) \times (-l_y, l_y)$ restricted to the E energy level is non-ergodic providing that $|l_{x_0} - l_x|, |l_{y_0} - l_y|, |E_0 - E|$ are all less than ε . The values of E_0, l_{x_0}, l_{y_0} can be made arbitrarily large.

We could also make small perturbations to the potential and still retain the stable elliptic orbit. Thus there exist non-symmetric, non-finite range potentials, close to our symmetric, finite range Lennard-Jones potentials, for which the single particle on the torus is non-ergodic. This issue is discussed further in [15, Section 5].

We have seen that for a fixed energy level, we can produce non-ergodicity by choosing a torus of a particular size. It is possible that if we choose other sizes for the torus, the flow would be ergodic. Finding a torus with a partially focusing disk for which the flow is ergodic looks to be a

very difficult problem. A partially focusing disk takes an infinitesimal family of trajectories that was diverging and makes it converging. Furthermore, these families can converge for an arbitrarily long time. If such a family were to become periodic before converging, it would be elliptic. Thus for a general torus, there are lots of trajectories that, if they were to become periodic, would be elliptic and thus they would destroy ergodicity. In the explicit examples we construct, we choose the size of the torus so as to guarantee periodicity of a particular orbit. For a general torus, it would be a very difficult problem to determine if any of the potentially elliptic orbits are indeed periodic.

For a smooth, repelling potential, the rotation function will be partially focusing for every energy level. Since the potential goes smoothly to zero at the edge of the disk, $\Delta\theta'_E(0) = 2$. For small ϕ , the repelling nature of the potential implies that $\Delta\theta'_E(\phi) < 2$. Although the rotation function is partially focusing, it does not satisfy condition (1) since $\phi^* = 0$ and $\Delta\theta_E(\phi^*) = 0 = 2\phi^*$. When we construct a periodic orbit (Section 2), we find that the length of this orbit is very large and as a result the orbit is hyperbolic rather than elliptic.

Our methods do not suffice to show that a system with a smooth, repelling potential is non-ergodic. However, because such a system is partially focusing, there are lots of potentially elliptic trajectories as the above argument shows and we conjecture that in a typical case, the system will have an elliptic orbit. This is in marked contrast to the hard sphere gas which can never contain elliptic orbits.

Remark 3.3. Turaev and Rom-Kedar⁽¹²⁾ look at systems with smooth repelling potentials that are approximations of scattering planar billiard systems. It is not clear whether their methods can be applied directly to our situation to produce a non-ergodic billiard with smooth, repelling potential. For this problem, the corresponding scattering billiard consists of a single circular obstacle on the two torus while they consider billiards in bounded regions in the plane. If there exists a periodic orbit (or homoclinic orbit) on the torus that lifts to a simple singular periodic orbit (or simple singular homoclinic orbit) on the plane, then we could consider that this orbit on the plane was produced by a billiard inside a bounded region and try to apply their methods.

4. REDUCTION OF 2 PARTICLE SYSTEM TO 1 PARTICLE SYSTEM

We consider two particles of masses m_1, m_2 moving on a two-dimensional torus $T^2 = (-l_x, l_x) \times (-l_y, l_y)$. The positions of the particles are $q_1, q_2 \in T^2$ with momentums $p_1 = m_1 \dot{q}_1, p_2 = m_2 \dot{q}_2$. The particles interact

under a symmetric potential V of finite range R . The Hamiltonian for the system is

$$H(q_1, q_2, p_1, p_2) = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(\|q_1 - q_2\|) \tag{3}$$

The equations of motion for the system are given by Hamilton's equations;

$$\begin{aligned} \frac{dq_i}{dt} &= \frac{\partial H}{\partial p_i} = \frac{p_i}{m_i} \\ \frac{dp_i}{dt} &= -\frac{\partial H}{\partial q_i} = -\frac{\partial V}{\partial q_i}(\|q_1 - q_2\|) \end{aligned} \tag{4}$$

There are three conserved quantities for this motion: the total energy

$E = H(q_1, q_2, p_1, p_2)$ and the x and y components of total momentum $P = (P_x, P_y) = p_1 + p_2$.

The phase space for this system is eight-dimensional, a subset of $T^2 \times T^2 \times R^2 \times R^2$. The existence of these three conserved quantities implies that any given trajectory $(q_1, q_2, p_1, p_2)(t)$ is restricted to moving within a five-dimensional level set on which the energy and total momentum are constant. For each of these energy-momentum level sets, we ask whether the flow restricted to that level set is ergodic or non-ergodic.

We will show that under appropriate change of variables, the motion of this system can be reduced to that of one particle moving on a torus \tilde{T}^2 on which there is a symmetric potential of finite range (i.e., a generalized Sinai billiard). We give three approaches to the problem. The first one works when the ratio of the masses m_2/m_1 is rational (Section 4a). In this case, the system is equivalent to a Cartesian product of two lower dimensional systems and one of these systems is a generalized Sinai billiard. The second reduction, which works for all masses, shows that the system contains a lower dimensional factor consisting of a generalized Sinai billiard. The third reduction (Appendix), that works in the special case of equal masses and zero total momentum $P=0$, has the advantage of being geometric and hence allows one to more easily visualize the relationship between the one-particle system and the original two-particle system.

4a. Rational Ratio of Masses

For the system described above, we will make a canonical linear change of variables

$$(Q_1, Q_2, P_1, P_2) = L(q_1, q_2, p_1, p_2) \tag{5}$$

We start by defining a change of variables on the configuration space: $L_1: T^2 \times T^2 \rightarrow \tilde{T}_1^2 \times \tilde{T}_2^2$ given by $L_1(q_1, q_2) = (Q_1, Q_2)$ with

$$\begin{aligned} Q_1 &= c_1 \left(\frac{m_1 q_1 + m_2 q_2}{m_1 + m_2} \right) \\ Q_2 &= q_1 - q_2 \end{aligned} \quad (6)$$

where the constant c_1 is determined below. The variables P_1, P_2 will be the conjugate momentum for Q_1, Q_2 .

This change of variables is the standard way to simplify the Kepler problem of two bodies interacting under a potential on the plane.⁽¹⁶⁾ In our case, the particles are moving on a torus which complicates the analysis. In particular, if the ratio of the masses m_2/m_1 is irrational, then the change of variables (6) is not well defined for q_1, q_2 on a torus. Specifically, the center of mass $Q_1/c_1 = (m_1 q_1 + m_2 q_2)/(m_1 + m_2)$ is not a well defined quantity.

We show that for the ratio of the masses rational, the change of variables is well defined. Assume that $m_2/m_1 = a/b \in \mathbb{Z}$. The two particles q_1 and q_2 move on the torus $T^2 = (-l_x, l_x) \times (-l_y, l_y)$. Let $v_1 = (2l_x, 0)$, $v_2 = (0, 2l_y)$ be a standard basis for the lattice generating T^2 . Let

$$\begin{aligned} \bar{q}_1 &= q_1 + N_1 v_1 + M_1 v_2 \\ \bar{q}_2 &= q_2 + N_2 v_1 + M_2 v_2 \end{aligned} \quad (7)$$

for $N_i, M_i \in \mathbb{Z}$ be any two lifts of q_1, q_2 in \mathbb{R}^2 . The values of Q_1 and Q_2 must be independent of which representatives of q_1 and q_2 are taken.

For Q_1 to be well defined on a torus \tilde{T}_1^2 defined by basis vectors $\{w_1, w_2\}$, we need that

$$c_1 \left(\frac{m_1 \bar{q}_1 + m_2 \bar{q}_2}{m_1 + m_2} \right) - c_1 \left(\frac{m_1 q_1 + m_2 q_2}{m_1 + m_2} \right) = z_1 w_1 + z_2 w_2 \quad (8)$$

for some $z_i \in \mathbb{Z}$ and for some vectors $w_i, i = 1, 2$.

If we take

$$c_1 = \frac{b(m_1 + m_2)}{m_1} \quad (9)$$

then we can solve equation (8) by setting $w_i = v_i$ and $z_1 = bN_1 + aN_2, z_2 = bM_1 + aM_2$. If we took a different value for c_1 , then there would still be a

solution but w_i would then be a scalar multiple of v_i with the scalar not equal to one.

If the ratio of the masses is irrational, then we can not solve (8) for general N_i, M_i values.

For $Q_2 = q_1 - q_2$ to be well defined on a torus \tilde{T}_2^2 defined by basis vectors $\{u_1, u_2\}$, we must have that

$$(\bar{q}_1 - \bar{q}_2) - (q_1 - q_2) = z_1(u_1) + z_2(u_2)$$

which holds for $u_1 = v_1, u_2 = v_2, z_1 = N_1 - N_2$ and $z_2 = M_1 - M_2$.

With c_1 given by (9), the change of variables $L_1(q_1, q_2) = (Q_1, Q_2)$ reduces to

$$Q_1 = bq_1 + aq_2, \quad Q_2 = q_1 - q_2 \tag{10}$$

The tori $\tilde{T}_1^2, \tilde{T}_2^2$ have the same size as the original torus T^2 . The linear map $L_1: T^2 \times T^2 \rightarrow \tilde{T}_1^2 \times \tilde{T}_2^2$ is given by a 4×4 matrix with integer entries and determinant $(a + b)^2$ and hence is a $(a + b)^2$ -to-one covering map. For the case of equal masses, $a = b = 1$, we recover Sinai's original change of variables (for inelastic billiard collisions) [4, p.185] that was a four-to-one cover.

Once the change of variables is defined for the position variables, we determine the generalized momentum via the Legendre transform: $P_i = \partial \mathcal{L} / \partial \dot{Q}_i$ where \mathcal{L} is the Lagrangian.⁽¹⁶⁾ A calculation gives that

$$P_1 = \frac{p_1 + p_2}{a + b} \tag{11}$$

$$P_2 = \frac{a}{a + b} p_1 - \frac{b}{a + b} p_2$$

Combining (10) and (11) gives us a change of variables $(Q_1, Q_2, P_1, P_2) = L(q_1, q_2, p_1, p_2)$ that is canonical: $L'JL = J$ where J is the 8×8 matrix of the form

$$J = \begin{pmatrix} O & Id \\ -Id & 0 \end{pmatrix} \tag{12}$$

We get a new Hamiltonian

$$\tilde{H}(Q_1, Q_2, P_1, P_2) = \frac{P_1^2}{2C_1} + \frac{P_2^2}{2C_2} + V(\|Q_2\|) \tag{13}$$

with

$$C_1 = \left(\frac{b^2}{m_1} + \frac{a^2}{m_2} \right)^{-1}, \quad C_2 = \left(\frac{m_1 m_2}{m_1 + m_2} \right)$$

Under this change of variables, the energy is unchanged: $H(q_1, q_2, p_1, p_2) = \tilde{H}(L(q_1, q_2, p_1, p_2))$.

The Hamiltonian \tilde{H} can be viewed as a sum of two Hamiltonians

$$\tilde{H}(Q_1, Q_2, P_1, P_2) = \tilde{H}_1(Q_1, P_1) + \tilde{H}_2(Q_2, P_2) \quad (14)$$

with

$$\tilde{H}_1(Q_1, P_1) = \frac{P_1^2}{2C_1}, \quad \tilde{H}_2(Q_2, P_2) = \frac{P_2^2}{2C_2} + V(\|Q_2\|) \quad (15)$$

Thus the system is split into the Cartesian product of two independent pieces.

The (Q_2, P_2) piece is the motion of a point particle of mass C_2 moving on the torus \tilde{T}_2^2 and being influenced by a potential V centered at the origin and of finite range. Using the methods of Section 2, we can make this system non-ergodic.

Since the change of variables was canonical, it preserves the Hamiltonian structure: for $i = 1, 2$,

$$\frac{dQ_i}{dt} = \frac{\partial \tilde{H}_i}{\partial P_i}, \quad \frac{dP_i}{dt} = -\frac{\partial \tilde{H}_i}{\partial Q_i}$$

For $i = 1$, the equations become $dQ_1/dt = P_1/C_1$, $dP_1/dt = 0$ so that $Q_1(t) = Q_1(0) + tP_1/C_1$, $P_1(t) = P_1(0)$. We interpret these solutions as follows. The total momentum of the original system equals $P_1(a+b)$ and is invariant. Q_1 is a type of generalized center of mass; it undergoes straight line motion on the torus \tilde{T}_1^2 .

In conclusion, we see that under the canonical change of variables given by (10, 11), the dynamics of the system split into a Cartesian product of two Hamiltonian systems. The first system is linear motion on a torus. The second is the motion of a point particle being acted upon by a symmetric potential \tilde{V} of finite range.

4b. Reduction for All Masses

To present a reduction that works also for the case of irrational mass ratios, we follow the method of Simanyi and Wojtkowski⁽¹⁷⁾ who studied the case of two particles with inelastic collision.

We start by changing configuration space coordinates: $(Q_1, Q_2) = L_1(q_1, q_2)$ with

$$Q_1 = q_1, \quad Q_2 = q_2 - q_1 \tag{16a}$$

This linear map $L_1: T^2 \times T^2 \rightarrow \tilde{T}_1^2 \times \tilde{T}_2^2$ is well defined with \tilde{T}_i^2 , $i = 1, 2$, having the same size as the original T^2 and is one-to-one. Using the Lagrangian formulation, we determine the associated generalized momentum coordinates

$$P_1 = m_1 \dot{q}_1 + m_2 \dot{q}_2 = p_1 + p_2 = \text{total momentum}, \quad P_2 = m_2 \dot{q}_2 = p_2 \tag{16b}$$

This change of variables is canonical and transforms the Hamiltonian (3) into

$$\tilde{H}_1(Q_1, Q_2, P_1, P_2) = \frac{P_1^2}{2m_1} - \frac{P_1 P_2}{m_1} + \frac{P_2^2}{2m_\mu} + V(\|Q_2\|) \tag{17}$$

where $m_\mu = (m_1 m_2 / m_1 + m_2)$ is called the reduced mass.

Hamilton's equations give

$$\frac{dQ_2}{dt} = \frac{\partial \tilde{H}_1}{\partial P_2} = \frac{-P_1}{m_1} + \frac{P_2}{m_\mu}, \quad \frac{dP_2}{dt} = -\frac{\partial \tilde{H}_1}{\partial Q_2} = -\frac{\partial V}{\partial Q_2}(\|Q_2\|) \tag{18}$$

The total momentum $P_1 = p_1 + p_2$ of the system is conserved. If we fix the energy level $H = E$ and the total momentum $P_1 = I$, then on the level surface of constant energy and constant momentum, the equations of motion for (Q_2, P_2) become

$$\frac{dQ_2}{dt} = \frac{-I}{m_1} + \frac{P_2}{m_\mu}, \quad \frac{dP_2}{dt} = -\frac{\partial V}{\partial Q_2}(\|Q_2\|) \tag{19}$$

Thus on a level surface of fixed energy and momentum, the motion of $(Q_2(t), P_2(t))$ is independent of the variables Q_1, P_1 . In such a case, the flow $(Q_2(t), P_2(t))$ is said to be a factor of the original flow [29, Section 4.1g].

Taking the Hamiltonian \tilde{H}_2 defined by

$$\tilde{H}_2(Q_2, P_2) = -\frac{I P_2}{m_1} + \frac{P_2^2}{2m_\mu} + V(\|Q_2\|) \tag{20}$$

we have that the motion $(Q_2(t), P_2(t))$ is determined by the equations

$$\frac{dQ_2}{dt} = \frac{\partial \tilde{H}_2}{\partial P_2}, \quad \frac{dP_2}{dt} = -\frac{\partial \tilde{H}_2}{\partial Q_2}$$

We complete the square to produce another canonical change of variables:

$$Q_3 = Q_2, \quad P_3 = \left(P_2 - \frac{m_\mu}{m_1} I \right) \quad (21)$$

that converts (19) into

$$\frac{dQ_3}{dt} = \frac{1}{\mu} P_3 = \frac{\partial \tilde{H}_3}{\partial P_2}, \quad \frac{dP_3}{dt} = -\frac{\partial V}{\partial Q_3}(\|Q_3\|) = -\frac{\partial \tilde{H}_3}{\partial Q_3} \quad (22)$$

where \tilde{H}_3 is given by

$$\tilde{H}_3(Q_3, P_3) = \frac{P_3^2}{2m_\mu} + V(\|Q_3\|) \quad (23)$$

The energy level for this system is related to the energy $E = H(q_i, p_i) = \tilde{H}_1(Q_i, P_i)$ of the original system by

$$\tilde{H}_3(Q_3, P_3) = \tilde{H}_2 + \frac{m_\mu I^2}{2m_1^2} = E - \frac{I^2}{2(m_1 + m_2)} \quad (24)$$

Now we have a single particle Q_3 moving on a torus \tilde{T}_3^2 of the same size as the original torus T^2 under the influence of a single radially symmetric potential $V(\|Q_3\|) = V(\|Q_2\|) = V(\|q_2 - q_1\|)$.

In summary, for a fixed energy and momentum level surface, the original system $H(q_i, p_i)$ is equivalent to a system $\tilde{H}(Q_i, P_i)$. This new system has a factor which is equivalent to the flow of a single point particle of mass m_μ moving on the torus \tilde{T}_3^2 under the influence of a finite range potential.

5. NONERGODICITY OF 2 PARTICLES

We examine the motion of two particles of mass m_1 and m_2 interacting under the influence of a Lennard-Jones potential V of finite range R on a two-dimensional torus $T^2 = (-l_x, l_x) \times (-l_y, l_y)$ and show that under appropriate conditions, this system is non-ergodic.

For the change of variables used in Section 4a, the system was a many-to-one cover of a Cartesian product of two systems, one of which was a point particle moving on a torus with a finite range Lennard-Jones potential. If this latter system is non-ergodic, then the Cartesian product and hence the original system are also non-ergodic.

For the change of variables procedure described in Section 4b, the original system contained as a factor a one-particle system moving on a torus with a finite range Lennard-Jones potential. If this factor is non-ergodic, then it is a standard ergodic theory result that the original system is also non-ergodic [29, Section 4.1g]. We outline in some detail the precise relationship between the factor system and the original system.

Given a fixed potential V , we look at the factor system $\tilde{H}_3(Q_3, P_3)$ given by (23). The motion of Q_3 occurs on a torus \tilde{T}_3^2 of the same size as T^2 . On \tilde{T}_3^2 there is a Lennard-Jones potential of finite range R centered at the origin. For each energy level \mathcal{E} , the potential generates a rotation function $\Delta\theta_{\mathcal{E}}$. By the results of Section 2, there is a threshold energy \mathcal{E}_0 , such that for all energies $\mathcal{E}^* \geq \mathcal{E}_0$, the rotation function $\Delta\theta_{\mathcal{E}^*}$ is partially focusing. Take any such energy level \mathcal{E}^* that also satisfies the technical condition (1): $\Delta\theta_{\mathcal{E}^*}(\phi^*) \neq 2\phi^* \pmod{\pi}$, where ϕ^* is the critical angle for which $\Delta\theta'_{\mathcal{E}^*}(\phi^*) = 2$.

Theorem 5.1. For such an \mathcal{E}^* , we can then find a torus size $\{l_{x_0}, l_{y_0}\}$ such that for any value of total momentum I and energy E satisfying the relation

$$E = \mathcal{E}^* + \frac{I^2}{2(m_1 + m_2)}$$

the two-particle system generated by the Hamiltonian

$$H(q_1, q_2, p_1, p_2) = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(\|q_1 - q_2\|), \quad q_i \in T^2, \quad i = 1, 2$$

is non-ergodic on the (E, I) energy-momentum level surface.

Furthermore, there exists an $\varepsilon > 0$ such that when $|\mathcal{E} - \mathcal{E}^*|, |l_{x_0} - l_x|, |l_{y_0} - l_y|$ are all less than ε , then the two-particle system restricted to an $\{E, I\}$ level surface for which

$$E = \mathcal{E} + \frac{I^2}{2(m_1 + m_2)}$$

is non-ergodic on every torus with size $\{l_x, l_y\}$.

Proof. By the results of Section 2, we can choose lengths $\{l_{x_0}, l_{y_0}\}$ for the torus \tilde{T}_3^2 such that the one-particle system \tilde{H}_3 has a stable elliptic orbit and hence is non-ergodic. Elliptic islands are stable under small perturbations so nearby energy levels and torus sizes will also be non-ergodic.

The following standard argument shows that for any values of energy E and momentum I for which

$$E - \frac{I^2}{2(m_1 + m_2)} = \mathcal{E}^*$$

non-ergodicity will then also hold for the original system $H(q_i, p_i)$ on the (E, I) energy-momentum level surface.

In a neighborhood of the initial conditions for the stable periodic orbit for \tilde{H}_3 , there is a set of positive measure of initial conditions $(Q_3(0), P_3(0)) \subset \tilde{T}_3^2 \times R^2$ for which the orbit $(Q_3(t), P_3(t))$ moves in a restricted region of its phase space. Consider this positive measure set in (Q_2, P_2) coordinates. Now choose a fixed value $P_1 = I$ (since $dP_1/dt = 0$, this value will remain constant under the flow) and consider the energy level surface $E = \mathcal{E}^* + I^2/(2(m_1 + m_2))$. Let the initial position $Q_1(0)$ vary over all of T^2 . The orbits $(Q_1(t), Q_2(t), P_1(t) \equiv I, P_2(t))$ produced in this way will form a positive measure set of trajectories which have a restricted motion for the system \tilde{H}_1 on the (E, I) level surface. Thus \tilde{H}_1 will be non-ergodic on this energy-momentum level set and hence so will the original Hamiltonian system $H(q_i, p_i)$.

APPENDIX. SPECIAL CASE OF EQUAL MASSES AND ZERO TOTAL MOMENTUM

In the case of equal masses and zero total momentum, we can reduce the two-particle system to the motion of a single particle in a way that allows us to see geometrically the relation between a periodic orbit for the reduced system and for the original system.

We denote the common mass of the particles by $m = m_1 = m_2$ and have that total momentum $P = p_1 + p_2$ equals zero. We choose the position coordinate q so that the center of mass of the system

$$q_{cm} = \frac{mq_1 + mq_2}{2m} \tag{25}$$

is initially at the origin. Since

$$\frac{dq_{cm}}{dt} = \frac{m\dot{q}_1 + m\dot{q}_2}{2m} = \frac{p_1 + p_2}{2} = \frac{P}{2} \tag{26}$$

the condition $P = 0$ implies that $q_{cm}(t)$ stays fixed at the origin for all time. Hence

$$q_1(t) = -q_2(t) \tag{27}$$

The condition $P = p_1 + p_2 = 0$ further implies that $p_1 = -p_2$ and hence that

$$\dot{q}_1 = -\dot{q}_2 \tag{28}$$

Thus to determine the dynamics of the system $(q_1, q_2, p_1, p_2)(t)$, it is enough to know the dynamics of $(q_1, p_1)(t)$ and then use equations (27, 28) to recover the full motion. The equations of motion for $(q_1, p_1)(t)$ are

$$\begin{aligned} \frac{dq_i}{dt} &= \frac{p_i}{m_i} \\ \frac{dp_i}{dt} &= -\frac{\partial V}{\partial q_i}(\|q_1 - q_2\|) = -V'(\|q_1 - q_2\|) \frac{\partial(\|q_1 - q_2\|)}{\partial q_i} \\ &= -V'(\|q_1 - q_2\|) \frac{(q_1 - q_2)}{\|q_1 - q_2\|} = -V'(2\|q_1\|) \frac{q_1}{\|q_1\|} \end{aligned} \tag{29}$$

since $q_2 = -q_1$.

We will show that the trajectories $(q_1, p_1)(t)$ that come from solving (29) can also be obtained as the solutions of a new Hamiltonian $\tilde{H}(\tilde{q}_1, \tilde{p}_1)$ on T^2 which includes several disjoint symmetric potentials of finite range.

To determine the Hamiltonian \tilde{H} , we look at the original system. The first particle moves linearly whenever the separation $\|q_1 - q_2\| > R$. When the separation $\|q_1 - q_2\| < R$, the two particles will interact under the potential V . Since the motion is taking place on a torus, the first particle will interact with the second particle whenever

$$\|q_1 - (nl_x, ml_y)\| \leq R/2, \quad n, m \in \{-1, 0, 1\} \tag{30}$$

where the torus $T^2 = (-l_x, l_x) \times (-l_y, l_y)$. For then, since $q_2 = -q_1$, we have that $\|q_1 - q_2\| \leq R$ (Fig. 5).

Now imagine that the second particle is made invisible. Then we will see one particle, whose position we denote by \tilde{q}_1 , moving on T^2 . Most of

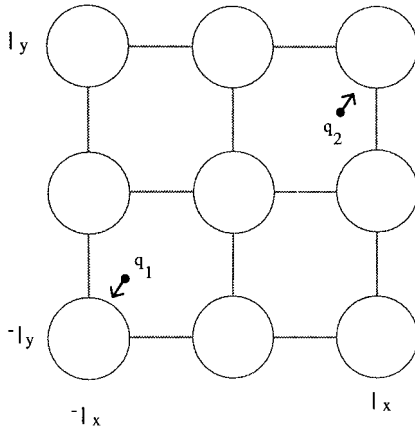


Fig. 5. Two particles on torus interacting by finite range potential.

the time, the particle moves in a straight line but, when it comes close to one of the lattice points of the torus, i.e., $\|\tilde{q}_1 - (nl_x, ml_y)\| \leq R/2$, $n, m \in \{-1, 0, 1\}$, it is deflected by some type of force. We will show that the force in a neighborhood of the lattice point (nl_x, ml_y) is generated by a symmetric potential $\tilde{V}_{(n,m)}$ of finite range $R/2$ given by

$$\tilde{V}_{(n,m)}(\tilde{q}_1) = \frac{1}{2} V(2 \|\tilde{q}_1 - (nl_x, ml_y)\|) \tag{31}$$

Assuming this result for the moment, we see that the solutions $(\tilde{q}_1, \tilde{p}_1)(t)$ of position and momentum of the point particle of mass m are generated by the Hamiltonian

$$\tilde{H}(\tilde{q}_1, \tilde{p}_1) = \frac{\tilde{p}_1^2}{2m} + \tilde{V}(\tilde{q}_1) \tag{32}$$

where \tilde{V} is a compound potential given by

$$\tilde{V}(\tilde{q}_1) = \sum_{m,n \in \{0,1\}} \tilde{V}_{(n,m)}(\tilde{q}_1) \tag{33}$$

Since our compound potential is defined on a torus, we have a choice as to where to base the potentials. We choose to take representatives of the potentials $\tilde{V}_{(n,m)}$ that are based at the lattice points $\{(0, 0), (1, 0), (0, 1), (1, 1)\}$ relative to the coordinate vectors $\{l_x, l_y\}$.

Note that the total energy of this one-particle system is exactly half the energy of the two-particle system (3).

To show that the force the single particle feels near a lattice point is indeed given by (31), we prove that the trajectories $(\tilde{q}_1, \tilde{p}_1)(t)$ generated by (32) agree with the trajectories $(q_1, p_1)(t)$ given by (29). We have that

$$\begin{aligned} \frac{d\tilde{q}_1}{dt} &= \frac{\partial \tilde{H}}{\partial \tilde{p}_1} = \frac{\tilde{p}_1}{m} \\ \frac{d\tilde{p}_1}{dt} &= -\frac{\partial \tilde{H}}{\partial \tilde{q}_1} = -\frac{\partial \tilde{V}}{\partial \tilde{q}_1}(\tilde{q}_1) \end{aligned} \tag{34}$$

Since the potential \tilde{V} has the same values about each lattice point, it is enough to consider the case that \tilde{q}_1 is close to the origin and interacts with the potential $\tilde{V}_{(0,0)}$. Then

$$\begin{aligned} \frac{d\tilde{p}_1}{dt} &= -\frac{\partial \tilde{V}_{(0,0)}}{\partial \tilde{q}_1}(\tilde{q}_1) = -\frac{1}{2} \frac{\partial V}{\partial \tilde{q}_1}(2 \|\tilde{q}_1\|) \\ &= -\frac{1}{2} V'(2 \|\tilde{q}_1\|) \frac{\partial(2 \|\tilde{q}_1\|)}{\partial \tilde{q}_1} = -V'(2 \|\tilde{q}_1\|) \frac{\tilde{q}_1}{\|\tilde{q}_1\|} \end{aligned} \tag{35}$$

Thus $(\tilde{q}_1, \tilde{p}_1)(t)$ and $(q_1, p_1)(t)$ satisfy the same equations of motion.

In conclusion, we have reduced the motion of the two-particle system (3) on T^2 in which the particles interact by means of a potential V to a one-particle system (32) on T^2 in which the particle interacts with a compound potential \tilde{V} consisting of four disjoint copies of a symmetric potential of finite range. A nice fundamental domain for T^2 is the region $(-l_x/2, 3l_x/2) \times (-l_y/2, 3l_y/2)$. With this choice of domain, each of the potentials $\tilde{V}_{(n,m)}$ based at the four lattice points $\{(0,0), (1,0), (0,1), (1,1)\}$ can be visualized without requiring identifications of the torus (Fig. 6). If the original potential V is of type Lennard-Jones, then the potentials $\tilde{V}_{(n,m)}$ are also of type Lennard-Jones.

We can make a further reduction in the system to produce a particle interacting with a single symmetric potential of finite range. Consider particle motion on the smaller torus

$$\tilde{T}^2 = (-l_x/2, l_x/2) \times (-l_y/2, l_y/2) \tag{36}$$

which contains one potential $\tilde{V}_{(0,0)}$ centered at the origin. Then the larger torus T^2 provides a four-fold cover of the smaller torus. The particle

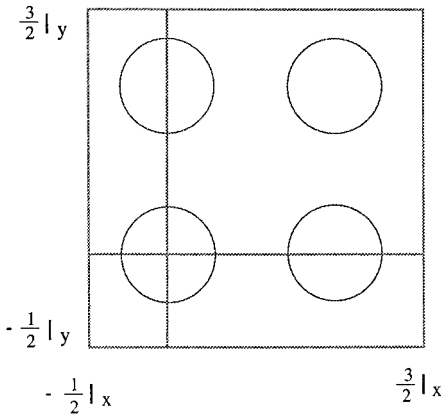


Fig. 6. Reduced system of one particle on torus with four disks.

motion on \tilde{T}^2 lifts to the particle motion on T^2 . This system seems to be closely related to the system $\tilde{H}_2(Q_2, P_2)$ of Section 4a.

Thus we have reduced our original two-particle system to a generalized Sinai billiard with one disk. We make the reduced system non-ergodic by constructing a stable elliptic periodic orbit. This orbit lifts using the relations $q_1(t) = -q_2(t)$, $\dot{q}_1(t) = -\dot{q}_2(t)$ to a stable periodic orbit for the two-particle system (Fig. 7). In this figure, we show the time evolution $\{q_i^t\}$, $i = 1, 2$ of the two particles at times $t = 0, 1, 2$.

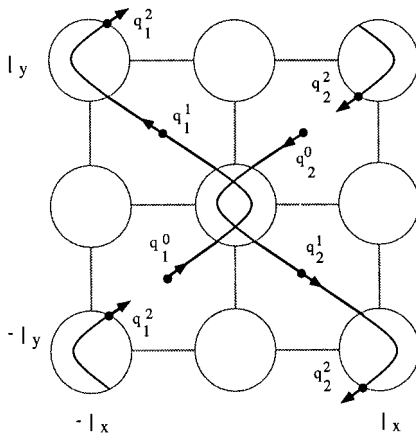


Fig. 7. Periodic orbit for two particles of equal mass and momentum zero on torus.

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