Threshold law for escaping from the Hénon-Heiles system

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We report a theoretical study of the escape rates of the Hénon-Heiles system above threshold. An analytic formula for the escape rate as a function of energy is presented. We also simulated the escaping process by following the motions of a large number of particles. Two algorithms are employed to solve the equations of motion. One is the Runge-Kutta-Fehlberg method, and another is a recently proposed fourth order symplectic method. Our simulations show the escape of Hénon-Heiles system follows exponential laws. We extracted the escape rates from the time dependence of particle numbers in the Hénon-Heiles potential. The extracted escape rates agree with the analytic result. Close to threshold we find the rate $\alpha(\Delta E)$ can be written as a series expansion, the first term of this expansion is $\frac{4}{3}\Delta E$.

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I. INTRODUCTION AND MODEL

The scaling laws are directly associated with the classical dynamics of the systems under study. Bauer and Bertsch [1] studied the decay laws of chaotic and nonchaotic billiards with windows. They found the number of particles remaining inside chaotic billiards decreases exponentially, but nonchaotic billiards decay according to power laws. The results suggest that the exponential law is connected to the chaotic dynamics. However, an exception is the circular billiard, which is integrable but decays exponentially [2]. Experimental studies on the decay laws of an elbow cavity using microwaves have also been reported [3]. We study the escape laws in the Hénon-Heiles system [4,5] with the following Hamiltonian:

$$H = \frac{1}{2}(p_x^2 + p_y^2) + U(x,y),$$

$$U(x,y) = \frac{1}{2}(x^2 + y^2) + x^2 y - \frac{1}{3}y^3, \tag{1}$$

where x and y are the coordinates and p_x and p_y are the momenta. The mass of the particle is set to one for convenience. This system exhibits both regular motion and chaotic motion depending on the energy of the system, and it has been studied from statistical, semiclassical and other perspectives [6–10]. Recently Brack *et al.* have calculated the density of states above threshold [11]. The escape laws have not been addressed so far.

Numerical studies show the motion of Hénon-Heiles system is regular for $E < 1/12$. When E is greater than 1/12, the fraction of chaotic region in phase space increases with increasing energy until $E = 1/6$ the whole phase space is chaotic. $E_{\mathrm{th}} = 1/6$ is the threshold energy of this system. When $E \geqslant E_{\mathrm{th}}$, a particle in the potential well can escape. Figure 1 shows the contours of the potential $U(x,y)$. There are three saddle points $P_1(x=0, y=1)$, $P_2(-\sqrt{3}/2, -1/2)$, and $P_3(\sqrt{3}/2, -1/2)$. All contours with energy less than 1/6 are closed. A particle with energy less than 1/6 always moves inside the closed contour and it remains in the well. The contour with $E = 1/6$ is the equilateral triangle $P_1P_2P_3$. The contours with energies larger than 1/6 are not closed. There are three openings at the three saddle points. A particle with energy above 1/6 can escape from the well via the three openings. Because this system is chaotic above threshold, we expect that the escape in the Hénon-Heiles system should also follow an exponential law. Assuming $N(0)$ random particles with the same energy in the Hénon-Heiles well at $t = 0$, the number of particles at t should be

$$N(t) = N(0)\exp(-\alpha t), \tag{2}$$

where α is an energy dependent decay rate. The purpose of this article is to verify Eq. (2) and to estimate α for different energies.

II. AN ESCAPE RATE FORMULA

We can derive a formula for the escape rate as a function of energy above threshold by assuming ergodicity in the

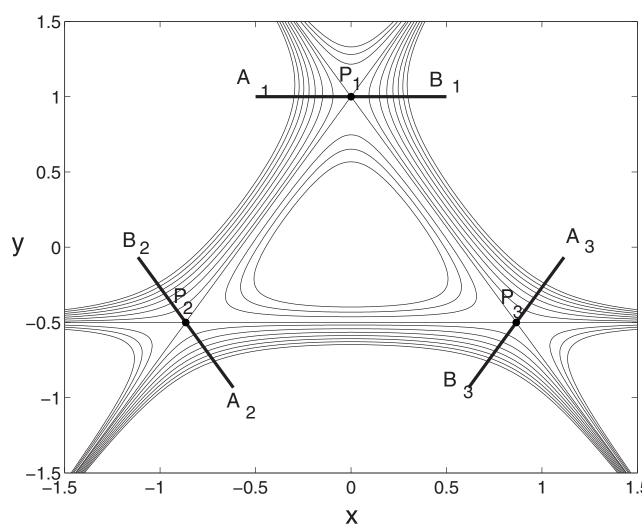

FIG. 1. Equipotential lines of the function $U(x,y)$ in Eq. (1). The points P_1, P_2, and P_3 are saddle points.

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Hénon-Heiles system above threshold. We draw a line perpendicular to the escape direction through each saddle point, they are lines A_1B_1, A_2B_2, and A_3B_3 in Fig. 1. For any energy E above threshold, we define the potential well of the Hénon-Heiles system to be the region restricted by the three disconnected contour lines and the three straight lines A_1B_1, A_2B_2, and A_3B_3. The motion in the well is assumed to be ergodic. For a given energy E, the phase space distribution is $\psi(q,p)=\frac{\delta(E-H(q,p))}{\int dqdp\,\delta(E-H(q,p))}$ [5], where q,p are the coordinates and momenta. For our two-dimensional system, it is easy to work out the results: the distribution in (x,y) is uniform inside the well, and once the particle's position is given, the magnitude of the momentum is fixed by the Hamiltonian in Eq. (1) and the direction of the momentum is uniformly distributed in $[0,2\pi]$. We define the energy above threshold by $\Delta E=E-E_{\mathrm{th}}$. We use θ to represent the direction of momentum relative to the y axis. We use $S(\Delta E)$ to denote the area of the well. Then the distribution in the variables (x,y,θ) can be expressed as $\rho(x,y,\theta)=\frac{1}{2\pi S(\Delta E)}$. Given N particles in the well, the number of particles leaving the well through the opening at the saddle point P_1 in unit time can be written as $N\int dx\int_{-\pi/2}^{\pi/2}d\theta\rho(x,y,\theta)|\mathbf{v}(x,y)|\cos(\theta)$, where the integral in x is along the line A_1B_1 and is restricted to the classical allowed part. We note the three openings of the system are symmetric. Therefore the number of particles leaving the well in unit time from three openings are just three times of the above result. The change of N with respect to t is

$$\frac{dN(t)}{dt}=-3N(t)\rho\int_{-\pi/2}^{\pi/2}\cos(\theta)d\theta\int_{-\sqrt{2\Delta E/3}}^{\sqrt{2\Delta E/3}}\sqrt{2(\Delta E-3x^2/2)}dx \tag{3}$$

$$=-2\pi\sqrt{3}\Delta E\rho N(t), \tag{4}$$

which gives the escape rate $\alpha(\Delta E)=\frac{\sqrt{3}\Delta E}{S(\Delta E)}$.

There is no analytical formula for the area of the well $S(\Delta E)$. We have applied Monte Carlo method to calculate the area as a function of ΔE. The numerical results are represented by dots in Fig. 2. We found the numerical results can be represented very well by the quadratic polynomial

$$S(\Delta E)=S_0+S_1\Delta E+S_2(\Delta E)^2, \tag{5}$$

where $S_0=\frac{3\sqrt{3}}{4}$ is the area of equilateral triangle $P_1P_2P_3$. By fitting Eq. (5) to the numerical results in Fig. 2 using least squares, we have determined the values for the other two coefficients $S_1=9.656$ and $S_2=-22.61$. The line in Fig. 2 is the fitted quadratic polynomial. We finally have the formula for the escape rate in the Hénon-Heiles system

$$\alpha(\Delta E)=\frac{\sqrt{3}\Delta E}{S_0+S_1\Delta E+S_2(\Delta E)^2}. \tag{6}$$

Very close to the threshold, a power expansion of Eq. (6) may be useful. Define

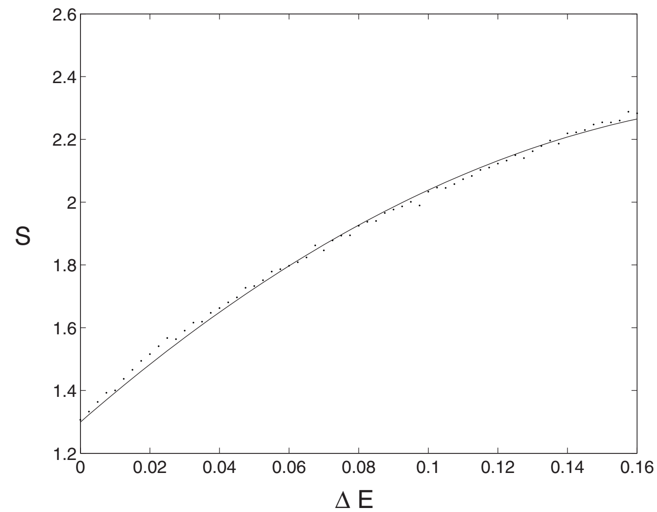

FIG. 2. The area of the well (region bounded by the three disconnected contour lines and the three straight lines A_1B_1, A_2B_2, and A_3B_3) as a function of energy above threshold ΔE. The dots are results calculated using Monte Carlo method. The solid line is the fitted quadratic polynomial in Eq. (5).

$$\alpha(\Delta E)=\sum_1^{\infty}B_i\Delta E^i. \tag{7}$$

The coefficients B_i can be expressed in S_0, S_1, and S_2. They are $B_1=\frac{\sqrt{3}}{S_0}$, $B_2=-\frac{\sqrt{3}S_1}{S_0^2}$, and others can be obtained from the following iteration formula $B_i=-\frac{S_1B_{i-1}+S_2B_{i-2}}{S_0}$, $i=3,4,\ldots$. The numerical values for the first four coefficients in the power expansion of Eq. (6) are $B_1=4/3, B_2=-9.9115, B_3=96.8743$, and $B_4=-892.547$. Keeping only the first term in the power expansion close to threshold, we obtain $\alpha(\Delta E)=\frac{4}{3}\Delta E$. The escape rate therefore increases linearly with the energy of the system near threshold. In contrast, the escaping rate for chaotic billiards with artificial windows depends on the square root of energy as shown by Bauer and Bertsch [1].

III. NUMERICAL SIMULATIONS OF ESCAPE

We now verify the exponential decay law in Eq. (2) and the escape rate formula in Eq. (6) using numerical simulations. In our numerical simulations of the escape process, we follow the positions of a large number of particles in time. The number of particles $N(t)$ remaining in the potential well as a function of time is monitored and used to extract the escape rate. For any energy above threshold, we initially place $N(0)$ particles in the well according to the distribution $\rho(x,y,\theta)=\frac{1}{2\pi S(\Delta E)}$. This distribution sets the initial conditions for the particles. The trajectory of each particle is then followed by numerically solving the Hamilton's equations. We used two algorithms to integrate Hamilton's equation. Runge-Kutta-Fehlberg (RKF) is the first algorithm [12]. In this algorithm the error in each step can be controlled by setting the relative tolerance and the absolute tolerance. In all our calculations, we set the absolute tolerance to 10^{-9}. The second algorithm (CC) was proposed recently by Chin and

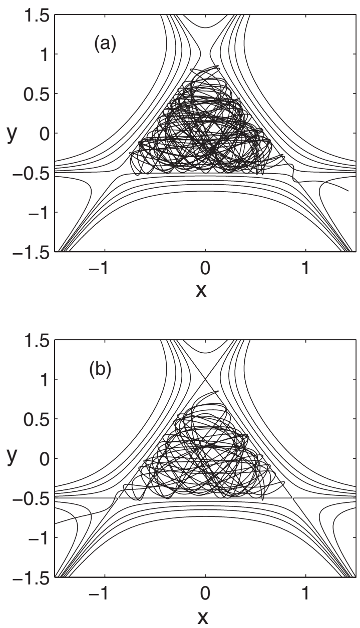

FIG. 3. Examples of trajectories calculated from the two algorithms in the Hénon-Heiles system. Both trajectories start from the position ($x=0$, $y=0.16$) with energy $E=0.18$, the initial direction of momentum points to the positive x axis. (a) RKF method [12] with relative tolerance 10^{-8} and time range (0–299). (b) CC method of Chin and Chen [13] with step 0.04 and time range (0–172).

Chen [13], it is a fourth order forward symplectic algorithm. It is generally believed that symplectic algorithms are better and can follow the true dynamics longer because they preserve the symplectic structures of Hamilton's equation. The explicit algorithm for advancing the system forward from t to $t+\epsilon$ is

$$\mathbf{p}_1 = \mathbf{p}(i) + \frac{1}{6}\epsilon\mathbf{F}(\mathbf{q}(i)),$$

$$\mathbf{q}_1 = \mathbf{q}(i) + \frac{1}{2}\epsilon\mathbf{p}_1,$$

$$\mathbf{p}_2 = \mathbf{p}_1 + \frac{4}{6}\epsilon\widetilde{\mathbf{F}}(\mathbf{q}_1),$$

$$\mathbf{q}(i+1) = \mathbf{q}_1 + \frac{1}{2}\epsilon\mathbf{p}_2,$$

$$\mathbf{p}(i+1) = \mathbf{p}_2 + \frac{1}{6}\epsilon\mathbf{F}(\mathbf{q}(i+1)). \quad (8)$$

Note $\mathbf{F}=-\boldsymbol{\nabla}U$ and $\widetilde{\mathbf{F}}=\mathbf{F}+\frac{1}{48}\epsilon^2\boldsymbol{\nabla}(|\mathbf{F}|^2)$ includes an correction to the original force. The time step size ϵ can be varied to control integration errors.

In Fig. 3 we show the two trajectories calculated using the two algorithms. The two trajectories start from the same initial condition: the position is at ($x=0$, $y=0.16$), the energy is $E=0.18$, and the direction of momentum is in the positive x axis. Figure 3(a) is the trajectory obtained using RKF algorithm with relative tolerance 10^{-8}. Figure 3(b) is the trajectory obtained using CC method with a time step size $\epsilon=0.04$. We have verified the accuracy of both calculations. When the time step size and relative tolerance were reduced further, the trajectories did not show noticeable change. Figures 3(a) and 3(b) show clearly the two trajectories obtained using the two algorithms stay close for some time and then separate. In Fig. 3(a), the particle escapes at $t=299$, while in Fig. 3(b), the particle escapes at $t=172$. The increased separation of the two trajectories calculated with two different algorithms starting with the same initial condition reflects the difficulty to follow chaotic motions for a long time. Nevertheless we can still extract accurate escape rates as shown below.

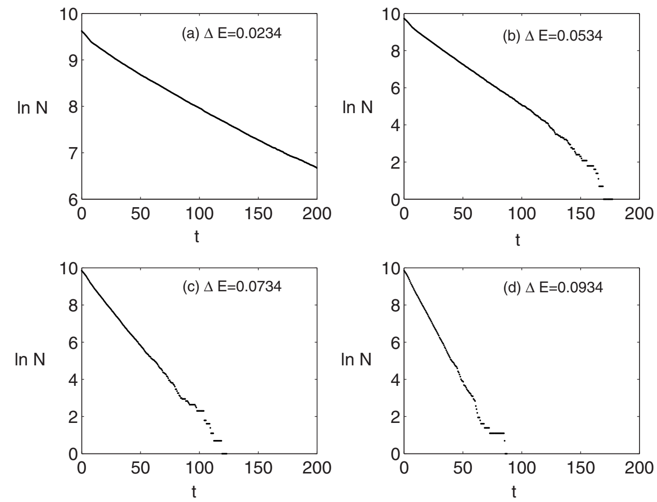

FIG. 4. The number of particles in the well as a function of time for four energies above threshold. (a) $\Delta E=0.0234$, $N(t=0)=15\,326$, (b) $\Delta E=0.0534$, $N(t=0)=17392$, (c) $\Delta E=0.0734$, $N(t=0)=18\,885$, (d) $\Delta E=0.0934$, $N(t=0)=19\,942$. The dots are numerical results obtained using RKF method [12] with a relative tolerance 10^{-8}.

A large number of particles are used in the simulations of escape process. For example, we initially put $N(0)=15326$ particles with the energy $\Delta E=0.0234$ above threshold according to $\rho(x,y,\theta)=\frac{1}{2\pi S(\Delta E)}$ in the well. We advanced this system by following the trajectory of each particle using RKF method with relative tolerance 10^{-8}. We recorded the number of particles $N(t_i)$ remaining in the well in time step $\Delta t=0.628$. Figure 4(a) shows $N(t)$ as a function of time in log-linear scale. Figures 4(b)–4(d) show similar results for different energies. We found the curves in Fig. 4 in all the cases are almost straight lines. The escape of Hénon-Heiles system therefore follows approximately exponential laws. For each energy, we can extract the escape rate from the simulated $N(t)$. We used the simulated $N(t)$ from time $t=0$ to a time when ten percent of the particles have escaped and fitted it to $\ln N(t)=c-\alpha t$ using least squares. The fitted parameter α is the extracted escape rate at the corresponding energy.

We compare in Fig. 5 the extracted escape rates and the analytic result in Eq. (6) as a function of energy above

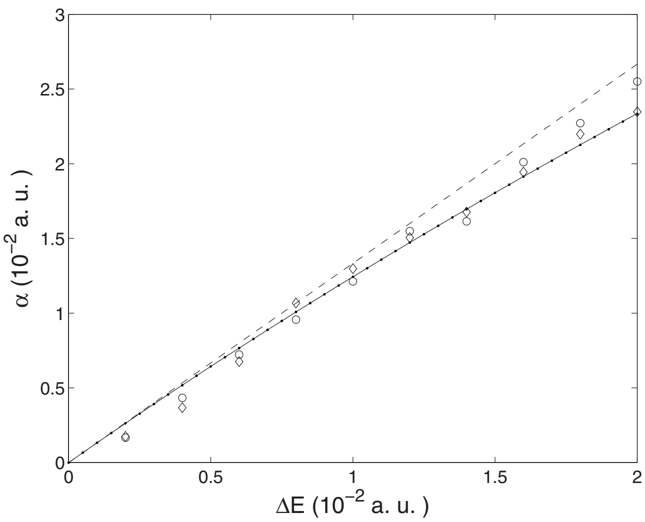

FIG. 5. The escape rate α as a function of energy above threshold for the Hé non-Heiles system. ΔE is the energy of the system above threshold. The solid line is the formula in Eq. (6). The circles are the numerical results from RKF method [12] with a relative tolerance 10^{-8}, and the diamonds are the numerical results obtained from CC method [13] with a time step 0.04. The dashed lines are the threshold scaling law $\alpha(\Delta E) = \frac{4}{3}\Delta E$. The dotted line is the power expansion of Eq. (7) with the first four terms only.

threshold. The solid line is from the formula in Eq. (6). The circles are the numerical results from RKF method with a relative tolerance 10^{-8}, the diamonds are the numerical results obtained from CC method [13] with time step 0.04. The numerical results from the two algorithms agree well. We verified the accuracy of simulations by using smaller tolerance and smaller step size, and we found that the numerical results did not change. The numerically extracted rate in Fig. 5 can be described quite well by the scaling law $\alpha(\Delta E) = \frac{4}{3}\Delta E$, which is shown as the dashed lines. The dotted line shows the power expansion of Eq. (6) with the first four terms. An improved agreement is achieved by the expansion.

IV. CONCLUSIONS

We have derived a formula in Eq. (6) for the escape rate of the Hénon-Heiles system. We also simulated the escape process by following a large number of trajectories. We used a symplectic algorithm and a nonsymplectic algorithm to advance each particle's trajectory in time. The numerically extracted escape rates using the two algorithms agree with each other, and they also agree with the analytic formula for Hénon-Heiles system in Eq. (6).

Close to threshold, we found the rate scales linearly with the energy of the system above threshold ΔE and can be written as $\alpha(\Delta E) = \frac{4}{3}\Delta E$. The linear dependence for Hénon-Heiles system differs from the $(\Delta E)^{1/2}$ dependence for chaotic billiards with artificial windows [1]. The derivation for the escape rate in Eq. (6) suggests that the linear scaling of escape rate should also apply to other two-dimensional chaotic systems with smooth openings.

ACKNOWLEDGMENT

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