

Regular and chaotic motions in Hénon–Heiles like Hamiltonian

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Abstract: The dynamics of a system subjected to a potential equal to the sum of the Hénon–Heiles potential and that of hydrogen in an electric field was studied. The 4 Hamilton's equations of motion follow from the Hamiltonian and they were integrated numerically using the Runge–Kutta fourth order method. The Poincaré surface of a section fixed at $x = 0$ and $p_x > 0$ was used to reduce the phase space to a 2-dimensional plane. The analysis of the Poincaré surface, the Lyapunov exponent, and the autocorrelation shows that as the constant of motion, E , increases from 0.30 to 0.45, the dynamics makes a transition from periodic and quasi-periodic to chaotic motions.

Key words: Hamiltonian, Hénon–Heiles, Poincaré section, Lyapunov exponent, autocorrelation

1. Introduction

A Hamiltonian form H for a dynamical system is very important in that a number of inquiries and sometimes conclusions can be made about the system without a prior solution of the dynamical equation. Many real problems coming from physics or chemistry are formulated as Hamiltonian systems and most of them admit a particular case that has just 2 degrees of freedom. In this situation, the numerical and analytical studies provide very detailed information about the behavior of the system [1].

The Hénon–Heiles potential has played a prominent role in the development of chaos theory. Suggested by Hénon and Heiles [2] as the simplest potential that produces all the complexities obtainable in any chaotic system, the potential has received a lot of attention from researchers, and has recently been referred to as the most famous open Hamiltonian system [1].

Hénon–Heiles' potential was constructed by adding 2 terms of third degree in coordinates to the potential of a planar harmonic oscillator. It also results from expansion of a potential function corresponding to an integrable system (resulting from some canonical transformations applied to a system modeling the motion of 3 particles on a circle under the influence of exponentially decreasing forces) to third degree terms [3,4].

The Hénon–Heiles Hamiltonian, H , is given as

$$H = \frac{1}{2} (p_x^2 + p_y^2) + V(xy) \quad (1)$$

with the potential energy $V(x,y)$ defined by

$$V(x,y) = \frac{1}{2} \left(x^2 + y^2 + 2x^2y - \frac{2y^3}{3} \right) \quad (2)$$

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where x and y are the coordinates of the oscillator, with corresponding momentum p_x and p_y .

The current trend in the study of nonlinear dynamical systems with state variables equal to or greater than 3 is to expose or characterize the nature of the trajectories of the system. The full graphical display of the state space (phase space) when dimension is ≥ 3 is difficult to visualize and interpret. The Poincaré surface of section is a well-known procedure for projecting the state space into a space of lower dimensions [5]. The Kolmogorov–Arnold–Moser (KAM) theory for conservative nonlinear systems has shown that a single dot in the Poincaré plane corresponds to a perfectly sinusoidal motion; a closed nonintersecting orbit represents a quasiperiodic motion, while dense scattered points are a measure of chaotic motion [6].

Our conjecture of a classical stark hydrogen atom in a gravitational field with Hamiltonian described in Eq. (9) to the best of our knowledge has not yet been reported in the literature.

2. Modified Hénon–Heiles potentials

Vesely and Podolsky [7] in describing the motion of free test particles in a vacuum gravitational pp-wave modified the Hénon–Heiles potential by interchanging the signs of the last 2 terms in Eq. (2) to obtain

$$V(x, y) = \frac{1}{2} \left(x^2 + y^2 - 2x^2y + \frac{2y^3}{3} \right) \quad (3)$$

This is different from the modified Hénon–Heiles system studied by Choudhury and Kalita [8]:

$$V(x, y) = \frac{1}{2} \left(x^2 - y^2 + 2x^2y - \frac{2y^3}{3} \right) \quad (4)$$

Also in [9] a different form of Hénon–Heiles potential given by

$$V(x, y) = \frac{x^2+y^2}{2} + \alpha \left(x^2y - \frac{y^3}{3} \right) \quad (5)$$

was studied.

The dynamics of a system subjected to a potential equal to the sum of the Hénon–Heiles potential and that of the hydrogen atom in a uniform magnetic field has been studied in [10] with the potential energy taking the form

$$V(x, y) = \frac{1}{2} \left(x^2 - y^2 + 2x^2y - \frac{2y^3}{3} \right) + \frac{5}{2}xy^2 + x^2 + y^2 - sx^2 + y^2, \quad (6)$$

where s is an energy scale parameter. The similarity in all the various forms of modification of Eq. (2) is that the coupling term(s) is of order 3 in space coordinates as in the original Hénon–Heiles potential.

Hydrogen, the simplest and most abundant element in the universe, is an energy carrier and is expected to play a critical role in new, decentralized energy infrastructures with many important advantages over other fuels [11].

The hydrogen atom has received a lot of attention from researchers, ranging from the classical electronic motion of the atom near a metal surface [12] and hydrogen atom in the presence of uniform magnetic and quadrupolar electric fields [13] to the hydrogen atom in parallel electric and magnetic fields [14].

In this paper, we consider a physical system in atomic physics, a hydrogen atom in a uniform electric field (a classical stark effect). The Hamiltonian in atomic units is [15]

$$H = \frac{p^2}{2} - \frac{1}{r} + \vec{F} \cdot \vec{r} \tag{7}$$

where F is the electric field force, taking to be $\vec{F} = F\hat{y}$ the electric field along the y axis

The Hamiltonian in 2 dimensions becomes

$$H = \frac{p_x^2 + p_y^2}{2} - \frac{1}{(x^2 + y^2)^{\frac{1}{2}}} + Fy, \tag{8}$$

where $r = (x^2 + y^2)^{\frac{1}{2}}$

$$V(x, y) = -\frac{1}{(x^2 + y^2)^{\frac{1}{2}}} + Fy. \tag{9}$$

3. Methodology

The sum of Hénon–Heiles potential (Eq. 2) and hydrogen atom in an electric field (Eq. 9) represents a physical system that may be called the classical stark hydrogen atom in a gravitational field. The Hamiltonian of the system is

$$H = \frac{p_x^2 + p_y^2}{2} + \frac{x^2 + y^2}{2} + x^2y - \frac{1}{3}y^3 - \frac{1}{(x^2 + y^2)^{\frac{1}{2}}} + Fy, \tag{10}$$

where $\frac{x^2 + y^2}{2}$ is the harmonic term of the electron motion in 2 dimensions, $-\frac{1}{(x^2 + y^2)^{\frac{1}{2}}}$ is the electrostatic potential energy between the fixed nuclear center and the electron, while Fy is the externally electric field energy, and $x^2y - \frac{1}{3}y^3$ plays the role of centrifugal energy that prevent the collapse of the electron into the nucleus.

The equations of motion are given by Hamilton’s equations:

$$\dot{p} = -\frac{\partial H}{\partial q} \tag{11}$$

$$\dot{q} = \frac{\partial H}{\partial p} \tag{12}$$

These are

$$\frac{dx}{dt} = p_x \tag{13}$$

$$\frac{dy}{dt} = p_y \tag{14}$$

$$\frac{dP_x}{dt} = -x - 2xy - \frac{x}{(x^2 + y^2)^{\frac{3}{2}}} \tag{15}$$

$$\frac{dP_y}{dt} = -y - x^2 + y^2 - \frac{y}{(x^2 + y^2)^{\frac{3}{2}}} + F. \tag{16}$$

The equations were integrated using the Runge–Kutta fourth order method. The Poincaré surface of the section was fixed at $x_0 = 0.0$ and $px_0 > 0$. This reduced the 4-dimensional phase space (x, y, px, py) to a 2-dimensional subspace in the (y, py) plane. The trajectories can intersect the Poincaré surface either way, but we followed positive orientation (anticlockwise). The Hamiltonian, H , (Eq. (9)), being explicitly time independent implies that it is a constant of motion and that the total energy $E \equiv H$ is conserved for all time, t . We considered the behavior of the system for energy, E , ranging from 0.30 to 0.45, and in all cases the electric field of the system was taken as $F = 0.45$. The Lyapunov exponent, λ , which is the averaged rate of divergence (or convergence) of 2 neighboring trajectories in the phase space, was computed using Eq. (16), while the autocorrelation, $\mathbf{R}_{\mathbf{x}\mathbf{x}}(\tau)$, was calculated using Eq. (17).

$$\lambda = \frac{1}{t} \log \frac{\delta \mathbf{z}(t)}{\delta \mathbf{z}(0)} \tag{17}$$

$$\mathbf{R}_{\mathbf{x}\mathbf{x}}(\tau) = \frac{1}{2T} \int_{-T}^T \mathbf{x}(t) \mathbf{x}(t + \tau) dt \tag{18}$$

4. Results and discussion

The Poincaré surfaces of sections for the modified Hénon–Heiles potential for various constants of motion or energies, E , are shown in Figures 1–5. For $E = 0.30$ (arbitrary units) and 0.35, 2 discernible egg/banana closed orbits in the py, y phase plane can be observed (Figures 1 and 2). The clear closed orbits correspond to quasiperiodic trajectories of the moving mass. When $E = 0.40$ (Figure 3), while the egg orbit remained closed, the banana orbit started losing shape. The banana orbit collapsed completely when $E = 0.44$ (Figure 4), while the egg orbit is still discernible. When $E = 0.45$, the 2 orbits merged and created many isolated orbits (islands) in the region right of the former egg orbit (Figure 5). No close orbits are discernible in the region of the former egg orbit. The phase space trajectories are thus fully chaotic for $E = 0.45$.

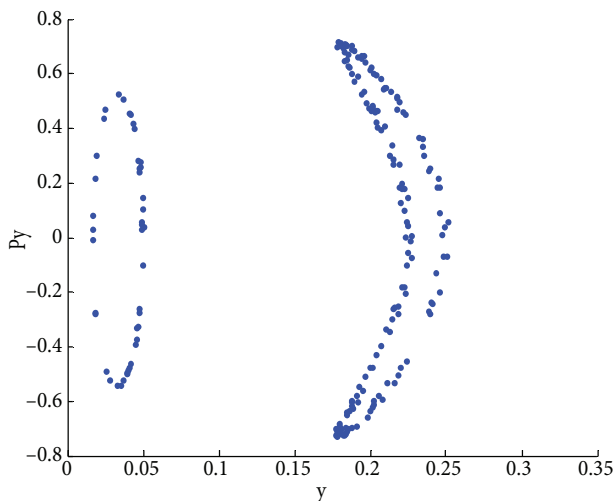


Figure 1. Poincaré surface of section, $E = 0.30$.

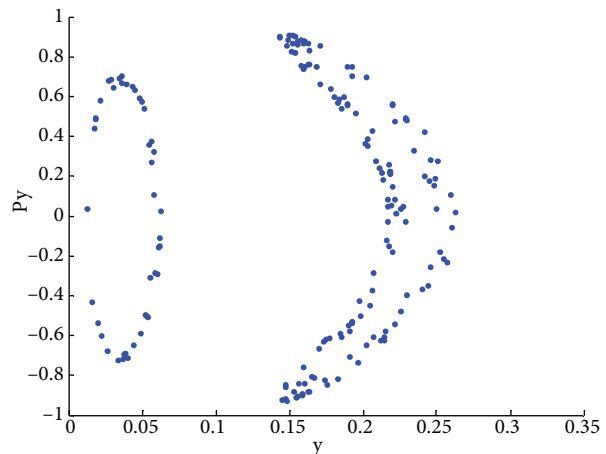


Figure 2. Poincaré surface of section, $E = 0.35$.

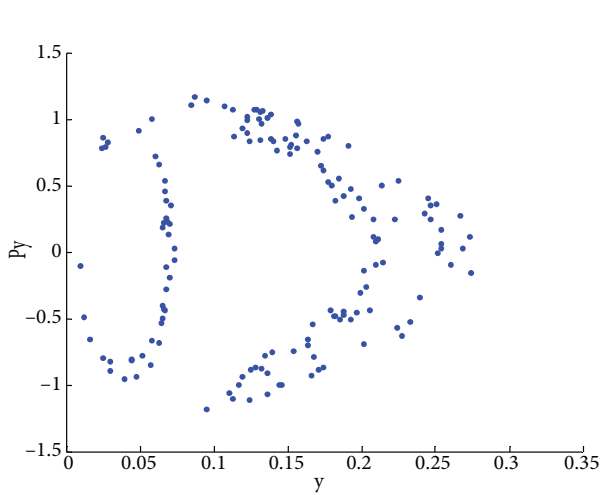


Figure 3. Poincaré surface of section, $E = 0.40$.

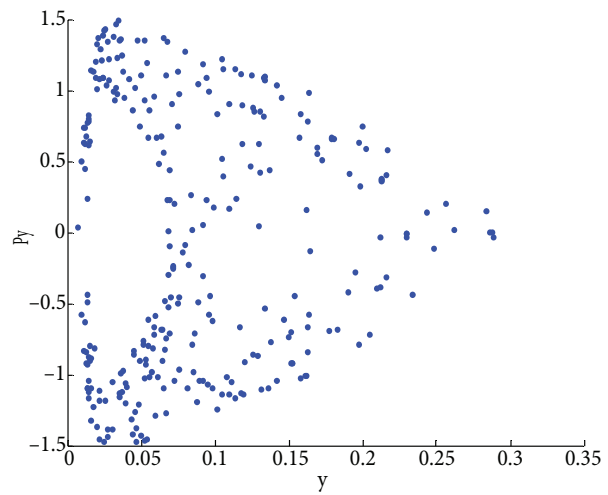


Figure 4. Poincaré surface of section, $E = 0.44$.

Lyapunov exponents for $E = 0.30$ and $E = 0.45$ corresponding to the regular and irregular trajectories are shown in Figures 6 and 7. The instantaneous slope of the graph for $E = 0.30$ (Figure 6) is less than zero for the greater part of the simulation time, while for $E = 0.45$ (Figure 7) the instantaneous slope is greater than zero. A positive Lyapunov exponent is one measure or signature of chaos and supports the Poincaré prediction of chaos at $E = 0.45$.

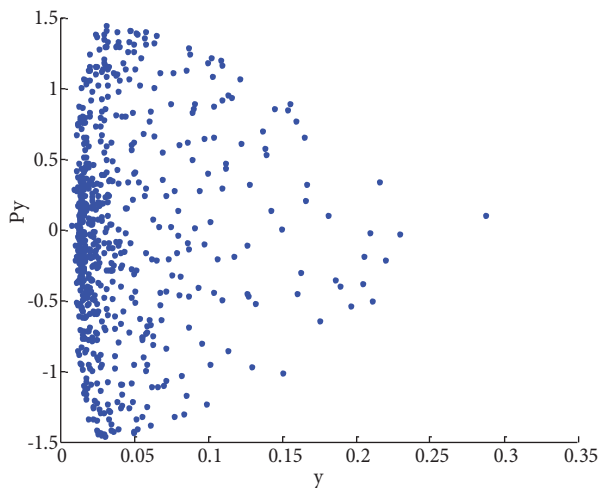


Figure 5. Poincaré surface of section, $E = 0.45$.

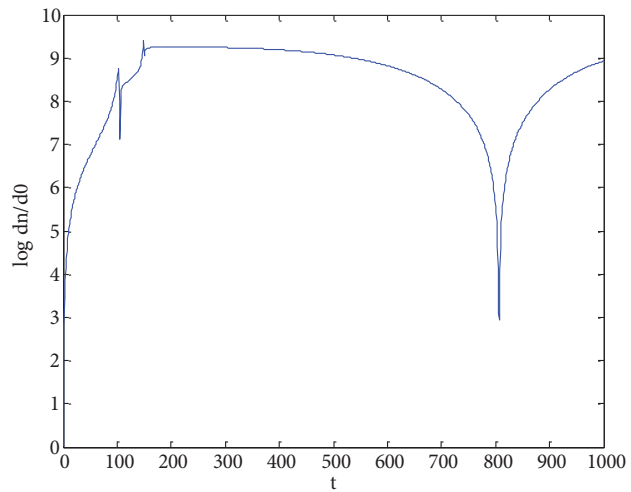


Figure 6. Lyapunov exponent, $E = 0.30$.

The autocorrelation of the system is shown in Figures 8–10. The small irregularity seen (Figure 8) indicates quasiperiodic motion like the Poincaré surface of the section (Figure 1). This irregularity continues at $E = 0.40$ (Figure 9) until it becomes completely irregular at $E = 0.45$ (Figure 10), showing a chaotic situation.

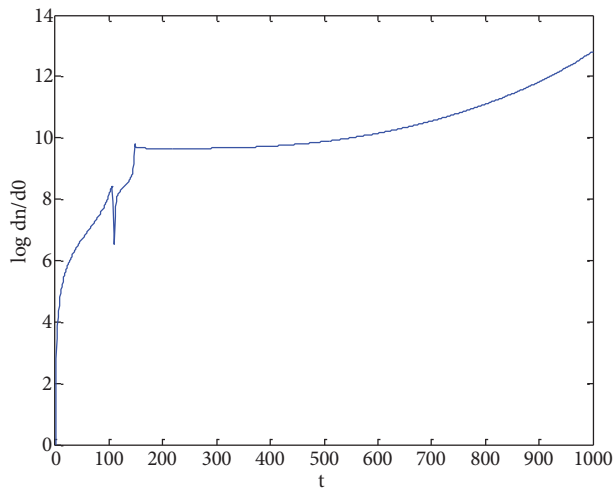


Figure 7. Lyapunov exponent, $E = 0.45$.

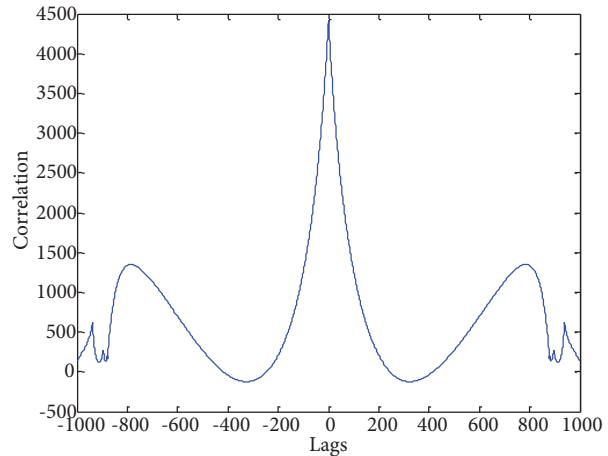


Figure 8. Autocorrelation, $E = 0.30$.

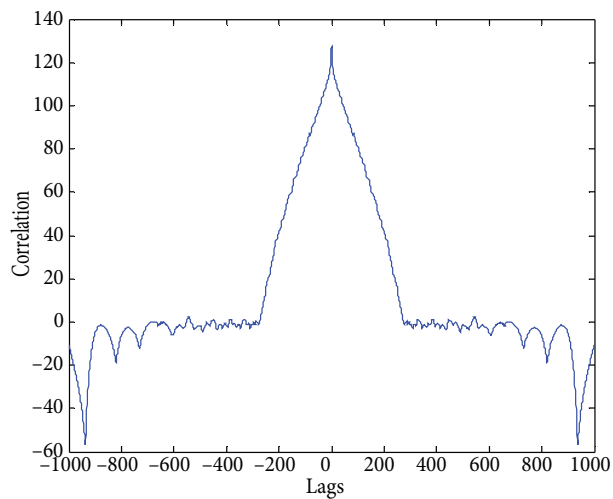


Figure 9. Autocorrelation, $E = 0.40$.

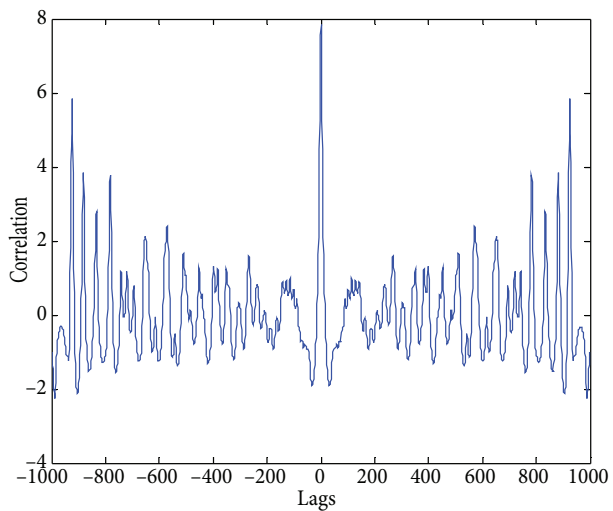


Figure 10. Autocorrelation, $E = 0.45$.

5. Conclusion

The investigation of a nonlinear dynamical system of state space dimension ≥ 3 is of great interest in physics because of the bizarre possibility of the motion degenerating from predictability to unpredictability (chaos). When a conservative nonlinear system is chaotic, it implies that the way the total energy, E , of the system is shared among the various degree of freedom (state variables) is unpredictable, even though the dynamical system is deterministic. We found in our study that classical stark hydrogen in a gravitational field becomes fully chaotic when $E = 0.45$. The 3 tools applied (Poincaré section, Lyapunov exponent, and autocorrelation) in the analysis of the trajectories all support the same conclusion.

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