A SIMPLE METHOD FOR DETERMINING THE NUMBER OF ISOLATING INTEGRALS IN MULTIDIMENSIONAL SYSTEMS: COMPUTATION OF THE POINTWISE DIMENSION

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The pointwise dimension is calculated for trajectories of two- and three-dimensional Hamiltonians, enabling the number of isolating integrals to be determined directly. Results for the Hénon–Heiles system are in agreement with recent calculations of the fractal and information dimensions by Stine and Noid.

1. Introduction

There is considerable current interest in the nature of the coexistence of regular (quasi-periodic) and irregular (chaotic, stochastic) motions in the phase space of generic classical Hamiltonian systems [1,2], especially the transition from predominantly regular to global chaotic behaviour found at high energies [1,2]. These ideas are widely recognized to be of fundamental importance for chemistry [3], insofar as classical dynamics provides an accurate description of intramolecular dynamics.

The classical mechanics of two-dimensional model potential surfaces has been intensively studied in recent years [2,3]. In particular, the Poincaré surface of section has been found to be a useful diagnostic for regularity or irregularity of a trajectory [3]. By contrast, very little is known at present concerning the detailed classical dynamics of multidimensional systems described by realistic potential surfaces (for recent work, cf. refs. [4–7]). Surface of section methods are difficult to apply for ($N \geqslant 3$)-dimensional systems, so that emphasis must be placed on intrinsic indicators of dynamical behaviour, such as the appearance of coordinate power spectra, or rate of divergence of nearby trajectories (cf. refs. [1,3]).

An important characteristic of any trajectory is the number of isolating integrals associated with it (in addition to the energy). This number determines the dimension of the trajectory, where a generalized notion of dimension such as the fractal dimension [8] must in general be used. The importance of the fractal dimension in this context has recently been emphasized by Reinhardt [9]. There are indications that for ($N = 3$)-dimensional coupled oscillator systems, for example, the chaotic region of phase space is divided at intermediate energies into disjoint "stochastic seas", each of which is characterized by a particular number of isolating integrals [10]. These disjoint regions then merge at higher energy into a single "big sea". It is clearly important for understanding the structure of chaos in multidimensional systems to have efficient methods for direct computation of the dimension of the trajectory in phase space.

Stine and Noid [11,12] have recently described methods for calculating both the fractal [11] and the so-called information dimension [12] of a trajectory [13]. These are summarized in section 2. Both techniques rely on computationally intensive bin-counting and sorting operations. In this letter we apply a conceptually and computationally simple approach for determining the *pointwise dimension* [13] of trajectories in two- and three-dimensional Hamiltonian systems. This method has previously been used by Guckenheimer [14] to characterize attractors. The definition [13] of the pointwise dimension (cf. section 3) relies on the existence of both a metric and a probability measure (density of points) in phase space. For Hamiltonian systems, the pointwise dimension is expected to be equal to both the information and the fractal dimension [12,13]. We have confirmed this result for the particular two- and three-dimensional potentials treated below.

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2. The fractal and information dimensions: methods of Stine and Noid

The idea for computing the fractal dimension of a trajectory [11] or attractor [13,15] is very simple: Phase space is divided into a large number of hypercubes (bins). The trajectory is then run for a time long enough to ensure that the number of bins visited by the trajectory converges to a constant value (no note is taken of the number of times a particular bin is visited by the trajectory). Plotting the log of the number of bins visited versus the log of the inverse size of the bin gives a straight line whose slope is the fractal dimension of the trajectory. Thus, let N be the number of bins in each direction of phase space, $2n$ the dimension of phase space, and N_{unique} the number of unique bins visited by the trajectory. We then have [11]:

$$\ln N_{\text{unique}} = (2n - k) \ln N + \text{constant}, \qquad (1)$$

where $2n - k$ is the fractal dimension of the trajectory with k the effective number of isolating integrals.

There are several drawbacks to this approach. For large N (corresponding to a large number N^{2n} of bins, necessary for accurate results) the trajectory must be run for a very long time to ensure that the number of unique hypercubes visited has reached its asymptotic value. In other words, the trajectory may tend to fill phase space very non-uniformly, which slows convergence of N_{unique}. The method also requires much computationally intensive bookkeeping to be done keeping track of bin occupations. Finally, all counting and sorting has to be done for a series of bin sized in order to determine k.

To alleviate the first problem mentioned above, Stine and Noid developed a method for calculating the information dimension of a trajectory. In this procedure, bins that are visited frequently by the trajectory are weighted more strongly than those visited less frequently. It is therefore possible to attain convergence with a shorter trajectory length than for the fractal dimension. In addition to a metric in phase space, a probability measure (number of trajectory points in a given bin/total number of points on trajectory) is required. If g_i is the probability of accessing hypercube i, a plot of the information entropy

$$S = \sum_i g_i \ln g_i \qquad (2)$$

versus $\ln N$ should give a straight line of slope $2n - k$ [12].

The above methods have been applied by Stine and Noid to calculate the number of isolating integrals k for quasi-periodic and chaotic trajectories of the 2D Hénon–Heiles system. Both approaches yield values $k = 2$ (quasi-periodic) and $k = 1$ (chaotic) within reasonable error limits. These results are expected on the basis of surface-of-section studies [2,3].

Nevertheless, both methods used by Stine and Noid rely on time-consuming bin-sorting operations. This factor becomes increasingly important for $(N > 2)$-dimensional systems. We have therefore applied a much simpler approach to determine the so-called pointwise dimension of a trajectory. This method, due to Guckenheimer [14] and described in the next section, has minimal sorting and storage requirements yet yields values in agreement with those of Stine and Noid for both two- and three-dimensional systems.

We note also the recent calculation of the so-called correlation exponent for attractors by Grassberger and Procaccia [16]. For the systems treated here the correlation exponent is identical with the pointwise dimension, but is computed using a different and (we found) more time-consuming algorithm.

3. Computation of the pointwise dimension

Suppose we have a probability measure μ (density of points on a trajectory) in phase space. The pointwise dimension d_p is then the exponent with which the total probability contained in a region (sphere) around a given point decreases as the radius of the sphere decreases [13]. More precisely, if $S_x(x_0)$ is a sphere of a radius x centered at point x_0 on the trajectory, then

$$d_p(x_0) \equiv \lim_{x \to 0} \frac{\ln \mu(S_x(x_0))}{\ln x}. \qquad (3)$$

If $d_p(x_0)$ is independent of x_0 for almost all x_0, then $d_p = d_p(x_0)$ is called the *pointwise dimension.*

A practical procedure for computing $d_p(x_0)$ is as follows [14]:

(i) Choose an initial point $x_0 = (q_0, p_0)$ in phase space.

(ii) Run a trajectory to obtain a series of points $x(t) = (q(t), p(t))$ with $x(t = 0) = x_0$. The trajectory

must be run for a time long enough to accumulate an appreciable density of points in the vicinity of x_0. This turns out to be quite feasible for two- and three-dimensional systems examined below, but is of course a major limitation of the method as applied to higher dimension problems, since it necessitates accurate integration over long times of trajectories having possible stochastic character.

(iii) At each point on the trajectory, calculate $D(t) = \|x(t) - x_0\|$, the distance of the point $x(t)$ from the reference point x_0. For a perturbed oscillator Hamiltonian of the form

$$H(q,p) = H_0 + V(q), \tag{4}$$

where

$$H_0 = \sum_{i=1}^{n} \tfrac{1}{2}(p_i^2 + \omega_i^2 q_i^2), \tag{5}$$

a natural metric in phase space is:

$$\|x(t) - x_0\|^2 = \sum_{i=1}^{n} [(p_i - p_0)^2 + \omega_i^2 (q_i - q_0)^2]. \tag{6}$$

For all the systems treated below $\omega_i = 1$ ($i = 1, 2$ and 3), so that the metric (6) reduces to the Cartesian distance in phase space. We have also verified that the precise form of the metric adopted is not crucial for computation of the pointwise dimension. For example, taking $0.5\,\omega_i^2$ instead of ω_i^2 in the metric (6) has no effect on the calculated value of d_p.

(iv) As the trajectory is run, the points $x(t)$ are binned according to the value of the distance $D(t)$. At the end of the run, this discrete distance distribution is integrated to give a binned distribution of the total number of points on the trajectory within a given distance of the reference point x_0. Note that no large-scale sorting operations are involved, regardless of the length of the trajectory or the dimension of phase space.

(v) The log of the number of points within a given distance is then plotted against the log of the distance. The slope of the straight line portion of the graph at small distances (see section 4) is $d_p(x_0)$.

(vi) Assuming that $d_p(x_0)$ is the same for all points x_0 on the trajectory, the pointwise dimension d_p can be defined as the average of $d_p(x_0)$ over a set of reference points $\{x_0\}$. We have used sets of 10 reference points (chosen by taking points at every 100th timestep at the beginning of a trajectory run; 100 timesteps is approximately 0.5 characteristic periods) to obtain the straight line plots shown in section 4. Keeping track of the distance along the trajectory from each reference point requires very little extra computational effort.

The assumption that $d_p(x_0)$ is constant over the whole trajectory allows us to improve statistics by averaging over a set of $\{x_0\}$. Examination of log–log plots for individual values of x_0 indicates that this assumption is valid for the trajectories shown in section 4, which have well defined regular or chaotic character. It would however be of great interest to study the variation of $d_p(x_0)$ with phase space point x_0 for a trajectory corresponding to a "patchy" torus, as suggested by Reinhardt [9]. Such a trajectory would presumably have local regions corresponding to different pointwise dimensions.

4. Results

4.1. Two-dimensional Hénon–Heiles potential

We have applied the method described in the previous section to calculate the pointwise dimension of trajectories for the standard degenerate two-dimensional Hénon–Heiles Hamiltonian:

$$H = \tfrac{1}{2}(p_1^2 + p_2^2) + \tfrac{1}{2}(q_1^2 + q_2^2) + (q_1^2 q_2 - \tfrac{1}{3} q_2^3). \tag{7}$$

Initial conditions were chosen to give three trajectories whose configuration-space projections are shown in fig. 1. They are of "precessing" quasi-periodic, "librating" quasi-periodic, and chaotic type, respectively. Hamilton's equation of motion were integrated using Gear's hybrid 6th order method [17], which has proved exceptionally stable for integration of long irregular trajectories [18].

For the calculations reported here a constant time step $\Delta t = 0.05$ was used for trajectory integration, and $x(t)$ computed for every point. Retaining a smaller fraction of points on the trajectory for the calculation of the pointwise dimension (for example, 1 point out of every 10) leaves the value of d_p essentially unchanged. We therefore keep all points on the trajectory in order to obtain better statistics for a given trajectory length.

A plot of the number of points within a given distance D versus $\log D$ is shown in fig. 2 for the precessing trajectory of fig. 1a. The trajectory was run for 1×10^5

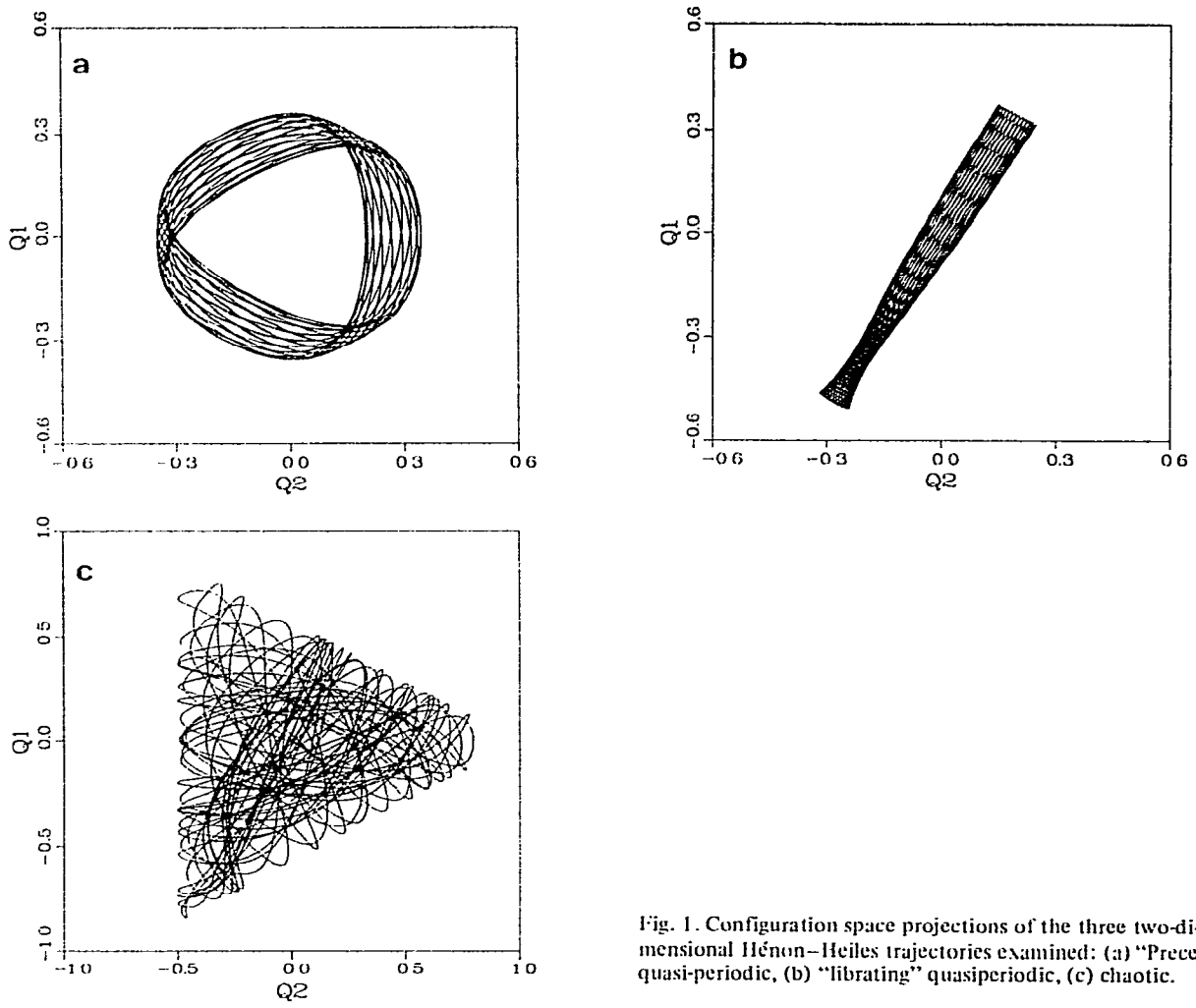

Fig. 1. Configuration space projections of the three two-dimensional Hénon–Heiles trajectories examined: (a) "Precessing" quasi-periodic, (b) "librating" quasiperiodic, (c) chaotic.

time steps. In this plot the distance D extends all the way to its maximum relevant value D_{max}, i.e. the size of the whole trajectory in phase space, as can be seen from the saturation of the number of points at large D. A well defined straight line portion of the plot is apparent at small values of D up to $\approx 0.1\ D_{max}$, and the slope of this section defines the pointwise dimension d_p. Regions of the plot for larger D up to D_{max} contain information on the global phase space structure of the torus, but are not analysed any further here. All plots shown from now on extend only up to $D \lesssim 0.1\ D_{max}$.

Log–log plots for each of the three trajectories of fig. 1 are shown in fig. 3. The plot of fig. 3a has least-squares slope 2.00, so that to the nearest integer value the pointwise dimension of the precessing quasi-periodic trajectory is 2. This corresponds to $k = 4 - 2 = 2$, so that there is one isolating integral in addition to the energy, as expected for a quasi-periodic trajectory on an invariant torus. The straight line portion of the curve for the librating trajectory does not extend as far as for the precessing case. Since the librating trajectory corresponds to a "long thin torus", this is a result of large local curvature of the trajectory manifold in phase space. The plot of fig. 3b corresponds to 2.5×10^5 points, and has least-squares slope 2.03. The librat-

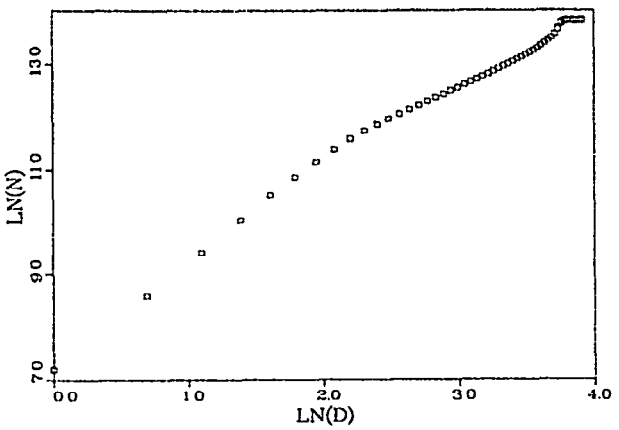

Fig. 2. Plot of log (number of trajectory points within a distance D of reference point) versus log D for the trajectory of fig. 1a, averaged over a set of 10 reference points. D extends all the way to D_{max}, the maximum extent of the trajectory in phase space. Note the well defined straight line portion at small D, and the saturation at large D. The pointwise dimension is the slope of the plot at small D.

ing trajectory therefore also has 2 isolating integrals. The plot for the chaotic trajectory is shown in fig. 3c (5×10^5 points) and has least-squares slope 2.98. The chaotic trajectory therefore has $k = 1$, and no isolating integrals in addition to the energy.

4.2. Three-dimensional model potential

To test the applicability of the method for three-dimensional systems, we follow ref. [11] and introduce an additional degree of freedom:

$$H' = H + \tfrac{1}{2}(p_3^2 + \omega_3^2 q_3^2), \qquad (8)$$

where we take $\omega_3 = 1.0$. Although the third degree of freedom is uncoupled, it serves to increase the dimensionality of phase space.

Trajectories were run for the three-dimensional system of eq. (8) with initial conditions for modes 1 and 2 identical with those of the trajectories of fig. 1; for mode 3, we set $q_3 = 0.0, p_3 = 0.3$. All trajectories were run for 1.0×10^6 time steps.

Log–log plots for the three trajectories run are shown in fig. 4. Least-squares values of d_p are 3.06, 2.99, and 3.94, corresponding to integer k values 3, 3, and 2, respectively. These values are just those expect-

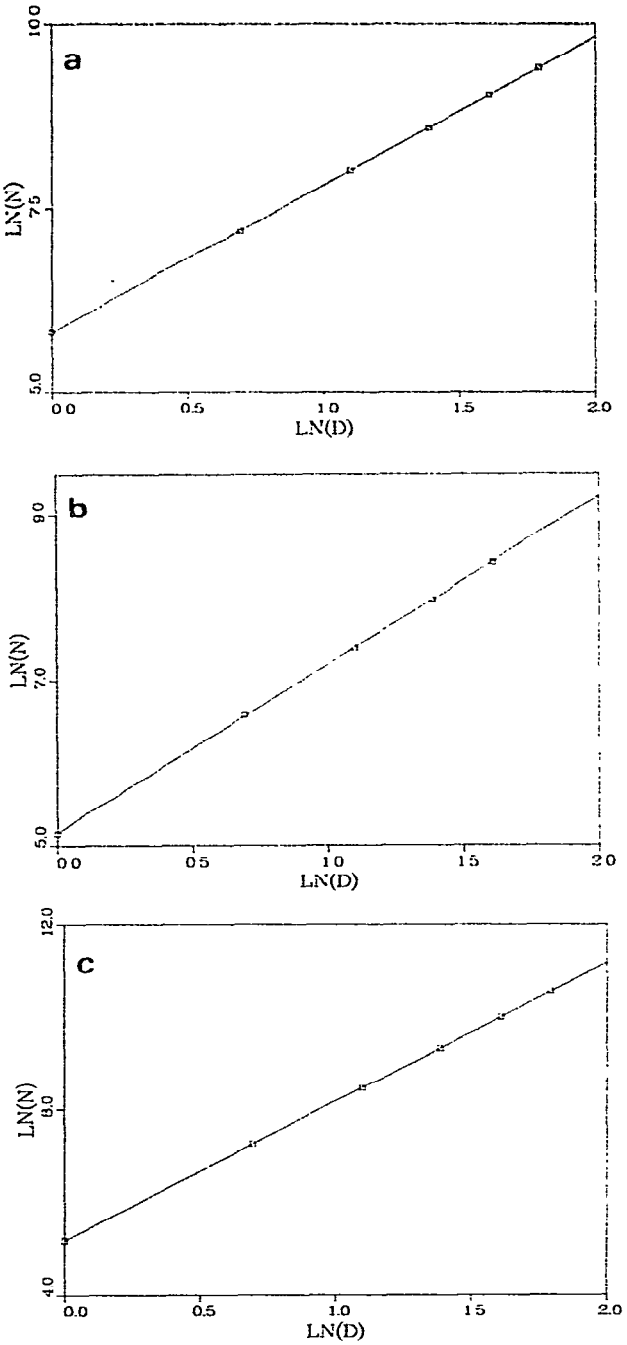

Fig. 3. Log (number of points) versus log D for the trajectories of fig. 1. The maximum value of D shown is $\lesssim 0.1\, D_{max}$. (a) Precessing quasi-periodic: least-squares slope = 2.00, (b) librating quasi-periodic: least-squares slope = 2.03, (c) chaotic: least-squares slope = 2.98.

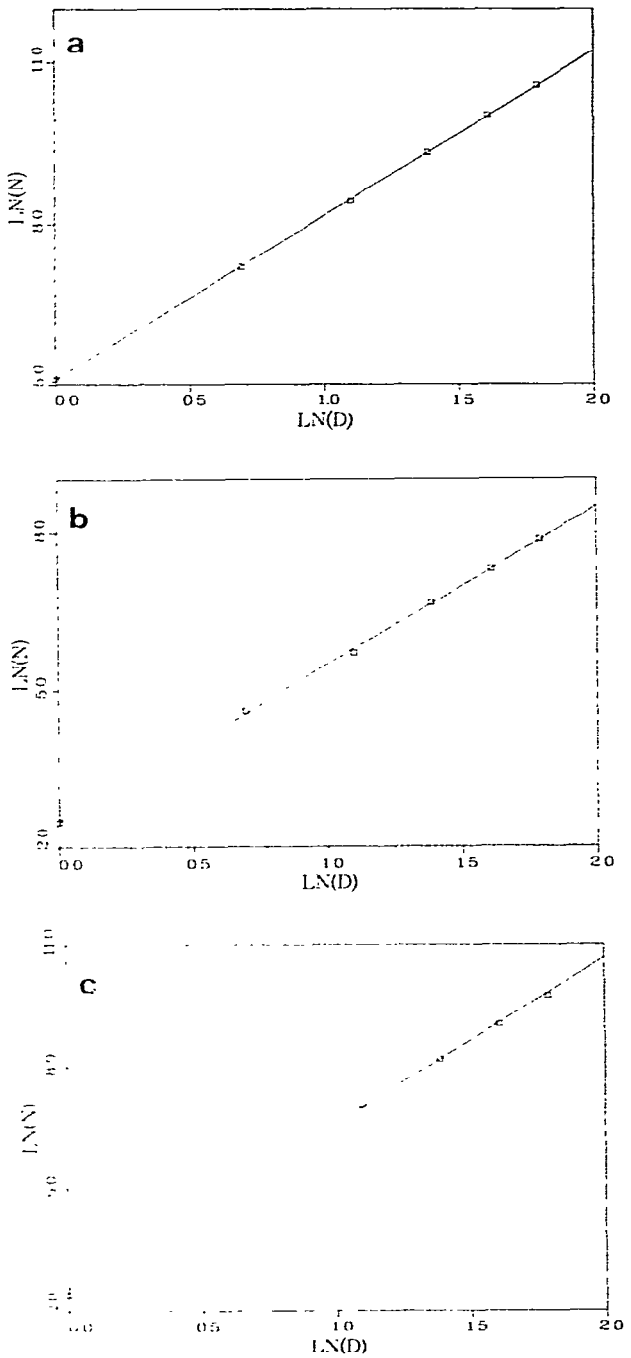

Fig. 4. Log (number of points within distance D) versus log D for the three trajectories of the (N = 3)-dimensional system discussed in section 4. (a) Least-squares slope = 3.06, (b) least-squares slope = 2.99, (c) least-squares slope = 3.94.

ed for the addition of an uncoupled degree of freedom to the two-dimensional system treated above.

These results establish the practicability of the method for three-dimensional Hamiltonian systems, and open the way for application to more realistic molecular potentials.

5. Conclusion

We have applied a conceptually and computationally simple method to calculate the pointwise dimension of trajectories of two- and three-dimensional Hamiltonian systems. The method provides the number of isolating integrals for the trajectory directly. Our calculations for the Hénon–Heiles potential confirm expectations based on surface of section studies, and are in agreement with the recent results of Stine and Noid [11,12]. We have also established the applicability of the method for $N = 3$ systems.

Work in progress is concerned with computation of the pointwise dimension for trajectories of realistic three-dimensional surfaces.

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References

[1] A.J. Lichtenberg and M.A. Lieberman, Regular and stochastic motion (Springer, Berlin, 1983).
[2] M. Tabor, Advan. Chem. Phys. 46 (1981) 73;
P. Brumer, Advan. Chem. Phys. 47 (1981) 201.
[3] D.W. Noid, M.L. Koszykowski and R.A. Marcus, Ann. Rev. Phys. Chem. 32 (1981) 267;
S.A. Rice, Advan. Chem. Phys. 47 (1981) 117.
[4] D. Carter and P. Brumer, J. Chem. Phys. 77 (1982) 4208.
[5] S.C. Farantos and J.N. Murrell, Chem. Phys. 55 (1981) 205;
S.C. Farantos, Chem. Phys. 71 (1982) 157; Chem. Phys. Letters 92 (1982) 379; J. Phys. Chem. 87 (1983) 5061.
[6] K.N. Swamy and W.L. Hase, Chem. Phys. Letters 92 (1982) 371.
[7] J. Santamaria and G.S. Ezra, unpublished.
[8] B.B. Mandelbrot, Fractals: form, chance and dimension (Freeman, San Francisco, 1977); The fractal geometry of nature (Freeman, San Francisco, 1982).

[9] W.P. Reinhardt, in: The mathematical analysis of physical systems, ed. R. Mickens (Van Nostrand, Princeton), to be published.
[10] G. Contoupoulos, L. Galgani and A. Giorgilli, Phys. Rev. A18 (1978) 1183.
[11] J.R. Stine and D.W. Noid, J. Phys. Chem. 87 (1983) 3038.
[12] J.R. Stine and D.W. Noid, Chem. Phys. Letters 100 (1983) 282.
[13] J.D. Farmer, E. Ott and J.A. Yorke, Physica 7D (1983) 153.
[14] J. Guckenheimer and G. Buznya, Phys. Rev. Letters 51 (1983) 346;
J. Guckenheimer, in: Contemporary mathematics, Vol. 28 (American Mathematical Society, 1984).
[15] H.S. Greenside, A. Wolf, J. Swift and T. Pignataro, Phys. Rev. A25 (1982) 3453.
[16] P. Grassberger and I. Procaccia, Phys. Rev. Letters 50 (1983) 346; Physica 9D (1983) 189.
[17] C.W. Gear, SIAM. J. Num. Anal. 2B (1964) 69.
[18] P. Brumer, J. Comput. Phys. 14 (1974) 391.