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## Numerical identification of regular and irregular spectra

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**Abstract.** Polyatomic molecules are described by nonintegrable Hamiltonians. For such systems it has been predicted (Percival 1973) that there are two regions of the quantal spectrum with contrasting properties. We obtain eigenvalues for the Hénon–Heiles non-integrable Hamiltonian and show that two regions of the quantal spectrum can be found which behave differently under a slowly changing perturbation. This behaviour is required by Percival for the existence of regular and irregular spectra.

### 1. Introduction

The quantal energy spectrum of a nonintegrable Hamiltonian is expected to exhibit two types of behaviour. At low energies the energy levels belong to a regular spectrum, and have the following property (Percival 1973).

A state with vector quantum number  $\mathbf{n}$  corresponds to regular phase space trajectories of the corresponding classical system, each of which lies on an  $N$ -dimensional toroid, where  $N$  is the number of degrees of freedom.

At higher energies it is predicted that energy levels exist belonging to an irregular spectrum. States belonging to an irregular spectrum have the following properties:

(a) A state of an irregular spectrum corresponds to irregular phase space trajectories of the classical system which fill a  $(2N-1)$ -dimensional volume of phase space in the  $(2N-1)$ -dimensional energy shell.

(b) The energy levels of an irregular spectrum are more sensitive to a slowly changing or fixed perturbation than those of the regular spectrum.

(c) The discrete bound state quantal spectrum must tend to a continuous classical spectrum in the classical limit. The energy differences

$$E(\Psi) - E(\Psi_0) = \hbar\omega$$

for fixed stationary  $\Psi_0$  and varying  $\Psi$  form a discrete distribution which tends to the continuous distribution in  $\hbar\omega$ . The distribution of levels of the irregular spectrum could take on the appearance of a random distribution.

These and other predictions were based on the KAM and Sinai theorems of classical dynamics, and also on the numerical experiments of various authors on classical non-integrable systems.

This paper presents preliminary results which show a division of the quantal energy spectrum of a simple nonintegrable Hamiltonian into two regions with contrasting properties. In particular, the behaviour of the energy spectrum under the influence of a fixed, and of a slowly varying perturbation is investigated.

## 2. Theory

The system considered in this communication has been studied classically by Hénon and Heiles (1964). By integrating the classical equations of motion for the potential

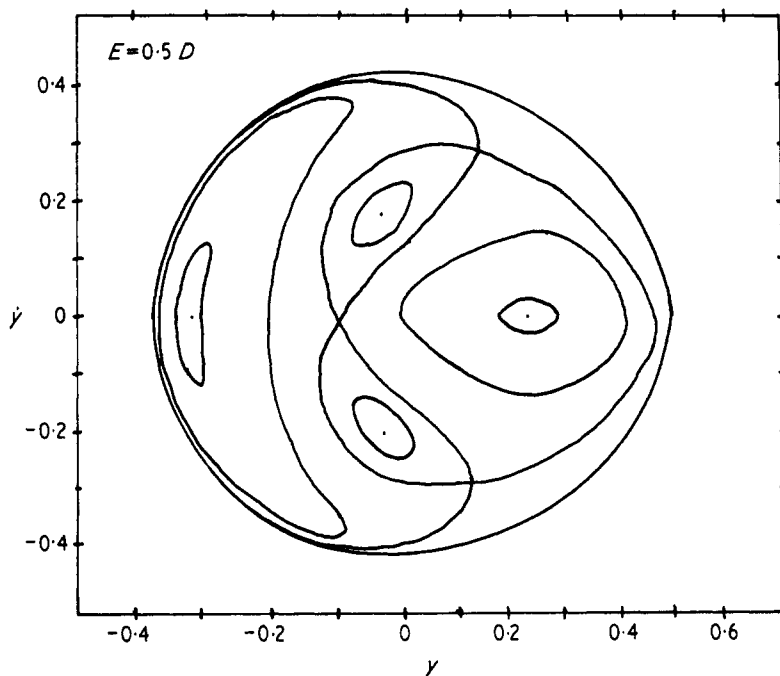
$$u(x, y) = \frac{1}{2}(x^2 + y^2) + \alpha(x^2y - \frac{1}{3}y^3) \quad (1)$$

with  $\alpha = 1$ , they found that for energies below a critical energy

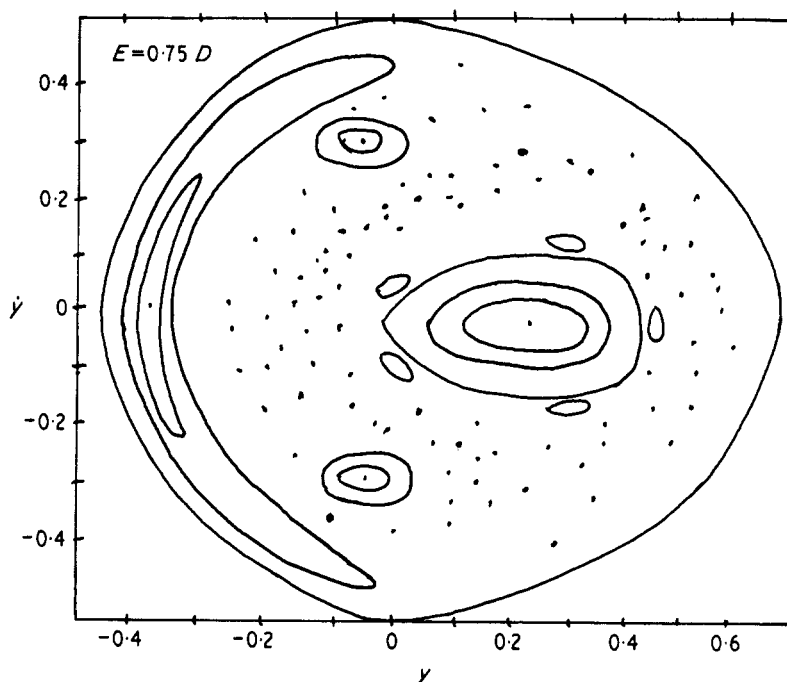
$$E^c \approx 0.68D \quad (2)$$

where  $D = 1/6\alpha^2$  is the depth of the potential well, all trajectories calculated lie on well-defined two-dimensional integral surfaces in the four-dimensional phase space (figure 1). For energies slightly above the critical energy however, trajectories are found which are unstable with respect to close starting conditions and fill a three-dimensional volume of phase space in the three-dimensional energy shell (figure 2). At still higher energies, this second type of trajectory dominates but some of the regular trajectories remain.

These results indicate a transition from nonstatistical (regular) to stochastic (irregular) behaviour as the energy is raised through the critical energy. Although the relatively crude computer calculations of Hénon and Heiles' 1964 paper indicate an abrupt transition to stochastic behaviour at an energy  $E^c \approx 0.11$ , in fact the transition is quite smooth over a small energy band. The narrow width of this energy band may be a characteristic of the Hénon-Heiles system.



**Figure 1.** A surface of section cut in the phase space for the Hénon-Heiles system taken at an energy  $E = 0.5 D$ . The closed curves correspond to classical trajectories which lie on two-dimensional toroids.



**Figure 2.** Surface of section at  $E = 0.75 D$  showing closed curves (as in figure 1) but also isolated points corresponding to a single trajectory.

The correspondence principle interpretation of these results leads us to suspect that the quantal spectrum of the Hamiltonian with potential (1) will show a transition from a regular to an irregular spectrum at an energy given approximately by equation (2).

We wish to find eigenvalues of the Hénon–Heiles Hamiltonian

$$H = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) + \alpha(x^2 y - \frac{1}{3}y^3) \quad (\hbar = 1, m = 1).$$

Preliminary numerical studies of the quantum mechanics of this Hamiltonian have been carried out by Rice and co-workers (private communication) in connection with the vibrational relaxation in isolated molecules. However, they concentrate on other nonlinear systems.

When written in polar coordinates the equilateral symmetry of the Hénon–Heiles potential becomes evident. In polar coordinates the Hamiltonian becomes

$$H = H^0 + \frac{\alpha r^3}{3} \sin 3\theta$$

where we have written as our unperturbed system the two-dimensional isotropic harmonic oscillator with unit frequency:

$$H^0 = \frac{1}{2}(p_r^2 + p_\theta^2) + \frac{1}{2}r^2.$$

A more flexible choice for our basis system is preferred however. Writing

$$H'^0 = \frac{1}{2}(p_r^2 + p_\theta^2) + \frac{1}{2}\omega^2 r^2$$

the full Hamiltonian becomes

$$H = H'^0 + \frac{\alpha r^3}{3} \sin 3\theta - \frac{1}{2}(\omega^2 - 1)r^2.$$

For computational purposes we choose the frequency  $\omega$  of our unperturbed system  $H'^0$  to be that value which minimizes the volume of the phase space required to represent the bound energy surfaces of the perturbed system. The optimum value of  $\omega$  was found to be  $\omega = (1/3)^{1/2}$ .

The basis functions are of the form

$$\phi_{vl} = N_{v|l|} F_{v|l|}(r) (e^{il\theta} \pm (-1)^l e^{-il\theta})$$

where  $v = n_1 + n_2$  and  $l = n_1 - n_2 = \pm v, \pm(v-2), \dots, 0$  or  $\pm 1$  have their usual meaning. These trigonometric functions are chosen because they have a symmetry in common with the Hamiltonian, viz invariance with respect to reflection in the  $y$ -axis.

Matrix elements of the perturbation were obtained using the well-known raising and lowering operator technique (Louck and Shaffer 1960). It is found that only states with  $l$  quantum number differing by multiples of three are coupled by the perturbation. There is consequently a splitting of the Hamiltonian matrix into three submatrices according to whether the matrix elements are derived from states of the unperturbed system with  $l = 0, +1$  or  $-1$ . A further splitting occurs because of the reflection symmetry mentioned above.

Separate diagonalization of each submatrix is possible, but for ease of computation we deal only with the two submatrices that are coupled to the  $|l| = 3$  states. These matrices have to be truncated. The order was chosen large enough to ensure convergence to at least four decimal places for all those eigenvalues of interest. The problem of resonance may be ignored for the same reason as in a treatment of the Stark effect.

For the five values of the perturbation parameter  $\alpha$  chosen for the computations, matrices of order  $N$  ranging between 176 and 234 were diagonalized. The method of diagonalization employed the Householder technique for reducing the input matrix to tridiagonal form, followed by the Sturm Sequence method for locating the roots. The calculations were performed on an IBM 370/155 computer using double precision arithmetic.

Three checks were performed on the eigenvalues:

- (i) With a small value of the perturbation parameter  $\alpha$ , the first few eigenvalues obtained using the program agree with second order quantum mechanical perturbation theory.
- (ii) Holding the Hamiltonian constant, the perturbation and basis system were altered by varying  $\omega$ . The resulting eigenvalues were found to be independent of  $\omega$  to the required precision.
- (iii) Convergence of the eigenvalues to four decimal places was checked by increasing the size of the basis set.

### 3. Results

The values of the perturbation parameter  $\alpha$  employed in the calculations and the corresponding well depths,  $D$ , are shown in the table below.

$\alpha$	0.090	0.089	0.088	0.087	0.086
$D$	20.58	21.04	21.52	22.02	22.53

For each value of  $\alpha$ , 71 eigenvalues were obtained which had converged to at least four decimal places. The behaviour of each eigenvalue with respect to increments  $\Delta\alpha = 0.001$  in  $\alpha$ , was studied by calculating the second differences  $\Delta$ , defined by

$$\Delta_i = |[E_i(\alpha + \Delta\alpha) - E_i(\alpha)] - [E_i(\alpha) - E_i(\alpha - \Delta\alpha)]|$$

where  $i$  denotes the particular eigenvalue under investigation. Perturbation theory yields

$$\Delta_i = O(\Delta\alpha^3).$$

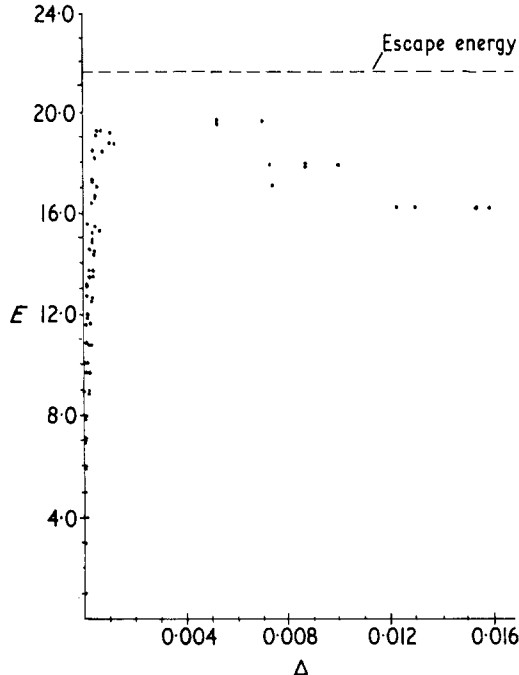
The values  $\Delta_i$  are shown as a function of the energy  $E_i$  in figure 3. For energies less than about  $E = 16.0 \approx 0.74 D$ , all second differences are very small.

For energies greater than  $E = 16.0$ , however, eigenvalues are found with corresponding  $\Delta_i$  values orders of magnitude larger. These eigenvalues are evidently very sensitive to small changes  $\Delta\alpha$  in the perturbation. High order terms in the perturbation expansion become important for these eigenvalues.

Thus two types of eigenvalue are distinguished by their behaviour under a slowly changing perturbation.

From the results of Hénon and Heiles (in particular see figure 7), the relative area  $\alpha_1$  of the surfaces of section covered by unstable trajectories is given approximately as a function of the energy  $E$ , by

$$\begin{aligned} \alpha_1(E) &= 0 & E < 0.68 D \\ &= 3.125(E/D) - 2.125 & E > 0.68 D. \end{aligned}$$



**Figure 3.** The second differences  $\Delta$  as a function of the energy  $E$ . (Since the eigenvalues are computed to four decimal places, the accuracy of the second differences, due to rounding errors, is  $\pm 0.0002$ .)

We can compare the integrals

$$I(E) = \int^E \alpha_1(E) dE$$

which are the total areas covered by unstable trajectories up to an energy  $E$ , with the quantities

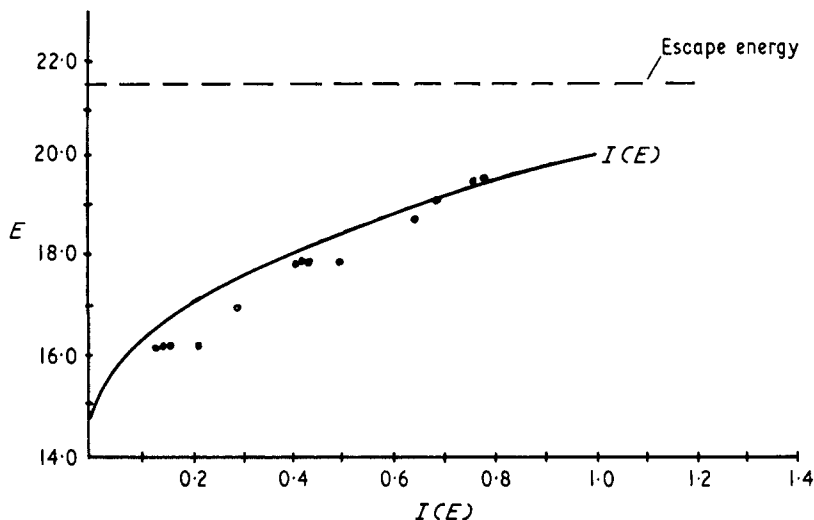
$$S(E) = \frac{1}{D} \sum_i^E n_i(E_i) \langle \Delta E_i \rangle$$

which are calculated from the quantal energy spectrum. In this sum, we set  $n_i(E_i) = 1$  if the eigenvalue  $E_i$  is very sensitive to the slight changes in the perturbation, and  $n_i(E_i) = 0$  otherwise.  $\langle \Delta E_i \rangle$  is a mean separation between an eigenvalue  $E_i$  and its two neighbouring eigenvalues  $E_{i-1}$  and  $E_{i+1}$

$$\langle \Delta E_i \rangle = \frac{1}{2}(E_{i+1} - E_{i-1}).$$

Figure 4 shows a plot of  $I(E)$  as a continuous curve and  $S(E)$  as a series of points. We see that qualitatively the points (quantal spectrum results) follow the shape of the curve (classical trajectory results). The two sets of results cannot hope to agree quantitatively since the sum  $S(E)$  corresponds to volumes of phase space while the integral is for areas. However, the energy at which the eigenvalues first become sensitive to the changing perturbation ( $\approx 0.74 D$ ) agrees well with the critical energy of Hénon and Heiles ( $\approx 0.68 D$ ).

Thus energy levels which are very sensitive to a slowly changing perturbation are identified as corresponding to the irregular unstable trajectories of Hénon and Heiles.



**Figure 4.** The integral curve  $I(E) = \int^E \alpha_1(E) dE$  as a function of the energy  $E$ . The points correspond to the sum

$$S(E) = \frac{1}{D} \sum_i^E n_i(E_i) \langle \Delta E_i \rangle.$$

#### 4. Conclusions

Eigenvalues of the Hénon and Heiles nonintegrable Hamiltonian with energy less than a critical energy  $E^c \approx 0.74 D$  were found to be insensitive to a slight change in the perturbation. These eigenvalues belong to a regular spectrum. Above the critical energy, which is known to within a narrow band of energy, eigenvalues are found which are very sensitive to a small change in the perturbation. These eigenvalues belong to an irregular spectrum.

Polyatomic molecules are examples of nonintegrable systems. The results presented above support the prediction of Percival (1973) that the vibrational energy spectrum of polyatomic molecules will show a regular progression which will terminate abruptly at a maximum energy below the dissociation limit. Modern lasers should have a sufficient resolution to detect irregular spectra.

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