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COMMENT

Chaotic behaviour of a Hamiltonian with a quartic potential

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Abstract. The Hamiltonian $H(x, p) = \frac{1}{2}p_1^2 + \frac{1}{2}p_2^2 + \frac{1}{2}x_1^2x_2^2$ is investigated. The different aspects (singular point analysis, stability analysis, numerical treatment etc) for studying chaotic behaviour are discussed. Moreover, we discuss the quantised version of the Hamiltonian.

The Hamiltonian

$$H(x, p) = \tfrac{1}{2}p_1^2 + \tfrac{1}{2}p_2^2 + \tfrac{1}{2}x_1^2x_2^2 \tag{1}$$

with the equations of motion

$$\begin{aligned} \dot{x}_1 &= p_1, & \dot{x}_2 &= p_2 \\ \dot{p}_1 &= -x_1x_2^2, & \dot{p}_2 &= -x_1^2x_2 \end{aligned} \tag{2}$$

or

$$\ddot{x}_1 = -x_1x_2^2, \qquad \ddot{x}_2 = -x_1^2x_2 \tag{3}$$

can be viewed as the simplest Hamiltonian showing chaotic behaviour.

In this comment we discuss this Hamiltonian from different points of view. Thus far different aspects have been studied in the literature (Martinyan *et al* 1981, Carnegie and Percival 1984, Steeb and Kunick 1985). This comment will complete these studies.

When we study a Hamiltonian the following approaches can be applied.

(i) The Painlevé test (Yoshida 1983) can be applied to test the algebraic integrability. The system under investigation is considered in the complex domain. To perform a Painlevé test for the autonomous system of first order $\dot{x}_i = F_i(x)$ the F_i's have to be rational functions. If the system under consideration passes the Painlevé test (note that this is not the case for the system given above) then we can look for further first integrals besides the Hamiltonian. If the system does not pass the Painlevé test, then we can study (numerically) the distribution of the singularities in the complex plane (Chang *et al* 1983). This gives us a possibility to decide whether or not the Hamiltonian shows chaotic behaviour.

(ii) The Painlevé test can fail when the first integrals are transcendental functions. To find this type of first integrals we can apply the Lie theory of extended vector fields (Leach 1981). Then from the symmetry generator and the Cartan form we can derive the first integrals. The technique can be extended to PDES and then we are able to find Lie Bäcklund vector fields (Steeb 1984).

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(iii) Explicit solutions (if any exist) can be constructed and then their stability can be studied. Two cases have to be distinguished. First, explicit solutions can arise when we impose certain initial conditions. Second, explicit solutions can arise when the Hamiltonian (in the present case the potential) have discrete symmetries. In the present model both types arise. From the second case we obtain periodic solutions.

(iv) The Toda–Brumer criterion (Toda 1974, Brumer and Duff 1976) (or extensions of it) can be applied for finding the onset of chaos. In certain cases this criterion can fail. A critical discussion of the Toda–Brumer criterion is given by Tabor (1981). We study the time-dependent eigenvalues of the 4×4 matrix

$$M=\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -V_{11}(t) & -V_{12}(t) & 0 & 0 \\ -V_{21}(t) & -V_{22}(t) & 0 & 0 \end{pmatrix} \tag{4}$$

where

$$(V(t))_{ij}=(\partial^2 V/\partial x_i\, \partial x_j)_{x=x(t)} \tag{5}$$

and $x(t)$ is the reference trajectory. The eigenvalues of M are given by $\lambda_\pm=\pm[-b\pm(b^2-4c)^{1/2}]^{1/2}$ where $b=\partial^2 V/\partial x_1^2+\partial^2 V/\partial x_2^2$ and $c=(\partial^2 V/\partial x_1^2)(\partial^2 V/\partial x_2^2)-(\partial^2 V/\partial x_1\,\partial x_2)^2$.

If any of the eigenvalues are real, the trajectory separation grows exponentially and the motion is deemed unstable. Imaginary eigenvalues correspond to stable motion. Notice that the eigenvalues are time dependent and therefore the stability of the motion can be a function of time. Toda (1974) removed the time dependence of $V(t)$ by replacing the time-dependent phase point $x(t)$ by the time-independent phase space coordinate x.

(v) Next we can perform numerical studies. For Hamiltonians with two degrees of freedom we can apply the surface of section technique. One follows the successive crossings of the trajectory through a surface intersecting the energy shell, for example, the (p_2, x_2) plane at the point $x_1=0$. If after a sufficient number of iterates, the resulting points form a closed curve, called an invariant curve, the trajectory corresponding to them lies on an invariant torus or KAM surface. If, instead, these points are dense in a two-dimensional area in the plane then the trajectory corresponding to them is irregular. Thus for a fixed energy E we are normally forced to calculate these points for a sufficiently high number of different initial values. Next we calculate the maximal one-dimensional Lyapunov exponent (Benettin *et al* 1976). For regular behaviour we have $\lambda=0$ and for chaotic behaviour $\lambda>0$. Here, too, we have to calculate (for a fixed energy E) a sufficiently large number of λ's for different initial conditions. As mentioned in (i) we can calculate the distribution of the singularities in the complex-t plane ($t=t_1+\mathrm{i}t_2$). Consider the cubically nonlinear oscillator $\ddot{x}+x^3=0$. This equation arises when we put $x_1=x_2=x$ in (3). The oscillator has a periodic solution described with Jacobi's elliptic functions. Its singularities (in the complex plane) are characterised as simple poles of order one (this tells us the Painlevé analysis) and are distributed doubly periodically in the whole complex-t plane. Such a regular distribution of singularities reflects faithfully on periodicity of the solution. When the system under investigation shows chaotic behaviour the singularities are distributed at random.

(vi) Finally we can study the system with respect to quantum chaos. This means the Hamiltonian can be quantised and then the eigenvalue equation $H\Psi=E\Psi$ can be studied. The various manifestations of the well defined classical chaos for Hamilton system do not transform in an unequivocal manner when passing to the quantised version. Percival (1977) proposed to adopt the terms regular and irregular to distinguish the quantal manifestations of quasiperiodic and ergodic classical motion. An approach to distinguish between regular and irregular spectral sequences is based on the distribution of nearest-neighbour spacings. In the generic regular case, the energy eigenvalues are distributed randomly, leading to a Poisson type distribution function. An irregular spectrum occurs when the energy levels are correlated resulting in a repulsion of adjacent levels. Then the nearest-neighbour spacings distribution function peaks at a finite value and exhibits the typical features of a Wigner distribution. It is assumed that the Hamiltonian is bounded from below and we have a discrete spectrum. Pullen and Edmonds (1981) and Haller *et al* (1984) studied the potential $V(x)=\frac{1}{2}x_1^2+\frac{1}{2}x_2^2+\frac{1}{2}kx_1^2x_2^2$.

Now let us perform our program described above.

(i) First we consider the Painlevé test. Inserting the ansatz $x_1(t)\propto a(t-t_1)^n$, $x_2(t)\propto b(t-t_1)^m$ into (3) we find that $n=m=-1$ and $a^2=b^2=-2$. Consequently, the autonomous system (2) is invariant under the similarity transformation $t\to\alpha^{-1}t$, $x_1\to\alpha x_1$, $x_2\to\alpha x_2$, $p_1\to\alpha^2p_1$, $p_2\to\alpha^2p_2$. Then $H(\alpha x,\alpha^2p)=\alpha^4H(x,p)$. Due to the results of Yoshida (1983) $r=4$ has to be one of the resonances (Yoshida calls them Kowalevski's exponents). The determination of the resonances yields $r_1=-1$, $r_2=4$, $r_{3,4}=\frac{3}{2}\pm\frac{1}{2}\mathrm{i}\sqrt{7}$. Due to the theorem of Yoshida (1983, p 381) 'In order that a given similarity system with rational right-hand side is algebraically integrable, every possible resonance must be a rational number', we conclude that the system (2) is not algebraically integrable.

(ii) The search for symmetry generators with the help of the theory of extended vector fields has no success. Only the symmetry generator $S=\partial/\partial t$ arises which is associated with the conservation of energy. Together with the result from point (i) we conclude that the system (2) is not integrable.

(iii) At once we find the particular solutions $x_1(t)=0$, $x_2(t)=C_1t+C_2$ and $x_1(t)=C_1t+C_2$, $x_2(t)=0$. The potential $V(x)=\frac{1}{2}x_1^2x_2^2$ is bounded from below and admits the C_{4v} symmetry. Due to the discrete symmetry $x_1\to x_2$, $x_2\to x_1$ of the equations of motion we can find an explicit solution by setting $x_1=x_2=x$. Then we obtain $\ddot{x}=-x^3$. The solution of this equation is given by $x(t)=A\,\mathrm{cn}(A(t-t_0),2^{-1/2})$ where A and t_0 are the constants of integration. The equations of motion (3) are also invariant under the discrete symmetry $x_1\to x_2$, $x_2\to -x_1$. Putting $x_1=-x_2=x$ again we obtain $\ddot{x}=-x^3$. Now we study the stability of these solutions. The variational equations are $(\dot{y}_1,\dot{y}_2,\dot{y}_3,\dot{y}_4)^{\mathrm{T}}=M(y_1,y_2,y_3,y_4)^{\mathrm{T}}$ where M is given by (4) and T means transpose. Then we find

$$\ddot{y}_1=-V_{11}(t)y_1-V_{12}(t)y_2 \qquad \ddot{y}_2=-V_{12}(t)y_1-V_{22}(t)y_2. \tag{6}$$

To perform a stability analysis we make the canonical transformation

$$\begin{aligned} x_1+\mathrm{i}x_2&=\exp(-\mathrm{i}\pi/4)(X_1+\mathrm{i}X_2)\\ p_1+\mathrm{i}p_2&=\exp(-\mathrm{i}\pi/4)(P_1+\mathrm{i}P_2). \end{aligned} \tag{7}$$

Then

$$H(P,X)=\tfrac{1}{2}P_1^2+\tfrac{1}{2}P_2^2+\tfrac{1}{8}(X_1^4+X_2^4-2X_1^2X_2^2). \tag{8}$$

The periodic solution $x_1=x_2=x$ with $\ddot{x}=-x^3$ is related to $X_1=0$. Then $\ddot{X}_2=-X_2^3$.

The variational equations are then

$$\ddot{y}_1 = (X_2(t))^2 y_1, \qquad \ddot{y}_2 = -3(X_2(t))^2 y_2 \tag{9}$$

where $X_2(t) = A\,\mathrm{cn}(A(t-t_0), 2^{-1/2})$. Without loss of generality we can put $t_0 = 0$ and $A = 1$. Let $\mathrm{Tr}\,M(T)$ be the index of stability (Whittaker 1927, Yoshida 1984). T denotes the period of the solution X_2. We find $\mathrm{Tr}\,M(T) = 8^{-1/2}\cosh(\sqrt{7}\pi/4)$. Now the solution is stable if $|\mathrm{Tr}\,M(T)| < 2$ and exponentially unstable if $|\mathrm{Tr}\,M(T)| > 2$. Consequently, the solution X_2 is unstable.

(iv) Let us now discuss the Toda–Brumer criterion. From the potential $V(x) = \frac{1}{2}x_1^2x_2^2$ we find $b = x_1^2 + x_2^2$ and $c = -3x_1^2x_2^2$. Let $x_1 \neq 0$ and $x_2 \neq 0$. Then $c < 0$. Since $b > 0$ this yields $E_c = 0$ (E_c is the threshold value) (Steeb and Kunick 1985).

Now (2) (or (3)) will be considered in the complex domain. We have calculated the singularities in the complex-t plane located nearest at the real-t_1 axis and the initial conditions have been chosen so that $x_1(0) \neq 0$, $x_2(0) \neq 0$, $x_1(0) \neq x_2(0)$ and $x_1(0) \neq -x_2(0)$. As mentioned above, the real solution is mainly determined by the singularities located nearest to the real-t_1 axis. We find that the singularities are distributed at random. The solution of (2) considered in the complex domain is given by the Lie series (Gröbner and Knapp 1967)

$$(x_1(t), x_2(t), p_1(t), p_2(t))^{\mathrm{T}} = \exp(tV)(x_1, x_2, p_1, p_2)^{\mathrm{T}}|_{x_1 \to x_{10}, \ldots, p_2 \to p_{20}} \tag{10}$$

where $|t|$ is sufficiently small and $x_{10} = x_1(t = 0)$. The vector field V is defined by the right-hand side of (2). The expression (10) can be used for numerical studies.

(v) We now discuss the numerical treatment. Let us exclude the particular solutions discussed at point (iii). Then we find that, for the trajectories under investigation, the one-dimensional Lyapunov exponent is positive. The surface of section technique has been widely described by Carnegie and Percival (1984). They conclude that the motion of a particle in the potential $V(x) = \frac{1}{2}x_1^2x_2^2$ is irregular everywhere except for a set of measure zero.

(vi) Let us now discuss quantum chaos. As mentioned above the potential V has the symmetry C_{4v} (Pullen and Edmonds 1981). The quantities A_1, A_2, B_1, B_2, and E label the different irreducible representations. The basic functions can now be chosen as a linear combination of the eigenfunctions of the unperturbed (two-dimensional) harmonic oscillator so that they transform according to the irreducible representations of C_{4v}. We have calculated the matrix representation of H for the subspaces which belong to A_1, A_2, B_1, and B_2. We are not able to diagonalise these infinite matrices exactly. Thus we are forced to truncate the matrices and calculate numerically the eigenvalues of these finite matrices. For actual calculation it is more suitable to introduce 'Bose creation b^+ and Bose annihilation operators b' according to $x_j = (b_j^+ + b_j)/\sqrt{2}$ and $p_j = \mathrm{i}(b_j^+ - b_j)/\sqrt{2}$. The order of our basis $|n_1, n_2\rangle$ ($n_1, n_2 = 0, 1, 2, \ldots$) will be $|0, 0\rangle$, $|1, 0\rangle$, $|0, 1\rangle$, $|2, 0\rangle$, $|1, 1\rangle$, $|0, 2\rangle$ and so on. Our truncated matrix is of the size 600×600. Then for calculating the histograms we have taken into account the first 300 energy levels. In all cases we find Wigner distributions which indicate quantum chaos. Since the threshold value is $E_c = 0$ we can take into account all 300 energy levels.

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