

## REGULAR AND CHAOTIC MOTION OF COUPLED ROTATORS

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Received 25 January 1983

Revised 11 May 1983

We consider a classical Hamiltonian  $H = L_z + M_z + L_x M_x$ , where the components of  $L$  and  $M$  satisfy Poisson brackets similar to those of angular momenta. There are three constants of motion:  $H$ ,  $L^2$  and  $M^2$ . By studying Poincaré surfaces of section, we find that the motion is regular when  $L^2$  or  $M^2$  is very small or very large. It is chaotic when both  $L^2$  and  $M^2$  have intermediate values. The interest of this model lies in its quantization, which involves finite matrices only.

Classical Hamiltonian systems with  $N$  degrees of freedom have two essentially different types of orbits [1, 2]. “Regular” orbits, such as those of integrable systems, are multiply periodic in time. They lie on  $N$ -dimensional tori in phase space and neighboring orbits separate at a rate which is roughly linear in time. On the other hand, “irregular” or “chaotic” orbits explore higher dimensional domains of phase space (possibly the entire energy hyper-surface) and neighboring orbits separate exponentially. Intermediate “pseudo-integrable” orbits may also exist [3].

There has been considerable controversy whether a similar distinction exists in quantum theory [4]. Classically chaotic systems, such as the Hénon–Heiles oscillator [5] or the Sinai billiard [6, 7] have quantum analogs with an *infinity* of states. Numerical simulations involving a truncation which leaves only a *finite* number of states may perhaps miss features which are essential for a meaningful comparison with the corresponding classical system [8]. In fact, any system with a finite number of states is almost periodic [9, 10].

The purpose of this paper is to present a classical system having both regular and chaotic motions. The quantum analog of this system is well defined and involves only a finite number of states. Its behavior will be discussed in a future publication.

Our system consists of two rotators, with angular momenta  $L$  and  $M$  respectively. (Here, a “rotator” means any physical system with dynamical variables having the same Poisson brackets – or commutators – as the components of angular momentum.) The Hamiltonian is

$$H = A(L_z + M_z) + BL_x M_x, \quad (1)$$

where  $A$  and  $B$  are numerical constants. Hamiltonians with a similar structure have been used to describe the interaction of quasi-spins in nuclear physics [11] and of pseudo-spins in solid state physics [12].

Although it is possible to write explicitly  $L = \mathbf{q}_1 \times \mathbf{p}_1$  and  $M = \mathbf{q}_2 \times \mathbf{p}_2$ , where  $\mathbf{q}_i$  and  $\mathbf{p}_i$  are conjugate canonical variables, it is far more convenient to consider a reduced phase space with only six dynamical variables  $L$  and  $M$ , having Poisson brackets

$$[L_m, L_n] = \sum \epsilon_{mns} L_s, \quad (2a)$$

$$[M_m, M_n] = \sum \epsilon_{mns} M_s, \quad (2b)$$

$$[L_m, M_n] = 0. \quad (2c)$$

(As usual,  $\epsilon_{mns} = \pm 1$  if  $mns$  is an even/odd permutation of 123, and  $\epsilon_{mns} = 0$  if any two indices are equal).

The variables  $L$  and  $M$  are not canonical but their reduced phase space can easily be handled by means of Martin's generalized dynamics [13]. In that formalism, Poisson brackets are defined as

$$[F, G] = \sum \eta^{mn} (\partial F / \partial z^m) (\partial G / \partial z^n), \quad (3)$$

where the  $\eta^{mn}$  are functions of the dynamical variables  $z^k$ . In the present case, we take

$$z^m = L_m, \quad (4a)$$

and

$$z^{m+3} = M_m, \quad (4b)$$

for  $m = 1, 2, 3$ . We then have

$$\eta^{mn} = -\eta^{nm} = \sum \epsilon^{mns} L_s, \quad (5a)$$

and

$$\eta^{m+3, n+3} = -\eta^{n+3, m+3} = \sum \epsilon^{mns} M_s, \quad (5b)$$

for  $m, n = 1, 2, 3$ . All other  $\eta^{mn}$  vanish.

The Hamiltonian evolution is

$$dL/dt = [L, H], \quad (6a)$$

$$dM/dt = [M, H], \quad (6b)$$

or, more generally,  $dF/dt = [F, H]$  for any function  $F(L, M)$ . It can be shown (see appendix) that this Hamiltonian evolution is *volume preserving* (Liouville's theorem is valid in the reduced phase space) but lower order Poincaré invariants do not seem to exist, because the  $\eta^{mn}$  matrix is singular.

In the 6-dimensional reduced phase space, there are three constants of motion:  $H$ ,  $L^2$  and  $M^2$ . There may be more if  $A = 0$  (then  $L_x$  and  $M_x$  are constant) or  $B = 0$  (then  $L_z$  and  $M_z$  are constant). If  $AB \neq 0$  we can rewrite

$$H = L_z + M_z + L_x M_x, \quad (7)$$

by choosing  $A^{-1}$  as the unit of time and  $AB^{-1}$  as

the unit of angular momentum. The KAM theorem [1, 2] then suggests that the motion should be regular if  $L^2$  and  $M^2$  are either very small or very large, when expressed in units of  $AB^{-1}$  as above (because, in these units they are very small or very large if  $B \rightarrow 0$  or  $A \rightarrow 0$ , respectively). Our numerical simulation indeed confirms this expectation, and also shows that intermediate values of  $L^2$  and  $M^2$  lead to chaotic motion.

The calculations were performed in double precision (16 digits) with a IBM 370/168 computer. The differential equations

$$dL_x/dt = -L_y, \quad (8a)$$

$$dL_y/dt = L_x - L_z M_x, \quad (8b)$$

$$dL_z/dt = L_y M_x, \quad (8c)$$

$$dM_x/dt = -M_y, \quad (8d)$$

$$dM_y/dt = M_x - L_x M_z, \quad (8e)$$

$$dM_z/dt = L_x M_y, \quad (8f)$$

were integrated by a Runge-Kutta method (subroutine DVERK of the IMSL library [14]). The time step  $\Delta t$  was chosen so that any reduction of  $\Delta t$  did not cause an appreciable change in the results. To test the accuracy of the calculation, we checked the constancy of  $H$ ,  $L^2$  and  $M^2$ .

Poincaré surfaces of section were obtained by plotting  $M_y$  versus  $L_x$  for  $L_y = 0$ , as in figs. 1 and 2. We have, at any point on such a section (for given  $H$ ,  $L^2$  and  $M^2$ )

$$L_z = \pm (L^2 - L_x^2)^{1/2}, \quad (9)$$

$$M_x = \{ (H - L_z) L_x \pm [(1 + L_x^2)(M^2 - M_y^2) - (H - L_z)^2]^{1/2} \} / (1 + L_x^2), \quad (10)$$

and

$$M_z = H - L_z - L_x M_x. \quad (11)$$

The  $\pm$  signs in (9) and (10) are independent so that each surface of section may contain up to four distinct classes of points, belonging to different

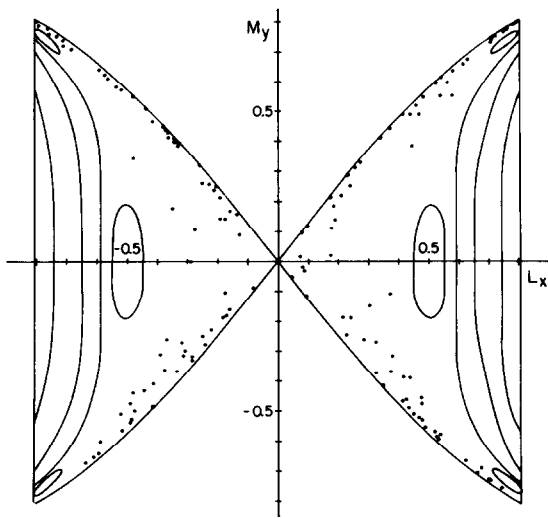


Fig. 1. Poincaré surface of section with  $H = 0$ ,  $L^2 = M^2 = 0.65$ ,  $L_y = 0$ . There are both regular and chaotic trajectories. (All the isolated dots belong to the same trajectory.)

regions of phase space. Figs. 1 and 2 were obtained by taking minus signs in both (9) and (10), i.e.,

$$L_z < 0 \tag{12a}$$

and

$$M_x < L_x M_z. \tag{12b}$$

Note that all values are real. Therefore, because of the square root in (9) and (10), the physical region is finite. It must satisfy both

$$|L_x| < L \tag{13}$$

and

$$(1 + L_x^2)(M^2 - M_y^2) > [H - (L^2 - L_x^2)^{1/2}]^2. \tag{14}$$

Moreover, for given  $L^2$  and  $M^2$ , the value of  $H$  itself is bounded:

$$H^2 \leq \begin{cases} (L + M)^2, & \text{if } LM < 1, \\ (L^2 + 1)(M^2 + 1), & \text{if } LM > 1. \end{cases} \tag{15}$$

(Proof. By symmetry, the largest value of  $|H|$ , for given  $L^2$  and  $M^2$ , is obtained when  $L_y = M_y = 0$  and, moreover, both  $L_z$  and  $M_z$  have the same sign as  $L_x M_x$ . Assume that all these signs are positive. We rewrite (7) as

$$H = (L^2 - L_x^2)^{1/2}(M^2 - M_x^2)^{1/2} - L_x M_x \tag{16}$$

and set  $\partial H / \partial L_x = \partial H / \partial M_x = 0$ . This gives two algebraic equations for  $L_x$  and  $M_x$ , whence (15) follows.)

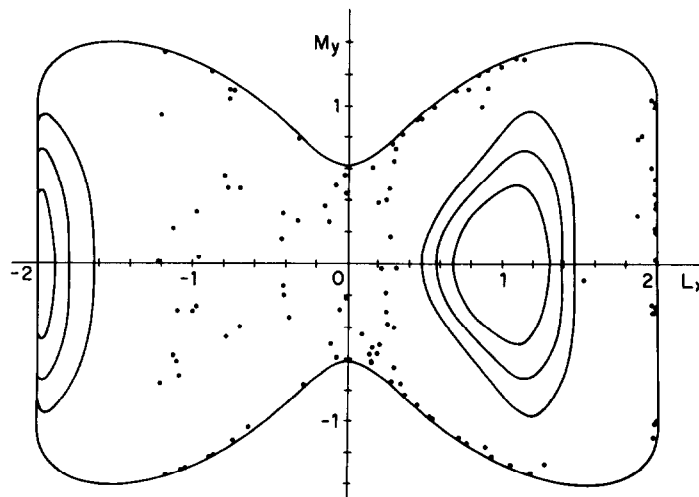


Fig. 2. Same as fig. 1, but with  $H = -3.9$  and  $L^2 = M^2 = 4$ .

Both fig. 1 and fig. 2 are symmetric with respect to a reflection of the  $M_y$ -axis. This is due to the fact that  $M_y \rightarrow -M_y$  and  $L_y \rightarrow -L_y$  (here  $L_y = 0$ ) correspond to a time reversal, as easily seen from (8).

Fig. 1 is also symmetric with respect to  $L_x \rightarrow -L_x$ , but fig. 2 is not. This is due to the following fact. The Hamiltonian (7) is invariant under a rotation of  $180^\circ$  around the  $L_z$  and  $M_z$  axes (namely  $L_x \rightarrow -L_x$ ,  $L_y \rightarrow -L_y$ ,  $M_x \rightarrow -M_x$  and  $M_y \rightarrow -M_y$ ). However, the criterion (12b) is *not* invariant under that transformation. The figure which is symmetric to fig. 2 would be obtained by taking the *opposite* criterion, and belongs to a different region of phase space.

Fig. 1, however, which corresponds to  $H = 0$ , has an additional symmetry, namely a combined rotation of  $180^\circ$  around the  $L_x$ -axis and the  $M_y$ -axis ( $L_y \rightarrow -L_y$ ,  $L_z \rightarrow -L_z$ ,  $M_x \rightarrow -M_x$  and  $M_z \rightarrow -M_z$ ). This rotation makes  $H \rightarrow -H$  and therefore it does not affect the surfaces of section for which  $H = 0$ .

Fig. 3 shows the behavior of surfaces of section for different values of  $L^2$  and  $M^2$ , and fixed  $H$ . The value  $H = 0$  was chosen for symmetry. It also gives the largest physical region in the  $L_x$ - $M_y$  plane. As expected, very small or very large values of  $L^2$  or  $M^2$  give (mostly) regular orbits; intermediate values give (mostly) chaotic orbits; and there is a

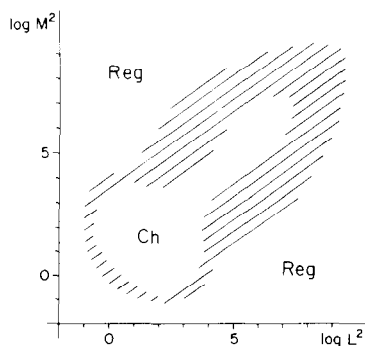


Fig. 3. Behavior of the surfaces of section for different values of  $L^2$  and  $M^2$ , and fixed  $H = 0$ . In the hatched region, there were both regular and chaotic trajectories. In the regions labelled Reg and Ch, we found only regular and chaotic trajectories, respectively.

transition region where both types of orbits co-exist, as in fig. 1.

Fig. 3 was constructed as follows. First, we note that each *point* of fig. 3 corresponds to an entire *surface of section* such as fig. 1. A point in fig. 3 was labelled regular, chaotic, or intermediate, by taking four orbits starting at equidistant points on the  $L_x$ -axis. When all four orbits were regular, or all chaotic, the corresponding point in fig. 3 was dubbed regular or chaotic, respectively. Otherwise, it was “intermediate”. This admittedly crude procedure—which nevertheless required many hours of computer time—was naturally unable to detect small chaotic domains in regular surfaces of section, and vice versa, although we do expect such domains to exist arbitrarily close to any point [15]. Therefore fig. 3 should be understood as having only qualitative validity.

By a similar procedure, we have tested the status of surfaces of sections for fixed  $L^2 = M^2 = 4$  and variable  $H$  (see, e.g., fig. 2). We found only regular orbits for  $4 < |H| < 5$ , mostly chaotic ones for  $|H| < 3$  and orbits of both types for  $3 < |H| < 4$ . Note that 5 is the maximum value of  $H$ , by virtue of eq. (15) and that the classification of orbits must be independent of the sign of  $H$ , because of the symmetry mentioned above. The importance of these results lies in the possibility of testing their quantum analogue, which we briefly discuss below.

In the quantized version of this model, we have  $L^2 = \hbar^2 l(l+1)$  and  $M^2 = \hbar^2 m(m+1)$ , where  $l$  and  $m$  are integers. The dynamical variables  $L$  and  $M$  are represented by hermitean matrices of order  $2l+1$  and  $2m+1$ , respectively (in fact, by standard numerical matrices [16] preceded by a factor  $\hbar$ ). The Hamiltonian  $H$ , which involves the direct product of these matrices, is itself a matrix of order  $(2l+1)(2m+1)$ . Obviously, the order of these matrices becomes very large in the semiclassical limit ( $L$  and  $M$  fixed,  $\hbar \rightarrow 0$  so that  $l$  and  $m$  are large). By analogy with the results of ref. 8, we expect the quantum energy spectrum to consist of families of nearly equidistant levels if the classical motion is regular, and to be “random” (possibly with some level repulsion) if the classical motion is

chaotic. Detailed numerical results will be the subject of another publication [17].

**Acknowledgments**

We are grateful to Prof. N.V. Berry for a clarifying discussion. This work, which is part of a thesis by M.F., was supported by the Israel Academy of Sciences and Humanities, the Lawrence Deutsch Fund, the Gerard Swope Fund, and the Fund for Encouragement of Research at Technion.

**Appendix A**

We shall now prove that the equations of motion (6) are *volume preserving* (Liouville’s theorem is valid in the reduced phase space) but not area preserving, because the  $\eta^{mn}$  matrix is singular. It is convenient to use notations similar to those of general relativity: Repeated indices will involve an implicit sum and  $U_{,m}$  will mean  $\partial U/\partial z^m$ .

From (3) and (6), the equations of motion can be written as

$$dz^m/dt = \eta^{mn} H_{,n} \tag{A.1}$$

Consider two neighboring points  $z^m$  and  $z^m + \zeta^m$ . The linearized deviation equation is [18]

$$d\zeta^m/dt = M_k^{m\gamma} \zeta^k, \tag{A.2}$$

where

$$M_k^m = (\eta^{mn} H_{,n})_{,k} = \eta^{mn}_{,k} H_{,n} + \eta^{mn} H_{,nk}. \tag{A.3}$$

Eq. (A.2) can be integrated as

$$\zeta(t) = S(t)\zeta(0), \tag{A.4}$$

where the transfer matrix  $S(t)$  satisfies

$$dS/dt = MS \tag{A.5}$$

and  $S(0) = I$ . We have

$$d(\det S)/dt = (\det S) \text{Tr}(S^{-1} dS/dt), \tag{A.6}$$

$$= (\det S) \text{Tr} M. \tag{A.7}$$

Now, from (A.3),

$$\text{Tr} M = \eta^{mn}_{,m} H_{,n} + \eta^{mn} H_{,nm}. \tag{A.8}$$

The first term on the right-hand side vanishes in our case, by virtue of (5), and the second term vanishes always, because  $\eta^{mn}$  is antisymmetric. It follows that  $\det S = 1$  is constant, so that the motion is volume preserving.

Are there lower order Poincaré invariants? We shall show that it is possible to prove in general an *area preserving theorem*, which unfortunately is vacuous in our case because the “area” as defined in it necessitates a nonsingular matrix  $\eta^{mn}$ .

Consider a third neighboring point  $z^m + \theta^m$ . We define the area spanned by the infinitesimal vectors  $\zeta$  and  $\theta$  as

$$A = \eta_{mn} \zeta^m \theta^n, \tag{A.9}$$

where  $\eta_{mn}$  is defined by  $\eta_{mn} \eta^{ns} = \delta_m^s$  (provided that the matrix  $\eta^{ns}$  is *not* singular). Eq. (A.9) coincides with the ordinary definition of an area in the case where the  $z^n$  are the standard canonical variables. Our problem is to show that  $dA/dt = 0$ .

We have, from (A.1),

$$d\eta_{mn}/dt = \eta_{mn,k} \eta^{ks} H_{,s}. \tag{A.10}$$

Combining this with (A.2), (A.3) and similar equations for  $d\theta/dt$ , we obtain, after some rearrangement

$$dA/dt = H_{,s} \zeta^m \theta^n (\eta_{mn,k} \eta^{ks} + \eta_{kn} \eta^{ks}_{,m} + \eta_{mk} \eta^{ks}_{,n}), \tag{A.11}$$

$$= H_{,s} \zeta^m \theta^n (\eta_{mn,k} + \eta_{nk,m} + \eta_{km,n}) \eta^{ks}. \tag{A.12}$$

However, the Jacobi identity implies that there exists a vector field  $V_m$  such that [13]

$$\eta_{mn} = V_{m,n} - V_{n,m}, \quad (\text{A.13})$$

and it follows that the parenthesis in (A.12) vanishes identically.

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