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Periodic and Aperiodic Orbits in the Hamiltonian Formulation of a Model Magnetic System

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1. Introduction

Classical dynamics and quantum dynamics have influenced each other since the idea of a quantum mechanics originated. Classical dynamics came first, so its influence on quantum theory almost goes without saying. Quantum mechanics grew out of classical mechanics. The converse influence is often referred to in the abstract, but rarely in detail. One finds statements [1] roughly to the effect that the classical theory was developed more fully in order to use it to further elucidate the corresponding quantum dynamics. But specific examples of classical calculations, which were suggested by quantum results or ideas, are not common. One of these rare examples [2] is 'rotators' or 'classical spins,' and that is the subject considered here.

This study makes contact with optimization theory at two places. First, the spin problem is initially expressed as an application of Hamiltonian dynamics; that is, it is simply an explicit particular example of the principle of least action. In the course of solution, we uncover two qualitatively different types of behavior, viz 'regular' and 'chaotic,' whose occurrence depends on the value of a (control) parameter. The chaotic solutions, moreover, are not equally chaotic; there is a more-or-less smooth progression into and back out of chaos as the parameter changes. The second contact with control theory then is a question; can the 'intensity' of the chaos be quantified, and if so, is there a value of the parameter for which the system is maximally chaotic?

The paper has four sections. Section 2 is a review of classical dynamics, including a description of numerical techniques for distinguishing regular from chaotic motion. Section 3 describes how the quantum mechanical form of a classical dynamics problem is produced. Section 4 discusses the exchange-type interactions relevant to classical spins and presents results of numerical integration for one specific such model.

2. Classical Dynamics

A problem in classical dynamics can be expressed in the Newtonian, Lagrangian, or Hamiltonian formalism [1,3]. Problems differ from each other by (or are specified by) choice of force, Lagrangian, or Hamiltonian, respectively. The formalism of the first two cases produces n, 2nd order ordinary differential equations, and, for the third, $2n$, 1st order ordinary differential equations. n is the number of 1degrees of freedom' of the problem. In each case, $2n$ initial values are needed. The problem is 'integrable' if explicit functions $q_i(q_{i0}, \dot{q}_{i0}, t)$ can be found which give the coordinates, at any time, in terms of the initial values and of t; if the functions are not known, but can be expressed as definite integrals, the problem has been merely 'reduced to quadrature,' but is still integrable. In the case of the Hamiltonian formulation, a necessary and sufficient condition for integrability is the existence of n independent functions I_i which are 'in involution' (defined below) with each other.

If the system is integrable, then all initial conditions lead to solutions which are periodic or quasiperiodic (a sum of periodic, but incommensurable, terms); there are n, possibly degenerate, frequencies. If the system is non-integrable, then at least some initial conditions lead to aperiodic

solutions; these aperiodic solutions are the famous chaotic orbits of the recent literature. The so-called KAM theorem [4] states (roughly) that if an integrable Hamiltonian system is perturbed by a small non-integrable term then a finite fraction of the initial condition space leads to periodic or quasiperiodic solutions; i.e., regularity persists in the face of a small departure from integrability. The quasiperiodic trajectories lie on surfaces called KAM tori, by generalization from the $n = 2$ case: there the phase space has 4 dimensions; if there is a conserved energy, as there usually is, the motion lies in a 3-d subspace; and if doubly, but incommensurably, periodic, covers a 2-d toroidal surface.

Whether a particular initial configuration leads to a regular or to a chaotic orbit cannot be decided easily. One possibility is to measure the divergence of two nearby trajectories: it is linear for regular ones, exponential for chaotic ones. We use here the method of the Poincaré surface of section, or Poincaré cut. The system is numerically integrated, and the intersections of the trajectory with a specified surface in the phase space (the cut plane) is graphed. The graphs are finite sets of points for periodic trajectories, smooth curves for quasiperiodic ones, and swarms of points for chaotic ones.

This technique is illustrated in figures 1 and 2. Figure 1 shows two trajectories and figure 2 the intersections of these with the plane $\theta_2 = \pi/2$ for the system

$$\begin{aligned}\dot{\theta}_1 &= J \sin\theta_2 \sin(\phi_1 - \phi_2) + (A_x - A_y)\cos\phi_1 \sin\phi_1 \sin\theta_1,\\ \dot{\phi}_1 &= \frac{J}{\sin\theta_1}\sin\theta_2 \cos\theta_1 \cos(\phi_1 - \phi_2) - \cos\theta_1(A_x \cos^2\phi_1 + A_y \sin^2\phi_1),\end{aligned} \tag{1}$$

and $1 \leftrightarrow 2$. The initial conditions are $\theta_{10} = 1.00$, $\theta_{20} = 2.00$, $\phi_{10} = 3.00$, $\phi_{20} = 1.26$ for (a) and $\phi_{20} = 1.29$ for (b). The parameters J, A_x, A_y are $1, 2, -1$, respectively. Study of the trajectories [5] (Fig. 1) gives no clue to the nature of the orbits: the pictures are effectively indistinguishable. Study of the intersections (Fig. 2) is hardly needed, nor is the reason for the use of the word chaos!

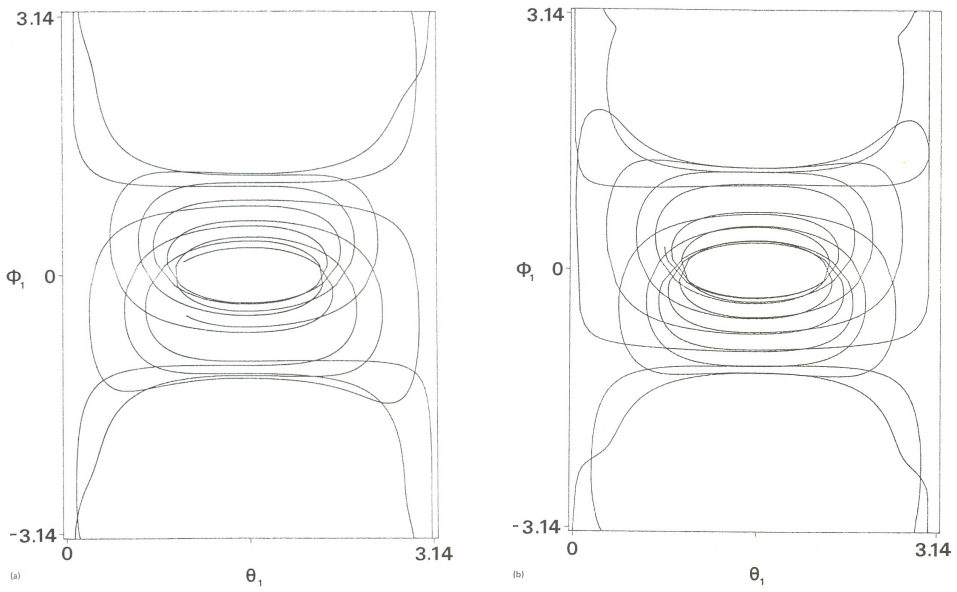

Figure 1. (a) Trajectory for the system given by Eq. (1) for initial data $(\theta_1, \theta_2, \phi_1, \phi_2) = (1.00, 2.00, 3.00, 1.26)$, projected onto the (θ_1, ϕ_1)-plane, for$0 \leq t \leq 50$. (b) As in (a), but with $(\theta_1, \theta_2, \phi_1, \phi_2) = 91.00, 2.00, 3.00, 1.29)$.

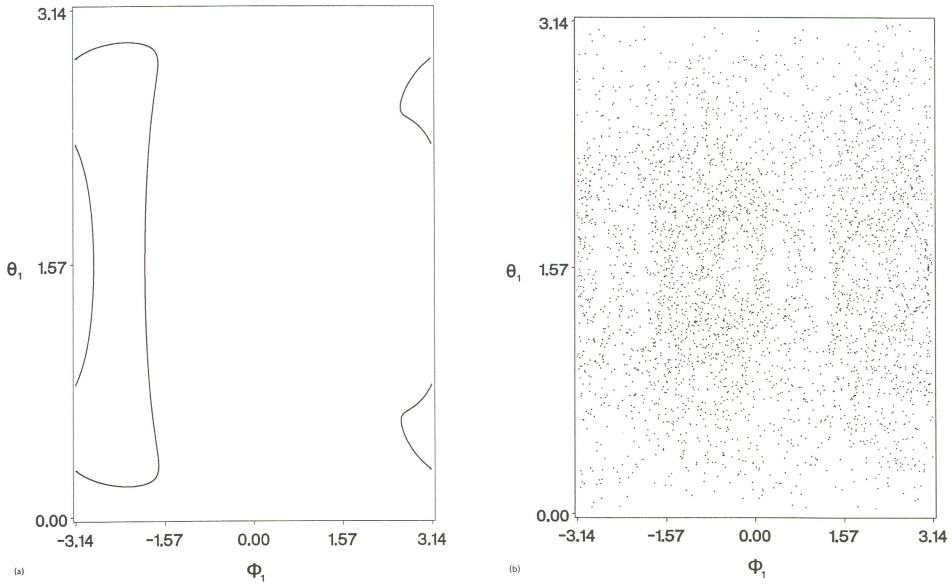

Figure 2. (a) Intersection of the trajectory of Fig. 1a qith the plane $theta_2 = \pi/2$, $0 \leq t \leq 18000$. (b) Intersection of the trajectory of Fig. 1a qith the plane $theta_2 = \pi/2$, $0 \leq t \leq 18000$.

Given a system described by a set of generalized coordinates q_i, $i = 1, \ldots, n$, the Lagrangian L is [kinetic energy − potential energy], expressed as a function of the q_i, their time derivatives, and time. The momentum canonically conjugate to q_i, called p_i, is given by

$$p_i = \frac{\partial L}{\partial \dot{q}_i}(q_i, \dot{q}_i, t). \tag{2}$$

The Hamiltonian function is

$$H = \sum_{i=1}^{n} p_i \dot{q}_i - L \tag{3}$$

expressed in terms of p_i, q_i and t. The equations of motion for the system, derivable from the principle of least action, are then

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}. \tag{4}$$

The time derivative of any function of q_i, p_i, t is given by

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \{F, H\}, \tag{5}$$

where

$$\{A, B\} = \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i}, \tag{6}$$

the 'Poisson Bracket' of A and B. Two functions whose Poisson Bracket is zero are said to be 'in involution' with each other.

3. From Classical to Quantum and Back

In quantum mechanics, dynamical variables are represented by (possibly) non-commuting operators. The prescription [6] for forming a quantum problem that corresponds to a specific classical

one is the replacement of Poisson brackets by commutators:

$$\frac{dA_c}{dt} = \{A, H_c\} + \frac{\partial A_c}{\partial t} \tag{7}$$

becomes

$$\frac{dA_q}{dt} = \mathrm{i}[A, H_q] + \frac{\partial A_q}{\partial t}, \tag{8}$$

where $[A, B] = AB - BA$ is the commutator of A and B. Here we deal with a problem in which the correspondence is used in the other direction; the classical problem is suggested by a quantum one; we know the commutator, and contrive classical variables whose Poisson brackets have the same algebraic structure. The Poisson bracket need not be explicitly dealt with; dq/dt can be written directly if the commutator is known in terms of the variables of the problem.

In the applications discussed here, the quantum variables are spin operators. Each one is a 3-vector and can be considered to represent an elementary magnet. If there are several spins, each is represented by its own vector (S_i^x, S_i^y, S_i^z). They satisfy the commutation rule

$$[S_i^x, S_i^y] = \mathrm{i}\delta_{ij} S_i^z \quad (x, y, z \text{ cyclic}). \tag{9}$$

A specific problem corresponds to a specific choice of Hamiltonian $H(\vec{S}_1, \vec{S}_2, \vec{S}_3, \ldots)$. For example, the simplest interaction between two spins is

$$H = -J\vec{S}_1 \cdot \vec{S}_2,$$

one spin in an external field $B\hat{e}_z$ has

$$H = -BS^z;$$

etc. A simple calculation shows that

$$\frac{d}{dt}\left[(S_i^x)^2 + (S_i^y)^2 + (S_i^z)^2\right] = 0$$

for general H, and therefore each spin is a fixed length vector with only two independent components. For a particular H, then, the time development of the spin is given by

$$\dot{S}_i^x = \mathrm{i}[S_i^x, H], \quad \dot{S}_i^y = \mathrm{i}[S_i^y, H], \quad \dot{S}_i^z = \mathrm{i}[S_i^z, H] \tag{10}$$

(for simplicity we presume no explicit time dependence). Now each commutator can be reduced to primitive commutators $[S_i^\alpha, S_j^\beta]$ and the replacement of each of these using equations (9), together with reinterpretation of the variables as classical ones, produces the classical problem from the quantum one.

This method of effecting the change from quantum to classical does not make explicit use of the canonical coordinates and momenta p and q. But if these are chosen to be $\cos\theta$ and ϕ, respectively, and if the components of the spin vectors are given in terms of θ and ϕ by

$$S^x = \sin\theta\cos\phi, \quad S_y = \sin\theta\sin\phi, \quad S^z = \cos\theta, \tag{11}$$

then the identical equations of motion follow from Hamiltonian's equations (4).

4. Choice of Interaction

The energy of one spin $\vec{S}_1$, interacting in a spherically symmetric way with a second spin $\vec{S}_2$, is $\vec{S}_1 \cdot \vec{S}_2$. A more general form for this interaction is

$$\sum_{i,j=1}^{n} J_{ij}\vec{S}_i \cdot \vec{S}_j + \sum_{i=1}^{n} \vec{h} \cdot \vec{S}_i.$$

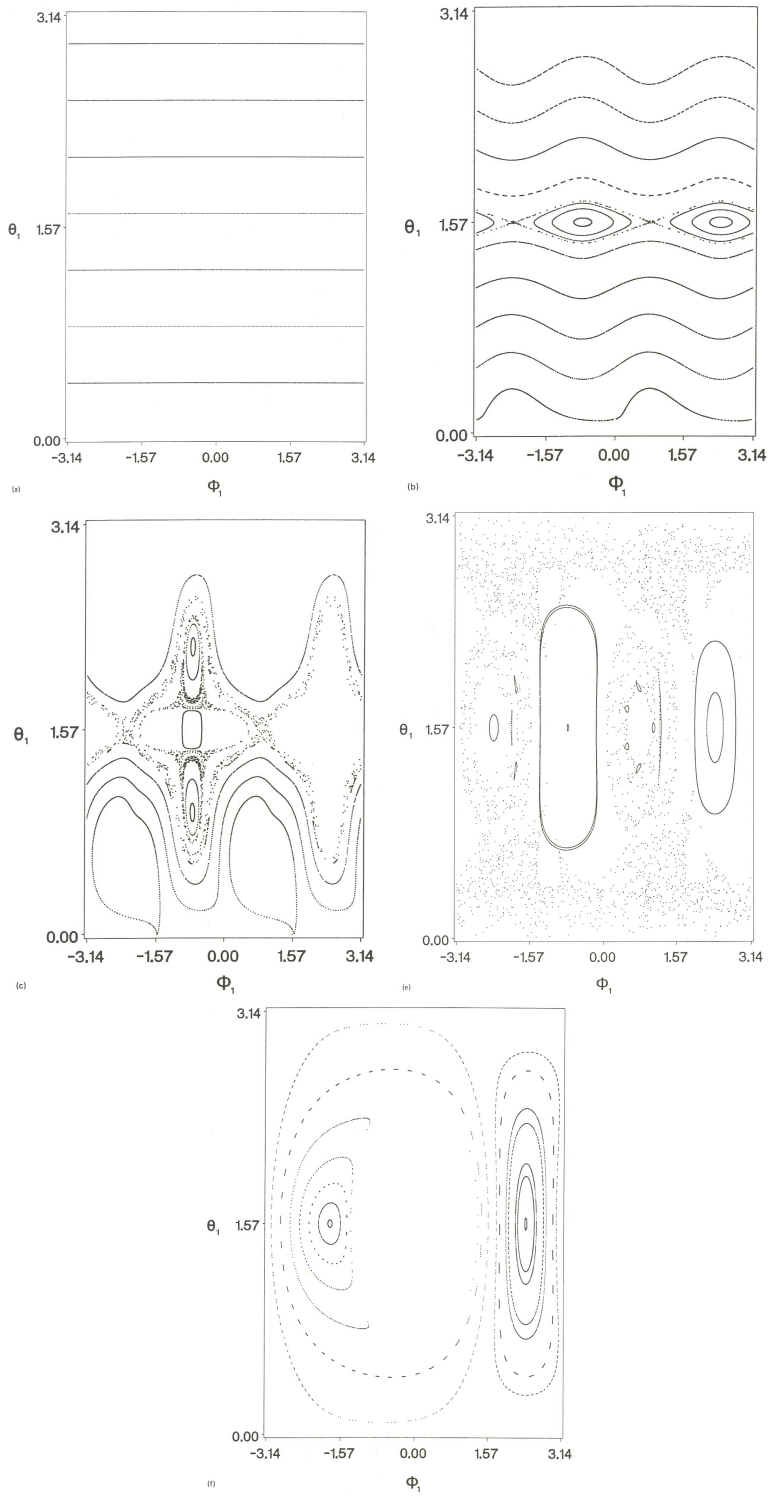

Figure 3. Projection onto the (θ_1, ϕ_1)-plane of the intersection of the trajectory of the system given by Eq. (13) with the plane $\theta_2 = \pi/2$. Only intersections for which $(d\theta_2/dt) < 0$ are plotted. (a) $\alpha = 0.0$, (b) $\alpha = 0.1$, (c) $\alpha = 0.5$, (d) $\alpha = 0.7$, (e) $\alpha = 0.85$, (f) $\alpha = 1.0$.

Specific choices of J_{ij} and $\vec{h}$ are known by particular names. For example, $H = -\vec{S}_1 \cdot \vec{S}_2$ is the two-spin Heisenberg model, $H = -S_1^z S_2^z$ the two spin Ising model, $H = -S_1^x S_2^x - S_1^y S_2^y$ the two-spin X-Y model, etc. Models defined by such Hamiltonians are known as lattice models because there is no kinetic energy in them; the primitive objects act as if fixed in position, nor do they have energy associated with the motion of changing orientation. And because we deal only with a small number of objects here, we speak of spin clusters rather than lattices. No explicit lattice structure is involved in our examples, however; the distance between spins plays no role. We have considered the dynamics for various $J_{ij}, \vec{h}$ in previous work [2,7]; here we present the results for the two-spin X-Y model with single-site anisotropy, defined by

$$H = -S_1^x S_2^x - S_1^y S_2^y + \frac{\alpha}{2}\left[(S_1^x)^2 + (S_2^x)^2 - (S_1^y)^2 - (S_2^y)^2\right], \tag{12}$$

for $0 < \alpha < 1$. The equations of motion which follow from this H are

$$\dot{S}_1^x = -S_1^z S_2^y - \alpha S_1^y S_1^z, \quad \dot{S}_1^y = S_1^z S_2^x - \alpha S_1^x S_1^z, \quad \dot{S}_1^z = S_1^x S_2^y - S_1^y S_2^x + 2\alpha S_1^x S_1^y \tag{13}$$

and $1 \leftrightarrow 2$. The problem is integrable for $\alpha = 0$ and for $\alpha = 1$. H provides one of the two necessary invariants; the second invariant is

$$S_1^z + S_2^z$$

for the case $\alpha = 0$; for $\alpha = 1$,

$$-S_1^x S_2^x + S_1^y S_2^y + S_2^z S_2^z$$

has zero time derivative and commutes with H. From $\alpha \neq 0$ or 1, the problem must be numerically integrated. Figures (3a) through (3f) show the results of numerical integration of these equations for $\alpha = 0, 0.1, 0.5, 0.7, 0.85$, and 1.0, each for a variety of initial conditions, for all of which H has the constant value $-.09957501$. Plotted are the intersections of the trajectories, with the plane $\theta = \pi/2$, for which $d\theta_2/dt < 0$, projected onto the (ϕ_1, θ_1) plane. The progression from integrability, into chaos, and back out to integrability, as α varies from 0 to 1, is evident. For $\alpha \simeq 0$, and $\alpha \simeq 1$, the equations are 'nearly' integrable, and almost all initial conditions shown lead to regular orbits, or tori. For $\alpha = 0.7$, a large fraction of the initial condition space apparently leads to chaotic orbits. For intermediate α, there is an intermediate fraction of the space covered by chaotic orbits.

These numerical statements suggest several questions. First, is there a convenient way to define the fraction (measure) of the initial condition space which leads to regular orbits? That is, is the measure easily extractable from the numerical information? Then, if so, is it expressible as a function of ex? Finally, if that function exists, we can study the controllability of the system as ex is changed. Specifically, we could find the value of ex for which this model is most chaotic.

Acknowledgments

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5. The integration times for Figures land 2 are 50 and 18000 units, respectively. If the trajectories in Figure 1 were shown for a longer time, almost all of the graphs would be covered, and no trajectory would be discernible.
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