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Regular and Chaotic Dynamics of Classical Spin Systems

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1. Introduction

In the context of the present discussion of the nature of quantum chaos [1], the dynamics of spin clusters has been the subject of several investigations [2-6] recently. The interest is focussed on the characteristic properties of quantum spin systems whose classical counterparts are nonintegrable. As a basis for the investigation of regular and chaotic spin motion. we have examined the problem of integrability of classical spin clusters [7,8].

We consider a system of N identical classical three-component spins $\vec{S}_l$, $l = 1, \dots, N$ of constant length $|\vec{S}_l| = S$ specified by a spin Hamiltonian $H(\vec{S}_1, \dots, \vec{S}_N)$. The time evolution of this system is governed by the equations of motion

$$\mathrm{d}\vec{S}_l/\mathrm{d}t = -\vec{S}_l \times (\partial H/\partial \vec{S}_l). \tag{1}$$

They coincide with the classical limit ($\hbar \to 0$, $|\vec{S}| \to \infty$, $\hbar|\vec{S}|$ finite) of the Heisenberg equations of motion of the spin operators $\hat{S}_l$ of the corresponding quantum system. Each spin $\vec{S}_l$ is confined to a sphere $|\vec{S}_l| = S$, and may be expressed in spherical coordinates $(\theta_l \phi_l)$,

$$\vec{S}_l = S(\sin\theta_l \cos\phi_l, \sin\theta_l \sin\phi_l, \cos\theta_l). \tag{2}$$

In terms of the variables $q_l = \phi_l$, $p_l = S\cos\theta_l$, the equations of motion (1) assume Hamiltonian form

$$\dot{q}_l = \partial H(\{q_l, p_l\})/\partial p_l, \quad \dot{p}_l = -\partial H(\{q_l, p_l\})/\partial q_l. \tag{3}$$

Therefore, an N-spin system represents a Hamiltonian system with N degrees of freedom, with a compact $2N$-dimensional phase space consisting of the product of N spheres $|\vec{S}_l| = S$. According to Liouville's theorem, such a system is completely integrable if there exist N independent constants of motion $I_k(\vec{S}_1, \dots, \vec{S}_N)$, $k = 1, \dots, N$, which are mutually in involution. A completely integrable system is characterized by the property that phase space is foliated into invariant N-tori which are obtained as the intersections of the N hypersurfaces $I_k(\vec{S}_1, \dots, \vec{S}_N) = \mathrm{const}$. Each trajectory is confined to one of these N-tori (regular motion). If fewer than N independent integrals of motion exist, the foliation into invariant tori is incomplete, leaving room for the occurrence of chaotic trajectories whose course through phase space is erratic and extremely sensitive to slight changes in initial conditions.

2. Integrability of Two-Spin Clusters

We have studied the integrability of spin motion in two-spin clusters specified by a Hamiltonian

$$H = -\sum_\alpha J_\alpha S_1^\alpha S_2^\alpha + \frac{1}{2} A_\alpha \Big[\big(S_1^\alpha\big)^2 + \big(S_2^\alpha\big)^2 \Big], \quad \alpha = x, y, z. \tag{4}$$

Since H is not explicitly time-dependent, it is itself conserved, and complete integrability requires the existence of one additional constant of motion $I(\vec{S}_1, \vec{S}_2)$. We have searched for integrals of the form

$$I = \sum_\alpha \left\{ -g_\alpha S_1^\alpha S_2^\alpha + \frac{1}{2} K_\alpha \left[\left(S_1^\alpha\right)^2 + \left(S_2^\alpha\right)^2 \right] \right\} \tag{5}$$

and have found the following results:
(i) For pure exchange anisotropy, i.e. $A_x = A_y = A_z = 0$, the two-spin cluster is always integrable, and the second constant of the motion is given by

$$I = -\sum_{\text{cycl}} J_\alpha J_\beta S_1^\gamma S_2^\gamma + \frac{1}{2} \sum_\alpha J_\alpha^2 \left[\left(S_1^\alpha\right)^2 + \left(S_2^\alpha\right)^2 \right]. \tag{6}$$

(ii) For nonzero single-site anisotropy (not all A_α equal), a second integral of the form (5) exists only if the parameters of the Hamiltonian (4) satisfy the condition

$$(A_x - A_y)(A_y - A_z)(A_z - A_x) + \sum_{\text{cycl}} J_\alpha^2 (A_\beta - A_\gamma) = 0. \tag{7}$$

It is then given by

$$I = -\sum_\alpha g_\alpha S_1^\alpha S_2^\alpha, \tag{8}$$

where

$$g_\alpha = (J_x + J_y + J_z) J_\alpha + (A_\alpha - A_\beta) J_\gamma + (A_\alpha - A_\gamma) J_\beta - (A_\alpha - A_\beta)(A_\alpha - A_\gamma). \tag{9}$$

As an example, we consider an XY-type model with

$$J_x = J(1+\gamma), \quad J_y = J(1-\gamma), \quad J_z = 0, \quad A_x = -A_y = J\alpha, \quad A_z = 0 \tag{10}$$

for which the condition (7) takes the form

$$\alpha^2 - \gamma^2 = 1. \tag{11}$$

We focus here on the general case of biaxial symmetry, where the existence of a second constant $I(\vec{S}_1, \vec{S}_2)$ is nontrivial. In the two limits $\alpha = 0$, $\gamma = 0$ (isotropic XY limit) and $\alpha = 0$, $\gamma = \pm 1$ (Ising limit), the system has rotational symmetry, and Noether's theorem guarantees the conservation of the total spin component M along the rotation axis. In fact, the combination $I - 4\gamma H$ of the two invariants H and I reduces to a quadratic function of M in these limits.

Our numerical calculations provide strong indication that a violation of the condition (7) or (11) renders the system nonintegrable. The behaviour of trajectories may be visualized by means of Poincaré surfaces of section. On such a surface, invariant tori are represented as closed curves, whereas chaotic trajectories fill two-dimensional areas. As an example, Fig. 1 shows the projection of the Poincaré surface of section defined by $\theta_2 = \pi/2$ onto the (θ_1, ϕ_1)-plane of the system (10) with $\gamma = 0$, $\alpha = -1/2$, and fixed energy for various initial conditions. One notices the coexistence of regular and chaotic regions. The chaotic trajectory acts as separatrix between two types of regular motion: precession of spin $\vec{S}_1$ about the z-axis (top and bottom), both accompanied by a considerable amount of nutation, and quasi-periodic oscillations of various complexity without precession about the z-axis (center).

The occurrence of chaotic trajectories for this model implies the nonexistence of a second analytic invariant. However, the abundance of invariant tori observed in the phase flow suggests that fragments of the second invariant I survive in some form.

Let us first consider a completely integrable case. If the second integral I were not known explicitly, it could be reconstructed numerically as follows: Pick any dynamical variable X which is independent of H. The time average of X over any trajectory is by construction time-independent, i.e. a constant of motion. It is in fact an analytic function of the initial conditions $(\vec{S}_1, \vec{S}_2)$, and may

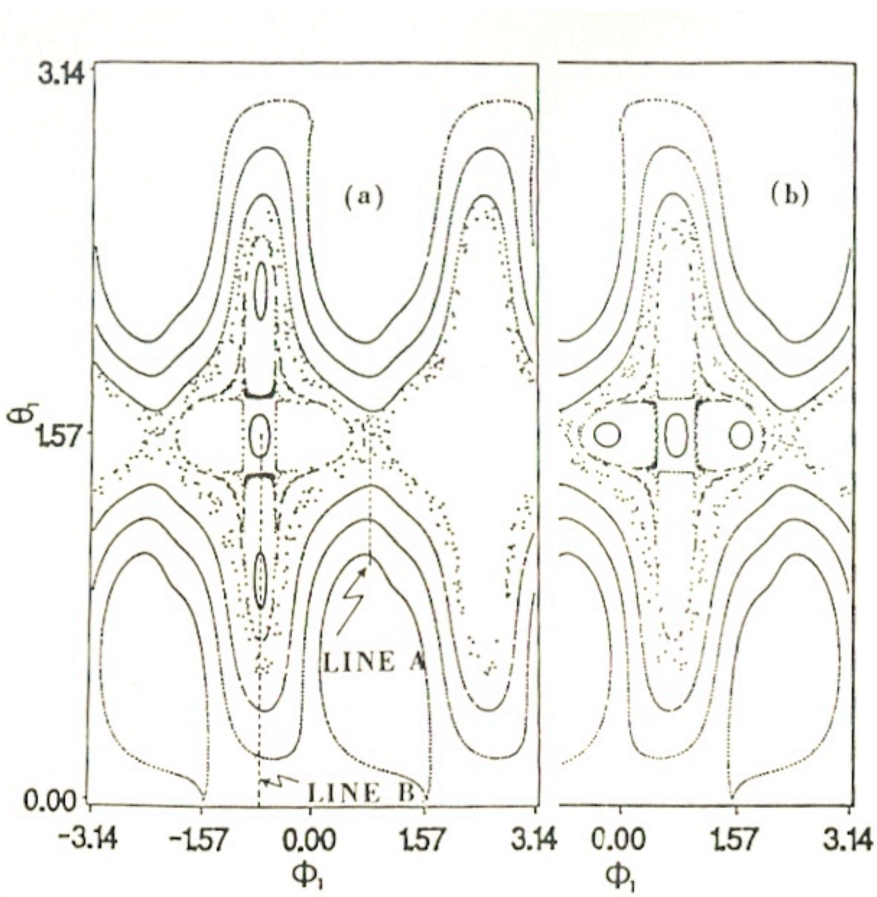

Figure 1. Projection of the Poincaré surfaces of section defined by (a) $\theta_2 = \pi/2$, $\dot{\theta}_2 < 0$ and (b) $\theta_2 = \pi/2$, $\dot{\theta}_2 > 0$ onto the (θ_1, ϕ_1)-plane for the nonintegrable two-spin model (10) with $\gamma = 0$, $\alpha = -0.5$ and $H = -0.09957501$.

therefore be identified as the second integral $\langle X \rangle = I(\vec{S}_1, \vec{S}_2)$. In nonintegrable cases, according to Birkhoff's theorem, the time average still exists for almost all trajectories, even chaotic ones. However, it is no longer an analytic function of the initial conditions: Its values for regular trajectories will represent the remains of the analytic invariant, whereas in regions filled densely by a chaotic trajectory, one may expect ergodic behaviour leading to a constant value of the average. Thus, as a function of the initial coordinates on a given energy shell, the time average would display a step-like behaviour, consisting of horizontal pieces in chaotic regions and isolated points on regular trajectories. In those parts where the chaotic regions are very thin, the graph of $\langle X \rangle$ will look like a smooth curve.

The calculation of time averages for a chaotic trajectory represents a highly nontrivial problem. Because of the positive Lyapunov exponent, numerical errors grow exponentially, i.e. two different integration procedures starting from the same initial condition will produce numerical orbits ("itineraries") which separate exponentially. Empirically, we find, however, that time averages calculated for different itineraries coincide within certain error bars. To obtain a measure of the convergence, we have calculated time averages over each of ten successive long time periods $T = 10^4 J^{-1}$) and determined the standard deviation.

In Fig. 2a, the time average $\langle (S_1^y)^2 \rangle$ is shown for a system with $\gamma = 0$, $\alpha = -0.5$ as a function of the initial value θ_1 along the line B marked in Fig. 1. In regions where invariant tori dominate, $\langle (S_1^y)^2 \rangle$ is found to converge rapidly, and looks like a well-behaved function of θ_1. In chaotic regions, on the other hand, the time average converges much more slowly, as indicated by the large error bars. This slow convergence has been shown to be caused by the existence of fragments of tori ("cantori") which act as barriers in phase space. In Fig. 2b, calculated for a system with $\gamma = 0$, $\alpha = -0.7$ along a corresponding line, such fragments are much rarer, and the convergence is better even in the chaotic region. Within numerical accuracy, the system appears to be ergodic in the chaotic region.

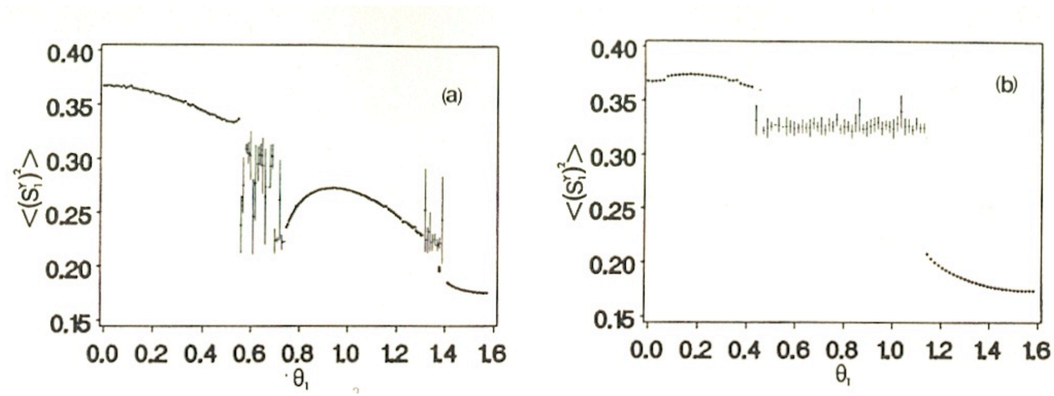

Figure 2. Time average $\langle (S_1^y)^2 \rangle$ over single trajectories as a function of initial value θ_1 for $\phi_1(t = 0) = -\pi/4$ (the line B of Fig. 1), for the model (10) with $\gamma = 0$, $\alpha = -0.5$ in (a) and $\gamma = 0$, $\alpha = -0.7$ in (b).

3. Integrable N-Spin-Clusters

As a contribution to the question of integrability of spin systems with $N > 2$, we list here a number of results (see Fig. 3). We have established complete integrability for a special class of N-spin systems which may be described as follows: The system consists of two arrays A and B of

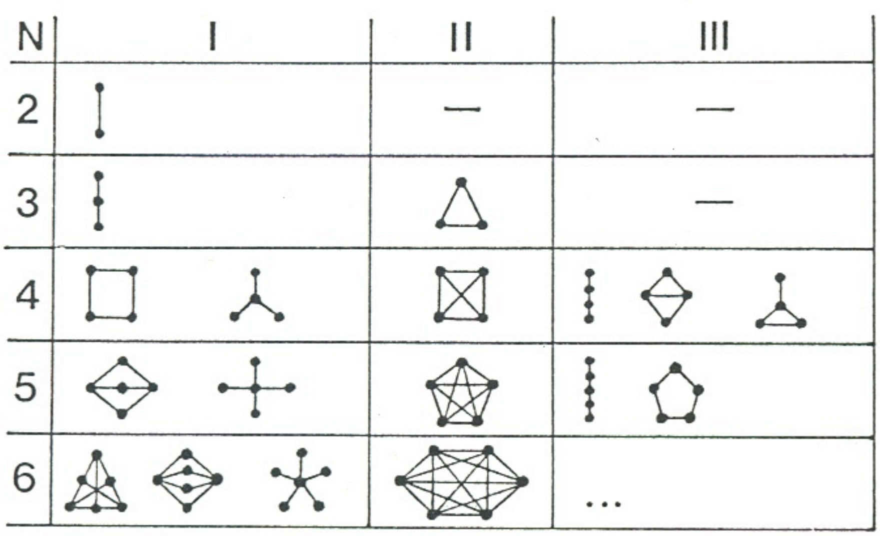

Figure 3. Table of integrable and nonintegrable N-spin clusters. Column I: Systems integrable for arbitrary anisotropic exchange coupling. Column II: Systems integrable only for isotropic exchange coupling. Column III: Nonintegrable systems.

N_A and N_B spins, respectively, such that every spin of array A is coupled to every spin of array B by a constant anisotropic exchange interaction J, but spins belonging to the same array do not interact directly (first column of Fig. 3). This class includes a two-sublattice model of an anti ferromagnet with constant inter-sublattice and zero intra-sublattice coupling.

Such as system is described by a Hamiltonian

$$H = -\sum_{\alpha} J_\alpha T_A^\alpha T_B^\alpha, \tag{12}$$

where $\vec{T}_{A,B}$ are the total spins of the arrays A, B,

$$\vec{T}_A = \sum_{l \in A} \vec{S}_l, \quad \vec{T}_B = \sum_{l \in B} \vec{S}_l. \tag{13}$$

The motion of the effective two-spin system $(\vec{T}_A, \vec{T}_B)$ is governed by the equations

$$\mathrm{d}\vec{T}_A/\mathrm{d}t = -\vec{T}_A \times (\partial H/\partial \vec{T}_A), \quad \mathrm{d}\vec{T}_B/\mathrm{d}t = -\vec{T}_B \times (\partial H/\partial \vec{T}_B). \tag{14}$$

It is completely integrable for arbitrary anisotropic J_α, since it is equivalent to the system described by Eq. (4) with $A_x = A_y = A_z = 0$, except for the fact that in general $|\vec{T}_A| \neq |\vec{T}_B|$. The motion of the individual spins in the two arrays A, B follows the motion of $\vec{T}_{A,B}$ in a rigid manner, such that all scalar products $\vec{S}_l \cdot \vec{S}_{l'}$, with l and l' belonging to the same array are constants of motion.

Another class of completely integrable N-spin systems are clusters in which every spin is coupled to every other spin by a constant isotropic exchange interaction (second column of Fig. 3). The Hamiltonian has the form

$$H = -\frac{1}{2} J \sum_{l \neq l'} \vec{S}_l \cdot \vec{S}_{l'}, \tag{15}$$

(Kittel-Shore model). In this case, the total spin

$$\vec{T} = \sum_{l} \vec{S}_l \tag{16}$$

is a constant of motion. The individual spins precess about $\vec{T}$ with constant frequency, such that all components parallel to $\vec{T}$ and all relative azimuthal angles are conserved. In the last column of Fig. 3, we have listed some spin clusters for which the numerical evidence indicates non-integrability.

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