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A quaternionic map for the steady states of the Heisenberg spin-chain

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ABSTRACT

We show that the steady states of the classical Heisenberg XXX spin-chain in an external magnetic field can be found by iterations of a quaternionic map. A restricted model, e.g., the xy spin-chain is known to have spatially chaotic steady states and the phase space occupied by these chaotic states is known to go through discrete changes as the field strength is varied. The same phenomenon is studied for the xxx spin-chain. It is seen that in this model the phase space volume varies smoothly with the external field.

1. Introduction

Magnets play an important role in our information technology dominated world. They are also physically interesting systems to study both in the classical and quantum domain. The low temperature study of some types of magnets is specially interesting, as it shows an unusual behavior of magnetization with cooling. While usually in magnetization problems, where disorder plays a role, the disorder is introduced externally, using lattice mismatch or impurities. It was shown in [1] that even when there is no external disorder, the classical xy spin-chain has stationary states which exhibit spatially chaotic spin patterns. In a later paper [2], it was shown that with change in the strength of the applied magnetic field the phase space occupied by the steady states goes through discrete changes which at low temperature may correspond to discrete change in the magnetization of the system. In the present paper we generalize the results reported in [2] to a full XXX spin-chain where all the three spin components take nonzero values. We note that while our model is classical, whereas the correct treatment of a magnetization problem has to be quantum, the classical phase-space structures are still expected to be important in the semiclassical studies of the problem.

Many physical systems can be modeled in terms of 2-dimensional area preserving maps [3,4]. In such systems the extremization condition for the energy gives rise to Hamiltonian evolution equations. The ground state belongs to the set of extremum energy solutions and so such models are useful in studying the commensurate (C)-incommensurate (IC) transitions. Apart from C and IC phases, chaotic configurations are also known to occur in such models. The chaotic configurations are interpreted as either an amorphous structure, or randomly pinned solitons [4]. In [5] an xy chain with power law interaction has been studied and steady states are used to predict phase-transitions. Here we study a map whose domain is the direct product of two two-spheres and whose range is a two-sphere. The orbits of this map are the spin configurations of the steady states of the ferromagnetic classical Heisenberg XXX spin-chain.

2. Evolution equations

Most of the area preserving maps studied in context of condensed matter systems have been two-dimensional. In the present paper we give evolution equations for the steady states of the ferromagnetic XXX Heisenberg spin-chain, which are in the form of a four-dimensional map. The Hamiltonian considered is

$$H = -J\sum \vec{S}_i \cdot \vec{S}_{i+1} - B\sum S_i^z \tag{1}$$

where we have assumed the magnetic field in the z direction without loss of generality. It is advantageous to work with a scaled Hamiltonian which is found by dividing H by $J|\vec{S}|^2$ and replace $B/(J|\vec{S}|)$ by B and consider $|\vec{S}|$ to be 1. The scaled Hamiltonian is of the form

$$H = -\sum \vec{S}_i \cdot \vec{S}_{i+1} - B\sum S_i^z. \tag{2}$$

Usually to find the extremum energy states of a Hamiltonian system $H(q_i, p_i)$ one has to solve the equations

$$\frac{\partial H}{\partial q_i} = 0 \tag{3}$$

which gives the extrema of the potential energy. We cannot apply the above conditions to find the stationary states of Hamiltonian

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in Eq. (2) because of the following. If the variables S^z and the projection (on the xy plane) angle ϕ are taken as momentum and coordinate variables respectively then the resulting Hamiltonian has momentum dependent potential and so steady states cannot be found by extremizing the potential with respect to z coordinates. One can get steady states by equating time derivatives $(\dot{z}, \dot{\phi})$ to zero, to get equations that are singular at $S^z = 1$. While it is possible to work with these equations, the quaternion map discussed by us below, has a more elegant mathematical structure and provides better geometrical insights.

To get the map, we write the evolution equations [1,2]

$$\frac{dS_i^j}{dt} = \epsilon_{lmn} \frac{\partial S_i^j}{\partial S_i^l} \frac{\partial H}{\partial S_i^m} S_i^n, \tag{4}$$

where i runs from 1 to n, the total number of spins and l, m, n refer to the spin components x, y, z. For stationary states we set the time derivatives to be zero, giving rise to

$$\vec{S}_i \times \vec{S}_{i+1} = (\vec{S}_{i-1} + \vec{B}) \times \vec{S}_i. \tag{5}$$

This equation fixes $\vec{S}_{i+1}$ in terms of the previous two spins $\vec{S}_i$ and $\vec{S}_{i-1}$. It turns out that there is a particularly neat way to find the steady states of the spin-chain using rotations through quaternions [6]. It can be seen that given $\vec{S}_i$ and $\vec{S}_{i-1}$ the next spin can be arrived at by rotating the spin $\vec{S}_i$ about the vector $\vec{R} = (\vec{S}_{i-1} + \vec{B}) \times \vec{S}_i$ by the angle $\alpha = \sin^{-1}(R)$. We write, the spin $\vec{S}_i$ as a quaternion with zero scalar part, $\tilde{S}_i$, and define the quaternion $\tilde{q} = \cos(\alpha/2) + \hat{R}\sin(\alpha/2)$ and $\tilde{q}^* = \cos(\alpha/2) - \hat{R}\sin(\alpha/2)$. The spin on the site $i+1$ can be calculated from the spin on the ith site, in quaternion notation as

$$\tilde{S}_{i+1} = \tilde{q}^* \tilde{S}_i \tilde{q}. \tag{6}$$

For details on the quaternion rotations see Appendix A. The process can be repeated to find the spin orientations along the chain if the initial two adjacent spins are given. If at some point in the iteration, the magnitude of $\vec{R}$ becomes more than 1, then it implies that a physical solution for the problem does not exist. In the study of the xy spin-chain it was found that with increase in the magnitude of the applied magnetic field, the phase space occupied by the steady states decreases. When a steady state which is chaotic (and so occupies phase space of nonzero measure) becomes inadmissible, the available phase space changes in a discrete manner. Disjoint island chains inside the phase space were also seen for the xy chain. Since the xy spin-chain is found by setting $S^z = 0$ at all sites in the xxx spin-chain, we expect to find similar chaotic states for the xxx chain as well. In the next section we show the numerical results.

3. Computation of the steady states

In the computation of steady states, we use spherical polar coordinates with

$$S^x = \sin\theta\cos\phi, \qquad S^y = \sin\theta\sin\phi, \qquad S^z = \cos\theta.$$

The initial conditions are chosen with $\phi_0 = 0$ because the first spin has a ϕ symmetry (for the first spin all the ϕ values are physically equivalent, as the magnetic field is in the z direction). Thus without loss of generality the first spin can be put in the x–z plane. The second spin has the angles θ_1 and ϕ_1.

In Figs. 1.1, 1.2 and 1.3, we show a regular spin-chain configuration, at the value $B = 0.1$, initial conditions $(\theta_0, \theta_1, \phi_0, \phi_1) = (0.1, 0.5, 0, 0.2)$ and chain length 600. Fig. 1.1 gives the (S^x, S^y) projection of the spins, Fig. 1.2 gives the (S^y, S^z) and Fig. 1.3 gives the (S^z, S^x) projection of the spins. Figs. 2.1, 2.2 and 2.3 show a chaotic spin-chain configuration at $B = 0.25$, initial conditions $(\theta_0, \theta_1, \phi_0, \phi_1) = (0.02, 0.03, 0, 0.05)$ and chain length 600.

In Fig. 3 we plot the fraction of phase space corresponding to admissible steady states as a function of the strength of the applied magnetic field. The initial points were chosen on a $60 \times 60 \times 60$ grid. It is known that the phase space changes in a discrete manner for the xy case. Since the xy chain is a restricted case of the xxx model, we expect the volume of the admissible phase space to go through similar discrete changes. However in comparison to the full four-dimensional phase space, the changes occurring in the admissible phases-space volume appears to be of measure zero. For a chain of length 500, the graph of the field strength against the phase-space fraction doesn't show any apparent discreteness. However, it can be seen that the change in the admissible phase space volume is not monotonic.

4. Summary

We have studied the steady states of the classical Heisenberg ferromagnetic spin-chain by writing the iteration equations for spin orientation in terms of a quaternionic map. In the quaternionic form, the map equations have a compact and geometrically more transparent form compared to vector form of the map. The quaternionic map also makes the group theoretic nature of the iterations evident. The map gives the orientation of spins along the chain if the initial two adjacent spins are given. The orbits of the map correspond to steady states of the spin-chain. The Numerical solutions show existence of regular and chaotic orbits. The existence of regular and chaotic orbits in the xxx model is consistent with existence of similar orbits in the xy model [2]. However in contrast to the xy model where the change in the admissible phase space volume is discrete, in the xxx model the admissible phase space is shown to change smoothly as a function of the applied field strength. This result is surprising to us and we believe that it is because the chaotic region in the phase space is not of measure 1. Our model studies deterministic chaos in a spin system, which is different from spin-glass behavior that results from quenched disorder. We believe that some of the experimental behavior of spatially chaotic steady states will be experimentally similar to that of a spin glass, for example the neutron diffraction patterns.

Our map, written using quaternions, makes the equations notationally simpler and makes the geometrical picture apparent. While our interest in this paper, is in the stationary states, it would be interesting to work with the quaternion picture for the dynamical problem too. The motivation of the present work was, (1) to show existence of spatial chaos in the steady states of classical ferromagnetic XXX spin-chain and (2) to see if the admissible phase space changes with field strength parameter B, in a discontinuous manner. We conclude from numerical evidence that non-planar chaotic orbits do exist in the XXX chain and the fractional change in the volume of the admissible phase space is continuous, but not monotonic.

Appendix A. Rotation of a vector using quaternions

Quaternions are four-dimensional generalization of complex numbers. A quaternion q is defined as $q = q_0 + iq_1 + jq_2 + kq_3$ where q_0, q_1, q_2 and q_3 are real numbers and i, j, k satisfy the multiplication laws $ij = -ji = k$, $jk = -kj = i$, $ki = -ik = j$ and $i^2 = j^2 = k^2 = -1$. An active rotation of a vector $\vec{V}$ by an angle α about an axis defined by a unit vector $\hat{n}$ can be achieved by [6]

$$\tilde{V}' = \tilde{q}\tilde{V}\tilde{q}^*, \tag{7}$$

where the vector $\vec{V}$ and the rotated vector $\vec{V}'$ are treated as quaternions with zero scalar parts and the unit vectors $\hat{x}$, $\hat{y}$, $\hat{z}$