Order and chaos in classical models of spin chains

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We study the ground state of one-dimensional classical spin chains with exchange and dipole interactions between nearest neighbors and with an anisotropy field at an arbitrary angle to the axis of the chain. We construct a mapping which connects the spin states at neighboring chain sites and we consider its properties in various limiting cases. We show that for a sufficiently high anisotropy field chaotic structures may appear. We give the spectral characteristics of these structures for the ferro- and antiferromagnetic cases.

1. INTRODUCTION

Experimental and theoretical studies of the last decade have shown that under well defined conditions there may occur in solids periodically modulated structures with a period which is incommensurate with the natural periods of the lattice. The appearance of incommensurate structures has the character of critical phenomena and can occur both in magnetic[1–3] and in elastic[3–8] systems.

An analysis of the incommensurate structures as a new class of structures turned out to be intimately connected with two general problems of a principal nature. Firstly, it turned out that in the one-dimensional case it was possible to formulate in a rather general form the problem of finding all equilibrium structures and distinguishing from among them those for which the free energy is a minimum.[3,4,9–12] More precisely, the meaning of this analysis consists in the following. Instead of studying the real trajectories of N individual particles ($N\to\infty$) one studies only the equilibrium positions of these particles. For the equilibrium positions one can write down equations connecting their values at neighboring chain sites. These coupling equations are in the form of a mapping acting in the space of the coordinates of the equilibrium positions of the atoms at the sites. The mapping obtained, in turn, determines some new dynamic system which differs, of course, from the initial one. Its trajectories give the coordinates of the atoms at the chain sites. Each trajectory corresponds to a well defined value of the free energy. The ground state of the chain corresponds to those trajectories for which the free energy has a minimum. Such an approach enabled one to incorporate into the analysis of possible structures of the chain modern methods in the theory of dynamic systems. In particular, it was shown in Refs. 10, 11 that an incommensurate structure is produced through nonlinear resonance in a specially constructed equivalent dynamic system.

The second general problem for which it turned out possible to consider it from a completely different angle is the problem of the formation of chaotic disordered, or amorphous, states of the chain.[3,4,10,12,13] On the one hand, an amorphous state arises as one of the invariant sets under the mapping for the equilibrium coordinates of the atoms in the chain. Of course, the occurrence of such sets is possible only in a well defined region of the values of the parameters of the system. On the other hand, the formation of an incommensurate structure always precedes the occurrence of amorphous structures.[10–13] One can easily understand this result from the point of view of the theory of dynamic systems. Moreover, just the results of this theory enable us to reach some general conclusions. For instance, there are no chaotic states in one-dimensional single-component dynamic systems in continuous models.[9]

The Frenkel'-Kontorov elastic model and some special forms of spin chains have been studied in rather much detail so far.[2,3,12,17] The present paper is devoted to the study of possible structures in a complex spin chain in which there is a planar Heisenberg (XY) interaction between the spins, a dipole (D) interaction, and an anisotropy (A) effect. We shall call this model in what follows the $XYDA$ model. One of the problems which will be considered below is connected with explaining the effect of one or other form of interaction in the $XYDA$ model on the formation of possible equilibrium structures. In particular, we shall elucidate the conditions under which in the $XYDA$ model an amorphous magnetic structure appears.

2. DESCRIPTION OF THE MODEL

We consider a one-dimensional chain of classical spins σ_i ($|\sigma_i| = 1$) positioned along the X axis. Let the vectors σ_i lie in the XY plane at an angle ϑ_i with the X axis. The Hamiltonian of the system with interactions between nearest neighbors can then be written in the form

$$H=D\sum_n[\boldsymbol{\sigma}_n\boldsymbol{\sigma}_{n+1}-3(\boldsymbol{\sigma}_n\mathbf{r}_{n,n+1})(\boldsymbol{\sigma}_{n+1}\mathbf{r}_{n,n+1})]-J\sum_n(\boldsymbol{\sigma}_n\boldsymbol{\sigma}_{n+1})+G\sum_n f(\boldsymbol{\sigma}_n), \quad (2.1)$$

where $\mathbf{r}_{n,n+1}$ is a unit radius vector between nearest neighbors, D the constant of the dipole interaction, J the exchange interaction constant, G the constant determining the anisotropy (or any other external) field, and $f(\boldsymbol{\sigma}_n)$ the function determining how the energy of the anisotropy field depends on the orientation of the spin of a single atom.

We rewrite (2.1) in terms of angular variables for the case $D\neq J$ in the form

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$$H=(D-J)\sum_n[\sin\vartheta_n\sin\vartheta_{n+1}+\alpha\cos\vartheta_n\cos\vartheta_{n+1}+\beta f(\vartheta_n)], \tag{2.2}$$

where

$$\alpha=(J+2D)/(J-D),\quad \beta=G/(D-J). \tag{2.3}$$

When $D=J$ ($\beta_1=G/J$)

$$H=3J\sum_n[\cos\vartheta_n\cos\vartheta_{n+1}+\beta_1 f(\vartheta_n)]. \tag{2.4}$$

The conditions for dynamic equilibrium of the chain have the form

$$\partial H/\partial\vartheta_j=0$$

for all j. This gives

$$\cos\vartheta_n(\sin\vartheta_{n+1}+\sin\vartheta_{n-1})$$
$$-\alpha\sin\vartheta_n(\cos\vartheta_{n+1}+\cos\vartheta_{n-1})+\beta f'(\vartheta_n)=0. \tag{2.5}$$

We write

$$\sin\varphi(\vartheta_n)=-\alpha\sin\vartheta_n/\rho(\vartheta_n),\quad \cos\varphi(\vartheta_n)=\cos\vartheta_n/\rho(\vartheta_n),$$
$$\rho(\vartheta_n)=[\cos^2\vartheta_n+\alpha^2\sin^2\vartheta_n]^{1/2},\quad \psi(\vartheta_n)=\beta f'(\vartheta_n)/\rho(\vartheta_n). \tag{2.6}$$

From (2.6) also follows the definition of the function $\varphi(\vartheta_n)$:

$$\varphi(\vartheta_n)=-\operatorname{arctg}\alpha\operatorname{tg}\vartheta_n\quad(|\vartheta_n|\leqslant\pi/2). \tag{2.7}$$

Using the definitions (2.6) and (2.7) we can write the conditions for equilibrium of the spins in the form of a recurrence relation:

$$\sin[\vartheta_{n+1}+\varphi(\vartheta_n)]=-\sin[\vartheta_{n-1}+\varphi(\vartheta_n)]-\psi(\vartheta_n). \tag{2.8}$$

The value of the two constants $(\vartheta_0,\vartheta_1)$ for the orientation angles of the initial spins determines all possible sequences $\{\vartheta_j\}$. We shall see in what follows that the specific features of Eq. (2.8) given, in general, a many-valuedness of possible "trajectories" $\{\vartheta_j|\vartheta_0,\vartheta_1\}$ for fixed $(\vartheta_0,\vartheta_1)$.

We write (2.8) in a more standard form. We introduce the variable

$$I_n=\vartheta_n-\vartheta_{n-1} \tag{2.9}$$

and the (I_n,ϑ_n) phase space. We can then write Eqs. (2.8), (2.9) in the form of a mapping

$$\hat T:\begin{cases} I_{n+1}=\Phi(I_n,\vartheta_n)-\vartheta_n, & \mod 2\pi\\ \vartheta_{n+1}=\vartheta_n+I_{n+1}, & \mod 2\pi\end{cases},$$

$$\Phi(I_n,\vartheta_n)=-\varphi(\vartheta_n)-\operatorname{Arcsin}\{\sin[\vartheta_n+\varphi(\vartheta_n)-I_n]+\psi(\vartheta_n)\}. \tag{2.10}$$

The mapping $\hat T$ determines a dynamic system in the (I,ϑ) phase space. The set of all trajectories $\{\vartheta_j,I_j|\vartheta_0,I_0\}_{(p)}$ of the system (2.10) is produced by the set of all initial conditions (I_0,ϑ_0) and the set (p) connected with possible bifurcations of the trajectories. One sees easily from Eqs. (2.5) and (2.9) that when $\beta\neq0$ the mapping $\hat T$ (2.10) can lead to ambiguity in the selection of one of two possible solutions. Each pair of initial conditions (I_0,ϑ_0) therefore generates, in general, 2^N trajectories. The index "p" labels one of these trajectories. The family of trajectories described here generates a set of values of the free energy of the system:

$$F=\lim_{N\to\infty}\frac{1}{N}H(\{\vartheta_j,I_j|\vartheta_0,I_0\}_{(p)}), \tag{2.11}$$

where N is the total number of spins in the chain. One can minimize expression (2.11) for F with respect to (I_0,ϑ_0) and (p). The result of minimization selects that trajectory which determines the equilibrium configuration (in the thermodynamic sense) of the spins.

We consider the Jacobian of the mapping (2.10):

$$\mathscr{D}_{n+1}=\left|\frac{\partial(I_{n+1},\vartheta_{n+1})}{\partial(I_n,\vartheta_n)}\right|$$
$$=\frac{|\cos(\vartheta_n+\varphi(\vartheta_n)-I_n)|}{|1-[\sin(\vartheta_n+\varphi(\vartheta_n)-I_n)+\psi(\vartheta_n)]^2|^{1/2}}. \tag{2.12}$$

It is clear from this that, generally speaking, when $\beta\neq0$, $\mathscr{D}\neq1$ and the mappping $\hat T$ does not conserve measure. We shall in what follows give a map of lines of constant $\mathscr{D}$ illustrating what we have just said.

One must, however, note that the substitution $\mathbf{r}_j\to-\mathbf{r}_j$ in (2.1) does not change the Hamiltonian H. This substitution is equivalent to the substitution $t\to-t$ in dynamics systems. The mapping $\hat T$ therefore refers to a class of so-called reversible, but non-Hamiltonian systems.[15] There are no attractors (limit points, limit cycles, and limit sets of other dimensionalities) in such systems, and the quantity $\mathscr{D}_n$ in the case of a regular (periodic or quasiperiodic) trajectory changes periodically as function of n. Reversible systems are in many of their properties analogous to Hamiltonian systems.[15] The classes of solutions possible in them are invariant tori which correspond to periodic trajectories and broken tori which corrspond to stochastic trajectories. We discuss them in sections 4 and 5.

3. EQUILIBRIUM STRUCTURES WHEN THERE IS NO ANISOTROPY FIELD

It is convenient to start the study of the mapping $\hat T$ with the case $\beta=0$. Using Eq. (2.7) the maping (2.10) takes the form

$$I_{n+1}=I_n-2\vartheta_n+2\operatorname{arctg}\alpha\operatorname{tg}\vartheta_n,\ \mod 2\pi,$$
$$\vartheta_{n+1}=\vartheta_n+I_{n+1},\ \mod\pi \tag{3.1}$$

on one branch of the function Φ. On the other branch we have from (2.8)

$$\vartheta_{n+1}-\vartheta_{n-1}=\pi, \tag{3.2}$$

whence we find the solution:

$$\vartheta_{2n}=\vartheta_0+n\pi,\quad \vartheta_{2n+1}=\vartheta_1+n\pi,\ \mod 2\pi,$$
$$I_n=(-1)^n(\vartheta_0-\vartheta_1)+(1+(-1)^n)\pi/2,\ \mod 2\pi. \tag{3.3}$$

The solution (3.3) corresponds to a two-fold continuous degeneracy in the parameters $(\vartheta_0,\vartheta_1)$ with energy $F\equiv0$. The period of the chain in this case becomes equal to four. The state with $F=0$ always is higher than the ground state and we shall not consider it in what follows.

We can associate with the mapping (3.1) the following equivalent dynamical system with Hamiltonian:

$$\mathscr{H}=I^2/2+\left(\vartheta^2-\int_0^{\vartheta}\operatorname{arctg}(\alpha\operatorname{tg}x)\,dx\right)\sum_{n=-\infty}^{\infty}\delta(z-n), \tag{3.4}$$

where the parameter z plays the role of the continuous time. The equation of motion

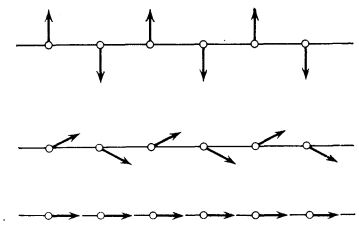

FIG. 1. Examples of different configurations with the same energy for $\alpha = -1, \beta = 0$.

$$dI/dz = -\partial\mathcal{H}/\partial\vartheta, \quad d\vartheta/dz = \partial\mathcal{H}/\partial I \tag{3.5}$$

after integration in the vicinity of the point $z = n$ leads to the mapping (3.1).

It is convenient in what follows to perform the analysis of the equivalent dynamic system (3.4), (3.5) instead of the analysis of the mapping (3.1). We note first of all the physical situations corresponding to different values of the parameter α. It is clear from (2.3) that $\alpha = 1$ when there is no dipole interaction ($D = 0$). The values of α in the vicinity of unity correspond to : a strong ferromagnetic interaction with an addition of a weak dipole interaction when $\alpha \gtrsim 1$ and a strong antiferromagnetic interaction with the addition of a weak dipole interaction when $\alpha \lesssim 1$. The value $\alpha = 0$ is reached when $J = -2D$ and $\alpha = -1$ when $J = -D/2$. A purely dipole interaction ($J = 0$) corresponds to $\alpha = -2$.

When $\alpha = 1$ we have from (3.1) the trivial case:

$$I_n = \text{const} = I_0,$$
$$\vartheta_{n+1} = \vartheta_n + \pi(1 - \operatorname{sign} J)/2 = \vartheta_0 + n\pi(1 - \operatorname{sign} J)/2, \mod 2\pi. \tag{3.6}$$

Minimizing F when solving (3.6) gives $I_0 = 0$ when $J > 0$ and $I_0 = \pi$ when $J < 0$. The parameter ϑ_0 is arbitrary.

When $\alpha = -1$ the energy of the dipole and of the antiferromagnetic interactions are equal ($J = -D/2$) and this leads to the following solution:

$$\vartheta_n = (-1)^n \vartheta_0, \quad I_n = (-1)^n 2\vartheta_0 \tag{3.7}$$

with a minimum of the energy $F = -3D/2$. This means a continuous degeneracy with respect to ϑ_0. Depending on the value of ϑ_0 the chain can change its order from antiferromagnetic ($\vartheta_0 = \pi/2$) to ferromagnetic ($\vartheta_0 = 0$) (Fig. 1). The physical meaning of this degeneracy can be understood also from the following considerations. In the case of complete ferromagnetic ordering $\vartheta_0 = 0$ for all n and according to (2.2) $F^+ = -J - 2D$. In the case of antiferromagnetic ordering $\vartheta_n = (-1)^n \pi/2$ and correspondingly $F^- = J - D$. Degeneracy with respect to these two kinds of ordering corresponds to the point J_0 which is a solution of the equation $F^+ = F^-$, i.e., $J_0 = -D/2$.

When $\alpha = 0$ ($J = -2D$) the mapping (3.1) takes the form

$$I_{n+1} = I_n - 2\vartheta_n, \mod 2\pi,$$
$$\vartheta_{n+1} = \vartheta_n + I_{n+1}, \mod 2\pi.$$

The minimized solution is trivial: $\vartheta_n = (-1)^n \pi/2$ and corresponds to antiferromagnetic order.

We analyzed the general situation for arbitrary values of α numerically. Phase portraits corresponding to the equivalent dynamical system (3.4), (3.5) are given in Fig. 2. For all values of α the minimum of the free energy is reached in the hyperbolic points of the system (3.4), (3.5).[1)] When $\alpha > 1$ this point occupies the position (0,0) in the (I,ϑ) plane and corresponds to ferromagnetic order.

When $-1 < \alpha < 1$ the ground state is reached in the point $(\pi,\pi/2)$ corresponding to antiferromagnetic order.

When $\alpha < -1$ ferromagnetic order is again realized in the point (0,0). We note the following nontrivial fact. In the range of parameter values $-2 < \alpha < -1$ the dipole interaction leads to the formation of ferromagnetic order notwithstanding the antiferromagnetic nature of the exchange interaction in that range.

In concluding this section we note the following features of the *XYDA* model for $\beta = 0$.

1. In the parameter value range $-100 < \alpha < 100$ no stochastic structure is observed. This enables us to assume that the mapping (3.1) refers to an integrable case.

2. In the same range no modulated structures of the ground state are observed. This, in particular, means the absence of incommensurate structures.

3. In the vicinity of the point $\alpha = -1$ small fluctuations can change the ground state configuration strongly, changing it from ferromagnetic to antiferromagnetic.

4. EQUILIBRIUM STRUCTURES WHEN THERE IS NO DIPOLE INTERACTION

Let $D = 0$ ($\alpha = 1$) and let the anisotropy field be chosen in the simplest form:

$$f(\vartheta) = \cos^2(\vartheta - \gamma), \tag{4.1}$$

where γ is an angle fixing the position of the anisotropy axis relative to the chain. The Hamiltonian (2.2) then takes the form

$$H = -J \sum_{n=0}^{N-1} [\cos(\vartheta_{n+1} - \vartheta_n) + \beta \cos^2(\vartheta_n - \gamma)]. \tag{4.2}$$

Hamiltonians with this structure were considered in Ref. 11. We write

$$S_n = \sin(\vartheta_n - \vartheta_{n-1}). \tag{4.3}$$

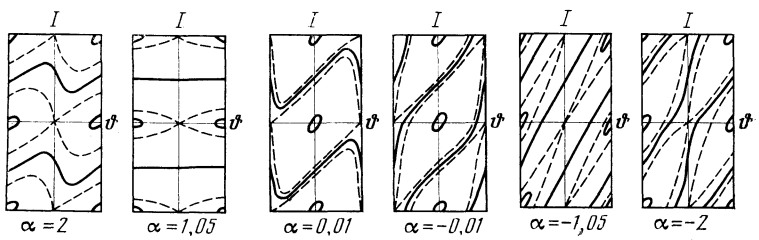

FIG. 2. Phase portraits of the equivalent dynamic system for $\beta = 0$; $-\pi/2 \leqslant \vartheta \leqslant \pi/2$; $-\pi \leqslant I \leqslant \pi$. The separatrix is indicated by a dashed line.

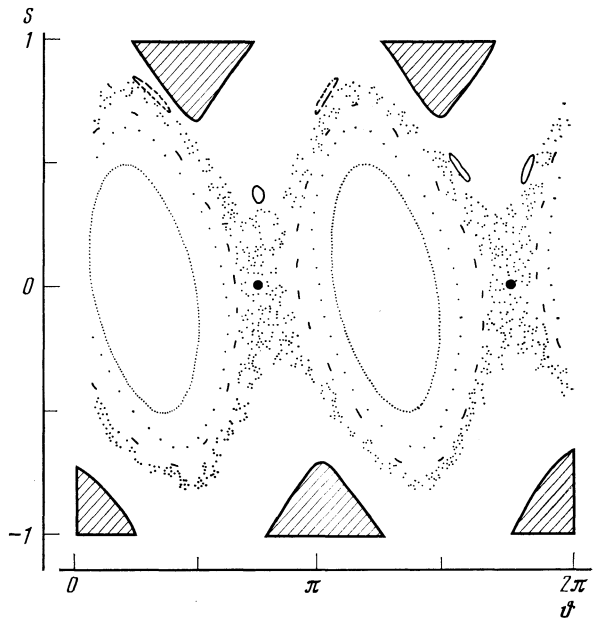

FIG. 3. Phase portrait of the *XYDA* model for the case of antiferromagnetic exchange ($J<0$): $\alpha=1$, $\beta=0.3$, $\gamma=\pi/4$. The forbidden regions are shaded; the dark filled circles are the fixed hyperbolic points.

In the variables (S,ϑ) the mapping $\hat{T}$ (2.10) then takes the form

$$S_{n+1}=S_n+\beta\sin 2(\vartheta_n-\gamma),\quad \vartheta_{n+1}=\vartheta_n+\omega_\nu(S_{n+1}),\qquad (4.4)$$

where

$$\omega_\nu(S_n)=\nu\pi+(-1)^\nu\arcsin S_n\quad(\nu=0,1),\qquad (4.5)$$

and the index ν determines the choice of one of the possible branches of the mapping $\hat{T}$. It follows from (4.4) that $\hat{T}$ conserves measure, independent of ν.

To begin with we consider the properties of the mapping (4.4) for each of the branches separately. One sees easily that the equivalent dynamic system with the Hamiltonian

$$\mathcal{H}=H_0(S)+\beta\cos^2(\vartheta-\gamma)\sum_{n=-\infty}^{\infty}\delta(z-n),\qquad (4.6)$$

$$H_0(S)=\nu\pi S+(-1)^\nu[S\arcsin S+(1-S^2)^{1/2}]$$

and the equations of motion

$$dS/dz=-\partial\mathcal{H}/\partial\vartheta=\beta\sin 2(\vartheta-\gamma)\sum_{n=-\infty}^{\infty}\delta(z-n),\qquad (4.7)$$

$$d\vartheta/dz=\partial\mathcal{H}/\partial S=\omega_\nu(S)$$

generates the mapping (4.4).

The system (4.7) describes a non-linear pendulum with frequency $\omega_\nu(S)$ perturbed by impacts with unit period. The role of the time is, as before, played by the variable z. The stability properties of the solutions of the system (4.7) are determined by the characteristic Lyapunov multipliers λ for the mapping (4.4). We have

$$\lambda=1+K(S,\vartheta)\pm[(1+K(S,\vartheta))^2-1]^{1/2},\qquad (4.8)$$

where

$$K(S,\vartheta)=\beta(1-S^2)^{-1/2}\cos 2(\vartheta-\gamma).\qquad (4.9)$$

The dynamics of the system is thus determined by the parameter K and for sufficiently large $K<K_c\lesssim 1$ there appears chaos.

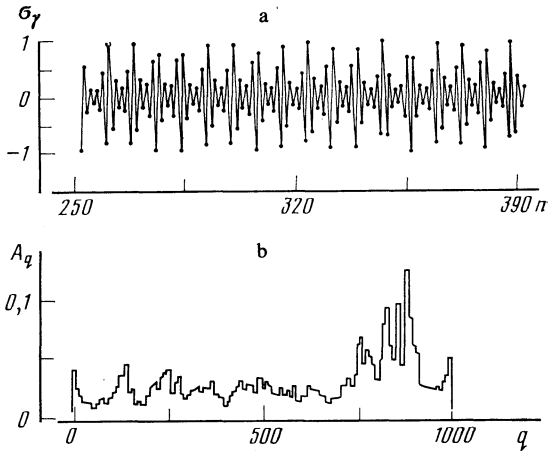

FIG. 4. Chaotic structure of an antiferromagnetic ($J<0$) chain ($\alpha=1$, $\beta=0.3$, $\gamma=\pi/4$, $N=2048$): a: spin component along the ansiotropy axis; b: Fourier spectrum of the angle ϑ_n.

We give in Fig. 3 the phase portrait of the system (4.7) for $J<0$, $\beta=0.3$, and $\gamma=\pi/4$. We depict the points of the trajectories corresponding to five different initial conditions. One of these trajectories is stochastic. All trajectories correspond to energies $F>F_0$, the free energy of the ground state. The latter corresponds to a periodic trajectory (heavy dots in Fig. 3) with a period 2 and with $S_0=S_1=0$ and $\vartheta_0=3\pi/4$, $\vartheta_1=7\pi/4$. The structure of the ground state is antiferromagnetic. The stochastic trajectory has the F value closes to F_0. This is connected with the fact that it spends the longest "time" as compared to the other (periodic) trajectories near the hyperbolic points determining the trajectory of the ground state.

In the regions shaded in Fig. 3 the denominator $[1-\{\sin(\vartheta+\varphi(\vartheta)-I)+\psi(\vartheta)\}^2]^{1/2}$ in expression (2.12) for the Jacobian becomes imaginary. This corresponds to those segments of the trajectories of the mapping (4.4) which in some step m may lead to a value $S_m>1$. In other words, there is a space, which is invariant under the $\hat{T}$ mapping (4.4) which is a subspace of the cylinder $S\in(-1,1)$, $\vartheta\in(0,2\pi)$. This subspace clearly does not include the shaded regions in Fig. 3. In reality the actual boundary of this subspace has a more complex form due to the existence of stochastic trajectories.

We consider in more detail the chaotic structure. It is convenient to introduce the quantity

$$\sigma_\gamma=\cos(\vartheta-\gamma),$$

which determines the spin component along the anisotropy axis. For the stochastic structure the n-dependence of σ_γ is given in Fig. 4a. The spectral properties of this structure can be described by the Fourier transform of the phase:

$$\vartheta_q=\frac{1}{N}\sum_{n=0}^{N-1}\vartheta_n\exp\left\{-\frac{2\pi i n q}{N}\right\},\quad q\in\left(-\frac{N}{2},\frac{N}{2}\right).$$

The quantity $A_q=|\vartheta_q|$ for the stochastic trajectory is shown in Fig. 4b. The maximum in the vicinity of the value $q=N/2$ shows the formation of an amorphous structure

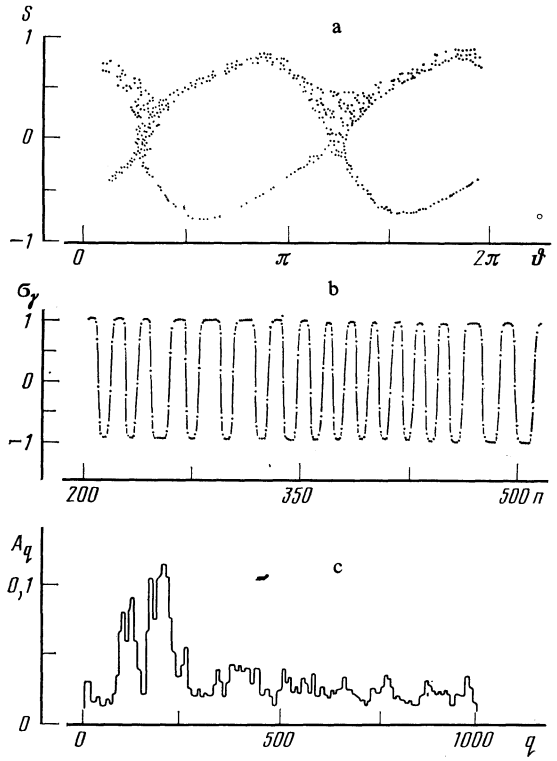

FIG. 5. Chaotic structure of a ferromagnetic ($J>0$) chain ($\alpha=1, \beta=0.3$, $\gamma=\pi/4$, $N=2048$): a: points of the trajectory in the phase plane ($\vartheta_0=3.927$, $S_0=0$); b): spin component along the anisotropy axis; c: Fourier spectrum of the angle ϑ_n.

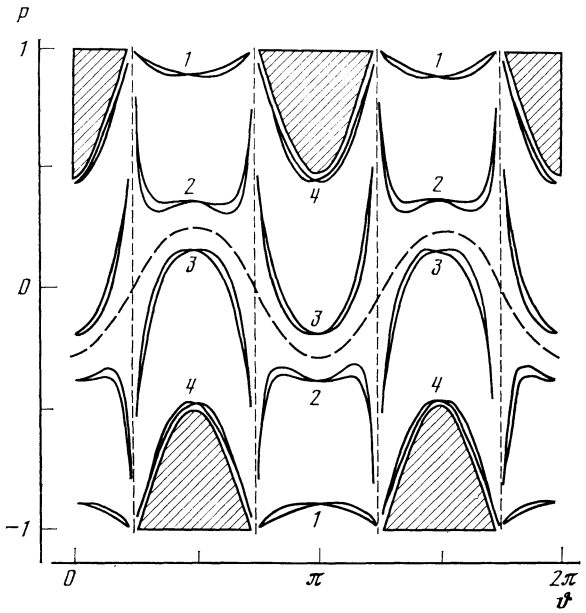

FIG. 6. Lines of constant Jacobian (2.12) for $\alpha=-1.05$, $\beta=0.55$, $\gamma=\pi/4$: 1: $\mathscr{D}=0.5$; 2: $\mathscr{D}=0.95$; 3: $\mathscr{D}=1.05$; 4: $\mathscr{D}=5$; dashed lines are those where $\mathscr{D}=1$.

with short-range antiferromagnetic order with a period close to 2.

The appearance of an amorphous structure for sufficiently large values of β occurs also in the case of a ferromagnetic kind of interaction ($J>0$). For the same values $\beta=0.3$ and $\gamma=\pi/4$ the points of the stochastic trajectory $\{S_n, \vartheta_n\}$ are given in Fig. 5a. The analogous picture for the DNK model with a mapping of the kind (4.4) was obtained in Ref. 16. It is clear from Fig. 5b that the amorphous structure is a disordered sequence of structures of the Block domain wall type. The spectrum of the system has a maximum close to the period 8 (Fig. 5c). This corresponds to a structure in which the direction of the spin along the anisotropy axis ($\gamma=\pi/4$) is specially selected.

The results of this section show that for a sufficiently strong anisotropy amorphous structures occur which may conserve approximate short-range order. The latter is determined by the relation between the parameters of the interaction of the spins and the anisotropy constant.

5. STUDY OF THE GENERAL CASE

In the general model (2.2) it is useful to distinguish from the beginning some special cases in which all three forms of interaction—the exchange, the dipole, and the anisotropy field interactions—are present.

We introduce for the case $\alpha=-1$ ($J=-D/2$) the new variable

$$P_{n+1}=\sin(\vartheta_{n+1}+\vartheta_n). \tag{5.1}$$

The $\hat{T}$ mapping (2.10) then takes the form of the measure conserving mapping

$$P_{n+1}=-P_n+\beta f'(\vartheta_n), \quad \vartheta_{n+1}=-\vartheta_n+\operatorname{Arcsin} P_{n+1}, \tag{5.2}$$

For arbitrary α, however, the mapping (2.10) does not conserve measure. It is therefore convenient to start the analysis of the case (2.10) with the range of α values lying close to $\alpha=-1$.

We give in Fig. 6 in the (P,ϑ) phase plane the lines on which $\mathscr{D}=$ const and the variable P is as before determined by Eq. (5.1) but now (when $\alpha\neq-1$) depends on the point in phase space. The corresponding phase portrait of the system (2.10) in the variables (P,ϑ) is given in Fig. 7 for five different initial conditions. The fixed points in it can be determined from the general condition (see (2.10)):

$$(\bar{P}, \bar{\vartheta})=\hat{T}(\bar{P}, \bar{\vartheta}). \tag{5.3}$$

With the use of Eqs. (2.6), (2.7), and (2.10) Eq. (5.3) leads in the general case to the following result:

$$\bar{P}=\sin 2\bar{\vartheta}=\beta f'(\bar{\vartheta})/(\alpha-1),$$

or, for the anisotropy (4.1) and $\gamma=\pi/4$

$$\bar{P}=\sin 2\bar{\vartheta}, \ \operatorname{tg} 2\bar{\vartheta}=\beta/(\alpha-1). \tag{5.4}$$

Hence

$$\bar{\vartheta}=\tfrac{1}{2}\operatorname{Arctg}[\beta/(\alpha-1)] \tag{5.5}$$

and the expression for the free energy F is found after substitution of (5.4), (5.5), into (2.2):

$$F=\tfrac{1}{2}(D-J)\{1+\alpha+\beta+(-1)^{\nu}\operatorname{sign}(\alpha-1)[(\alpha-1)^2+\beta^2]^{1/2}\} \quad (\nu=0,1). \tag{5.6}$$

In particular, if there is no single-particle anisotropy ($\beta=0$) we have

$$F(\beta=0)=\tfrac{1}{2}(D-J)\alpha^{1-\nu} \quad (\nu=0,1). \tag{5.7}$$

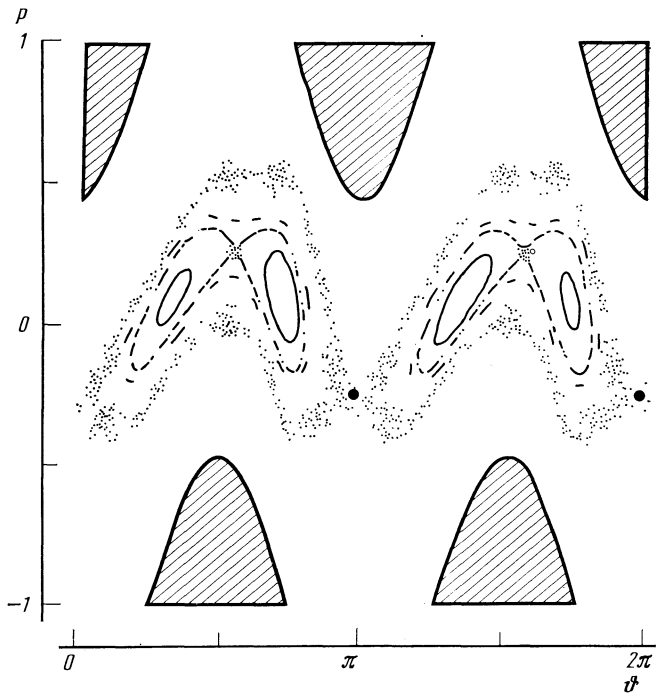

FIG. 7. Phase portrait of the *XYDA* model for $\alpha = -1.05$, $\beta = 0.55$, $\gamma = \pi/4$; the forbidden regions are shaded; the black filled circles are fixed hyperbolic points.

The choice of branch, i.e., the value of ν is determined by the condition that F have a minimum in the point (5.5). The latter, in turn, depends on the values of α and β. For instance, when $\beta = 0$ the branch with $\nu = 0$ is always realized according to (5.7).

The minimum of F in Fig. 7 corresponds to the heavy point (it is repeated with period π). The stochastic set of points corresponds to one random trajectory with parameters $\{\alpha = -1.05;\ \beta = 0.55;\ \gamma = \pi/4;\ \vartheta_0 = -0.1111;\ \vartheta_1 = -0.1211\}$.

The two sets of points of a "figure of eight" type with a smeared out region near the point of intersection are also a single trajectory. It corresponds to the lowest value of the energy from all the trajectories shown in Fig. 7 (except for the points determined by Eq. 5.5)).

In the general case of the *XYDA* model (2.1), as in the case when there is no dipole interaction ($D = 0$), there is thus the possibility of chaotic structures.

6. DISCUSSION OF THE RESULTS

The analysis given in the foregoing requires a discussion of a number of problems which are a matter of principle and of methodology.

1. First of all, one must pay attention to the avoidance of confusion in the use of the concept of an "equilibrium state." The state which is an equilibrium one in the thermodynamic sense, satisfies the conditions for a minimum of the quantity F of (2.11). The determination of a structure corresponding to the minimum of F is connected with the determination of trajectories of a mapping (2.10) (or the trajectory of an equivalent dynamic system). This trajectory is not necessarily stable for the mapping which generates it. Moreover, in all nonstochastic cases the minimizing trajectory is a hyperbolic (i.e., an unstable) point of the mapping. This feature of the model had also been noted in the other models.[13,17,18]

2. The paradox that the energetically stable state corresponds to an unstable fixed point of the mapping generating the distribution of the elements of the chain requires a more detailed discussion.

Let initially the interaction constants (α, β, γ) of the problem be such that stochastic trajectories either do not exist or can appear only in exponentially small regions of the phase space of the mapping. It is then relevant to pose the problem of the effect of a small perturbation on the state of the system to which the coordinates of the hyperbolic point corresponds. The answer is well known in this case. The trajectory of the mapping will leave the hyperbolic point because of its unstable nature. As the system considered performs in phase space a finite motion the perturbed trajectory will be periodic and will periodically approach and go away from the equilibrium position. As the perturbation is small the period of the trajectory will be very large. The perturbed trajectory therefore corresponds to a modulated structure of the chain with a very small deviation of the energy from its equilibrium value (of the order of the magnitude of the perturbation) and with a very long period. In that sense we can say that small perturbations of the trajectory of the mapping even in the vicinity of its unstable fixed point lead also to small perturbations in the structure of the chain.

The position is completely changed if the values of the parameters are such that there occurs an appreciable region in phase space in which the trajectories of the mapping are stochastic. First of all, the vicinity of the hyperbolic point is subjected to a stochastic disruption. Any arbitrarily small perturbation of the trajectory near the hyperbolic point leads to the occurrence of a stochastic trajectory with a probability close to unity. The ground state of the system becomes thus really unstable. Moreover, the energy of the chaotic structure corresponding to the stochastic trajectory of the mapping differs from the ground state energy by a finite amount which is not connected with the magnitude of the perturbation of the initial conditions (the latter may, as we mentioned already, be arbitrarily small).

3. The basic feature of a stochastic (amorphous) structure is the stochastic disruption of long-range order with a partial conservation (if one is not too far from criticality) of short-range order. The latter is just determined by the amount one is away from criticality, e.g., by $|\beta - \beta_c|$, where β_c is the boundary of stochasticity in the parameter β. The connection between short-range order and the amount one is away from criticality was for the standard mapping established in Ref. 19 In the given case the short-range order is easily seen from the spectral histograms in Figs. 4, 5. It determines the characteristic average size of the domains in the amorphous structure of the spin chain. We emphasize that we are dealing here only with such stochastic structures which are generated by stochastic trajectories which fill an exponentially small volume in the phase space of the mapping.

4. One should pay special attention to the form of the invariant set of points of the mapping in which the stochastic

trajectory lies. This set has a very complex but everywhere dense structure of a hierarchical nature. A more detailed description of it must be given separately.

5. We note, in particular, that when $\alpha = 0$ ($J = -2D < 0$) the mapping (2.10) takes the form

$$I_{n+1} = I_n - 2x_n - \beta f'(\operatorname{Arcsin} x_n), \qquad x_{n+1} = x_n + I_{n+1} \quad (|x_n| \leqslant 1) \tag{6.1}$$

in the variables

$$x_n = \sin \vartheta_n, \quad I_n = x_n - x_{n-1}$$

and conserves measure. When $\alpha = \infty$ ($J = D > 0$) the mapping (2.10) has the same form (6.1) with the substitution $x_n = \cos \vartheta_n$. This mapping can turn out to be useful in the analysis of the order-disorder transition in pseudo-spin ferroelectric systems.

6. We have already mentioned that the many-valuedness of the mapping (2.10) is a specific property of spin chains. It produces, generally speaking, for each initial condition 2^N trajectories in the phase space of the mapping (N is the number of particles). However, a numerical analysis shows that in all cases considered the "local minimization" condition selects the trajectory corresponding to only a single well defined branch of the mapping (2.10). In other words, the branch index ν is an invariant of the mapping. The choice of the value of ν is determined by the parameters (α, β, γ) (see end of section 5).

The local minimization consisted in the following two conditions: a) $\partial^2 H / \partial \vartheta_n^2 > 0$ for all n; b) when condition "a" is satisified one must choose at a given stop in the iteration n such a $\nu = \nu_1$ for which $H_n^{\nu_1} < H_n^{\nu_2}$; H_n^{ν} is the density of the Hamiltonian H^{ν} for the branch ν:

$$H^{\nu} = \sum_{n=0}^{N-1} H_n^{\nu}.$$

Of course, such a choice of the minimizing trajectory does not exhaust all possible 2^N cases. In particular, in phase space the "forbidden" regions of initial conditions are those for which either the mapping (2.10) has no meaning or for which condition "a" cannot be satisfied for $n = 2$. Generally speaking, one does not exclude those regions of phase space such that a trajectory starting from them arrives at a step $n > 2$ at a case for which condition "a" is not satisfied.

[1)]We note that the points of stable equilibrium of the initial system (3.1) are not the same as the points of equilibrium of the equivalent dynamic system. The statement made here does therefore not contain a contradiction.

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Note added in proof (31 May 1984): In the general case (arbitrary α) the variables in terms of which there arises a measure preserving mapping have the form

$$I_n = \rho(\vartheta_n) \sin[\vartheta_{n-1} + \varphi(\vartheta_n)], \quad \tilde{\vartheta}_n = \vartheta_n.$$

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