PHYSICAL REVIEW B VOLUME 57, NUMBER 10 1 MARCH 1998-II

Magnetic superlattices, classical spin chains, and the Frenkel-Kontorova model

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(Received 25 July 1997)

An equivalence between a simple magnetic model subject to an intrinsically nonconvex Heisenberg interaction and a Frenkel-Kontorova-type model is formulated. The magnetic model is able to reproduce the experimental results obtained on Fe/Cr(211) superlattices and for this reason has already attracted theoretical attention. The problem is formulated via a two-dimensional area-preserving map and the effect of the surfaces in the magnetic model, which are introduced by appropriate boundary conditions, is shown to be equivalent to the introduction of a discommensuration in a Frenkel-Kontorova-type chain. Further analogies between the two models are presented. The analysis is used to reconsider and clarify some of the features of the magnetic model and to add some contributions to its phase diagram in the space of parameters. [S0163-1829(98)02009-8]

I. INTRODUCTION

In the last decade great attention has been devoted to magnetic films and superlattices;[1] this interest has been driven by the enormous experimental advances in the growth and characterization techniques of these materials, as well as in the investigation ones, which have led to the realization of high quality samples and the discovery of many new and interesting phenomena, such as the oscillatory exchange coupling between ferromagnetic films separated by nonmagnetic spacers,[2] the giant magnetoresistence effect,[3] and the biquadratic exchange coupling.[4]

Additional interest in magnetic superlattices comes from their lack of translational invariance in the direction normal to the surfaces and by the high-ratio surface to volume of these systems, so that they are ideal candidates to investigate the effect of surfaces and/or interfaces.[5]

In this framework, Fe/Cr(211) superlattices have recently received consistent attention. These superlattices, grown by a sputtering technique as single-crystal samples with a uniaxial anisotropy, show an antiferromagnetic interlayer coupling for a suitable choice of the Cr thickness (11 Å).[6] Magnetic measurements[7] performed via magneto-optical Kerr effect (MOKE) and superconducting quantum interference device (SQUID) techniques showed two main peaks in the magnetic susceptibility at the so-called surface and bulk spin-flop transitions and other minor peaks in the intermediate region, in the case of an even number of Fe layers. In the considered situation, the system is isomorphic to a classical two-sublattice antiferromagnet, with ferromagnetic planes antiferromagnetically coupled, and it is suitably described by a simple uniaxial antiferromagnetic model. Starting from this model, the behavior of the system with an even number of planes was explained, using a numerical self-consistent approach, as due to jumps of a Bloch wall.[7] The occurrence of this series of experimentally detected phase transitions stimulated further theoretical work: a determination of the ground state of the system formulated as a two-dimensional area preserving map emphasized the importance of the discreteness of the magnetic lattice and of the chaotic nature of the map,[8] due to the high ratio between the uniaxial anisotropy and the exchange interaction; a very recent study using effective potential methods produced the phase diagram of the same model in the space of parameters.[9]

One of the essential characteristics of the Fe/Cr(211) superlattices is the competition between the antiferromagnetic exchange interaction and the Zeeman interaction. The first one favors an antiparallel orientation of neighboring spins, i.e., a difference of π in their orientation, while the second one tends to align all the spins in the field direction, with a zero (or equivalently 2π) difference in the orientation of neighboring spins.

On a general grounds, competitive interactions can make the determination of the ground state far from trivial, as the internal degrees of freedom are frustrated by two or more interactions, which favor different equilibrium configurations.[10] A clear example of such a difficulty is given by the ground-state properties and the spectacular phase diagram of the Frenkel-Kontorova[11,12] model and of the axial next-nearest-neighbor Ising (ANNNI) model,[13] both of these models being characterized by two natural length scales, just as the uniaxial antiferromagnet in the presence of an applied field.

As a consequence of this simple observation, it is obviously tempting to describe the magnetic system in the wider framework of frustrated models,[12] and this is exactly what is done in this paper.

In fact, I will show in the following how it is possible to establish an equivalence between a Frenkel-Kontorova-type model and the uniaxial antiferromagnet with an external magnetic field in the direction of the easy magnetization axis. The equivalence I am going to formulate connects an intrinsically nonconvex interaction—such as the Heisenberg interaction in the magnetic model considered—with the paradigmatic convex one given by the interparticle interaction in the Frenkel-Kontorova model. In particular, I will show that the effect of the surfaces in the magnetic model is equivalent to the introduction of a *discommensuration* in a Frenkel-Kontorova chain. The importance of the concept of discommensuration in the analysis of the considered magnetic system was foreseen by Micheletti *et al.*[9] My approach goes in the well-estabilished path in statistical mechanics of reducing a wide series of observations to a restricted number of models, and the analysis performed is also used to reconsider and clarify some of the many interesting features of the magnetic system and to add some contributions to its phase diagram in the space of parameters.

The paper is then organized as follows: In Sec. 2, for the sake of completeness, some of the basic properties of the Frenkel-Kontorova model are recalled; in Sec. III the magnetic model is introduced, and the determination of its ground state is formulated by means of a two-dimensional area-preserving map. The equivalence between the magnetic model and a Frenkel-Kontorova-type model is then shown. The interpretation of the magnetic field dependence of the ground-state configuration and of the magnetic susceptibility of the Fe/Cr(211) superlattices given the established equivalence and using the concept of discommensuration is presented in Sec. IV, whereas the low anisotropy case for the film and the semi-infinite system is considered in Sec. V. Conclusions are drawn in Sec. VI.

II. FRENKEL-KONTOROVA MODEL

In this section I will outline some of the basic properties of the ground state of the Frenkel-Kontorova model;[15] as the subject is extensively treated in numerous papers and reviews (see, for example, Refs. 11, 12, and 16–23), my description will be no more than schematic.

The Frenkel-Kontorova model describes a chain of elastically coupled atoms submitted to a periodic potential (at zero temperature). The energy of the system can be written as

$$U=\frac{1}{2}\sum_i (u_{i+1}-u_i-\mu)^2+\frac{\lambda}{2}\sum_i \left(1-\cos\frac{\pi u_i}{a}\right), \qquad (1)$$

where u_i is the abscissa of the ith particle.

The goal is to determine the ground state of this system and its properties, which turns out to be a far from trivial task as the harmonic interaction and the sinusoidal potential favor different equilibrium positions of the particles. All the equilibrium configurations of the system are given by

$$\frac{\partial U}{\partial u_i}=0 \quad \forall i. \qquad (2)$$

Introducing the new variable $p_i \equiv u_i - u_{i-1}$, Eq. (2) can be written as a two-dimensional recursive mapping:

$$p_{i+1}=p_i-\frac{\lambda\pi}{2a}\sin\frac{\pi u_i}{a}, \qquad (3)$$

$$u_{i+1}=u_i+p_{i+1}, \qquad (4)$$

which is known as the *standard map*.[24–26]

The standard map is area preserving, since its Jacobian $|J|=1$, and setting $\theta_i=u_i(\mathrm{mod}2a)$ the mapping can be folded onto a torus $[0,2a]\times[0,2a]$. As the map is derived from Eq. (2), any trajectory in its phase space is associated with an equilibrium configuration of the system.

By the analysis of the standard map Aubry was able to determine the properties of the ground state of the system. First of all he introduced a distinction between the concept of minimum energy configuration and the concept of ground state.[11,18,19] The concept of a ground state is restricted to minimum energy configurations which can be represented by recurrent trajectories in the associated map. A recurrent trajectory returns to any neighborhood of any point of the trajectory. The reason for this distinction is that under certain boundary conditions, for example,

$$\lim_{N-N'\to\infty}\frac{u_N-u_{N'}}{N-N'}=2a, \qquad (5)$$

the equilibrium configuration which has the lowest energy is a *discommensuration*, which is not associated with a recurrent trajectory and is not considered as a ground state, since this kind of solution is a zero-measure set in the map representation. Despite their zero measure, discommensurations play an essential role in understanding the generation of stochasticity in the map phase space. For our purposes, they have even a greater importance, since they are the configurations providing the ground state of the magnetic system in the presence of surfaces, as I will show in the following sections. A rigorous definition of discommensuration will be given in a moment.

Any ground state is specified by the *winding number* $l/2a$ of the corresponding trajectory in the standard map,[11,18,19] where

$$l=\lim_{N-N'\to\infty}\frac{u_N-u_{N'}}{N-N'}. \qquad (6)$$

The winding number represents the mean number of revolutions around the cylinder per iteration of the map, and it can be either rational or irrational. In the first case the ground state is commensurate with the lattice:

$$u_i=il+\alpha_i, \qquad (7)$$

where α_i is an arbitrary phase factor; the corresponding trajectory is associated with fixed points[27] (i.e., periodic cycles) in the standard map. Moreover, the set of commensurate ground states can be either continuous or discontinuous. In the former situation it can be parametrized by a set of functions $\{u_i(\alpha)\}$, where α is a continuous factor, varying from $-\infty$ to $+\infty$. In the latter situation this is not possible and there exist two ground state configurations

$$v_i^-=il+\alpha_i^-, \quad v_i^+=il+\alpha_i^+, \qquad (8)$$

such that no other ground state exists in between them. This is a sufficient and necessary condition for the existence of a discommensuration, that is, a minimum energy configuration u_i, such that

$$v_i^-<u_i<v_i^+, \qquad (9)$$

and (for an advanced discommensuration) (see Fig. 4 in Ref. 19)

$$\lim_{i\to\pm\infty}|u_i-v_i^{\pm}|=0. \qquad (10)$$

The continuous case is an exceptional situation, which occurs only in integrable maps; it corresponds to the absence of a lattice locking of the commensurate ground state. On the contrary, in the discontinuous case, the lattice does apply a locking effect, and this means that none of the particles can be at a maximum of the sinusoidal potential in physically stable solutions.[11,22] It was proved by Aubry[11,18,19] that a discommensuration corresponds with the set of homoclinic intersections associated to the corresponding fixed points.

In the case with $l/2a$ irrational, Aubry proved[11,17–19] that a transition exists at a well-defined value λ_c of the constant λ (depending on the value of l), which he called *transition by breaking of analyticity*. This transition can be related to the discrete nature of the structure and the existence of a nonvanishing Peierls-Nabarro barrier,[28] i.e., the smallest energy barrier that has to be overcome to move a domain wall along a chain. The transition by breaking of analyticity is associated with the breaking of a Kolmogorov-Arnold-Roser (KAM) curve of the standard map, and precisely of a KAM curve which encircles the torus; a curve with such a characteristic is called nonhomotopic to zero, since it cannot be reduced to a point on the toroidal surface by a continuous deformation.

The number of results proven by Aubry applies not only to the Frenkel-Kontorova model, but also to any chain of particles with a nearest-neighbor interaction, such that its energy can be written as

$$E=\sum_i L(u_i,u_{i+1}), \tag{11}$$

provided that the function L satisfies some conditions;[11,18] the most restrictive of these conditions is that $L(x,y)$ is twice differentiable and satisfies for all x and y

$$-\frac{\partial^2 L(x,y)}{\partial x \partial y}>c>0, \tag{12}$$

which means that the interparticle interaction must be strictly convex. This condition ensures that the corresponding map is unambiguously determined.

On the other hand, the work by Aubry was not devoted to the determination of the actual ground state of the system for different values of the parameters. This determination is due to Griffiths and Chou,[20,21] which developed and employed an effective potential method which works for both convex and nonconvex interactions W, given the energy of the system in the form

$$E=\sum_i [V(u_i)+W(u_i-u_{i-1})]. \tag{13}$$

Using the effective potential method, Griffiths and Chou were able to produce the phase diagram of the model in the space of parameters.[20,21]

An interesting variation of the Frenkel-Kontorova model is the one in which the potential V is a Fourier series:[20,21]

$$V(u_i)=\frac{K}{(2\pi)^2}\sum_{k=1}^{\infty} \epsilon_k(1-\cos 2\pi k u_i), \tag{14}$$

where the coefficients ϵ_k are assumed to be sufficiently small that no other minima or maxima are introduced in the potential V with respect to the Frenkel-Kontorova case (which is obtained for $\epsilon_k=0$ with $k\geqslant 2$). The phase diagram of the above model with $\epsilon_1=1$, $\epsilon_2=0.1$, and $\epsilon_k=0$ for $k\geqslant 3$ was again obtained numerically by Griffiths and Chou.[20,21] Their analysis shows that in this situation one can distinguish two different types of commensurate ground state with the same winding number P/Q, where P and Q are irreducible positive integers. The two phases, labeled A and B, are separated by horizontal lines corresponding to first-order transitions. In states of type A there are particles at the minima of the potential V if Q is odd, while if Q is even the phase is characterized by the absence of particles at the minima of V; in the phase B, on the contrary, there are particles at the maxima of V, regardless of the parity of Q.

III. MAGNETIC MODEL

Consider now a magnetic superlattice composed by ferromagnetic films separated by nonmagnetic spacers, in the condition of antiferromagnetic coupling between the ferromagnetic films. Suppose that the only effect of the intrafilm interaction, which is usually much stronger than the interfilms one, is to keep all the spins belonging to the same film parallel to each other and that each film can be represented by a single layer. Under these assumptions, the determination of the ground state of the three-dimensional superlattice reduces to a one-dimensional problem in the direction normal to the films surfaces.

In the case of Fe/Cr(211) superlattices,[7,6] the system is isomorphic to a classical two-sublattice, uniaxial, antiferromagnet, so that, denoting by ϕ_i the angle formed by the magnetization of the ith layer with the direction of the applied field, the energy of the system at $T=0$ can be written as

$$\frac{E}{N_\parallel S}=\sum_i [H_E \cos(\phi_i-\phi_{i-1})-H_A \cos^2 \phi_i-2H \cos \phi_i], \tag{15}$$

which is equivalent to the energy of a classical spin chain. H_E and H_A are the exchange interaction and the uniaxial anisotropy constants, and H is the external magnetic field. For an infinite system (with $i=0,\pm 1,\pm 2,\ldots$), a first-order phase transition occurs when H exceeds a critical value, driving the system in the so-called bulk spin-flop phase.[29] In this phase, the spins belonging to the two sublattices form an angle $\phi\simeq\pm\pi/2$ with the direction of the applied field. The antiferromagnetic (AF) phase and the bulk spin-flop (BSF) phase have equal energy for $H=H_B\equiv\sqrt{2H_EH_A-H_A^2}$. The upper and lower boundaries of the metastability region associated with the first-order nature of the transition are $H_{\mathrm{BSF}}\equiv\sqrt{2H_EH_A+H_A^2}$ and $H_B'\equiv(2H_EH_A-H_A^2)/\sqrt{2H_AH_E+H_A^2}$, respectively.[30] For $H=H_{\mathrm{sat}}=2H_E-H_A$ the saturation regime, with all the spins aligned with the magnetic field, is reached.

All the equilibrium configurations are obtained by

$$\frac{\partial E}{\partial \phi_i}=0 \quad \forall i, \tag{16}$$

which leads to

$$H_E[\sin(\phi_{i+1}-\phi_i)+\sin(\phi_{i-1}-\phi_i)]+2H \sin \phi_i +H_A \sin(2\phi_i)=0. \tag{17}$$

Introducing $\xi\equiv H/H_E$, $\zeta\equiv H_A/H_E$, and $s_i=\sin(\phi_i-\phi_{i-1})$, Eq. (17) can be rewritten as a two-dimensional recursive mapping

$$s_{i+1}=s_i-2\xi \sin \phi_i-\zeta \sin(2\phi_i), \tag{18a}$$

$$\phi_{i+1}=\phi_i+\sin^{-1}(s_{i+1}), \tag{18b}$$

The map is area preserving, since its Jacobian $|J|=1$, and it is invariant with respect to the transformation $(\phi,s)\rightarrow(-\phi,-s)$. Its domain is $[0,2\pi)\times[-1,1]$, once the variable ϕ is defined as mod(2π). Trajectories in the (ϕ,s) space are associated with equilibrium configurations. The AF and BSF phases are reproduced by second-order fixed points, such that $(\phi_{n+2},s_{n+2})=(\phi_n,s_n)$. They are $P_-^{\mathrm{AF}}=(0,0)$, $P_+^{\mathrm{AF}}=(\pi,0)$, $P_-^{\mathrm{BSF}}=(-\overline{\phi},-\sin 2\overline{\phi})$, and $P_+^{\mathrm{BSF}}=(\overline{\phi},\sin 2\overline{\phi})$, where $\cos\overline{\phi}=\xi/(2-\zeta)$. A linear stability analysis shows that the AF fixed points P_-^{AF} and P_+^{AF} are hyperbolic for $H\leqslant H_{\mathrm{BSF}}$ and elliptic for higher fields. On the other hand, the BSF fixed points P_-^{BSF} and P_+^{BSF} are hyperbolic for $H\geqslant H_B'$ and elliptic for lower fields. In the metastability region, both the AF and the BSF fixed points are hyperbolic. In this region we can still distinguish two regimes; for $H<H_B$ the stable and unstable manifolds associated with the BSF fixed points are enclosed by the stable and unstable ones associated to the *AF* fixed points, and the opposite happens for $H>H_B$.[31]

Let us now turn to the semi-infinite and the film cases. In the semi-infinite situation Eq. (17) for $i=1$ is modified in

$$H_E \sin(\phi_2-\phi_1)+2H \sin \phi_1+H_A \sin(2\phi_1)=0, \tag{19}$$

which introduces a boundary condition for the map of the infinite system; this condition is taken into account[32,14] with the introduction of a fictitious plane for $i=0$ such that

$$s_1=\sin(\phi_1-\phi_0)=0. \tag{20}$$

For an N-planes film, two fictitious planes must be introduced,[14] for $i=0$ and $i=N+1$, respectively, so that in this case the boundary conditions are

$$s_1=\sin(\phi_1-\phi_0)=0, \tag{21}$$

$$s_{N+1}=\sin(\phi_{N+1}-\phi_N)=0. \tag{22}$$

Only those trajectories of the map Eq. (18) which satisfy the boundary conditions represent therefore equilibrium configurations of the system in the presence of surfaces. For the semi-infinite system, it is possible to obtain a nonuniform ground state if the inflowing orbit to a hyperbolic fixed point intersects the boundary condition line $(s=0)$; in fact, far from the surface the system must have the same configuration as the bulk. For the film, the trajectories associated with equilibrium configurations must have two intersections with the $s=0$ line, exactly separated by N steps.

It is interesting to consider the effect of an applied magnetic field on the semi-infinite system and the film. The semi-infinite system, in the limit of small external field and small anisotropy with respect to the exchange interaction, was analyzed several years ago.[33,34] In a uniaxial semi-infinite antiferromagnet with the surface spins *antiparallel* to the magnetic field $(\mathrm{AF}_{\uparrow\downarrow})$, a surface transition occurs at a field $H_{\mathrm{SSF}}\equiv\sqrt{H_AH_E+H_A^2}\simeq H_{\mathrm{BSF}}/\sqrt{2}$, as pointed out by the softening at $H=H_{\mathrm{SSF}}$ of the surface mode.[33,35] This instability was predicted to drive the system in the so-called surface spin-flop state.[33] In this phase, the spins were predicted[33] to turn by nearly $\pi/2$ near the surface and asymptotically reach the antiferromagnetic configuration in the bulk. It was also suggested[34] that the extension of the region of turned spins should increase continuously with increasing H, until the onset, for $H=H_{\mathrm{BSF}}$, of a uniform bulk spin-flop state, with all the spins rotated by nearly $\pi/2$.

For a film with an even number of planes, one finds an analogous behavior of the excitations. There are two surface modes, and for $H=H_{\mathrm{SSF}}$ the one localized at the surface with the spins antiparallel to H shows a complete softening.[36] The surface transition is again a first-order phase transition. H_{SSF} is therefore the upper boundary of the associated metastability region, whose lower boundary will be H_S', below which no nonuniform configuration can be minima for the system. In between these two values, H_S is the field of energetic equivalence between nonuniform configurations and the antiferromagnetic one. Both H_S' and H_S have to be determined numerically. From the analysis of the map phase portrait at different values of the field, one can find the ground-state configurations for the semi-infinite system and for the film, as will be shown in Secs. IV and V.

Equivalence with the Frenkel-Kontorova model

Consider for the moment the infinite system. In the mapping, Eq. (18) the presence of the $\sin^{-1}$ function is due to the Heisenberg interaction between neighboring spins, and it makes the map multivalued, as a direct consequence of the nonconvexity of the Heisenberg interaction. At each step two choices are possible:

$$\phi_{n+1}=\phi_n+(-1)^\nu\Psi+\nu\pi, \quad \nu=0,1, \tag{23}$$

where $\Psi=\sin^{-1}(s_{n+1})$ is the principal value of the trigonometric function $\sin^{-1}$ and ν is the branch index. Each pair of initial conditions generates 2^N trajectories after N iterations of the map. The choice of the branch index is trivial only for bulk systems characterized by low periodic configurations. Anyway, in the case of small parameters $(\xi,\zeta\ll 1)$, i.e., when the exchange interaction is largely dominant with respect to the Zeeman and the anisotropy ones, there is a natural choice of the branch index to obtain the ground state. Neighboring spins tend to align in a nearly antiparallel way, and this situation is reproduced by the choice $\nu=1$ at each step. The same reasoning does not hold for comparable interactions, which turns out to be the case pertinent to the experimental situation. Several years ago, Belobrov *et al.*[37] proposed a *local minimization* criterion to select the branch index. The criterion consisted in two conditions: (a) $\partial^2E/\partial\phi_n^2>0$ for all n, and (b) when condition (a) is satisfied by both the branches, one has to choose the branch which gives the lowest energy *at that step*. Unfortunately, we verified that this criterion, and more generally any local criterion, does not apply in our situation: we followed all the trajectories for which condition (a) was satisfied, and it usually happened that the configuration with the lowest energy for $n=n_2$ did not originate from the lowest-energy one for $n=n_1$, with $n_1<n_2$.

Myself and co-workers proposed[38] a different criterion: the branch index is always a *constant* of the mapping, once the parameters are fixed, and the choice to adopt is the one which reproduces the correct ground state for the associated infinite system.

In the infinite system there exists a threshold value $H_{\rm th}=(2H_E-H_A)\cos(\pi/4)$ for which the angle formed by two neighboring spins is exactly $\pi/2$. So, for $H\leqslant H_{th}$ the choice one has to fulfill to reproduce the uniform bulk spin-flop configuration is $\nu=1$, while for $H\geqslant H_{\rm th}$ it is $\nu=0$. For $H=H_{\rm th}$, the two choices are equivalent. We believe the constancy of the branch to hold for finite and semi-infinite systems, too, and we have numerical evidence for all the situations we considered, although we were not able to give an analytical explanation. The criterion is expected to hold as far as the uniaxial anisotropy becomes so large that the system is more adequately described by an Ising model rather than a Heisenberg one.

The invariance of the branch index under map iteration has important consequences: as is apparent considering the form of the Heisenberg interaction and Eq. (23), as far as $\nu=1$ the coordinates ϕ_i are subject only to the convex part of the Heisenberg interaction, while for $\nu=0$ they are subject only to the nonconvex part of the interparticle interaction. This is equivalent to say that, when $\nu=1$, the map, Eq. (18), satisfies the *twist* condition[39] which, given the definition of the variable s_i, is

$$\left(\frac{\partial\phi_{i+1}}{\partial s_i}\right)_{\phi_i}<0. \tag{24}$$

Since the coordinates are subject only *either* to the convex part of the Heisenberg interaction *or* to the nonconvex one, it is possible to introduce a harmonic approximation, which is expected to be correct for values of the magnetic field sufficiently far from $H_{\rm th}$. The energy of the system in this approximation becomes

$$H<H_{\rm th},\quad E=\sum_i\left[\frac{1}{2}(\phi_i-\phi_{i-1}-\pi)^2-2\xi\cos\phi_i-\zeta\cos^2\phi_i\right], \tag{25}$$

$$H>H_{\rm th},\quad E=\sum_i\left[-\frac{1}{2}(\phi_i-\phi_{i-1})^2-2\xi\cos\phi_i-\zeta\cos^2\phi_i\right]. \tag{26}$$

Consider the first case, which is the one defined in the interesting range of H, $H_{\rm th}$ being much higher than $H_{\rm BSF}$ and close to the saturation value $H_{\rm sat}$. For $\zeta=0$ our system is now equivalent to the Frenkel-Kontorova model (1), with $\mu=a$ [or, equivalently, with $d\equiv|(\mu-2a)/2a|=1/2$] and

$$\frac{\pi u_i}{a}\rightarrow\phi_i,\quad \lambda\rightarrow4\xi\frac{a^2}{\pi^2}, \tag{27}$$

or, in the notation of Griffiths and Chou,[20] with $\gamma\equiv(1-d)=1/2$ and $K\rightarrow2\xi$. The presence of the uniaxial anisotropy makes the system equivalent to a Frenkel-Kontorova model with a second-harmonic contribution to the sinusoidal potential [Eq. 14]. The second-order fixed points $P^{\pm}_{\rm AF}$ and $P^{\pm}_{\rm BSF}$ are the periodic configurations with winding number $w=1/2$ which give the ground state for $\gamma=1/2$. The A phase is equivalent to the bulk spin-flop one, and the B phase to the antiferromagnetic configuration. The horizontal line separating the A and B phases is equivalent to the bulk spin-flop transition. Identified 2ξ with $K\epsilon_1$ and ζ with $2K\epsilon_2$ [see Eqs. (14) and (15)], this transition, for $\gamma=1/2$, is located at

$$K=\frac{16\epsilon_2}{\epsilon_1^2+16\epsilon_2^2}. \tag{28}$$

The condition which ensures no additional minima or maxima in the potential V becomes in our case $H>H_A$, which is again the interesting region of our system.[9]

Although in the following only the $\nu=1$ choice will be considered, it is interesting to take briefly into account the regime in which the particles are subject to the nonconvex part of the Heisenberg potential. First of all, it must be stressed that this region is ''explored'' only due to the presence of the external magnetic field. Actually, Griffiths and Chou[20] showed that the ground state of a system with an energy given by Eq. (13), with a Heisenberg interaction form for W and the following one for V,

$$V(\phi_i)=h\cos(p\phi_i), \tag{29}$$

never experiences the nonconvex part of W for any $p\geqslant2$, putting on a rigorous ground an earlier hypothesis by Banerjea and Taylor[40] for the $p=2$ case. The presence of a $p=1$ contribution makes the nonconvex part accessible, as actually happens for the chiral model[41] or other types of models.[42,43] In our model, too, for very high values of the magnetic field, i.e., near the saturation value, all the spins are canted in the field direction and the ground state is provided by a trajectory obtained with the $\nu=0$ choice.[38]

To summarize, the *constant branch index criterion* we have introduced has two main consequences: the equivalence, for a wide range of the applied field H, of the magnetic model with a Frenkel-Kontorova-type model with a misfit $d=1/2$ and the possibility to tackle a series of models with nonconvex interparticle interactions, like the *Josephson junction arrays*[44,45] which seemed precluded, up to now, from a map approach analysis.

IV. Fe/Cr(211) SUPERLATTICES

Consider for the moment the situation in which $\xi,\zeta\leqslant1$. The phase portrait (see Fig. 1) is extremely regular and this means that we are in a quasi-integrable limit.

On the contary, Fe/Cr(211) superlattices are characterized by a relatively high ratio between the uniaxial anisotropy and the exchange interaction. A reasonable estimate is $H_E=2.0$ kG and $H_A=0.5$ kG, and the corresponding phase portrait for a magnetic field in the range of interest is shown in Fig. 2. Strong nonintegrability effects and, in particular, the homoclinic intersections between the inflowing and the outflowing orbits from the antiferromagnetic fixed points are apparent. Moreover, these manifolds oscillate and intersect the boundary condition line $s=0$. This means that several metastable configurations coexist and the ground state must

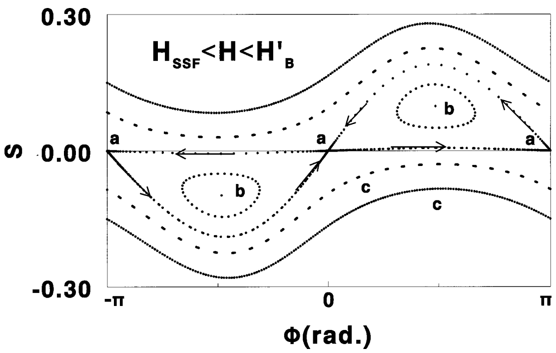

FIG. 1. Phase portrait obtained from mapping Eq. (18) for small anisotropy $\zeta=0.01$ and an applied field such that $H_{\rm SSF}<H<H_B'$. The various labels denote (a) hyperbolic fixed points $P_{\pm}^{\rm AF}$, (b) elliptic fixed points $P_{\pm}^{\rm BSF}$, and (c) nonhomotopic to zero trajectories. Arrows denote inflowing and outflowing orbits associated with the hyperbolic fixed points.

be determined by a comparison of their energy. The presence of metastable states is intimately connected with the strong nonintegrability of the map and the pinning effect produced by the lattice.[22] It is interesting to note that the stable and unstable manifolds ''cover'' all the domain of the variable s, so that nonhomotopic to zero curves cannot exist. This is the characteristic of the stocasticity regime defined by Greene[25] in his analysis of the standard map.

Nonetheless, the determination in an accurate way of the equilibrium configurations of a film is still possible, given a limited number of planes, and it was performed for $N=22$ and, for a restricted range of H, for $N=16$, too. At the growing of the magnetic field some intersections of the manifolds with the $s=0$ line disappear, or a previously metastable state becomes the ground-state; this causes abrupt changes in the ground-state configuration and consequently in the magnetization $M(H)$ of the system. Correspondingly to the jumps of $M(H)$, one has spikes in the magnetic susceptibility $\chi=dM/dH$ (see Fig. 3).

The first peak for $H>H_S$ (at $H\simeq1.045$ kG) was not present in our earlier version[8,38] of Fig. 3, as the true ground-state for this and lower values of H is embedded in a very chaotic region of the map phase portrait, and we missed it. This is a clear example of the difficulties of a map approach to the ground-state determination. In fact, using the map

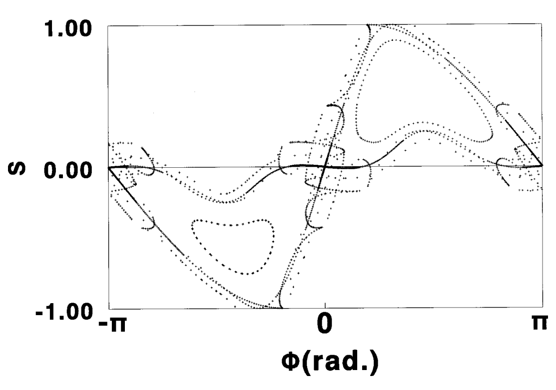

FIG. 2. Phase portrait obtained from mapping Eq. (18) for $H_E=2.0$ kG, $H_A=0.5$ kG, and $H=1.073$ kG. The inflowing and outflowing orbits associated with the AF fixed points are shown, and their homoclinic intersections are apparent.

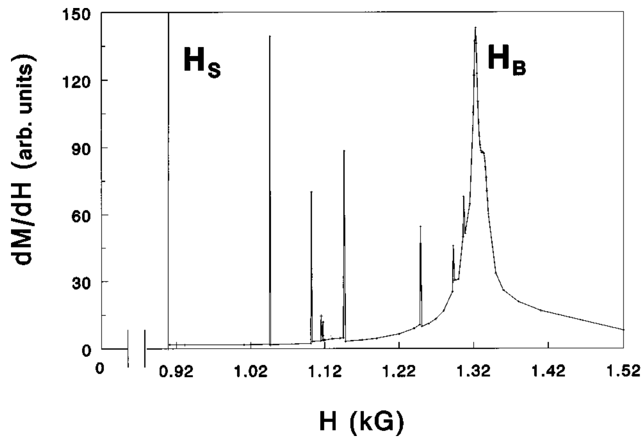

FIG. 3. Magnetic susceptibility as a function of the applied filed for a $N=22$ film, with $H_E=2.0$ kG and $H_A=0.5$ kG.

method, the problem is more complex than the actual ground-state one, as each trajectory in the map phase diagram is associated to an equilibrium configuration, regardless of its energetic stability or of its energy. The determination of the ground state is possible only once *all* the stable equilibrium configurations have been determined, by a comparison of their energies. Moreover, energetic stable configurations correspond to topologically unstable trajectories.[11,16,46,47] The advantage is that a map is an exact representation of the equilibrium configuration space and displays in a graphical way the various kinds of solution the system can have, the presence of possible metastable configurations, the importance of effects due to the discreteness and to the nonintegrability of the system, and the occurrence of strongly chaotic regimes, which is exactly the present situation.

The behavior of the system becomes comprehensible in a more direct way if one considers the connection existing between the mestastable configurations and the homoclinic intersections. As it is shown in Figs. 4 and 5, the ground state is provided *almost* exactly by a subset of the homoclinic intersections between the manifolds relative to the AF fixed points. The only coordinates which slightly deviate from this subset are the ones on the first and last planes.

If we take for a moment $\{\phi_i\}$ as a coordinate along a chain rather than on a circumference, it is clear that the ground state is represented by a discommensuration (see Fig. 6). The explanation is straightforward: the spins on the sur-

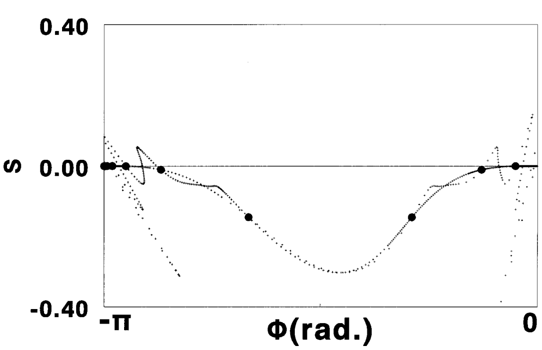

FIG. 4. Inflowing orbit in $(-\pi,0)$, outflowing one from (0,0), and ground-state configuration (solid circle) for the odd planes of a $N=22$ film, with $H_E=2.0$ kG, $H_A=0.5$ kG, and $H=1.113$ kG.

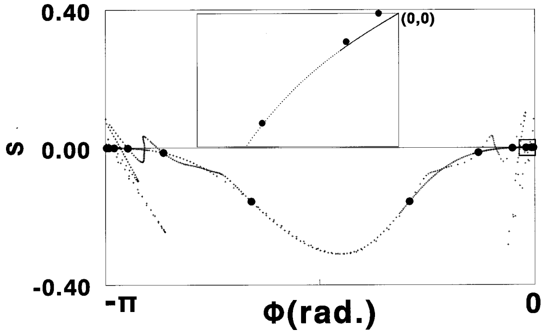

FIG. 5. The same as in the previous figure, with $H=1.120$ kG. The inset shows the outflowing orbit and the ground-state configuration in the proximity of (0,0).

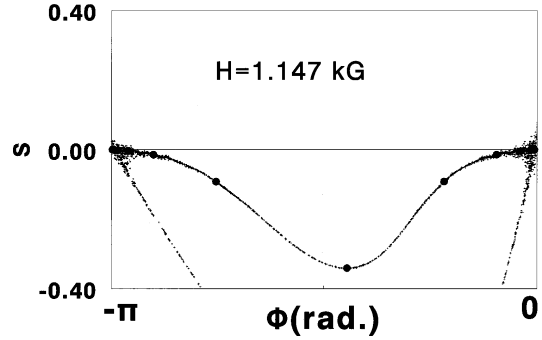

FIG. 7. Inflowing orbit in $(-\pi,0)$, outflowing one from (0,0), and ground-state configuration (solid circle) for the odd planes of a $N=22$ film, with $H_E=2.0$ kG, $H_A=0.5$ kG, and $H=1.147$ kG.

faces have a reduced number of neighbors, so that they are the most influenced by the magnetic field, which tends to make them parallel to its direction; these spins belongs to opposite sublattices (N is even) and this means that a rotation of nearly 2π between the first and last spins of the chain must intervene. This is exactly the definition of discommensuration in the Frenkel-Kontorova model [see Eq. (5)], given the substitution $u_i(\pi/a)=\phi_i$ [see Eq. (27)]. The effect of the surfaces is then to introduce a discommensuration.

Micheletti *et al.*[9] were the first to use the concept of discommensuration in the analysis of this system. Using the effective potential method, they studied the phase diagram of a film with an even number of planes and of a semi-infinite system in the parameter space (ξ,ζ). Their results for $\zeta=0.25$ are in excellent agreement with ours.

Together with the presence of a discommensuration, the other key ingredient is the high value of the anisotropy. For $H<H_{SSF}\simeq1.118$ kG, the magnetic field fixed, all the metastable configurations (and the ground state) are characterized by a ''forbidden zone'' around the maximum energetic cost for the anisotropy: the homoclinic intersection around $\pm\pi/2$ is always avoided (see Figs. 4 and 5). This means that the ''particles'' are pinned by the lattice. The high value of the anisotropy determines a Peierls-Nabarro barrier which forbids a continuous evolution of the ground state at the increasing of the magnetic field, and the discontinuities occur when H forces the particles to overcome the barrier. So, for $H_S<H<H_{SSF}$, the ground-state evolution is the following: at H_S a discommensuration[48] nucleates at the surface with spins antiparallel to the applied field in the AF phase; at the increasing of H the discommensuration proceeds discontinuously into the film, until a symmetric configuration is reached for $H\simeq H_{SSF}$.[7,9] This description is confirmed by the analysis of the $N=16$ situation. In this case a reduced number of discontinuities are detected, since the ground state reaches the symmetric configuration with fewer jumps. For a film with $N>22$ a similar behavior is expected, with the discontinuities accumulating at H_{SSF}.[9]

For $H>H_{SSF}$ the effect of the magnetic field starts to overcome the other interactions and the spin configuration in the middle of the sample resembles the bulk spin-flop phase, which is close to the top of the energy barrier produced by the uniaxial anisotropy (see Fig. 7). The transitions in this range of the magnetic field increase the number of spins in this position (see Fig. 8). The change from a configuration with neighboring spins almost mutually antiparallel to a configuration with an increasing number of spins near the bulk spin-flop phase is responsible for the steep increase of the background magnetization,[7,8] to which the jumps are superimposed. The transitions occurring for $H>H_{SSF}$ were interpreted[9] as due to the enlargement of the core of what was called a bulk discommensuration, positioned between two tails reaching the AF phase. In this description the discontinuities cease when the two AF-BSF interfaces reach the surfaces. Our description is substantially equivalent, even if a growing of the core is still observed after that the last jump takes place. From a mapping perspective it is instead worthwhile to stress that the transitions cease when the trajectory providing the ground state is distinct from a subset of the homoclinic points not only in the proximity of the surfaces, but for all layers, and reduces to a regular nonhomotopic to zero curve.[49]

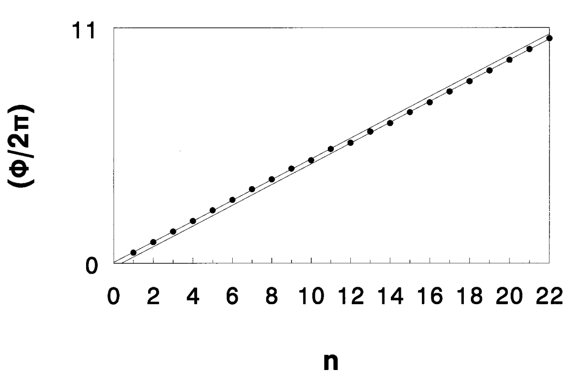

FIG. 6. Ground-state configuration for a $N=22$ film, with $H_E=2.0$ kG, $H_A=0.5$ kG, and $H=1.118$ kG.

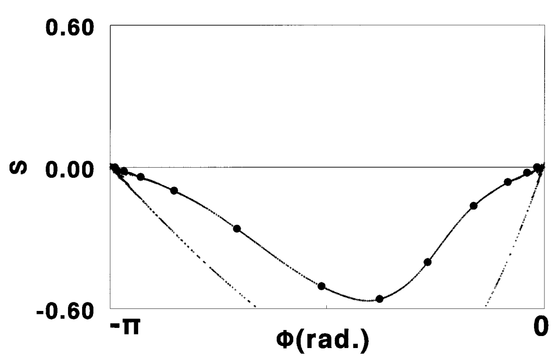

FIG. 8. The same as in the previous figure, with $H=1.294$ kG.

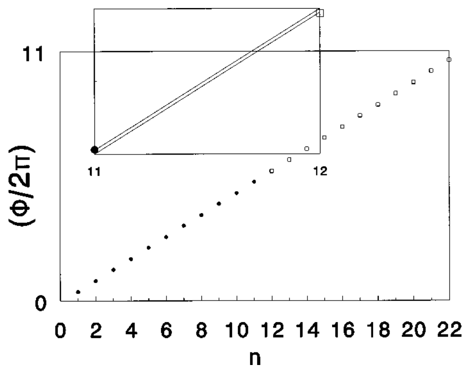

FIG. 9. Ground-state configuration for a $N=22$ film, with $H_E=2.0$ kG, $H_A=0.02$ kG, and $H=0.201$ kG; the lines in the inset are the best fit of the coordinates in the first and second halves of the film.

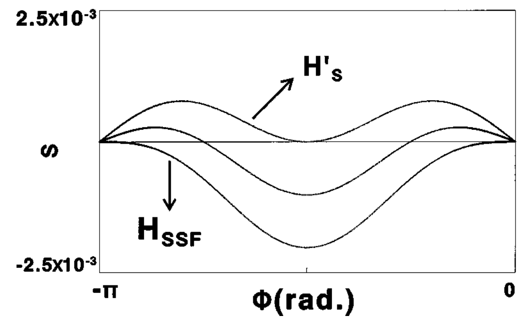

FIG. 10. Inflowing orbits in $(-\pi,0)$, for $\zeta=0.01$ and different values of the magnetic field in the metastability region of the surface transition.

V. LOW-ANISOTROPY CASE

Let us now turn to the low-anisotropy case. As we already noted the map phase portrait is extremely regular, reflecting the quasi-integrability of the system. Due to the low value of the anisotropy, the dimensions of both the surface and the bulk spin-flop metastability regions are greatly reduced. For $H_E=2.0$ kG and $H_A=0.02$ kG we have, for example, $H_{SSF}\simeq 0.201$ kG and we found $H_S\simeq 0.200$ kG.

Consider initially the effect of the magnetic field on the semi-infinite system $AF_{\uparrow\downarrow}$, for $H>H_{SSF}$. This is the regime in which the existence of a surface spin-flop configuration was originally proposed. The analysis of the map showed that this is impossible as the inflowing orbit does not intersect the $s=0$ line,[14] which is the necessary condition to have a surface localized nonuniform configuration. It was then inferred by energetic arguments that the system becomes unstable with respect to the nucleation of a domain wall which produces an interchange of the two sublattices, making the spins on the surface layer parallel to the applied field.[14] This result was recently confirmed.[9]

Consider now the film case in the same regime of the magnetic field. A nonuniform ground state is provided by nonhomotopic to zero curves. The effect of the surface is still to introduce a discommensuration (see Fig. 9), but in this case the notion itself of discommensuration for the finite system must be reconsidered. In fact, at variance with the high-anisotropy case, even for large values of N, the ground state is now provided by a nonhomotopic to zero curve which is clearly distinct from the set of homoclinic points. Actually, the considered trajectory is likely to be a KAM curve so that there would be no discommensuration, and on the contrary there would be particles arbitrarily near the maximum of the sinusoidal potential, if this curve were considered for the infinite system. Moreover, at variance again with the high-anisotropy case and confirming the connection between metastability and pinning effects, the ground state is the only stable equilibrium configuration given our boundary conditions; following Aubry's notation,[18] the ground state is then said to be *undefectible*. As a consequence its evolution with the magnetic field is continuous.

Some attention is then necessary considering the phase diagram of the system. In this range of fields it was argued[9] that the transitions between configurations with a different length of the BSF core joining the AF tails exist all the way down to $\zeta=0$. Actually, these transitions may exist if one considers the homoclinic intersections, or subsets of them, which exist as soon as $\zeta>0^+$ being associated with the nonintegrability of the map, but no transition is indeed possible if one considers the actual ground state.

In other words, the form of the ground state as a discommensuration and the impossibility to have particles at the top of the sinusoidal potential mirror the finite size effect,[22] but this does not necessarily mean that the ground-state evolution is discontinuous (and we numerically verified that it is certainly not for N up to 100, for $\zeta=0.01$).

Let us now turn to magnetic field values lower than H_{SSF}. In this regime there is a range of magnetic field in which the inflowing orbits intersect the $s=0$ line (see Fig. 10).

This is the metastability region for the semi-infinite system. Its lower bound is given by the condition that the inflowing orbit be tangent to the $s=0$ axis; this happens for $H=H'_S\simeq\sqrt{H_EH_A-H_A^2}$. Surface-localized, nonuniform, configurations, i.e., a true surface spin-flop phase (see Fig. 11), of lower energy than the AF configuration are obtained[9,38] for $H_S<H<H_{SSF}$.

The surface spin-flop configuration has the form of a discommensuration, even if the discontinuity is too small to be detected in Fig. 11; the distance of the discommensuration from the surface grows with the magnetic field, until it is pushed to infinity, accomplishing the interchange of the two sublattices, at $H\to H_{SSF}$.

The question addressing the continuity or the discontinuity of the motion of the discommensuration from the surface

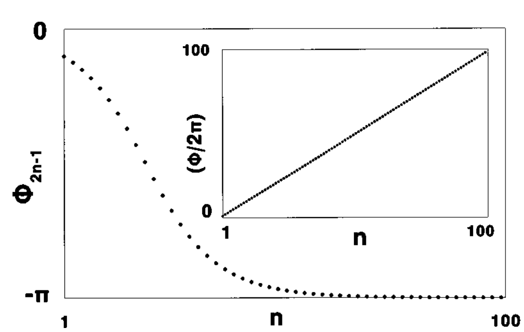

FIG. 11. Stable equilibrium configuration on the odd planes of a semi-infinite system, for $\zeta=0.01$ and a magnetic field in between H_S and H_{SSF}.

for $H_S < H < H_{SSF}$ may be answered considering the film case. The surface localized configuration for the semi-infinite system has a counterpart in nonsymmetric ground-state configurations for films with a sufficiently high value of N (for example, the $N=22$ ground state is always symmetric). These nonsymmetric ground states are characterized by the same distance of the discommensuration from the surface as the semi-infinite system. The evolution of these configurations to the symmetric one at the increasing of the magnetic field is continuous. This is inferred by a numerical analysis of the corresponding magnetization, which shows no jumps, but above all by the fact that the ground state is always undefectible; no pinning effects and consequent discontinuities are therefore expected. We then argue that the evolution of the spin-flop configuration for the semi-infinite system is continuos too; i.e., no Peierls-Nabarro barrier exists either in this region or in the $H > H_{SSF}$ range for $\zeta = 0.01$.

VI. CONCLUSIONS

I showed in this paper how it is possible to establish an equivalence between a simple and realistic magnetic model and a Frenkel-Kontorova model with an additional second-harmonic contribution to the sinusoidal potential and a fixed misfit $d=1/2$. The determination of the ground state of the magnetic model—a uniaxial antiferromagnet in the presence of an applied field H—was formulated as a two-dimensional area-preserving map; the results are consistent with the experimental data on Fe/Cr(211) superlattices[7] and other theoretical works.[7,9] The effect of the surfaces, introduced by appropriate boundary conditions, is shown to be equivalent to the introduction of a discommensuration, whose meaning both in the high- and low-anisotropy cases is discussed, together with its connection with metastability and pinning effects. Discommensurations, which are usually neglected as ground states in the analysis of the Frenkel-Kontorova model due to their zero measure in the equilibrium configurations set, are therefore of the greatest importance for the considered magnetic model.

Moreover, the results for the low-anisotropy case seem to indicate the existence of a threshold line $\zeta = \zeta(\xi)$ in the model parameter space, separating an unpinned and undefectible ground-state region from one in which a nonvanishing Peierls-Nabarro barrier forbids the continuous evolution of the ground state. In the ‘‘noncontinuous’’ regime, the ground state is provided almost exactly by a subset of homoclinic intersections, and the discontinuities cease when the trajectory associated with the ground state becomes a regular nonhomotopic to zero curve, as in the low-anisotropy case. This could suggest a possible connection with the transition by breaking of analyticity in the Frenkel-Kontorova model, whose investigation is beyond the scope of this paper. Actually, it must be stressed that the transition by breaking of analitycity occurs at a fixed, and irrational, winding number; the analysis I performed is different, as I focused on the ground-state problem of the system once the surfaces are properly taken into account, rather than on a peculiar winding number.

My analysis obviously applies also to finite Frenkel-Kontorova chains, with an even number of sites. To my knowledge, this problem was treated only by Braiman *et al.*,[50] for a pure Frenkel-Kontorova model (i.e., without the second-harmonic contribution). A comparison with their results emphasized the importance of the uniaxial anisotropy in our model; in fact, for an even number of sites they always found only symmetric configurations.

ACKNOWLEDGMENTS

Many interesting discussions with M.G. Pini, P. Politi, and A. Rettori, and their critical reading of the manuscript, are gratefully acknowledged.

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