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Phase transition in a domain wall

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Résumé. — On étudie une paroi de domaine dans un modèle XY tridimensionnel en fonction de l'anisotropie K et de la température T . On montre que la paroi présente une transition de phase dans le plan (K, T) , le paramètre d'ordre étant la chiralité. C'est un système à deux états analogue à un système d'Ising. La transition peut être du second ordre avec modes mous. Dans l'état ordonné, la paroi peut posséder des domaines de chiralités opposées séparés par des lignes singulières.

Abstract. — We study a domain wall in a three dimensional XY model as a function of anisotropy (K) and temperature (T). It is shown that the wall undergoes a phase transition in the K, T plane, the order parameter being the chirality. Thus it is a two state system analogous to an Ising system. The phase transition can be of the second order and exhibits soft modes. In the ordered state the wall can exhibit domains of opposite chirality separated by singular lines.

We consider a three dimensional XY [1] model ($n = 2$) with two dimensional rotators, the rotation axis being the Z direction. The rotators are located at the vertices of a simple cubic lattice, the interaction being between first neighbours. The Hamiltonian of the system can be written :

$$\begin{aligned} H &= -J \sum_{ii'} \mathbf{S}_i \cdot \mathbf{S}_{i'} - K \sum_i (S_i^Y)^2 \\ &= -J \sum_{ii'} \cos(\theta_i - \theta_{i'}) - K \sum_i \cos^2 \theta_i \end{aligned} \quad (1)$$

θ_i : angle between \mathbf{S}_i and the Y axis

i : represents the three-dimensional (p, q, r) indices.

When we vary the temperature this system undergoes a bulk phase transition — ferromagnetic ordering — which, because of the anisotropy K , is of Ising character ($n = 1$).

Let us consider a domain wall perpendicular to the Z direction at $T = 0$. When K is large, the domain wall width, δ , is of the order of $a\sqrt{J/K}$ (a : lattice parameter); so this relation loses its meaning when δ is smaller than $a(J/K \ll 1)$ [2]. In this regime ($J/K \ll 1$), the domain wall is one unit cell spacing, the spins being up for $Z \leq 0$ and down for $Z \geq 1$ (up refers to the Oy direction). Let us call this configuration (I).

The equilibrium conditions for the wall are :

$$2J \sum_{i'} \sin(\theta_i - \theta_{i'}) + K \sin 2\theta_i = 0 \quad (2)$$

with the boundary conditions :

$$\theta(z = -\infty) = 0; \quad \theta(z = +\infty) = \pi.$$

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These conditions are fulfilled in (I) because $\theta_i = 0$ or π . To investigate its stability let us now study small movements around this configuration. The equations of motion are :

$$I \frac{d^2 \theta_i}{dt^2} = -2J \sum_{i'} \dot{\sin}(\theta_i - \theta_{i'}) - K \sin 2\theta_i \quad (3)$$

(I is the moment of inertia of each rotator).

Let us write $\theta_i = \theta_i^0 + \varphi_i$ (θ_i^0 equilibrium angles) and linearize (3) :

$$I \frac{d^2 \varphi_i}{dt^2} + 2J \sum_{i'} (\varphi_i - \varphi_{i'}) + 2K\varphi_i = 0 \quad \text{when } r \text{ or } r' \neq 0 \text{ or } 1 \quad (4)$$

$$I \frac{d^2 \varphi_{p,q,0}}{dt^2} + 2J[4\varphi_{p,q,0} - \varphi_{p+1,q,0} - \varphi_{p-1,q,0} - \varphi_{p,q+1,0} - \varphi_{p,q-1,0} - \varphi_{p,q,-1} + \varphi_{p,q,1}] + 2K\varphi_{p,q,0} = 0 \quad (4.1)$$

$$I \frac{d^2 \varphi_{p,q,1}}{dt^2} + 2J[4\varphi_{p,q,1} - \varphi_{p+1,q,1} - \varphi_{p-1,q,1} - \varphi_{p,q+1,1} - \varphi_{p,q-1,1} - \varphi_{p,q,2} + \varphi_{p,q,0}] + 2K\varphi_{p,q,1} = 0 \quad (4.2)$$

obviously the solutions have the form

$$\varphi_{\mathbf{K}_{\parallel}}(p, q, r) = \exp[i(\omega_{\mathbf{K}_{\parallel}} t - \mathbf{K}_{\parallel} \mathbf{R}_{(p,q)})] \psi_{\mathbf{K}_{\parallel}}(r).$$

For a given value of \mathbf{K}_{\parallel} , we have a full spectrum consisting of a localized mode (in the Z direction), ω_L , and a branch of delocalized modes $\omega_{\mathbf{K}_{\parallel}}(K_{\perp})$:

$$\omega_L^2 = \omega_L^{02} + \frac{4J}{I} [2 - \cos K_X a - \cos K_Y a] \quad (5)$$

with

$$\omega_L^{02} = \frac{2J}{I} \left(\frac{K}{J} - \frac{4}{3} \right)$$

and

$$\omega_{\mathbf{K}_{\parallel}}^2(K_{\perp}) = \frac{2K + 4J(1 - \cos K_Z a)}{I} + \frac{4J}{I} [2 - \cos K_X a - \cos K_Y a]. \quad (6)$$

The expression (5) has meaning only if $K/J - 4/3$ is positive. So the condition of stability of configuration (I) is $K/J \geq 4/3$ [3, 4, 5]. If we look at ω_L^{02} as a function of K/J , we have a typical soft mode behaviour, the eigenvector corresponding to this mode near the threshold value $(K/J)_c = 4/3$ being :

$$\begin{aligned} \varphi(p, q, r) &= \left(\frac{1}{3}\right)^{-r} A & r \leq 0 \\ \varphi(p, q, r) &= -\left(\frac{1}{3}\right)^{r-1} A & r \geq 1 \end{aligned} \quad (7)$$

with a typical width of the order of $2a$.

Just below the threshold, the solution of (2) in the third order in θ gives

$$\begin{aligned} \theta(p, q, r) &= \varepsilon \left(\frac{1}{3}\right)^{-r} \frac{9}{\sqrt{32}} \left(\frac{4}{3} - \frac{K}{J}\right)^{1/2}, & (\varepsilon = \pm 1), & r \leq 0 \\ \theta(p, q, r) &= \pi - \theta(p, q, 1 - r) & r \geq 1 \end{aligned} \quad (8)$$

which is a narrow domain wall with a helicoidal structure (Bloch character). This is another stable configuration (II) which was prefigured by the eigenvector (7). If we look at the domain wall as a function of K/J , we see a phase transition with a soft mode. The order parameter is the amplitude of the localized modes given by the value of $\theta(r = 0)$ which varies typically as $(K/J - (K/J)_c)^{1/2}$. This value of the critical exponent is due to the molecular field approximation (we have neglected quantum fluctuations).

1. **Thermodynamic behaviour.** — We want to study this system as a function of T . From an heuristic point of view, we know that for a given value of T , near T_c , K is a relevant quantity and will impose an Ising behaviour for the system. Thus just below T_c , the domain wall must have an Ising character (without chirality). On the other hand at low temperature we know that the domain wall will have a Bloch character, so we must have a phase transition within the domain wall as a function of T .

To study this problem, we will look at two limiting regimes $T \simeq 0$ and $K \simeq 0$.

1.1 T NEAR 0, $\frac{K}{J} = \frac{4}{3} - \varepsilon$. — We can associate with each line of spins, n , perpendicular to the wall a quantity ε_n ($\varepsilon_n = \pm 1$) which characterizes the chirality of the line. The « θ » angles of the line are given by (8). The interaction energy between two neighbouring lines n and n' can be written, knowing Hamiltonian (1), in the form :

$$\tilde{\mathcal{H}} = \tilde{J} \varepsilon_n \varepsilon_{n'} \quad (9)$$

where

$$\tilde{J} = \frac{9^3}{32} J \left(\frac{4}{3} - \frac{K}{J} \right)$$

this Hamiltonian (9) exhibits clearly the features of a two-dimensional Ising model with a critical temperature

$$kT^* = \frac{\tilde{J}}{\text{Arctanh}(\sqrt{2} - 1)}$$

1.2 K NEAR 0. — We know that the domain wall width varies as $a\sqrt{J/K}$, so we will go to a continuum description. Let us call X and Y the magnetization components. The three-dimensional Ginzburg-Landau Free Energy corresponding to the Hamiltonian (1) is of the form :

$$F_L = Ja^2[(\text{grad } X)^2 + (\text{grad } Y)^2] - (6J - kT + K)(X^2 + Y^2) + KX^2 + B(X^2 + Y^2)^2 \quad (10)$$

The uniform solution corresponds to a paramagnetic case for $T > T_c$ ($T_c = \frac{6J + K}{k}$) and a ferro-

magnetic case for $T < T_c$. We look at a domain wall perpendicular to the Z direction in such a way that the « grad » terms are $\partial/\partial z$.

The Euler-Lagrange equations associated with our problem have been solved by Sarker *et al.* [6]. We have two regimes :

i) $\frac{k(T_c - T)}{2K} < 1$ the domain wall exhibits an Ising character

$$\begin{cases} X = 0 \\ Y = \pm \sqrt{\frac{k(T_c - T)}{2B}} \tanh \left[\frac{1}{2} \frac{k(T_c - T)}{J} \right]^{1/2} \frac{z}{a} \end{cases}$$

ii) $\frac{k(T_c - T)}{2K} > 1$ the domain wall exhibits a Bloch character (with definite chirality)

$$\begin{cases} X = \mp \sqrt{\frac{k(T_c - T) - 2K}{2B}} \text{sech} \frac{z}{\lambda} \\ Y = \pm \sqrt{\frac{k(T_c - T)}{2B}} \tanh \frac{z}{\lambda} \end{cases}$$

where λ is the characteristic width of a Bloch wall ($\lambda = a\sqrt{J/K}$).

The transition temperature is given by

$$kT^* = kT_c - 2K \quad (11)$$

It is easy to show, that if we take a Ginzburg-Landau time dependent expansion, we have also soft modes connected to this transition [7]. All the critical exponents are of mean field character as a result of the approximations. It is obvious that, in this case, we have the exponents of a two dimensional Ising model except at $T = 0$ where we can conjecture that the critical exponents will be those of a three-dimensional Ising model.

The results are summarized in figure 1.

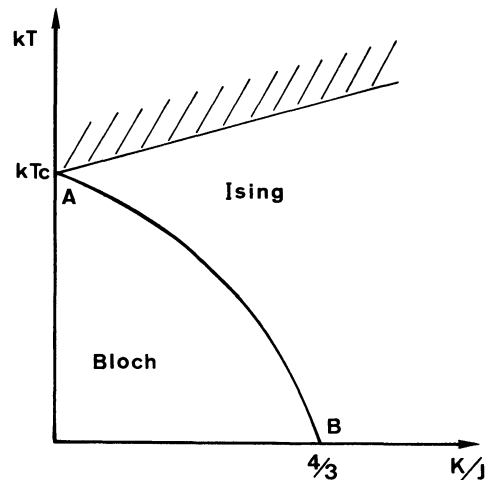


Fig. 1. — The AB line is the transition line between a domain wall of Ising type and a domain wall of Bloch type (chiral). The shaded region corresponds to the bulk paramagnetic state.

2. **Other type of ordered state.** — We will show in one definite example that the structure of the ordered domain wall can be more complex. We now limit the discussion to $T = 0$. The frequency (5) of the localized mode associated with configuration (I) depends on ω_L^0 on one hand and on the dispersion relations of the excitations of spin wave type in the (X, Y) plane on the other hand. So, if one introduces in our model an antiferromagnetic exchange between next nearest neighbours in the X and Y directions, one modifies the dispersion relations in these directions in such a way that ω_L can be zero when ω_L^0 is still nonzero. Thus, now, we are going to consider a Hamiltonian of the same kind as that used by Redner and Stanley [8] :

$$H = -2J \sum_{\langle ij \rangle} \mathbf{S}_i \mathbf{S}_j + 2J_2 \sum_{\langle ij \rangle}^{XY} \mathbf{S}_i \mathbf{S}_j - K \sum_i (S_i^Y)^2$$

where the second term represents an exchange between next nearest neighbours in the (X, Y) plane.

In this case, the frequency of the localized mode becomes :

$$\omega_L^2(K_X, K_Y) = \omega_L^{02} + \frac{4J}{I} \left\{ [2 - \cos K_X a - \cos K_Y a] - \frac{J_2}{J} [2 - \cos 2K_X a - \cos 2K_Y a] \right\} \quad (12)$$

and we have two regimes :

— if $\frac{4J_2}{J} < 1$, $\omega_L = 0$ for $\frac{K}{J} = \frac{4}{3}$ ($\omega_L^0 = 0$) the soft mode has a uniform structure in the (X, Y) plane and the wall which appears for $\frac{K}{J} = \frac{4}{3} - \varepsilon$ is of uniform Bloch type;

— if $\frac{4J_2}{J} > 1$, $\omega_L(K_X, K_Y)$ is minimum for

$$(K_X, K_Y) = (q_X, q_Y)$$

with $\cos q_Y a = \cos q_X a = \frac{J}{4J_2}$. It is easy to show that $\omega_L(q_X, q_Y)$ is zero when

$$\frac{K}{J} = \frac{4}{3} + \frac{J}{2J_2} \left(1 - \frac{4J_2}{J} \right)^2, \quad (13)$$

the soft mode exhibiting a modulated structure associated with the wave vectors q_X and q_Y in the X and Y directions. Consequently the wall which appears for $\frac{K}{J}$ just below $\frac{4}{3} + \frac{J}{2J_2} \left(1 - \frac{4J_2}{J} \right)^2$ has a modulated structure. In such a situation if one has a bulk phase transition from a ferromagnet to a helimagnet (III \rightarrow IV), as the domain wall of the ferromagnet has already an helical character, the nucleation of the bulk helicoidal state will occur in the domain wall (the width of the wall diverges on line c). Such an

hypothesis has already been made to interpret experimental results [9].

These results show that there must also exist a line, in the $\left(\frac{K}{J}, \frac{4J_2}{J} \right)$ plane, giving the transition between Bloch wall and modulated Bloch wall. The results summarized in figure 2 indicate the presence of a Lifshitz point [10].

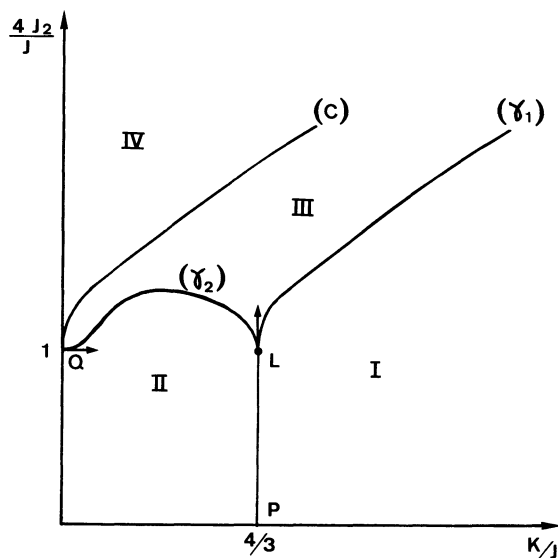


Fig. 2. — Phase Diagram at $T = 0$. The region I corresponds to configuration (I); The region II corresponds to uniform Bloch wall; The region III corresponds to modulated Bloch wall; The region IV corresponds to a bulk helicoidal type of state; L is a Lifshitz point; (γ_1) is given by (13); (γ_2) is a numerically calculated; (C) characterizes the transition between uniform and modulated structures in the bulk and is parallel to (γ_1) . One can show that LP, (γ_1) , (γ_2) have a vertical tangent at L. At Q, (C) has a vertical tangent, and γ_2 a horizontal one.

3. **Conclusion.** — We have shown that a ferromagnetic domain wall can undergo a two-dimensional phase transition in space with parameters (J, J_2, K, T) . The broken symmetry is the chiral symmetry (right-left). In the ordered state, singularities associated with the broken symmetry are Bloch lines. This transition is associated with the fact that the dimensionality, n , of the order parameter is greater than one and is different from the roughening transition [11]. The bulk phase transition locks one of the components of the order parameter; the transition then occurs in the space of the $(n - 1)$ other components. This shows that the singularities associated with ordered media [12] can change their nature in a cooperative way. Thus their degree of universality is less than that of the bulk transition; that is to say they are more sensitive to the structure of the Hamiltonian. We have presented another example of a phase transition in two dimensions [13].

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Footnotes and references

- [1] This model can be used for a Heisenberg system with strong planar anisotropy in the XY plane induced by magnetostatic interactions. The usual localized spin waves are degenerated in the absence of dipolar interactions. In fact this interaction is a relevant one; it splits the degeneracy and so we consider only (near the transition) the lowest branch. Physically the spins cannot get out of the XY plane because of the pole field. This amounts to an associated moment of inertia $I \sim \frac{\hbar^2 V^{-1}}{M_s^2}$ where V is the volume of the unit cell (one magnetic moment by unit cell) and M_s the spontaneous magnetization.
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