Theory of the soliton-induced phase transition in quasi-one-dimensional magnets

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It is shown that the phase transition occurring in quasi-one-dimensional systems of weakly coupled magnetic chains with solitons in the form of π kinks is closely related to the properties of these solitons. The critical behavior of the systems considered corresponds to the critical behavior of the Ising model with the same dimension. The model describing the behavior of solitons below and above the critical temperature is presented. This model explains the experimental field dependence of the magnetization direction in the spin-flopping configuration for antiferromagnetic K_2FeF_5. Application of the theory proposed here to the antiferromagnetic tetramethylammonium manganese trichloride (TMMC) allows one to explain the experimental field dependence of the Néel temperature.

I. INTRODUCTION

During the past ten years much interest has been focused on the various phenomena in solid-state physics and statistical mechanics connected with the concept of solitons.[1] Two main branches of the theoretical part of this interest are (a) searching for classical and quantum models that are governed by nonlinear equations of motion, and looking for the solutions in the form of solitary waves or solitons,[2] (b) investigations of the role of soliton excitations for thermodynamical properties of nonlinear systems.[3,4]

Magnetic systems seem to be very interesting objects both from the point of view of (a) (Ref. 5) as well as (b).[6] A majority of the works published to date in this area are connected with the one-dimensional models. However, real magnetic systems, such as $CsNiF_3$ or tetramethyl ammonium manganese trichloride (TMMC) compounds, are in an obvious way quasi-one-dimensional in character in the sense that they consist of the weakly coupled chains of spins. Therefore, it is valuable to investigate the role of soliton excitations in such quasi-one-dimensional spin models. Particularly, the role of solitons for phase transitions in quasi-one-dimensional systems seems to be one of the most interesting problems.

In our previous works we showed that solitons, in the form of so-called π kinks, can play a crucial role for the soliton-induced phase transition appearing in certain cases of quasi-one-dimensional magnetic systems, namely, in the systems with the Ising-like symmetry[7] and in the systems governed by the sine-Gordon equation.[8] The situation is similar to that in the weakly coupled chains with the φ^4 potential.[9]

In this paper the complete theory of soliton-induced phase transition in systems of weakly coupled anisotropic magnetic chains with π kinks is presented. All considerations are performed here for systems with the local anisotropy taken in a more general form than in Refs. 7 and 8, and consisting of the uniaxial anisotropy of the easy axis type and the anisotropy corresponding to the sine-Gordon symmetry. Moreover, using the concept of the field-induced anisotropy, the theory is extended to the quasi-one-dimensional anisotropic antiferromagnets with external magnetic field. The predictions of our theory for the critical temperature are compared successfully with experimental data for antiferromagnetic quasi-one-dimensional TMMC compounds in the presence of a magnetic field. Moreover, the model of the soliton-induced phase transition proposed here very well explains the experimental data for spin flop in antiferromagnetic K_2FeF_5.

The plan of the work is as follows: In Sec. II we analyze the problem of the single soliton-bearing ferromagnetic spin chain with the required form of the local anisotropy and the external magnetic field applied along the easy axis of the anisotropy. The results of Sec. II are applied in Sec. III where the phase transition in the system of weakly coupled anisotropic ferromagnetic spin chains is analyzed and a single model explaining the behavior of kinks in this system is proposed. In Sec. IV a system of weakly coupled antiferromagnetic chains with an external field is considered. Comparison of theoretical predictions with experimental data is presented. Section V contains the main conclusions.

II. SINGLE ANISOTROPIC MAGNETIC CHAIN WITH SOLITONS IN AN EXTERNAL MAGNETIC FIELD

In this section we want to consider the role of solitons for some properties of the single chain of classical spins, described by the following Hamiltonian:

$$\mathcal{H}=\sum_{i=1}^{I}\left[-J\mathbf{S}_i\cdot\mathbf{S}_{i+1}+A(S_i^z)^2-C(S_i^x)^2-BS_i^x\right], \qquad (2.1)$$

where $B=Hg\mu_B/\hbar$, $J, A, C>0$. $H\geq 0$ is the external magnetic field applied along the easy axis and $J\gg C\gg B/S$ is assumed ($S=|\mathbf{S}_i|$). The first term describes the exchange interaction, the second term corresponds to the easy plane anisotropy, and the third to the uniaxial anisotropy.

It is well known that if the external field is equal to zero, the continuous version of the system described by

(2.1) is completely integrable and the Landau-Lifshitz equations of motion for spins have solutions in the form of kinks, spin waves, and breathers.[10] The kinks can be described as follows:

$$\cos\theta(x,t)=\tanh[\pm\zeta(x-x_0-vt)/d]\ , \tag{2.2a}$$

$$\Phi(x,t)=\Phi_0=\text{const}\ , \tag{2.2b}$$

$$\zeta=[1+(A/C)\cos^2\Phi_0]^{1/2}\ , \tag{2.2c}$$

$$v=ASd\zeta^{-1}\sin2\Phi_0\ , \tag{2.2d}$$

$$d=(J/2C)^{1/2}a\ , \tag{2.2e}$$

where a denotes the lattice constant and the coordinate system is assumed in such a way that

$$\mathbf{S}(x,t)=S(\cos\theta,\ \sin\theta\sin\Phi,\ \sin\theta\cos\Phi)\ . \tag{2.2f}$$

One can see that these π kinks correspond to the rotation of the spin vector between two directions which are equivalent to degenerate ground states of the Hamiltonian (2.1): $S^x=-S$ and $S^x=S$. The energy of kinks (2.2) is equal to

$$E_k(\Phi)=E_{k_0}\zeta,\quad E_{k_0}=2(2CJ)^{1/2}S^2\ , \tag{2.3}$$

and the velocity v of kinks depends on the angle Φ. The π kinks (2.2) play the role of domain walls dividing the chain into domains (segments) in which the magnetization is $S^x=-S$ or $S^x=S$.

The second type of solutions for $H=0$ are the low-amplitude periodic waves (spin waves) corresponding to small oscillations of the spin vectors around one of the ground states. The dispersion relation for these spin waves is

$$\omega(k)=2S\{[C+A+2J\sin^2(ka/2)]\times[C+2J\sin^2(ka/2)]\}^{1/2}\ . \tag{2.4}$$

The third type of solutions possible for $H=0$ corresponds to the so-called breathers; however these will not be considered in our investigations.

With the external field H different from zero, the solutions of the Landau-Lifshitz equations of motion are modified substantially. In the static limit these equations of motion can be reduced to the static version of the double-sine-Gordon equation which has the special solution in the form[11]

$$\theta(x)=\pm2\arcsin\{[\cosh^2(d_1x)-d_2\sinh^2(d_1x)]^{-1/2}\}\ , \tag{2.5a}$$

$$\Phi(x)=n\pi/2,\quad n-\text{integer}\ , \tag{2.5b}$$

where

$$d_1=[(2C+2A\cos^2\Phi+BS^{-1})/Ja^2]^{1/2}\ , \tag{2.5c}$$

$$d_2=[1+B/2S(C+A\cos^2\Phi)]^{-1}\ . \tag{2.5d}$$

Here, the static solution is obtained for n odd only. If $B\ll CS$, this solution can be treated as a kind of 2π kink, being a coupled pair of slightly modified static π kinks. If B/CS tends to zero, such a pair dissociates into a pair of two noncoupled static π kinks and the energy corresponding to the solution (2.5) tends to two energies of the static π kinks. Contrary to π kinks, the 2π kinks do not divide the chain into domains with opposite directions of the magnetization because for the 2π kinks one has $S^x=S$ for $|x|\to\infty$ and $S^x=-S$ at $x=0$ (the point $x=0$ denotes here the central point of the 2π kink). The approximate time-dependent solutions in the form of moving 2π kinks can also be found, but only for $|B|\ll SA$.[11]

Now, consider the thermodynamic properties of the classical spin chain described by the Hamiltonian (2.1). The partition function of the system is

$$Z=\int\exp(-\beta\mathcal{H})\prod_{i=1}^{I}d\mathbf{S}_i,\quad \beta=1/k_BT\ , \tag{2.6a}$$

where the coordinate system is assumed in such a way that

$$\mathbf{S}_i=S(\cos\vartheta_i\cos\varphi_i,\ \cos\vartheta_i\sin\varphi_i,\ \sin\vartheta_i)\ , \tag{2.6b}$$

$$d\mathbf{S}_i=\sin\vartheta_i d\vartheta_i d\varphi_i\ , \tag{2.6c}$$

and periodic boundary conditions are superimposed. Using the transfer integral method, one obtains

$$Z=\sum_n\exp(-\beta\bar{E}_nI)\ , \tag{2.7}$$

where $\bar{E}_n$ are defined by means of the transfer integral equation

$$\int d\mathbf{S}_i\exp[-\beta h(\mathbf{S}_{i+1},\mathbf{S}_i)]\psi_n(\mathbf{S}_i)=\exp(-\beta\bar{E}_n)\psi_n(\mathbf{S}_{i+1})\ , \tag{2.8a}$$

$$h(\mathbf{S}_{i+1},\mathbf{S}_i)=-J\mathbf{S}_i\cdot\mathbf{S}_{i+1}+\tfrac{1}{2}[A(S_i^z)^2+A(S_{i+1}^z)^2-C(S_i^x)^2-C(S_{i+1}^x)^2-BS_i^x-BS_{i+1}^x]\ . \tag{2.8b}$$

In the thermodynamic limit ($I\to\infty$), the partition function is dominated by the lowest eigenvalue $\bar{E}_0=\min(\bar{E}_n)$ and the free energy of the system per one spin is equal to

$$F=-\lim_{I=\infty}[(\beta I)^{-1}\ln Z]=\bar{E}_0\ . \tag{2.9}$$

To find $\bar{E}$, Eq. (2.8) is replaced by the differential equation. To this purpose, the continuous version of the Hamiltonian (2.1) is taken and $\psi_n(\mathbf{S}_i)$ is developed in a Taylor series around the point $\mathbf{S}_{i+1}$, so that Eq. (2.8a) can be integrated. The result is as follows:

$$(L^2/2\beta^2JS^2+AS^2\sin^2\vartheta-CS^2\cos^2\vartheta\cos^2\varphi-BS\cos\vartheta\cos\varphi)\psi_n(\vartheta,\varphi)=E_n\psi_n(\vartheta,\varphi)\ , \tag{2.10a}$$

where E_n is defined by

$$\bar{E}_n = E_n + \Delta E, \quad \Delta E = -S^2 J + \beta^{-1} \ln(\beta J S^2/2\pi) , \tag{2.10b}$$

and L^2 is the operator analogous to the square angular momentum operator

$$L^2 = -\frac{1}{\cos\vartheta}\frac{\partial}{\partial\vartheta}\left[\cos\vartheta\frac{\partial}{\partial\vartheta}\right] - \frac{1}{\cos^2\vartheta}\frac{\partial^2}{\partial\varphi^2} . \tag{2.10c}$$

Equation (2.10a) has the form of the perturbed Schrödinger equation for a quantum rotator with the potential

$$V(\vartheta,\varphi) = S^2(A\sin^2\vartheta - C\cos^2\vartheta\cos^2\varphi) , \tag{2.11a}$$

and with

$$\Delta V(\vartheta,\varphi) = -BS\cos\vartheta\cos\varphi \tag{2.11b}$$

as a perturbation.

It is fruitful to present here, first, the solution of the unperturbed problem, i.e., the case with $B=0$ ($H=0$) found in Ref. 12. The potential $V(\vartheta,\varphi)$ has two degenerate minima at ($\vartheta=0$, $\varphi=0$), and at ($\vartheta=0$, $\varphi=\pi$). In the low-temperature region, i.e., for $m^* = 2\beta^2 CJS^4 \gg 1$, the classical WKB approximation can be used. As a result, the energies of the two lowest levels are obtained[12]

$$E_0 = \tilde{E}_0 - t_0 \text{ and } E_1 = \tilde{E}_0 + t_0 , \tag{2.12a}$$

where

$$\tilde{E}_0 = CS^2\{-1 + (m^*)^{-1/2} \times[(1+\lambda)^{1/2}+1]\}, \quad \lambda = A/C \tag{2.12b}$$

$$t_0 = 8CS^2[1+(1+\lambda)^{1/2}] \times\exp[-2(m^*)^{1/2}]\exp(-\alpha)I_0(\alpha) . \tag{2.12c}$$

Here, $\alpha = (m^*)^{1/2}\lambda/2$, $I_0(\alpha)$—the modified Bessel function. In (2.10a)–(2.10c), the lowest eigenvalue for a problem with a single potential well centered in one of the minima of $V(\vartheta,\varphi)$ is approximated by the lowest energy of the two-dimensional anisotropic harmonic oscillator. The quantity t_0, given by (2.12c), denotes the tunneling splitting which is the consequence of the existence of two wells in $V(\vartheta,\varphi)$ and is calculated with the "improved" WKB method.[13] It is important that for the low-temperature region ($m^* \gg 1$), the tunneling contribution t_0 is very small as compared with terms ΔE and $\tilde{E}_0$. Finally, taking into account (2.9) and (2.10b), the free energy of the system with $B=0$ is equal to

$$F(t, B=0) = \tilde{E}_0 + \Delta E - t_0 . \tag{2.13}$$

It is interesting to note here that this result was obtained without any use of the solutions of the equations of motion. The same result can also be obtained with the use of the so-called collective gas phenomenological model.[12] This allows us to interpret the formula (2.13) physically. In such an approach the free energy is calculated as a sum of the ground-state energy and free energies corresponding to particular types of excitations, with interaction between various types taken into account by means of the so-called phase shifts. To do this, the free energy of kinks and spin waves can be calculated directly using the formula for energies of these excitations, and the role of the breathers is assumed to be negligible.[12] To show this, the free energy (per one spin) of spin waves

$$F_{SW} = k_B T(2\pi)^{-1}\int dk \ln\{1-\exp[-\beta\hbar\omega(k)]\} , \tag{2.14}$$

with $\omega(k)$ defined by (2.4), is calculated within the classical approximation ($\beta\hbar\omega \ll 1$) and with use of the assumption $J/C \gg 1$. The result is as follows:[12]

$$F_{SW} = (1/\beta)\ln(\beta J S^2/2\pi) + CS^2[1+(1+\lambda)^{1/2}](m^*)^{-1/2} . \tag{2.15}$$

On the other hand, the free energy (per one spin) of kinks can be calculated as a free energy of noninteracting quasiparticles with a chemical potential $\mu=0$ and energy $E_k + \Sigma_k$, where E_k is the energy of a kink (2.3) and Σ_k describes a change in kink energy connected with kink spin waves interaction described in the frame of the phase shift formalism.[12] As a consequence of the change in the spin-wave density caused by a kink, the free energy of spin waves changes by the amount ΔF_{SW}. It is usually assumed that $\Delta F_{SW} = \Sigma_k$. Thus, $E_k + \Sigma_k$ represents the thermally renormalized energy of a kink. In view of a low density of kinks (in the low-temperature region), the influence of kink-kink interaction can be neglected.[12] Then, the grand partition function of kinks is as follows:

$$Z_k(T,L,\mu) = \sum_{N_k=0}^{\infty} \exp(\beta\mu N_k)(N_k!)^{-1}\left[\int_0^L dx_k \int_{-2\pi}^{2\pi} dp_k \cdot \exp\{-\beta[E_k(p_k)+\Sigma_k]\}\right]^{N_k} , \tag{2.16}$$

where L is the length of the chain, x_k a position of the kink, $p_k = 2(\pi/2 - \Phi_{0k})$ the impulse of the kink, Φ_{0k} the spherical angle between the plane of rotation of spins in the kink, and the hard axis [see Eq. (2.2)]. After integration, a thermodynamic potential

$$\Omega_k = -(1/\beta L)\ln Z_k ,$$

and the average kink density

$$n_k = -(\partial\Omega_k/\partial\mu)_{T,L} ,$$

(with $\mu=0$) are calculated. The resulting free energy of the kinks is as follows:[12]

$$F_k = -n_k k_B T = -t_0 . \tag{2.17}$$

If one adds the ground-state energy $E_g=-S^2(J+C)$ of the Hamiltonian (2.1) with $B=0$, the spin-wave free energy F_{SW} (2.15), and the kink free energy F_k (2.17), one obtains that the energy of the system ($B=0$), calculated by means of the collective gas phenomenological model, is exactly equal to the free energy calculated by means of the transfer integral method

$$F(T,B=0)=E_g+F_{SW}+F_k=\tilde{E}_0+\Delta E-t_0 \ . \quad (2.18)$$

Now, the full problem with the perturbation ΔV (2.11b) different from zero, i.e., $B\neq 0$, can be discussed. In view of the low-temperature assumption $m^*\gg 1$, the difference of energies between the lowest levels E_0 and E_1 split by tunneling is very small as compared with those for the next levels. Moreover, the matrix element of the perturbation ΔV, taken for the states corresponding to the levels E_0 and E_1, is very large as compared with all other nonvanishing matrix elements. Therefore, to calculate the perturbed lowest level energy $\bar{E}_0$, one can take into account only the lowest two levels (2.12a) of the unperturbed system. Assuming that the eigenfunctions corresponding to these two levels form a complete orthonormal set (we call this assumption the two-level approximation), the lowest energy of the perturbed system can be found and the result is as follows:[14]

$$\bar{E}_0=\Delta E+\tilde{E}_0-(t_0^2+p^2S^2B^2)^{1/2} \ , \quad (2.19a)$$

$$p=1-[4(m^*)^{1/2}]^{-1}[1+1/(1+\lambda)^{1/2}] \ , \quad (2.19b)$$

where a power series in $(m^*)^{-1/2}$ was applied. Taking into account formula (2.9), the free energy (per one spin) of the system is equal to

$$F(T,B)=\Delta E+\tilde{E}_0-(t_0^2+p^2S^2B^2)^{1/2} \ . \quad (2.20)$$

In order to interpret this result, one can expand the free energy (2.20) with respect to t_0/SBp, assuming $p\approx 1$ and $t_0/SB\ll 1$. (Note that the conditions $SB/t_0\gg 1$ and $B/CS\ll 1$—necessary for the earlier used perturbation method—can be fulfilled together because, in view of the low-temperature region $m^*\gg 1$, one has $CS^2/t_0\gg 1$.) In this case a term proportional to t_0^2 appears in the free-energy expression. In view of the fact that

$$t_0\sim\exp[-2(m^*)^{1/2}]$$

is proportional to $\exp(-\beta E_{k0})$, where E_{k0} is the static kink energy (2.3), the considered term in the free-energy expansion is proportional to $\exp(-2\beta E_{k0})$, showing that the excitations with energy $2E_{k0}$ exist in the system. When $B/CS\ll 1$, these excitations correspond to the 2π kinks discussed previously. Moreover, there is no term linear in t_0, i.e., there is no contribution to the free energy coming from the π kinks.

Now, the average magnetization (per spin) $\langle S^x\rangle=-\partial F/\partial B$ can be calculated, and the result is

$$\langle S^x\rangle=B(pS)^2[t_0^2+(BpS)^2]^{-1/2} \ , \quad (2.21a)$$

and for $BpS\ll t_0$

$$\langle S^x\rangle=[B(pS)^2/t_0][1-(BpS/t_0)^2/2] \ . \quad (2.21b)$$

Moreover, the initial susceptibility

$$\chi_{xx}=(\partial\langle S^x\rangle/\partial B)_{B=0}$$

is

$$\chi_{xx}=(Sp)^2/t_0 \ . \quad (2.22)$$

The same formula for the susceptibility could be obtained from the fluctuation-dissipation theorem

$$\chi_{xx}=\beta\int_{-\infty}^{+\infty}\langle S^x(0)S^x(x)\rangle dx \ , \quad (2.23)$$

if the correlation function in (2.23) would be calculated by means of the transfer integral method. In this case one obtains

$$\langle S^x(0)S^x(x)\rangle=pS\exp(-2\beta t_0\,|\,x\,|\,/a) \ , \quad (2.24)$$

which means that the correlation range for the easy axis spin components is

$$\xi_x=a/2t_0\beta \ . \quad (2.25)$$

In view of (2.17), the formula (2.22) shows that, because $F_k\neq 0$ for $T>0$ K, thus $\chi_{xx}<\infty$ for all $T>0$ K. This means that the existence of π kinks in our system for $H=0$ is the reason for the lack of nonzero spontaneous magnetization at $T>0$ K. This last property is, of course, the well-known property of one-dimensional systems with short-range interaction. However, what is important for us is the part the π kinks play in this crucial role.

This critical role is connected with the property of π kinks in that they divide the chain into domains with $S^x=S$ and $S^x=-S$. When the external field is equal to zero, the π kinks are distributed randomly along the chain so that the average size of the domains with $S^x=+S$ is the same as of those with $S^x=-S$, thus the spatial average of the magnetization, $\langle S^x\rangle=0$.

III. SOLITON-INDUCED PHASE TRANSITION IN QUASI-ONE-DIMENSIONAL FERROMAGNET

Up to this point we have considered only a single chain of spins. We will now show that in three-dimensional systems of weakly coupled chains of spins (with the same type of local anisotropy as in Sec. II), where the long-range ordering exists in low temperatures as a result of a coupling between chains, the static π kinks extending along the chains are responsible for the disappearance of the long-range ordering above a critical temperature, but below that temperature the π kinks are coupled into pairs which are, in fact, deformed 2π kinks.

For this purpose we consider a D-dimensional system ($D=2$ or 3) of weakly coupled parallel chains of classical spins with interactions between the spins belonging to different chains taken into account. The system is described by the following Hamiltonian:

$$\mathcal{H}^D=\sum_k\mathcal{H}_k^1-\tfrac{1}{2}J_\perp\sum_{k,k'}{}'\sum_l\mathbf{S}_{k,l}\cdot\mathbf{S}_{k',l} \ , \quad (3.1a)$$

where

$$\mathcal{H}_k^1=\sum_l[-J_\parallel\mathbf{S}_{k,l}\cdot\mathbf{S}_{k,l+1}-C(S_{k,l}^x)^2+A(S_{k,l}^z)^2] \ . \quad (3.1b)$$

Here, $\mathcal{H}_k^l$ represents the Hamiltonian of the kth chain, l labels the position of spin inside the chain, and the second term in $\mathcal{H}^D$ describes the interchain interactions of the spin which are the nearest neighbors but belong to the nearest neighboring chains labeled by indices k and k' ($k \neq k'$). For simplicity, we assume that the array of spins forms the simple cubic lattice (for $D=3$) or the quadratic lattice (for $D=2$) with a lattice constant taken as the length unit. We assume also that the intrachain ($J_\parallel$) and interchain ($J_\perp$) exchange constants as well as the local anisotropy constants A and C fulfill the relations

$$J_\parallel \gg C \gg J_\perp > 0, \quad A \geq 0 . \tag{3.1c}$$

Due to the first part of this inequality ($J_\parallel \gg C$), at temperatures so low that $\beta J_\parallel S^2 \gg 1$, the continuous approximation can be used in the description of intrachain interactions. $C>0$ denotes that the X axis is an easy axis of uniaxial anisotropy and $A \geq 0$ denotes the XY easy plane anisotropy. Finally, $J_\parallel \gg J_\perp$ corresponds to the special kind of exchange interaction anisotropy which appears in systems of weakly coupled chains of spins.

To study the thermodynamical properties of the system considered here, we want to calculate the classical partition function

$$Z = \int \exp(-\beta \mathcal{H}^D) \prod_{l=1}^{L} \prod_{k=1}^{K} d\mathbf{S}_{k,l} , \tag{3.2}$$

where L is the number of spins in a chain, K is the number of chains,

$$d\mathbf{S}_{k,l} = \sin\vartheta_{k,l} d\vartheta_{k,l} d\varphi_{k,l}$$

and angles $\vartheta_{k,l}$ and $\varphi_{k,l}$ define a direction of the spin $\mathbf{S}_{k,l}$. We use the transfer integral method along the axis of chains so that in low temperatures the discrete form of the intrachain interactions can be replaced by a continuous version. We superimpose the periodic boundary conditions and for simplicity introduce the following quantities:

$$\boldsymbol{\mu}_l = (\mathbf{S}_{1,l}, \mathbf{S}_{2,l}, \ldots, \mathbf{S}_{K,l}) , \tag{3.3a}$$

$$h(\boldsymbol{\mu}_l, \boldsymbol{\mu}_{l+1}) = -J_\parallel \boldsymbol{\mu}_l \cdot \boldsymbol{\mu}_{l+1} - (C/2)[(\mu_l^x)^2 + (\mu_{l+1}^x)^2] + (A/2)[(\mu_l^z)^2 + (\mu_{l+1}^z)^2] - \tfrac{1}{4} J_\perp \sum_{k,k'}{}' (\mathbf{S}_{k,l} \cdot \mathbf{S}_{k',l} + \mathbf{S}_{k,l+1} \cdot \mathbf{S}_{k',l+1}) . \tag{3.3b}$$

Now the Hamiltonian can be written as

$$\mathcal{H} = \sum_{l=1}^{L} h(\boldsymbol{\mu}_l, \boldsymbol{\mu}_{l+1}) \tag{3.4}$$

and the partition function as

$$Z = \sum_n \exp(-\beta L E_n') , \tag{3.5}$$

where E_n' are defined by means of the transfer integral equation

$$\int d\boldsymbol{\mu}_l \exp[-\beta h(\boldsymbol{\mu}_l, \boldsymbol{\mu}_{l+1})] \psi_n(\boldsymbol{\mu}_l) = \exp(-\beta E_n') \psi_n(\boldsymbol{\mu}_{l+1}) . \tag{3.6}$$

In a thermodynamic limit ($L \to \infty$), the free energy (per one spin) of the system is equal to

$$F = -\lim_{L=\infty} (1/\beta K L) \ln Z = (1/K) E_0' , \tag{3.7}$$

where E_0' is the lowest value of the set $\{E_n'\}$. One can see that the transfer integral equation has a similar form to that used in Sec. II for the case of a single chain. Thus, one can expand $\psi_n(\boldsymbol{\mu}_1)$ into the Taylor series about $\psi_n(\boldsymbol{\mu}_{l+1})$ and integrate the transfer integral equation. The result is as follows:

$$\left[(1/2\beta^2 J_\parallel S^2) L_{\mu_l}^2 + A(\mu_l^z)^2 - C(\mu_l^x)^2 - \tfrac{1}{2} J_\perp \sum_{k,k'}{}' \mathbf{S}_{k,l} \cdot \mathbf{S}_{k',l} \right] \psi_n(\boldsymbol{\mu}_l) = E_n \psi_n(\boldsymbol{\mu}_l) , \tag{3.8}$$

where $\beta J_\parallel S^2 \gg 1$ and $J_\parallel / C \gg 1$ were applied. Here

$$L^2 = \sum_k L_{k,l}^2 = \sum_k \left[-\frac{1}{\cos\vartheta_{k,l}} \frac{\partial}{\partial \vartheta_{k,l}} \left[\cos\vartheta_{k,l} \frac{\partial}{\partial \vartheta_{k,l}} \right] - \frac{1}{\cos^2\vartheta_{k,l}} \frac{\partial^2}{\partial \varphi_{k,l}^2} \right] , \tag{3.9a}$$

$$(\mu_1^z)^2 = \sum_k (S_{k,l}^z)^2, \quad (\mu_l^x)^2 = \sum_k (S_{k,l}^x)^2 , \tag{3.9b}$$

$$E_n = E_n' - K \Delta E, \quad \Delta E = -S^2 J_\parallel + (1/\beta) \ln(\beta J_\parallel S^2 / 2\pi) . \tag{3.9c}$$

The operator in the large parentheses in (3.8) can be treated as the Hamiltonian of a (D-1)-dimensional system of weakly coupled quantum rotators in an anisotropy field. The free energy (per one spin) of the system considered is therefore equal (up to the additive constant) to the energy (per rotator) of the ground state $\psi_0(\mu_1)$ of the system of rotators. Thus, to investigate the thermodynamic properties of the D dimensional system of weakly coupled chains of spins, it is necessary to analyze the ground state of the (D-1)-dimensional system of weakly coupled rotators. To do this analysis we treat the interaction between rotators as a small perturbation. We denote $|\psi^s_{m,n}\rangle$ and $|\psi^a_{m,n}\rangle$ the eigenfunctions corresponding to the, respectively, symmetric and antisymmetric combinations formed from the mth and nth eigenstates of the unperturbed rotator. Here, $|\psi^s_{0,0}\rangle$ corresponds to the ground state of the unperturbed rotator. First and higher-order corrections are coming from the first ($|\psi^a_{0,0}\rangle$) and higher eigenstates of the unperturbed rotator. These corrections depend on the matrix elements of the perturbation operator and on the difference between higher eigenvalues and the eigenvalue corresponding to the ground state of the unperturbed rotator. Taking into account the form of the perturbation operator ($J_\perp \mathbf{S}_k \cdot \mathbf{S}_{k'}$), one can see that it is necessary to calculate the matrix elements of the type $\langle \psi^s_{0,0} | S^{x,y,z} | \psi^{s,a}_{n,m} \rangle$. For temperatures so low that $m^* = 2\beta^2 J_\parallel C S^2 \gg 1$, the main contribution comes from $|\psi^a_{0,0}\rangle$. Therefore, to find the ground state of the Hamiltonian (3.8) for temperatures so low that $m^* \gg 1$, and with the assumption that the interactions between rotators are so weak that $J_\perp \ll C$, it is enough to use the two-level approximation[9] in which the basis consists of only the two lowest eigenfunctions $\psi^s_{0,0}$ and $\psi^a_{0,0}$. We call this approximation the pseudospin (or spinor) approximation. Moreover, in view of the fact that $\langle \psi^s_{0,0} | S^{y,z} | \psi^a_{0,0} \rangle = 0$, the Y and Z spin components of interactions play only a minor role as compared with the easy axis X spin component. In our pseudospin approximation the eigenfunction $|\psi^s_{0,0}\rangle$ is replaced by spinor $\binom{1}{0}$, and $|\psi^a_{0,0}\rangle$ by spinor $\binom{0}{1}$. Thus, the part of the Hamiltonian (3.8) corresponding to noninteracting rotators can be transformed in the following way:

$$\sum_{k=1}^{K} [(1/2\beta^2 J_\parallel S^2)(L_k)^2 - C(S^x_k)^2 + A(S^z_k)^2] \rightarrow \sum_{k=1}^{K} [-(\Gamma/2)\sigma^z_k + (\Gamma/2 + E^s_{0,0}) I_k] , \tag{3.10a}$$

$$\Gamma = 2t_0 , \tag{3.10b}$$

where

$$\sigma^z_k = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad I_k = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} .$$

To prove this transformation, it is enough to note that the matrix elements of the operators on both sides of this transformation are the same due to the fact that the eigenvalue $E^s_{0,0}$ corresponds to the eigenvector $|\psi^s_{0,0}\rangle$, and the eigenvalue $E^a_{0,0} = E^s_{0,0} + 2t_0$ corresponds to the eigenvector $|\psi^a_{0,0}\rangle$. Similarly, the interaction part of the Hamiltonian (3.8) can be transformed as follows:

$$-\tfrac{1}{2} J_\perp {\sum_{k,k'}}' \mathbf{S}_k \cdot \mathbf{S}_{k'} \rightarrow -\tfrac{1}{2} J_\perp {\sum_{k,k'}}' S^x_k S^x_{k'} \rightarrow -\tfrac{1}{2} p^2 J_\perp S^2 \sigma^x_k \sigma^x_{k'} , \tag{3.11}$$

where

$$\sigma^x_k = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

and

$$p = 1 - [4(m^*)^{1/2}]^{-1} [1 + 1/(1+\lambda)^{1/2}], \quad \lambda = A/C . \tag{3.12}$$

To prove (3.11), it was useful to note that the matrix elements $\langle \psi^a_{0,0} | S^x | \psi^a_{0,0} \rangle$, $\langle \psi^s_{0,0} | S^x | \psi^s_{0,0} \rangle$, and $\langle \psi^{s,a}_{0,0} | S^{y,z} | \psi^{s,a}_{0,0} \rangle$ vanish.

In this way our problem of the ground state of the system of weakly coupled rotators is reduced to the problem of the ground state of the following Hamiltonian:

$$\mathcal{H}^\sigma_{\text{eff}} = -\frac{\Gamma}{2} \sum_{k=1}^{K} \sigma^z_k - \tfrac{1}{2} p^2 S^2 J_\perp {\sum_{k,k'}}' \sigma^x_k \sigma^x_{k'} , \tag{3.13}$$

where the unimportant term

$$(\Gamma/2 + E^s_{0,0}) \sum_k I_k = \tilde{E}_0 \sum_k I_k$$

is omitted [$\tilde{E}_0 = E^s_{0,0} + t_0$—according to (2.12a)]. The Hamiltonian (3.13) represents the so-called Ising model with a transverse field, the ground state of which is well recognized. Note that while the Hamiltonian (3.1) described a D dimensional system of spins, the effective Hamiltonian (3.13) represents a (D-1)-dimensional system of pseudospin. In the ground state of the last Hamiltonian, in the thermodynamic limit ($K \rightarrow \infty$), a phase transition appears.[15] For values of the transverse field Γ smaller than a critical value Γ_c, the long-range ordering appears ($\langle \sigma^x_k \rangle \neq 0$), but for Γ larger than Γ_c the long-range ordering vanishes ($\langle \sigma^x_k \rangle = 0$). Using solutions obtained in Ref. 15, we have

$$\Gamma_c = g(D) J_\perp p^2 S^2 , \tag{3.14a}$$

$$\langle \sigma_k^x \rangle = [1-(\Gamma/\Gamma_c)^2]^{\beta^*}, \quad \text{for } \Gamma \lesssim \Gamma_c , \tag{3.14b}$$

$$\chi_{XX}^{\sigma} \sim (\Gamma - \Gamma_c)^{-\tau^*}, \quad \text{for } \Gamma \gtrsim \Gamma_c , \tag{3.14c}$$

where χ_{XX}^{σ} represents the initial easy axis susceptibility; we also have for $D=2$: $g(2)=2$, $\beta^*=1/8$, and $\tau^*=\frac{7}{4}$, and for $D=3$: $g(3)\approx 6.2$, $\beta \approx \frac{5}{16}$, and $\tau^* \approx \frac{5}{4}$.

One can see now that there is a one-to-one correspondence between the Hamiltonians (3.8) and (3.13): The order parameter $\langle \sigma_k^x \rangle$ in the system described by (3.13) corresponds to the order parameter $\langle S_k^x \rangle$ in the system described by (3.8)—because the matrix elements of σ_k^x taken in the basis of spinors $\binom{1}{0}$ and $\binom{0}{1}$ are the same (up to the multiplicative constant) as the matrix elements of S_k^x in the basis of eigenvectors $|\psi_{0,0}^s\rangle$ and $|\psi_{0,0}^a\rangle$. Similarly, the initial susceptibility χ_{XX}^{σ} for the Hamiltonian (3.13) corresponds to the initial susceptibility χ_{XX}^{σ} for the Hamiltonian (3.8). It is so because the application of the external magnetic field along the X axis to the system of coupled rotators corresponds to the application of the external field along the X axis to the Hamiltonian (3.13). Moreover, the critical properties of the ground state of the Hamiltonian (3.13) correspond to those of the system described by (3.8). Finally, in view of the relation (3.7), all properties of the ground state of the system described by the Hamiltonian (3.8) correspond to the properties of the system of weakly coupled chains of spins described by the Hamiltonian (3.1). We can now put the relations (3.10b) and (2.17) together

$$\Gamma = 2t_0 = -2F_k = 2n_k k_B T , \tag{3.15}$$

which means that the transverse field Γ in (3.13) is defined by the free energy of π kinks or the density n_k of π kinks [calculated for a single chain described by the Hamiltonian (3.1b)]. Concluding, we find that for the system of weakly coupled chains of spins described by the Hamiltonian (3.1a), there exists a critical temperature T_c, and corresponding to this temperature the critical density of π kinks $n_k^c = n_k(T_c)$, such that at T_c the following relations are fulfilled:

$$-F_k(T_c) = n_k^c k_B T_c = \tfrac{1}{2} g(D) J_\perp p^2 S^2 . \tag{3.16a}$$

The critical temperature T_c is therefore defined as a temperature at which the value of the free energy of π kinks (calculated for a single chain of spins) is comparable with the value of interchain interactions. Below T_c, in view of the relation (3.14b), there exists a long-range magnetic ordering described by the nonvanishing spontaneous magnetization along the easy axis

$$\langle S^x \rangle = \left[1 - \left(\frac{n_k(T) T}{n_k^c T_c} \right)^2 \right]^{\beta^*} pS, \quad T \lesssim T_c . \tag{3.16b}$$

Above T_c, the long-range magnetic ordering vanishes, and in view of the relation (3.14c) the initial susceptibility can be written as

$$\chi_{xx}^s \sim \left[1 - \frac{n_k^c T_c}{n_k(T) T} \right]^{-\tau^*}, \quad T \gtrsim T_c . \tag{3.16c}$$

If the relations (3.16b) and (3.16c) are expanded in a power series of $|T - T_c|$, then one finds that the critical behavior of the weakly coupled chains of spins is identical to that of the D-dimensional Ising model, i.e., $\langle S^x \rangle \sim (T_c - T)^{\beta}$, $\chi_{XX}^s \sim (T - T_c)^{-\tau}$, where the critical exponents β, τ are the critical exponents of the D-dimensional Ising model. To conclude this, it was useful to know that the critical exponents of the ground state of the $(D-1)$-dimensional Ising model with transverse field are exactly the same as the critical exponents of the D-dimensional Ising model without any transverse field, which was proven in Ref. 16, i.e., $\beta(D) = \beta^*(D-1)$ and $\tau(D) = \tau^*(D-1)$. The results obtained earlier are in good agreement with the universality hypothesis for critical phenomena, because due to the existence in our system of the easy axis uniaxial anisotropy, the dimension of the order parameter is the same as for the Ising model.

One can see that below T_c the density n_k of thermally activated π kinks is smaller than n_k^c, but above T_c the density n_k is larger than n_k^c. The decrease of n_k to the value n_k^c as $T \to T_c$ is the reason for the singularity χ_{XX}^s at T_c. In this way there appears a dominant influence of π kinks on the critical properties of the quasi-one-dimensional system considered here. The situation is, to some extent, similar to that for the one-dimensional systems, but contrary to the one-dimensional systems, where the existence of π kinks is responsible for the lack of spontaneous magnetization for $T > 0$ K, in the quasi-one-dimensional systems the critical temperature is different from 0 K.

In conclusion, the phase transition occurring in the quasi-one-dimensional systems of weakly coupled chains of spins with a proper local anisotropy considered here is induced by π kink solitons. The situation is fully analogous to that appearing in weakly coupled chains with the φ^4 potential.[9]

Now we propose a simple model explaining the behavior of π kinks in a system under consideration.[8,17] Above the critical temperature T_c, the quasi-one-dimensional system behaves as a system of single one-dimensional chains. π kinks and spin waves together form a collective gas of elementary excitations in which the π kinks are distributed randomly along each chain so that the correlation range (2.25) is inversely proportional to the mean density of π kinks. Therefore, there are domains with $S^x = S$ and domains with $S^x = -S$ in each chain, and these domains are bounded by walls (π kinks) distributed randomly. The mean sizes of domains with $S^x = S$ and of those with $S^x = -S$ are the same, thus $\langle S^x \rangle = 0$. Below T_c, π kinks along each chain are coupled into pairs which are deformed 2π kinks in a very similar way as in a single chain with the external magnetic field applied along the easy axis (see Sec. II). In our quasi-one-dimensional system, the role of the external field is played by the internal field coming from the weak interchain interactions.

To illustrate such a model, one can apply the molecular field approximation to the weak interchain interac-

tions while the strong intrachain interactions are taken into account exactly. Thus, the Hamiltonian

$$\mathcal{H}^{\mathrm{MF}}=\sum_{l=1}^{L}[-J_{\parallel}\mathbf{S}_{k,l}\cdot\mathbf{S}_{k,l+1}+A(S_{k,l}^{z})^{2} -C(S_{k,l}^{x})^{2}-B^{\mathrm{MF}}S_{k,l}^{x}], \tag{3.17a}$$

may be used for the kth chain, where

$$B^{\mathrm{MF}}=zJ_{\perp}\langle S_{k,l}^{x}\rangle . \tag{3.17b}$$

Here z denotes the number of nearest-neighboring spins belonging to the nearest-neighboring chains [for $D=2$ or 3, $z=2(D-1)$, because we assumed that our chains form a quadratic or simple cubic lattice, respectively). Only interactions between S^{x} components are included to B^{MF} in view of the easy axis uniaxial anisotropy. Using the results (2.21a) obtained for $\langle S_{k,l}^{x}\rangle$ with B^{MF} substituted instead of B, one can calculate

$$B^{\mathrm{MF}}=\pm[(zp^{2}S^{2}J_{\perp})^{2}-t_{0}^{2}]^{1/2}/Sp , \tag{3.18}$$

(apart from the trivial solution corresponding to the molecular field vanishing). The relation (3.18) allows us to find the equation defining the critical temperature T_{c}^{MF}

$$t_{0}(T_{c}^{\mathrm{MF}})=zS^{2}J_{\perp}p^{2}(T_{c}^{\mathrm{MF}}) . \tag{3.19}$$

The molecular field B^{MF} can also be used as an applied field for the equations of motion for the spins in each chain. For the continuous version of the Hamiltonian (3.17a), the solutions of these equations of motion were found in the form (2.5). These solutions represent the static 2π kinks, which for $B^{\mathrm{MF}}\ll CS$ (it holds, due to $J_{\perp}\ll C$) have a form of the pair of coupled and slightly deformed, static π kinks. For $B^{\mathrm{MF}}\ll CS$, the coupling energy of π kinks in such a pair is much smaller than the energy of a single π kink, thus the energy of 2π kink is equal approximately to two energies of π kinks. We remember from Sec. II that for the 2π kinks, the mean sizes of domains with $S^{x}=S$ and domains with $S^{x}=-S$ are not equal, thus $\langle S^{x}\rangle\neq 0$. Such a situation exists below T_{c}. When $T\to T_{c}^{-}$, then $\langle S^{x}\rangle\to 0$ and $B^{\mathrm{MF}}\to 0$, thus the distance between π kinks in a pair tends to infinity, which can be interpreted as a dissociation of a 2π kink into a pair of uncoupled π kinks.

Resuming, apart from the critical region, above T_{c} we have a gas of free π kinks, but below T_{c} a gas of 2π kinks.

It is interesting that some indications of the existence of 2π kinks below T_{c} can be also obtained in some rigorous way—from the transfer integral method instead of the molecular field approximation. Namely, the free energy (per one spin) of the weakly coupled chains of spins, according to formulae (3.7), (3.9c), (3.10)–(3.11), can be written as

$$F=\Delta E+\tilde{E}_{0}+E_{g} , \tag{3.20}$$

where ΔE is given by (3.9c), $\tilde{E}_{0}$ by (2.12b), and E_{g} corresponds to the ground energy (per one lattice point) of the Hamiltonian (3.13). The sum $\Delta E+\tilde{E}_{0}$ represents the free energy of spin waves in a single chain plus the ground-state energy of such a chain (per one spin). On the other hand, the exact expression for E_{g}, approximated by the perturbative series with respect to z^{-1} [z, the coordinate number for a system (3.13) in Ref. 18], can be written as follows:

$$E_{g}=-\Gamma/2+O(1/\Gamma)=-t_{0}+O(1/t_{0}) , \quad \text{for } \Gamma>2zS^{2}p^{2}J_{\perp} , \tag{3.21a}$$

$$E_{g}=-zp^{2}S^{2}J_{\perp}/2-t_{0}^{2}/2zJ_{\perp}S^{2}p^{2}+O(t_{0}^{4}) , \quad \text{for } \Gamma<2zS^{2}p^{2}J_{\perp} . \tag{3.21b}$$

Expression (3.21a) shows that for the system of weakly coupled chains above a critical temperature there exists a contribution to the free energy, having the same form as the free energy corresponding to π kinks in a single chain. On the other hand, (3.21b) shows that below this critical temperature there exists a term proportional to $t_{0}^{2}\sim\exp(-2E_{k_{0}}\beta)$, where $E_{k_{0}}$ is the free energy of the static π kink. The existence of this term suggests that the excitations with energy $2E_{k_{0}}$ exist in the system in a situation considered. These excitations correspond just to 2π kinks, being, in fact, pairs of coupled π kinks. It is important here that no term of the series (3.21b) is proportional to t_{0}, which shows that there are no free π kinks below T_{c}.

The model proposed here was described by us earlier for the case of sine-Gordon chains[8] and was later used successfully by Rettori[19] to explain the recent experimental results on the quasi-one-dimensional antiferromagnet $K_{2}FeF_{5}$. Namely, the field dependence of the mean angle between the hyperfine field and the antiferromagnetic axis in the spin flopping configuration (magnetic field applied parallel to the initial direction of antiferromagnetism), measured in the Mössbauer effect, agrees surprisingly well with theoretical predictions based on our model despite the particular simplicity of the model which shows that the solitons responsible for the great variation of the angle mentioned earlier (when the field approaches the spin flop field) are very similar to our 2π kinks.

IV. SOLITON-INDUCED PHASE TRANSITION IN WEAKLY COUPLED ANISOTROPIC ANTIFERROMAGNETIC CHAINS IN AN EXTERNAL FIELD

Theory presented in Sec. III can be easily applied to systems of weakly coupled anisotropic antiferromagnetic chains with the external field applied to the system. One example of such a system is the quasi-one-dimensional antiferromagnetic TMMC compound. The existence of π kinks in this compound was confirmed experimentally.[20–22]

The quasi-one-dimensional TMMC compound can be described by the following Hamiltonian:

$$\mathcal{H}^{\mathrm{3D}}=\sum_{k}\mathcal{H}_{k}^{\mathrm{1D,AF}}-\tfrac{1}{2}J_{\perp}\sum_{k,k'}{}'\sum_{l}\mathbf{S}_{k,l}\cdot\mathbf{S}_{k',l} , \tag{4.1a}$$

$$\mathcal{H}_{k}^{\mathrm{1D,AF}}=\sum_{l}[2J_{\parallel}(\mathbf{S}_{k,l}\cdot\mathbf{S}_{k,l+1}-\delta S_{k,l}^{z'}S_{k,l+1}^{z'}+\epsilon S_{k,l}^{x'}S_{k,l+1}^{x'}) -g\mu_{B}H^{\alpha}S_{k,l}^{\alpha}] , \tag{4.1b}$$

where X', Y', Z' are the axes of the coordinate system, H^α is the external magnetic field applied along the α axis, $\alpha=X'$ or Y'; $J_\parallel=6.7Kk_B$, $|S|=\frac{5}{2}$, $g=2$, $\delta\approx 0.01-0.02$, $\epsilon\approx 2.6\times 10^{-4}$, $J_\perp\approx(10^{-5}-10^{-4})Kk_B$ (the exact values of parameters δ and $J_\perp$ are not uniquely known).[22,23] If no external field is applied, the (X',Y') plane is the easy plane and the X' axis is the easy axis in that plane.

It was shown[23] that the static properties of such an antiferromagnetic Hamiltonian (4.1b) (for $H^\alpha g\mu_B/4J_\parallel S \ll 1$) are the same as static properties of the following ferromagnetic Hamiltonian:

$$\mathcal{H}_k^{\mathrm{1D,F}}=\sum_l [-J_\parallel \mathbf{S}_{k,2l}\cdot\mathbf{S}_{k,2l+2}-c(S_{k,2l}^{x'})^2 + a(S_{k,2l}^{z'})^2+b(S_{k,2l}^{\alpha})^2] , \tag{4.1c}$$

with $a=4\delta J_\parallel$, $b=g\mu_B H^\alpha/8J_\parallel S^2$, and $c=4\epsilon J_\parallel$. The lattice constant in the last case is equal to two lattice constants of the previous case, thus the free energy (per one spin) for the former is two times larger than that for the latter. It is worth noting that the square field $(H^\alpha)^2$ plays the role of the uniaxial anisotropy with the hard axis. Now the calculations of Sec. III can be applied to the present case, leading to the following result for the free energy at the critical temperature:

$$-F_k(T_N)=eg(D)\tilde{J}_\perp S^2 p^2(T_N)/2 , \tag{4.2}$$

where $g(3)\approx 6.2$, e is a factor of order of unity, dependent on the type of the crystallographic lattice, and $\tilde{J}_\perp=2J_\perp$. Using the relations (2.17) and (2.12c), one obtains the equation which defines a dependence of the critical temperature for TMMC on the direction and value of the external field H^α

$$[C+(C^2+AC)^{1/2}]\exp(-2m_N^{*1/2})\exp(-w_N)I_0(w_N) = J_\perp(6.2/8)\{1-[1+(1+A/C)^{-1/2}]/4m_N^{*1/2}\}^2 , \tag{4.3}$$

where $w_N=m_N^{*1/2}A/2C$, $m_N^*=2CJ_\parallel S^4/(k_B T_N)^2$, and A and C are the H^α dependent combinations of constants a, b, and c. For example, if H^α is directed along the Y' axis and $b\le a$, then $A=a-b$, and $C=b+c$, but if $b\ge a$, then $A=b-a$, and $C=a+c$. If, however, H^α is directed along the X' axis and $b\le c$, then $A=a$, and $C=c-b$, but for $a+c\ge b\ge c$ one has $A=a+c-b$, and $C=b-c$, and for $b\ge a+c$ one has $A=b-a-c$, and $C=a$. The results of numerical computations for $\delta=0.024$ and $eJ_\perp=0.53\times 10^{-4}Kk_B$ are depicted in Fig. 1, with experimental data[24,25] together. Good agreement of the theory and experiment is obtained. It is necessary to mention at this point that similar phase diagrams for TMMC were, in part, obtained earlier, theoretically, with the use of the molecular field approximation used to describe the interchain interactions.[24,25] The constant $J_\perp^{\mathrm{MF}}$ however, necessary to obtain good agreement with experiment in this case, is smaller by a factor of 1.3 than our constant $J_\perp$. In view of the more rigorous treatment of the interchain interaction in our approach (the pseudospin approximation), the temperature T_N, obtained from the molecular field calculation for the same values of $J_\perp$ must be treated as too large.

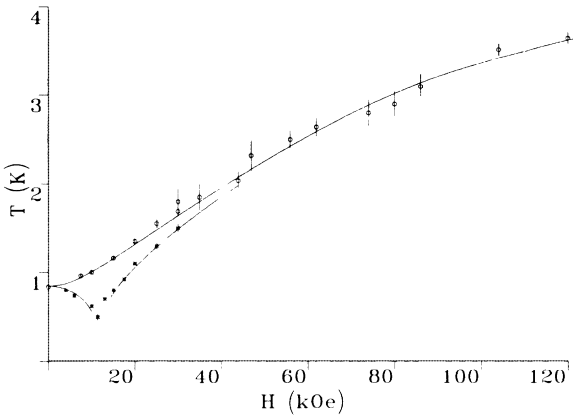

FIG. 1. Field dependence of the critical temperature for the antiferromagnetic TMMC compound. Continuous curve—the result of our theory with experimental points taken from Refs. 24–26. Circles and asterisks correspond to the field directed along the hard axis and the easy axis, respectively.

V. CONCLUSIONS

Our analysis of some of the properties of quasi-one-dimensional systems of weakly coupled magnetic chains with the solitons in the form of π kinks shows that the phase transition appearing in such systems is related closely to properties and behavior of solitons. We call such phase transitions soliton-induced phase transitions. The critical role of solitons in systems considered here appears in the following way: As compared with one-dimensional systems, where the existence of solitons in the form of π kinks determines the finite value of the correlation range and makes the magnetic susceptibility finite for $T>0$ K, i.e., leads to the lack of phase transitions for $T>0$ K, in quasi-one-dimensional systems of weakly coupled chains the existence of π kinks leads to the appearance of the phase transition at some $T_c>0$ K and to the appropriate expressions for magnetic susceptibility at $T>T_c$ and for nonvanishing spontaneous magnetization below T_c. The critical temperature T_c is obtained as a temperature at which the free energy of π kinks (calculated for a single chain) is comparable with the energy of interchain interactions. The critical behavior of the system considered corresponds to the critical behavior of the Ising model with the same dimension—in complete agreement with the universality hypothesis.

The important result of our analysis is connected with our model of the behavior of π kinks below the critical temperature. We showed here that below T_c, the π kinks are coupled into pairs corresponding to the 2π kinks (along each chain). The reason for such a pairing is the interchain interaction, the effect of which is similar to that of the external field in the single chain case. As the critical temperature is approached from below, the dis-

tances between π kinks of one pair increase, and at T_c the 2π kinks dissociate into free π kinks. Above T_c, only free π kinks exist. Such a model explains the experimental field dependence of the magnetization direction in the spin flopping configuration obtained for antiferromagnetic K_2FeF_5 by means of the Mössbauer technique.

Application of our theory to the antiferromagnetic TMMC compound allows us to obtain the field dependence of the Néel temperature of this compound, which is in good agreement with experimental data.

Possibilities of further experimental verification of our theory may be searched for in various types of experiments, e.g., on specific heat on the one hand, and on critical exponents on the other hand.

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