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Soliton-induced magnetic phase transition in three-dimensional systems of weakly coupled magnetic chains with local anisotropy

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Thermodynamical properties of weakly coupled magnetic chains, consitituting three-dimensional classical ferromagnets with special exchange and local anisotropies, are considered. The transfer-operator method and pseudospin approach are used. It is shown that the phase transition connected with the disappearance of three-dimensional magnetic ordering is induced here by static kink solitons obtained for one-dimensional systems.

Recently, there is a great progress in solid-state physics connected with quasi-one-dimensional crystals with excitations described by nonlinear equations of motion. In such crystals, represented in the simplest case of theory by noninteracting one-dimensional systems, besides the usual low amplitude and extended excitations (like phonons, magnons, etc.), the special exact stable high amplitude and localized excitations, called solitons, can appear. These solitons play a dominant role in many physical events in such systems.[1-3] In particular, it is well established that in the one-dimensional classical ferromagnets with an easy axis local anisotropy, the solitons in a form of static kinks or domain walls can exist.[4,5] Thermodynamical properties of the last systems were analyzed in papers[6-8] and it was shown there that the existence of these kinks is responsible for the fact that the correlation length does not ever become infinite for any finite temperature. It means simultaneously that the existence of kinks is responsible for a lack of long-range ordering in these one-dimensional systems.

Here, we show that in the three-dimensional systems of weakly coupled magnetic chains with the local uniaxial anisotropy, where the long-range ordering exists in low temperatures as a result of coupling between chains, the similar static kinks extending along the chains are responsible for the disappearance of the long-range ordering above a critical temperature. This situation is similar to those in analogical systems with structural phase transitions,[9] in weakly coupled linear conductors,[10] etc. Only results are presented here, the full calculations will be published in a separate paper.

We consider a three-dimensional[11] system of weakly coupled magnetic chains of classical spins with interactions described by the following Hamiltonian:

$$H=-\sum_{i=1}^{I}\sum_{k=1}^{K}\sum_{l=1}^{L}\{\vec{S}_{i,k,l}[J_{\parallel}\vec{S}_{i,k,l+1}+J_{\perp}(\vec{S}_{i,k+1,l}+\vec{S}_{i+1,k,l})]+B(S^{z}_{i,k,l})^{2}\}\ , \tag{1}$$

where the exchange constants $J_{\parallel}$ and $J_{\perp}$ and the local anisotropy constant B are assumed to fulfill

$$J_{\parallel}>>B>>J_{\perp}>0\ . \tag{2}$$

Spins with a special pair of indices (i,k) form a chain and different chains are labeled by various sets (i,k). For simplicity of formulas we consider the array of spins in a form of the simple cubic lattice with the lattice constant taken as the length unit and we put $|\vec{S}_{i,k,l}|=1$. Of course $I,K,L>>1$ are assumed. In a view of inequality (2), at low temperatures the continuous approximation can be used for interactions of spins inside a chain (the so-called displacive limit), but cannot be used for interactions of spins belonging to different chains (the so-called order-disorder limit).

To study thermodynamical properties of the system considered, we use the transfer operator method originally applied to one-dimensional systems,[2,7,12] and then generalized to weakly coupled systems of chains.[9,10,13] According to this method the transfer operator acts along the axis of chains. Thus the classical partition function Z of our system can be written as

$$\exp(-\beta F)=Z=\int\exp(-\beta H)\prod_{i=1}^{I}\prod_{k=1}^{K}\prod_{l=1}^{L}d\vec{S}_{i,k,l}=\sum_{n}\exp(-\beta E_{n}L)\ , \tag{3}$$

where $\beta=(k_{B}T)^{-1}$, T is a temperature and k_{B} is the Boltzmann constant, F denotes the free energy of the system, and E_{n} are eigenvalues of the following effective Hamiltonian, up to some irrelevant additive constant

$$H_{\text{eff}}=\sum_{i=1}^{I}\sum_{k=1}^{K}\left[-J_{\perp}\vec{S}_{i,k}(\vec{S}_{i,k+1}+\vec{S}_{i+1,k})-B(S^{z}_{i,k})^{2}+\frac{1}{2\beta^{2}J_{\parallel}}(\mathcal{L}_{i,k})^{2}+\left[-J_{\parallel}+\frac{\ln(2\beta J_{\parallel})}{\beta}\right]\right]\ , \tag{4}$$

where $\mathcal{L}_{i,k}$ denotes the angular momentum operator for a chain labeled by (i,k). In a derivation of (4) the condition (2) (concerning the values of $J_{\parallel}$ and B) was used and $\beta J_{\parallel}>>1$ was assumed as well.

The effective Hamiltonian (4) describes a two-dimensional (2D) system of coupled hindered quantum rotators. We need to find its ground energy and the ground-state wave function. This is in general rather a difficult task but simple analytical solutions can be obtained for a low-temperature region defined by

$$\beta(BJ_{\parallel})^{1/2}>>1\ . \tag{5}$$

Using the condition (2) a diagonalization of Hamiltonian (4) can be performed in a truncated basis consisting of the two lowest states of noninteracting rotators. The eigenvalue problem for a single rotator can be transformed to a pseudo-Schrödinger equation with a potential consisting of two symmetric wells. In the low-temperature approximation [Eq. (5)], these two lowest energies of the rotator considered correspond to the "tunnel-split" lowest energy of a single well. The value of this splitting, in a standard WKB

approximation, is twice the free energy of static kinks[7,8] and it can be expressed in terms of the average density $n(T)$ of kinks at the temperature considered. Fortunately, the next levels of a single rotator are much higher than these split levels and this allows us to consider the two-states basis. For weak interactions between chains [condition (2)], the ground state for the coupled rotators system can be approximately found in this truncated basis.[9,10,13] These facts allow us to use the so-called pseudospin representation in which the Hamiltonian (4) is transformed to the following form, up to some additive constants,

$$H_{\text{eff}} = -\sum_{i=1}^{I}\sum_{k=1}^{K}\left[\tfrac{1}{2}\Gamma\sigma_{ik}^{z} + J_{\perp}\sigma_{i,k}^{x}(\sigma_{i+1,k}^{x}+\sigma_{i,k+1}^{x})\right] , \tag{6}$$

where $\sigma_{i,k}^{x}$ and $\sigma_{i,k}^{z}$ are the Pauli matrices connected with the chain (i,k). Here Γ denotes the WKB energy splitting for the lowest level of a single rotator and is equal to

$$\Gamma \simeq \frac{8e}{\pi d}E_0\exp(-\beta E_0)$$

$$= 2n(T)\beta^{-1} = -2F_k , \tag{7}$$

where $E_0 = 2(2BJ_{\parallel})^{1/2}$ is the energy of a static kink in a single chain, $d = [J_{\parallel}/(2B)]^{1/2}$ is a measure for the effective width of a kink, $n(T)$ is the average density of kinks (in noninteracting chains) as a function of temperature, and F_k denotes the free energy of kinks.[8]

Hamiltonian (6) represents a very well-known 2D Ising model with "a transversal field Γ," and is widely used for the description of phase transitions in ferroelectrics.[14] For our purpose, the ground-state properties of this Hamiltonian are interesting. For small values of Γ, there exists long-range ordering described by $\langle\sigma_{i,k}^{x}\rangle \neq 0$, but for Γ larger than a critical value Γ_c, the long-range ordering vanishes: $\langle\sigma_{i,k}^{x}\rangle = 0$. Using solutions found in Ref. 15 we have

$$\Gamma_c = 6.2J_{\perp} , \tag{8}$$

$$\langle\sigma_{i,k}^{x}\rangle \sim \left[1-\left(\frac{\Gamma}{\Gamma_c}\right)^{2}\right]^{0.32} \quad \text{for } \Gamma \lesssim \Gamma_c , \tag{9}$$

$$\chi_{\sigma}^{xx} \sim (\Gamma-\Gamma_c)^{-1.24} \quad \text{for } \Gamma \gtrsim \Gamma_c , \tag{10}$$

where χ_{σ}^{xx} is the static isothermal susceptibility of the system described by Hamiltonian (6). In view of relation (7) the solutions (8)–(10) mean that for our system, described by Hamiltonian (1), there exists a critical temperature T_c and a corresponding critical kink density

$$n_c = \frac{4eE_0}{\pi dkT_c}\exp\left(-\frac{E_0}{kT_c}\right) ,$$

such that in a critical point we have

$$n_c k_B T_c = 3.1J_{\perp} \tag{11}$$

and below this temperature there exists nonvanishing long-range order described by the spontaneous magnetization

$$\langle S^{z}\rangle \sim \left[1-\left(\frac{n(T)T}{n_cT_c}\right)^{2}\right]^{0.32} \quad \text{for } T \lesssim T_c . \tag{12}$$

Above T_c the long-range ordering vanishes and the static isothermic susceptibility χ_S^{zz} of the system is as follows:

$$\chi_S^{zz} \sim \left(1-\frac{n_cT_c}{n(T)T}\right)^{-1.24} \quad \text{for } T \gtrsim T_c . \tag{13}$$

A dominant meaning of kinks for the disappearance of spontaneous magnetization above T_c (of course, below T_c this spontaneous magnetization exists in our 3D system as a result of coupling between the chains) appears here in the same way as in the corresponding one-dimensional systems these kinks are responsible for the lack of spontaneous magnetization for all finite temperatures $T > 0$. The susceptibility (13) is finite above T_c but diverges as T_c is approached and $n(T)$ tends to n_c. The nonzero spontaneous magnetization (12) is limited to temperatures lower than T_c, so that the kink density is lower than their critical n_c. An influence of kinks on critical properties of our system is also easily seen: The characteristic $(T-T_c)$ expansion can be obtained and critical indices are nearly the same as those for the 3D Ising model.

In conclusion, the phase transition occurring in the considered here 3D (or 2D) systems, consisting of weakly coupled chains of spins with a proper local uniaxial anisotropy, is induced by static kink solitons obtained usually for 1D systems. This is the phase transition between the low-temperature phase with a three-dimensional long-range ordering dependent on the kink-soliton density and the phase characterized by quasi-one-dimensional behavior with susceptibilitiy also dependent on the kink-soliton density. The situation is fully analogical to those appearing in weakly coupled systems of conductors or in similar systems with structural phase transitions.

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