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Quasi-one-dimensional anisotropic Heisenberg model in a transverse magnetic field

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The phase diagram of weakly coupled XXZ chains in a transverse magnetic field is studied using the mean-field approximation for the interchain coupling and known exact results for an effective one-dimensional model. Results are applied to the quasi-one-dimensional antiferromagnet Cs_2CoCl_4 and the value of interchain interaction in this compound is estimated.

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The effects induced by magnetic fields in low-dimensional magnets are subjects of intensive theoretical and experimental research [1]. One of the striking effects is the dependence of magnetic properties of quasi-one-dimensional (Q1D) antiferromagnets with anisotropic interactions on the direction of the applied magnetic field. For example, the behavior of these systems in a transverse magnetic field is drastically different in comparison with the case of the longitudinal field applied along the anisotropy axis. In particular, the transverse field induces a gap in the spectrum and the antiferromagnetic long range order (AF LRO) in the perpendicular direction. A quantum phase transition takes place at some critical field, where the LRO and the gap vanish. The phase transition of this type has been observed in the Q1D antiferromagnet Cs_2CoCl_4 [2]. The simplest model of the one-dimensional anisotropic antiferromagnet in the transverse field is the spin-$\frac{1}{2}$ XXZ chain described by the Hamiltonian

$$\mathcal{H}_{1\mathrm{D}} = J\sum(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z) - - H\sum S_n^x, \qquad (1)$$

where Δ is an anisotropy parameter which assumed to be $0 \le \Delta < 1$.

It was proposed [2] that low-energy properties of Cs_2CoCl_4 is described by (1) with $J = 0.23\,\mathrm{meV}$ and $\Delta = 0.25$. In contrast to the case of the longitudinal field the symmetry-breaking transverse field does not commute with the XXZ Hamiltonian and the exact integrability of (1) is destroyed. The model (1) has been investigated using different approximate approaches [3 – 6]. The scaling estimates at small field [7] show that the transverse field generates the staggered magnetization $M_{st} = \langle(-1)^n S_n^y\rangle$ (AF LRO in the Y direction) and the gap in the spectrum m (at $H = 0$ the spectrum is gapless)

$$m \sim (H/J)^{\frac{1}{2-d}}, \qquad d = \frac{\eta}{2} + \frac{1}{2\eta},$$
$$M_{st} \sim (H/J)^{\frac{\eta/2}{2-d}}, \qquad \eta = 1 - \frac{1}{\pi}\arccos\Delta. \qquad (2)$$

To study the model (1), when the field H is not small, the mean-field approximation (MFA) has been proposed in [7] and elaborated in [8]. The MFA is based on the Jordan-Wigner transformation of spin-$\frac{1}{2}$ operators to the Fermi ones with the subsequent mean-field treatment of the four-fermion interaction term. As a result the arising Hamiltonian is quadratic in Fermi-operators and it is solved exactly. Transforming this MFA Hamiltonian back to spin variables we obtain a spin-$\frac{1}{2}$ XY model in the longitudinal field

$$\mathcal{H}_{XY} = J'\sum[(1-\gamma)S_n^x S_{n+1}^x + (1+\gamma)S_n^y S_{n+1}^y - hS_n^z], \qquad (3)$$

where parameters J', γ and h are determined by the MFA self-consistent conditions [7, 8].

The model (3) is exactly solvable and its properties are well studied [9]. This model undergoes the $T = 0$ phase transition of the 2D Ising universality class at $h = 1$ corresponding to the MFA value of the critical field $H_c^{1\mathrm{D}}(\Delta)$. In particular, in the vicinity of the critical field $M_{st} \sim \left|H_c^{1\mathrm{D}}(\Delta) - H\right|^{1/8}$. A comparison of the MFA results with those obtained in precise numerical DMRG calculations shows high accuracy of the MFA at $H \gtrsim J$ [8]. The dependence $M_{st}(H)$ for $\Delta = 0.25$ obtained with use of the MFA and scaling estimate (2) is shown on Fig.1 by dashed line. This magnetization curve is qualitative similar to that observed in neutron-scattering experiments on Cs_2CoCl_4. At the same time,

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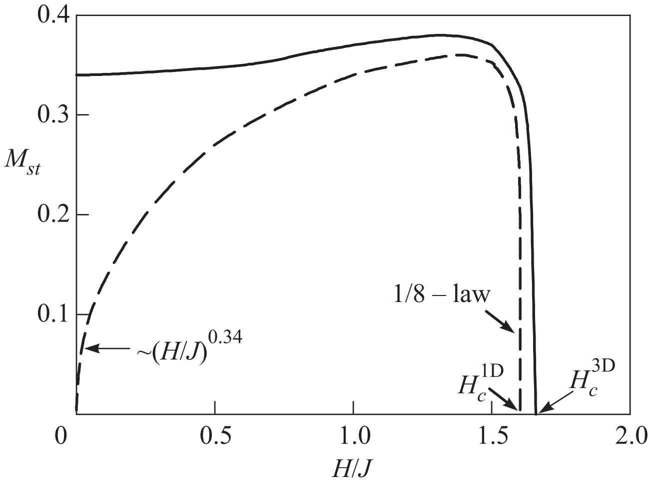

Fig.1. The dependence of $T = 0$ LRO parameter on magnetic field for 1D chain (dashed line) and Q1D system (solid line) for $\Delta = 0.25$

there is essential difference in the low-field behavior of M_{st}. The experimental AF ordered moment is finite at $H = 0$ while $M_{st} \to 0$ according to (2). This difference is due to weak interchain couplings in real systems and these couplings form a 3D magnetically ordered moment below a Neel temperature T_N. Besides, interchain couplings extend the 1D ordered phase with $M_{st} \neq 0$ to finite temperatures. Therefore, to describe low temperature properties of real Q1D compounds it is necessary to take into account interchain interactions.

In this latter we will consider the system of coupled parallel XXZ chains in the transverse field described by the Hamiltonian

$$\mathcal{H} = J\sum(S^x_{n,\mathbf{r}}S^x_{n+1,\mathbf{r}} + S^y_{n,r}S^y_{n+1,\mathbf{r}} + \Delta S^z_{n,\mathbf{r}}S^z_{n+1,\mathbf{r}}) + \\ + J_\perp\sum(S^x_{n,\mathbf{r}}S^x_{n,\mathbf{r}+\delta} + S^y_{n,\mathbf{r}}S^y_{n,\mathbf{r}+\delta} + \Delta S^z_{n,\mathbf{r}}S^z_{n,\mathbf{r}+\delta}) - \\ - H\sum S^x_{n,\mathbf{r}} \qquad (4)$$

where n and $\mathbf{r}$ label lattice sites along the chain and in perpendicular directions, δ is summed over two nearest neighbor vectors in the transverse directions, $J_\perp$ is a weak coupling between neighboring chains.

A standard method for treating the model (4) is to use the mean-field approximation for interchain coupling and to treat the resulting effective 1D problem as exactly as possible [10, 11] (we call this approach as chain mean-field theory (CMFT) to distinguish it from the MFA for the 1D model (1)). We assume that AF order in each chain to be oriented along the Y direction and the uniform magnetization along the X axis as it occurs in the pure 1D model (1). The quasi-1D model contains another mechanism to generate the LRO. If one of the chains is AF ordered, the interchain couplings induce an effective staggered field on the nearest chains. In the CMFT interchain coupling is replaced by effective fields and the Hamiltonian (4) reduces to an effective 1D Hamiltonian having the form

$$\mathcal{H}_{\text{eff}} = J\sum(S^x_n S^x_{n+1} + S^y_n S^y_{n+1} + \Delta S^z_n S^z_{n+1}) - \\ - (H - H_x)\sum S^x_n - H_y\sum(-1)^n S^y_n \qquad (5)$$

where fields H_x and H_y are determined by self-consistency relations

$$H_x = zJ_\perp\langle S^x_n\rangle, \quad H_y = zJ_\perp M_{st}, \qquad (6)$$

z is the transverse coordination number.

At first, we consider the model (5) at $H = 0$ and $T = 0$. It can be easily shown that the self-consistency relation gives $\langle S^x_n\rangle = 0$ and the model (5) reduces to the XXZ chain in the staggered field. The low-energy properties of this model are described by a quantum sine-Gordon model [12]

$$\mathcal{H} = \mathcal{H}_0 + V, \\ \mathcal{H}_0 = \frac{v(\eta)}{2}\int dx\{(\partial_x\Phi)^2 + (\partial_x\Theta)^2\}, \qquad (7) \\ V = -H_y\sqrt{2A(\eta)}\int dx\sin(\sqrt{2\pi\eta}\Theta),$$

where $\Phi(x)$ and $\Theta(x)$ are boson and dual fields respectively, $v(\eta) = J\sin(\pi\eta)/(2-2\eta)$ is the sound velocity and the coefficient $A(\eta)$ was found in [13].

The spectrum of $\mathcal{H}_0$ is gapless. The perturbation V has scaling dimension $\eta/2$ and generates the mass gap

$$m = v\left(\frac{CH_y}{v}\right)^{\frac{1}{2-\eta/2}}, \qquad (8)$$

where constant C is [14]

$$C = \frac{\sqrt{2A}\pi\Gamma\left(1-\frac{\eta}{4}\right)}{2\Gamma\left(\frac{\eta}{4}\right)}\left(\frac{2}{\sqrt{\pi}}\frac{\Gamma\left(\frac{\eta}{8-2\eta}\right)}{\Gamma\left(\frac{2}{4-\eta}\right)}\right)^{2-\eta/2}. \qquad (9)$$

The staggered magnetization M_{st} is related to a mass gap m as [13]

$$M_{st} = \sqrt{2A}\left\langle\exp\left(i\sqrt{2\pi\eta}\Theta\right)\right\rangle = D\left(\frac{m}{v}\right)^{\eta/2}, \qquad (10)$$

where

$$D = \frac{\sqrt{2A}\pi\Gamma\left(1-\frac{\eta}{4}\right)}{(16-4\eta)\sin\left(\frac{\pi\eta}{4-\eta}\right)\Gamma\left(\frac{\eta}{4}\right)}\times \\ \times\left(\frac{\Gamma\left(\frac{2}{4-\eta}\right)\Gamma\left(\frac{8-3\eta}{8-2\eta}\right)}{4\sqrt{\pi}}\right)^{\frac{\eta}{2}-2}. \qquad (11)$$

From the equations (8) and (10) we get

$$M_{st} = D\left(CD\frac{zJ_\perp}{v}\right)^{\frac{\eta/2}{2-\eta}}, \tag{12}$$

$$m = v\left(CD\frac{zJ_\perp}{v}\right)^{\frac{1}{2-\eta}}. \tag{13}$$

The AF LRO M_{st} survives at $T < T_N$. The Neel temperature T_N can be found using the random phase approximation (RPA). The RPA dynamical susceptibility of coupled chains in disordered phase ($T > T_N$) is

$$\chi^{yy}(\omega,k,k_\perp) = \frac{\chi^{yy}_{1\mathrm{D}}(\omega,k)}{1 - J_\perp(k_\perp)\chi^{yy}_{1\mathrm{D}}(\omega,k)}. \tag{14}$$

The condition determined T_N is

$$zJ_\perp\chi^{yy}_{1D}(0,\pi) = 1. \tag{15}$$

The dynamical susceptibility of the 1D XXZ model at $T \ll J$ is known [15]

$$\chi^{yy}_{1\mathrm{D}}(0,\pi) = \frac{B}{v}\left(\frac{v}{2\pi T}\right)^{2-\eta}, \tag{16}$$

where

$$B = A\sin(\pi\eta/2)\,\frac{\Gamma^2(1-\eta/2)\,\Gamma^2(\eta/4)}{\Gamma^2(1-\eta/4)}. \tag{17}$$

Using the condition (15) we extract the Neel temperature at $H = 0$

$$T_N(H=0) = \frac{v}{2\pi}\left(\frac{BzJ_\perp}{v}\right)^{\frac{1}{2-\eta}}. \tag{18}$$

We note that the ratio T_N/m does not depend on $J_\perp$ and is determined by 1D parameter η only.

An analysis of experimental data carried out in Ref.[2] has shown that the Q1D antiferromagnet Cs_2CoCl_4 consists of two interpenetrating sublattices with identical intrasublattice interactions. These sublattices are non-interacting on the CMFT level. Each sublattice has tetragonal symmetry and described by the model (4) with $z = 4$. However, no direct experimental data on the value of the interchain interaction $J_\perp$ is available. The Neel temperature in Cs_2CoCl_4 at $H = 0$ is $T_N = 0.0813\,J = 0.217$ K [2]. Using these data we can estimate unknown value of $J_\perp$ in Cs_2CoCl_4. Substituting $\Delta = 0.25$ ($A = 0.1405$) in (18) we find

$$\frac{J_\perp}{J} = 0.0147. \tag{19}$$

This value is really small, so that our assumption about Q1D behavior of the system is justified.

Further, using the found value of $J_\perp$ we can find the staggered magnetization M_{st} at $T = 0$. According to Eq.(12) $M_{st} = 0.348$. The experimental value of the AF ordered moment at $T \ll T_N$ is $M_{st} \approx 0.342$ [2]. Such a perfect coincidence confirms our estimate (19). Besides, the found value of $J_\perp$ gives us also the gap (13) $m = 0.78\,$K. It is remarkable that even so small interchain coupling as in Eq.(19) causes so large value of LRO and the gap.

At $H = 0$ and $T = 0$ the AF LRO is generated by the interchain couplings. At $H > 0$ the 'one-dimensional' mechanism is switched. The crude estimation of the value H^*, at which this mechanism becomes predominant, can be obtained by a comparison of (2) with (13)

$$H^* \sim J\,(zJ_\perp/J)^{\frac{2-d}{2-\eta}}. \tag{20}$$

At $H > H^*$ in the Hamiltonian (5) the mean field H_x can be neglected in comparison with H and at $T = 0$ the main effect of H_y consists in a small shift of the critical field $H_c^{1\mathrm{D}}$ (see below).

At $H = H_c^{1\mathrm{D}}$ and $H_y = 0$ the spectrum of the model (5) is gapless. The perturbation $H_y\sum(-1)^n S_n^y$ has scaling dimension 1/8 and generates the mass gap $m \sim (H_y/J)^{8/15}$ and AF LRO $M_{st} \sim (H_y/J)^{1/15}$ in the model (5). The self-consistency relations (6) therefore give

$$M_{st}(H_c^{1\mathrm{D}}) \sim (zJ_\perp/J)^{1/14},$$
$$m(H_c^{1\mathrm{D}}) \sim (zJ_\perp/J)^{4/7}. \tag{21}$$

To estimate the Neel temperature $T_N(H)$ in the RPA it is necessary to know the finite temperature staggered susceptibility $\chi^{yy}_{1\mathrm{D}}(0,\pi)$ for the model (1) at $H > 0$. Unfortunately, it is unknown. Instead, we consider the MFA model (3), for which the susceptibility can be found. As it was noted above the MFA describes correctly the ground state properties of the model (1) at $H \geq J$. We expect that the MFA gives a satisfactory description of (1) at low temperature ($T \ll J$) as well. The problem of finding $T_N(H)$ can be solved in the same manner as it was done by Carr and Tsvelik in [16] for Q1D quantum Ising model, which on the CMFT level reduces to (3) with $\gamma = 1$.

We are mainly interested in the region of the fields near the critical field $H_c^{1\mathrm{D}}(\Delta)$ or at $h \sim 1$ in terms of the MFA Hamiltonian (3). Exactly at $h = 1$, where the model (3) is critical, the staggered susceptibility at $T \ll J$ according to [15] is

$$\chi^{yy}_{1\mathrm{D}}(0,\pi) = R(\gamma)\frac{\pi}{v_c}\left(\frac{v_c}{2\pi T}\right)^{7/4}\frac{\Gamma(7/8)\,\Gamma^2(1/16)}{\Gamma(1/8)\,\Gamma^2(15/16)}, \tag{22}$$

where sound velocity at the critical field $v_c = \gamma J'$ is determined from the MFA self-consistent equations [7] and

$$R(\gamma) = \frac{e^{1/4} 2^{1/12} A^{-3}}{4} \frac{2\gamma^{3/4}}{1+\gamma} \qquad (23)$$

with Glaisher constant $A \simeq 1.282$.

The Neel temperature in the RPA is

$$T_N(H_c^{1D}) = \frac{v_c}{2\pi} \left[\frac{\pi z J_\perp}{v_c} \frac{R(\gamma)\Gamma(7/8)\Gamma^2(1/16)}{\Gamma(1/8)\Gamma^2(15/16)} \right]^{4/7}. \qquad (24)$$

For $\Delta = 0.25$ the critical field in the MFA is $H_c^{1D} \approx \approx 1.6\,\mathrm{J}$ and $v_c \approx 0.185\,\mathrm{J}$. Therefore, the estimated Neel temperature for Cs_2CoCl_4 is $T_N(H_c^{1D}) = 0.145\,\mathrm{K}$.

Near the critical field at $H \gtrsim H_c^{1D}$ (disorder region in the 1D model) the low-temperature staggered susceptibility is well approximated by the formula [1]

$$\chi_{1D}^{yy}(\omega, \pi - k) \approx \frac{\gamma^{3/4}}{1+\gamma} \frac{v(2m/v)^{1/4}}{v_c^2 k^2 + m^2 - (\omega + i/\tau_c)^2} \qquad (25)$$

where the gap $m = \left| H - H_c^{1D} \right|$ and the phase relaxation time $\tau_c = (\pi/2T)e^{m/T}$. In this case the RPA condition of the phase transition (15) reads

$$m^2 + \tau_c^{-2} = \frac{(\gamma v_c)^{3/4}}{1+\gamma} (2m)^{1/4} z J_\perp. \qquad (26)$$

At first we estimate the shift of the critical field $\delta H_c = H_c^{3D} - H_c^{1D}$ caused by interchain couplings. This shift is determined by the condition $T \to 0$ in Eq.(26)

$$\delta H_c = 2^{1/7} \frac{(\gamma v_c)^{3/7}}{(1+\gamma)^{4/7}} (z J_\perp)^{4/7}. \qquad (27)$$

For $\Delta = 0.25$ and found value of $J_\perp$ (19) the shift of the critical field is about 3%. We note that in the vicinity of the critical point H_c^{3D} the low-energy properties of Q1D model (4) belong to the universality class of the (3+1)-dimensional classical Ising model.

Eq.(26) gives also the behavior of Neel temperature near the 3D critical point $H_c^{3D} - H \ll \delta H_c$

$$T_N(H) \approx 2(\delta H_c) \ln^{-1} \left(\frac{\delta H_c}{H_c^{3D} - H} \right) \qquad (28)$$

At intermediate fields $H^* < H < H_c^{1D}$ (the 1D ordered region) the low temperature $T \ll m$ staggered susceptibility has an exponential form [1]

$$\chi_{1D}^{yy}(0, \pi) \sim (m/v)^{1/4} \xi_c \tau_c \sim \frac{v^{3/4}}{m^{1/4} T^{3/2}} e^{2m/T} \qquad (29)$$

with correlation length $\xi_c = v\sqrt{\pi/2mT}e^{m/T}$ [1]. Thus, for $zJ_\perp \ll m(m/v)^{3/4}$ the RPA criteria (15) yields

$$T_N(H) \sim 2m(H) \ln^{-1} \left(\frac{m(H)}{zJ_\perp} \right). \qquad (30)$$

Combining the found expressions for Neel temperature in different regions (18), (24), (28), (30) we arrive at the phase diagram schematically shown on Fig.2. Since the gap $m(H)$ in the AF ordered region has a maximum

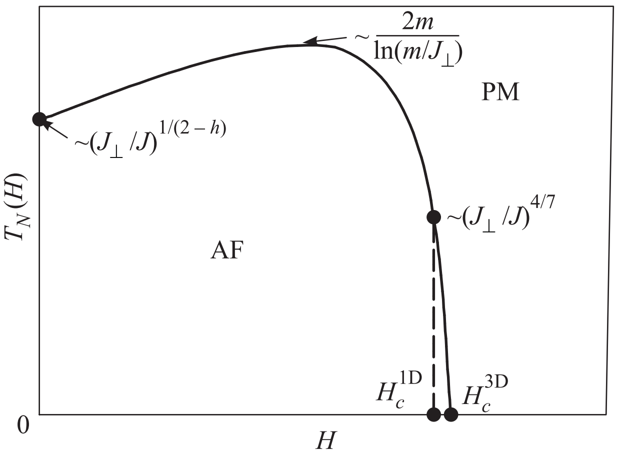

Fig.2. Schematic phase diagram of the model (4). The phase boundary separates the antiferromagnetic phase with $M_{st} \neq 0$ from the paramagnetic phase without AF LRO

at some intermediate value of field [7, 8], then according to Eq.(30) the function $T_N(H)$ also has a maximum as shown on Fig.2. This fact was experimentally observed in Cs_2CoCl_4 [2].

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