

Quantum chiral phases in frustrated easy-plane spin chains

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The phase diagram of antiferromagnetic spin- S chain with XY -type anisotropy and frustrating next-nearest-neighbor interaction is studied in the limit of large integer S with the help of a field-theoretical approach. It is shown that the existence of gapless and gapped chiral phases found in recent numerical studies [M. Kaburagi *et al.*, J. Phys. Soc. Jpn. **68**, 3185 (1999); T. Hikihara *et al.*, J. Phys. Soc. Jpn. **69**, 259 (2000)] is not specific for $S=1$, but is rather a generic large- S feature. Estimates for the corresponding transition boundaries are obtained, and a sketch of the typical phase diagram is presented. It is also shown that frustration stabilizes the Haldane phase against the variation of the anisotropy.

In recent years, the problem of possible nontrivial ordering in frustrated quantum spin chains has attracted considerable attention.¹⁻⁵ Nersisyan *et al.* predicted¹ that in an anisotropic (easy-plane) antiferromagnetic $S=\frac{1}{2}$ chain with sufficiently strong frustrating next-nearest-neighbor (NNN) coupling, a new phase with a broken parity would appear, which would be characterized by the nonzero value of *chirality*

$$\kappa_n^z \equiv \langle (\mathbf{S}_n \times \mathbf{S}_{n+1})_z \rangle; \quad (1)$$

note that definition (1) differs from the other, so-called scalar chirality $\tilde{\kappa} \propto \mathbf{S}_{n-1} \cdot (\mathbf{S}_n \times \mathbf{S}_{n+1})$ which is often discussed in the context of the isotropic spin chains.⁶ This prediction was made on the basis of the bosonization technique combined with a subsequent mean-field-type decoupling procedure. A similar conclusion can be reached⁷ by means of a mean-field decoupling of the quartic terms in the Jordan-Wigner transformed fermionic version of the Hamiltonian, in the spirit of the Haldane's treatment of a spontaneously dimerized phase.⁸ Up to now, however, this prediction for $S=\frac{1}{2}$ was not confirmed in numeric studies.^{4,2} On the other hand, *two* different types of chiral ordered phases, gapped and gapless, were found numerically in the $S=1$ easy-plane frustrated chain.^{4,5} At present, to our knowledge, there is no theoretical analysis addressing the problem of chiral ordered phases for the $S \geq 1$ case.

The aim of the present Communication is to study the generic large- S behavior of antiferromagnetic easy-plane integer- S chain with frustrating NNN interaction, described by the following Hamiltonian:

$$\hat{H} = J \sum_n \{ (\mathbf{S}_n \mathbf{S}_{n+1})_\Delta + j (\mathbf{S}_n \mathbf{S}_{n+2})_\Delta + D (S_n^z)^2 \}. \quad (2)$$

Here, $(\mathbf{S}_1 \mathbf{S}_2)_\Delta \equiv S_1^x S_2^x + S_1^y S_2^y + \Delta S_1^z S_2^z$, \mathbf{S}_n denotes the spin- S operator at the n th site, the lattice spacing a has been set to unity, $J > 0$ is the nearest-neighbor exchange constant, $j > 0$ is the relative strength of the NNN coupling, and $0 < \Delta < 1$ and $D > 0$ are, respectively, the dipolar (inter-ion) and the single-ion anisotropies.

We argue that the existence of gapless and gapped chiral phases found in Refs. 4 and 5 is not specific for $S=1$, but is

rather a generic large- S feature. Estimates for the corresponding transition boundaries are obtained, and a sketch of the typical phase diagram is presented. As a side result, we also show that the domain of stability of the Haldane phase against the anisotropy variation grows when the frustrating coupling j is increased, in accordance with the numerical results.⁹

We use the well-known technique of spin coherent states^{12,13} which effectively replaces spin operators by classical vectors $(S_n^+, S_n^z) = S(\sin \theta_n e^{i\varphi_n}, \cos \theta_n)$ and incorporates the quantum features by means of the path integral over all space-time configurations of (θ, φ) . The classical ground state of Eq. (2) is well known: the spins always lie in the easy plane (xy) , i.e., $\theta = (\pi/2)$, for $j < \frac{1}{4}$ the alignment of spins is antiferromagnetic, $\varphi_n = \varphi_0 + \pi n$, and for $j > \frac{1}{4}$ a helical structure with incommensurate magnetic order develops, $\varphi_n = \varphi_0 \pm (\pi - \lambda_0)n$, where $\lambda_0 = \arccos(1/4j)$, and the \pm signs above correspond to the two possible chiralities of the helix.

In one dimension the long-range helical ordering is impossible since it would imply a spontaneous breaking of the continuous in-plane symmetry; in contrast to that, the existence of the finite chirality $\kappa_n^z = \langle \sin(\varphi_{n+1} - \varphi_n) \rangle$ is not prohibited by the Mermin-Wagner theorem.

The classical *isotropic* system has for $j > \frac{1}{4}$ three massless modes with wave vectors $q=0$, $q=\pm\delta$, where $\delta \equiv \pi - \lambda_0$ is the pitch of the helix. The effective field theory for the isotropic case is the so-called $SO(3)$ nonlinear sigma model, with the order parameter described by the local rotation matrix.^{10,11} The physics becomes simpler in the presence of anisotropy since the modes with $q=\pm\delta$ acquire a finite mass. Our starting point will be the following ansatz for the angular variables θ, φ :

$$\begin{aligned} \theta_n &= \pi/2 + p_n + (\xi_n e^{i\delta n} + \xi_n^* e^{-i\delta n})/2, \\ \varphi_n &= \pi n + \psi_n + (w_n e^{i\delta n} + w_n^* e^{-i\delta n})/2. \end{aligned} \quad (3)$$

We assume that the fluctuations p, ξ, w are small and that they are smooth functions of n , slowly varying over the characteristic distance $l_0 = 2\pi/\lambda_0$; the same property is assumed for the function $\lambda_n \equiv \psi_{n+1} - \psi_n$ which can be viewed as a dual variable to ψ .¹⁴

After passing to the continuum in the effective Lagrangian $L = \int dx \mathcal{L} = \hbar S \sum_n (1 - \cos \theta_n) \partial_t \varphi_n - H(\theta, \varphi)$ we average over l_0 , making the oscillating terms disappear. The resulting expression for \mathcal{L} is

$$\begin{aligned} \mathcal{L} = & \hbar S \{ p(\partial_t \psi) (1 - |\xi|^2/4) + [w^*(\partial_t \xi) + w(\partial_t \xi^*)]/4 \} \\ & - JS^2 \{ V[\lambda] (1 - |\xi|^2/2) + A_0 p^2 + (A_1/2) |w|^2 \} - (JS^2/4) \\ & \times \{ M |\xi|^2 + F \Delta |\partial_x \xi|^2 \}, \end{aligned} \quad (4)$$

where the following notation has been used:

$$\begin{aligned} V[\lambda] = & j \cos 2\lambda - \cos \lambda - U_0 + (j/2) \cos 2\lambda (\partial_x \lambda)^2, \\ U_0 = & j \cos 2\lambda_0 - \cos \lambda_0, \quad F = \cos \lambda_0 - 4j \cos 2\lambda_0, \\ A_0 = & D + \Delta(1+j) - U_0, \quad M = 2[D - (1-\Delta)U_0], \\ A_1 = & \cos^2 \lambda_0 + j \cos^2 2\lambda_0 - U_0. \end{aligned} \quad (5)$$

Integrating out the ‘‘slave’’ fields $p \simeq -(\hbar/2JSA_0) \partial_t \psi$, $w \simeq (\hbar/2JSA_1) \partial_t \xi$, and passing to the imaginary time $y = ict$, $c = JS(2A_0)^{1/2}/\hbar$, we obtain the effective Euclidean action

$$\begin{aligned} \mathcal{A}_E = & \frac{1}{g_0} \int \int dx dy \{ \frac{1}{2} (\partial_y \psi)^2 + V[\lambda] \} (1 - \frac{1}{2} |\xi|^2) \\ & + \frac{\tilde{E}}{4g_0} \int d^2 X \{ (\partial_\mu \xi^*) (\partial_\mu \xi) + m_0^2 |\xi|^2 \}, \end{aligned} \quad (6)$$

where $(X_1, X_2) = (x, ict)$, $c' = JS(A_1 F \Delta)^{1/2}/\hbar$, $\partial_\mu = \partial/\partial X_\mu$, and the constants g_0 , \tilde{E} , m_0 are given by

$$g_0 = \frac{\sqrt{2A_0}}{S}, \quad \tilde{E} = \left(\frac{A_0 F \Delta}{A_1} \right)^{1/2}, \quad m_0^2 = \frac{M}{F \Delta}. \quad (7)$$

Further, integrating out the massive ξ yields the effective action for ψ only, with a renormalized coupling g_{eff} :

$$\begin{aligned} \mathcal{A}_E = & \frac{1}{g_{\text{eff}}} \int \int dx dy \{ \frac{1}{2} (\partial_y \psi)^2 + V[\lambda] \}, \\ g_{\text{eff}} = & g_0 \left/ \left(1 - \frac{g_0}{2\pi \tilde{E}} \ln(1 + \Lambda^2/m_0^2) \right) \right., \end{aligned} \quad (8)$$

where $\Lambda = \pi$ is the lattice cutoff. A similar derivation may be carried out for $j < 1/4$: starting from the ansatz of the type (3) with *real* ξ , w and $\delta = \pi$, one arrives at the same result (8), but with λ_0 set to zero in all quantities defined in Eq. (5) and (7).

We have mapped the initial quantum one-dimensional (1D) model to the 2D classical XY helimagnet at effective ‘‘temperature’’ g_{eff} described by the effective action (8). The validity of this mapping is determined by the requirements $g_0 \ll 1$, $|w| \ll |\xi| \ll 1$, $p \ll 1$, which translate into

$$S \gg (2A_0)^{1/2}, \quad \Lambda e^{-\pi \tilde{E}/g_0} \ll m_0 \ll S g_0 / \tilde{E}. \quad (9)$$

The first inequality above means that we are not allowed to consider large $j \gtrsim S^2/2$, and the second one requires the anisotropy to be within a certain range. We will be mainly

interested in the behavior of Eq. (8) for j close to the Lifshitz point $j_L \equiv \frac{1}{4}$, then the condition for the anisotropy transforms into

$$\zeta \pi^2 \varepsilon e^{-2\pi S \sqrt{\zeta \varepsilon}} \ll 3\mu/8 \ll 1, \quad (10)$$

where $\mu \equiv 1 - \Delta + 4D/3$, $\varepsilon \equiv |j - j_L|$, and the constant $\zeta = 1$ for $j < j_L$ and $\zeta = 2$ for $j > j_L$, respectively.

The model (8) possesses two basic types of topological defects:¹⁵ (i) domain walls connecting regions of opposite chirality, and (ii) vortices, existing inside the domains with certain chirality and destroying the long-range helical magnetic order (only quasi-long-range helical order is possible at finite g_{eff}). Thus one may expect two phase transitions: Ising-type transition (‘‘freezing’’ of the domain walls) which corresponds to the onset of the chiral order, and the Kosterlitz-Thouless (KT) transition (vortex unbinding) corresponding to the transition from the gapless chiral phase with algebraically decaying helical magnetic correlations $\langle \cos \psi(x) \cos \psi(0) \rangle \propto (1/x)^{g_{\text{eff}}/2\pi}$ to the gapped chiral phase with only short-range helical order (but still with the long-range chiral order $\langle \kappa^z(x) \kappa^z(0) \rangle \rightarrow \text{const}$, $x \rightarrow \infty$). For the *two* transitions to be possible, one has to assume that the critical temperature of the Ising-type transition is *higher* than the corresponding temperature of the KT transition. In the opposite case, only *one* chiral phase, namely the gapless one, will exist.

Inside the phase with broken chiral symmetry one can set $\psi = \pm \lambda_0 x + \phi_\pm$, then $\lambda \simeq \pm \lambda_0 + \partial_x \phi_\pm$ and $V[\lambda] \simeq \frac{1}{2} F (\partial_x \phi_\pm)^2$. One then obtains the following estimate for the KT temperature:

$$g_c^{KT} \simeq (\pi/2) \sqrt{F}. \quad (11)$$

The equation $g_{\text{eff}} = g_c^{KT}$ determines the transition from the chiral gapless to the chiral gapped phase at $j > j_L$, as well as the transition from the nonchiral ($\lambda_0 = 0$) gapless XY phase to the nonchiral gapped Haldane phase at $j < j_L$. Note that Eq. (11) is still valid away from the Lifshitz point $j = j_L$, since the field ϕ remains smooth far from the vortex core, and the KT transition temperature is determined by the logarithmic divergence in the free vortex energy at large distances.

In order to estimate the critical temperature of the Ising transition, let us first make some observations concerning the properties of chiral domain walls. The domain wall (DW) energy can be easily calculated in the vicinity of the Lifshitz point, where $\lambda \ll 1$, so that the potential $V[\lambda] \simeq (1/8) \{ (\lambda^2 - \lambda_0^2)^2 + (\partial_x \lambda)^2 \}$ takes the form of the ϕ^4 model, and one readily obtains the static DW solution $\lambda = \lambda_0 \tanh \{ \lambda_0 (x - x_{DW}) \}$ and the corresponding energy (per unit length in the y direction)

$$E_{DW} \simeq \lambda_0^3/3, \quad j - j_L \ll 1. \quad (12)$$

Further, it is easy to see that the chiral DW cannot move freely, since the infinitesimal displacement of the DW coordinate x_{DW} would cause global change of the phase ψ at $x \rightarrow \infty$. The DW can only ‘‘jump’’ by the integer multiples of π/λ_0 , then the phase at infinity changes by the integer multiples of 2π . The jump by $n\pi/\lambda_0$ involves formation of n

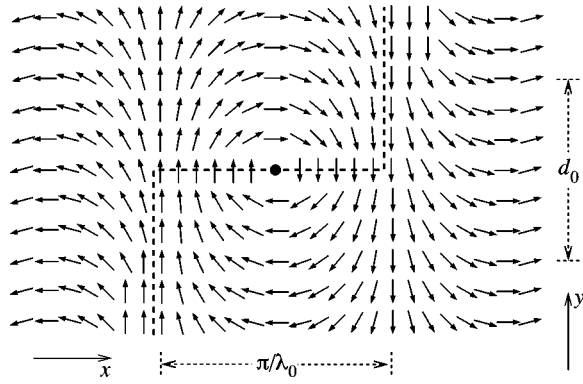


FIG. 1. Elementary “kink” of the chiral domain wall interface, corresponding to the jump of the wall by π/λ_0 . The arrows show the angle ψ ; the vortex in ψ corresponds to the two “half-vortices” in the fields $\phi_{\pm} = \psi \mp \lambda_0 x$ living at the opposite sides of the boundary. The position of the domain wall is indicated with the dashed line.

vortices bound on the DW, the elementary $n=1$ jump is schematically shown in Fig. 1. The energy per such a bound vortex can be estimated as

$$E_{bv} \approx \pi\sqrt{F} \ln(\pi/\lambda_0), \quad \lambda_0 \ll 1. \quad (13)$$

Since the Ising transition is governed by the discrete fluctuations of the DW interface, it is natural to use the so-called Müller-Hartmann-Zittartz (MHZ) approximation.¹⁶ In this approach the transition temperature is determined by looking for the point where the free energy σ of the DW interface becomes zero; a simple calculation yields the following equation for the critical coupling $g = g_c^I$:

$$\sigma = E_{DW} - \frac{g}{d_0} \ln \left[1 + d_0 \left[\coth \frac{E_{bv}}{2g} - 1 \right] \right] = 0, \quad (14)$$

where $d_0 \approx \pi/(\lambda_0\sqrt{F})$ is the characteristic size of the bound vortex in the y direction (in the derivation of Eq. (14) we have assumed that the distance along the y axis between two successive “jumps” should be greater than d_0). This equation can be solved numerically, and for $j \leq 0.26$ the solution is well fitted with the function $g_c^I \approx 1.62\lambda_0 + 0.28\lambda_0^2$, thus at $j \rightarrow j_L$ the Ising transition temperature is larger than the KT one, $g_c^I > g_c^{KT} \approx (\pi/2)\lambda_0$.

Away from the Lifshitz point the above discussion of the Ising transition is no longer valid, because the characteristic size of the bound vortex and the DW thickness become comparable with the lattice constant, and the continuum description breaks down. However, it is known¹⁴ that E_{DW} saturates at $C_{DW} \approx 0.87$ for $j \geq 0.8$; one could also speculate that for $j \rightarrow \infty$ the energy of the bound vortex $E_{bv} \rightarrow C_{bv}\sqrt{j}$, where C_{bv} is some constant, and then from Eq. (14) one obtains $g_c^I \approx C_{bv}\sqrt{j}/\ln j$ at $j \rightarrow \infty$. On the other hand, according to Eq. (11), $g_c^{KT} \rightarrow \pi\sqrt{j}$ in the same limit. Thus, one may expect that above a certain critical value of j the Ising transition temperature g_c^I becomes lower than g_c^{KT} , and the gapped chiral phase disappears.

The resulting conjectured phase diagram of the 2D helimagnet (8) is shown in Fig. 2. It should be mentioned that our picture of the transitions in the 2D XY helimagnet dis-

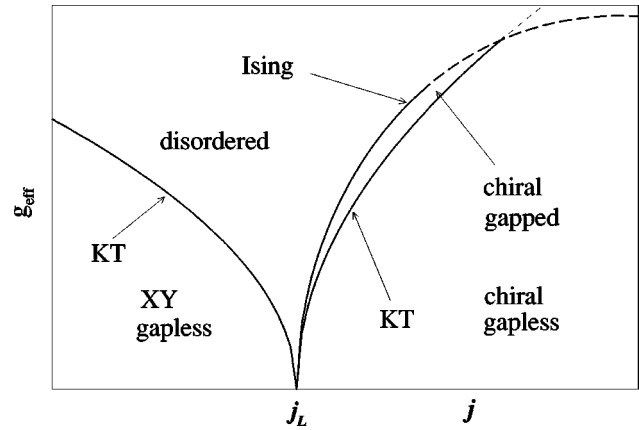


FIG. 2. Sketch of the conjectured phase diagram of the 2D helimagnet described by Eq. (8).

agrees strongly with that presented in Ref. 15. In the latter work, using the arguments of Ref. 17, it was concluded that at low temperatures the vortices are bound by strings, which would suppress the KT transition and make the Ising transition occur first with increasing the temperature. However, the argument of Ref. 17 is adequate only for systems with broken *in-plane* symmetry, which is not the case here. Another point is that in the description used in Ref. 15, the fields ϕ^{\pm} , measuring the deviations from the two *different* possible helix states with opposite chirality, are allowed to live and interact at the *same* space-time point, which, in our opinion, is rather unphysical.

The above picture of the transitions in the 2D XY helimagnet is now easily translated into the phase diagram of the frustrated spin chain, which is schematically shown in Fig. 3 for $D=0$. Very close to j_L , where $m_0 \gg \Lambda$, which in terms of $\varepsilon \equiv |j - j_L|$ and $\mu \equiv (1 - \Delta) + \frac{4}{3}D$ means $\varepsilon \ll 3\mu/(8\zeta\pi^2)$, the renormalization of the coupling constant is small, $g_{\text{eff}} \approx g_0$, and the transition boundaries are approximately given by

$$\varepsilon_c^a = \frac{K_a}{\pi^2 S^2} \left(D + \frac{3 + 5\Delta}{4} \right). \quad (15)$$

Here the coefficient $K_{C:C} \approx 1$ for the transition between gapless and gapped chiral phases, $K_{C:H} \approx 0.94$ for the transition

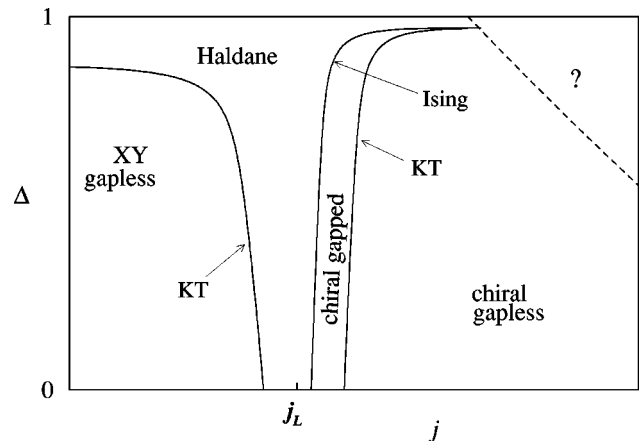


FIG. 3. Schematic phase diagram of the anisotropic frustrated spin chain (2).

from the chiral gapped to the Haldane phase, and $K_{H:XY} \approx 2$ for the Haldane-XY transition. One can see that the slope of the transition lines in the vicinity of j_L is very large (proportional to S^2), and the boundaries move closer and closer to the classical Lifshitz point $j = j_L = \frac{1}{4}$ as $S \rightarrow \infty$.

At larger deviations from $j = j_L$, when $m_0 \ll \Lambda$, one has the following equations for the phase boundaries:

$$\mu_c^a = \frac{8\zeta\pi^2}{3}\varepsilon e^{-2\pi S\sqrt{\zeta}(\sqrt{\varepsilon} - \sqrt{\varepsilon_0^a})}, \quad \varepsilon_0^a = \frac{2K_a}{\pi^2 S^2}, \quad (16)$$

which are valid for $\sqrt{\varepsilon} - \sqrt{\varepsilon_0^a} \gg 1/S$. One can see that the chiral gapped phase shrinks with increasing j . It is interesting to note that for $j < j_L$ the Haldane phase is stabilized by the frustration, in accordance with the numerical results.⁹ Further away from j_L , when λ_0 becomes of the order of 1, the theory breaks down; however, from the above arguments concerning the behavior of g_c^I we expect that the chiral gapped phase disappears above a certain critical value of j .

Certain limitations of the present theory should be mentioned. Our approach does not distinguish between integer and half-integer S , since we have integrated out the out-of-plane components, and the only remaining topological charge, in-plane vorticity, plays no role. The topological term present in the full theory of the unit vector field contains another quantum number, the so-called Pontryagin index; for $j < j_L$ this term is known¹³ to suppress the KT transition for half-integer S , preventing the appearance of the

Haldane phase. At $j > j_L$ there is no topological term,^{10,11} and one may expect that the KT transition for $j > j_L$ survives also for half-integer S . However, this point is not so clear since the ground state of a half-integer spin chain at sufficiently strong frustration is spontaneously dimerized,⁸ and our approach does not allow one to capture this feature. Another limitation is that we cannot describe the hidden (string) order in any way, and thus it is not possible to analyze the coexistence of the string order and chirality in the gapped chiral phase observed in Refs. 4 and 5 nor to study the transition to the so-called double Haldane phase characterized by the absence of the string order.¹⁸

Note added in proof. Recently, we noted that several important results on the topic have appeared. It is now believed that at least one chiral phase exists in the $S = \frac{1}{2}$ case.¹⁹ New types of chiral phases were observed numerically in the $S = 1$ chain with single-ion uniaxial anisotropy.²⁰ Chiral phase in the Josephson-junction ladder was reported.²¹ A general- S XY version of model (2) was studied via the bosonization approach,²² the results being basically in agreement with those presented here.

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