Effective field theory for the $S=1$ quantum nematic

B. A. Ivanov[1,*] and A. K. Kolezhuk[1,2,†]
[1]*Institute of Magnetism, National Academy of Sciences and Ministry of Education, 36(b) Vernadskii Avenue, 03142 Kiev, Ukraine*
[2]*Institut für Theoretische Physik, Universität Hannover, Appelstraße 2, D-30167 Hannover, Germany*
(Received 3 February 2003; revised manuscript received 22 May 2003; published 4 August 2003)

For the $S=1$ system with general isotropic nearest-neighbor exchange, we derive the low-energy description of the spin nematic phase in terms of the RP^2 nonlinear σ model. In one dimension, quantum fluctuations destroy long-range nematic (quadrupolar) ordering, leading to the formation of a gapped spin liquid state being an analog of the Haldane phase for a spin nematic. Nematic analog of the Belavin-Polyakov instanton with π_2 topological charge 1/2 is constructed. In two dimensions the long-range order is destroyed by thermal fluctuations and at finite temperature the system is in a renormalized classical regime. Behavior in external magnetic field is discussed.

DOI: 10.1103/PhysRevB.68.052401 PACS number(s): 75.10.Jm, 75.40.Cx, 75.40.Gb

Low-dimensional spin systems have been attracting permanent attention of researchers over more than half a century. A rich palette of their physical properties determined by the essential role played by quantum fluctuations makes them a very attractive playground for testing various theoretical concepts. In the last two decades, this interest has got a considerable impact, motivated particularly by the increasing availability of quasi-low-dimensional magnetic materials. A number of exotic "quantum spin liquid" states has been discovered, the most widely known example being the famous Haldane phase in integer-spin antiferromagnetic (AF) chains.[1]

A generic example of the Haldane phase is the isotropic Heisenberg spin-1 AF chain. However, the most general isotropic exchange interaction for spin $S=1$ includes biquadratic terms as well, which naturally leads to the model described by the following Hamiltonian:

$$\hat{H}=\sum_{\langle n\delta\rangle}\cos\theta(\boldsymbol{S}_{\boldsymbol{n}}\cdot\boldsymbol{S}_{\boldsymbol{n}+\boldsymbol{\delta}})+\sin\theta(\boldsymbol{S}_{\boldsymbol{n}}\cdot\boldsymbol{S}_{\boldsymbol{n}+\boldsymbol{\delta}})^2, \qquad (1)$$

where $\boldsymbol{S}_{\boldsymbol{n}}$ are spin-1 operators at the lattice site $\boldsymbol{n}$, and summation over the nearest neighbors is implied. There are indications[2,3] that moderate biquadratic exchange is present in the quasi-one-dimensional compound $LiVGe_2O_6$. The points $\theta=\pi$ and $\theta=0$ correspond to the Heisenberg ferro- and antiferromagnet, respectively. In one dimension (1D), the model (1) is studied rather extensively, and a number of analytical and numerical results for several particular cases are available.[1,4–19] It is firmly established that the Haldane phase with a finite spectral gap occupies the interval $-\pi/4<\theta<\pi/4$, and the ferromagnetic state is stable for $\pi/2<\theta<5\pi/4$, while $\theta=5\pi/4$ is an SU(3) symmetric point with highly degenerate ground state.[20]

Exact solution is available[14] for the Uimin-Lai-Sutherland (ULS) point $\theta=\pi/4$ which has SU(3) symmetry. The ULS point was shown[12] to mark the Berezinskii-Kosterlitz-Thouless (BKT) transition from the massive Haldane phase into a massless phase occupying the interval $\pi/4<\theta<\pi/2$ between the Haldane and ferromagnetic phase; this is supported by numerical studies.[13]

The properties of the remaining region between the Haldane and ferromagnetic phase are more controversial. The other Haldane phase boundary $\theta=-\pi/4$ corresponds to the exactly solvable Takhtajan-Babujian model;[15] the transition at $\theta=-\pi/4$ is of the Ising type and the ground state at $\theta<-\pi/4$ is spontaneously dimerized with a finite gap to the lowest excitations.[4–9,13] The dimerized phase extends at least up to and over the point $\theta=-\pi/2$ which has a twofold degenerate ground state and finite gap.[16–18]

Chubukov[11] used the Holstein-Primakoff-type Bosonic representation of spin-1 operators[10] based on the quadrupolar ordered "spin nematic" reference state with $\langle\boldsymbol{S}\rangle=0$, $\langle S_{x,y}^2\rangle=1$, $\langle S_z^2=0\rangle$, and suggested, on the basis of the renormalization group (RG) arguments, that the region with $\theta\gtrsim5\pi/4$ is a disordered nematic phase. Early numerical studies[21] seemed to have ruled out this possibility, and a common belief now[22,23] is that the dimerized phase extends all the way up to the ferromagnetic phase, i.e., that it exists in the entire interval $5\pi/4<\theta<7\pi/4$. However, recent numerical results[24] indicate that the dimerized phase ends at certain $\theta_c>5\pi/4$, casting doubt on the conclusion reached nearly a decade ago.

The aim of the present paper is to show that the low-energy dynamics of the model (1) for $\theta\gtrsim5\pi/4$ can be effectively described by the nonlinear σ model for a unit *director* field (i.e., a unit vector whose opposite directions are physically identical). The coupling constant becomes small in the vicinity of the ferromagnetic phase boundary $\theta=5\pi/4$. This formulation allows one to establish many properties of the nematic phase by using extensive results available for the standard (vector field) O(3) nonlinear σ model. We also study the effect of external magnetic field, which can be easily incorporated in our formalism. We argue that in 1D the ground state is disordered, in a complete analogy with the Haldane phase in case of the vector O(3) model, and its elementary excitation is a massive triplet. In 2D, long-range nematic order exists only at $T=0$. An explicit solution for the Belavin-Polyakov instanton with *half integer* charge in a $(1+1)$-dimensional isotropic nematic is presented.

We start by introducing the following set of coherent states for $S=1$:

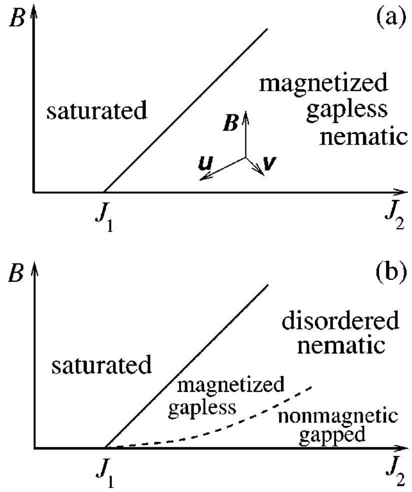

FIG. 1. Schematic $T=0$ phase diagram of the model (1) in the vicinity of the critical point $J_2=J_1$: (a) in dimension $D\geqslant 2$; (b) in one dimension.

$$|\boldsymbol{u},\boldsymbol{v}\rangle=\sum_j (u_j+iv_j)|t_j\rangle, \quad j\in(x,y,z), \tag{2}$$

where $|t_j\rangle$ are three ''Cartesian'' spin-1 states:

$$|\pm\rangle=\mp(1/\sqrt{2})(|t_x\rangle\pm i|t_y\rangle), \quad |0\rangle=|t_z\rangle. \tag{3}$$

The coherent state is characterized by vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ satisfying the normalization constraint $\boldsymbol{u}^2+\boldsymbol{v}^2=1$. The freedom to choose an overall phase factor can be fixed by setting $\boldsymbol{u}\cdot\boldsymbol{v}=0$. It is easy to check that the resolution of identity $(3/4\pi^2)\int\mathcal{D}(\boldsymbol{u},\boldsymbol{v})|\boldsymbol{u},\boldsymbol{v}\rangle\langle\boldsymbol{u},\boldsymbol{v}|=1$ holds.

In what follows we are interested in the region around $\theta=5\pi/4$, hence it is convenient to use the notation

$$\cos\theta\equiv -J_1, \quad \sin\theta\equiv -J_2, \quad J_2\gtrsim J_1>0.$$

Using the states (2), one can construct the coherent state path integral, and the effective Lagrangian will have the form

$$L_{\text{eff}}=-2\hbar\sum_{\boldsymbol{n}} \boldsymbol{v}_{\boldsymbol{n}}\cdot\partial_t\boldsymbol{u}_{\boldsymbol{n}}-\sum_{\langle \boldsymbol{n}\boldsymbol{\delta}\rangle}\langle\hat{h}_{\boldsymbol{n},\boldsymbol{n}+\boldsymbol{\delta}}\rangle, \tag{4a}$$

where the average of the local Hamiltonian for two neighboring sites 1 and 2 is, up to a constant, given by

$$\begin{aligned}\langle\hat{h}_{12}\rangle=&-4J_1\{(\boldsymbol{u}_1\cdot\boldsymbol{u}_2)(\boldsymbol{v}_1\cdot\boldsymbol{v}_2)-(\boldsymbol{u}_1\cdot\boldsymbol{v}_2)(\boldsymbol{v}_1\cdot\boldsymbol{u}_2)\}\\ &-J_2\{(\boldsymbol{u}_1\cdot\boldsymbol{u}_2-\boldsymbol{v}_1\cdot\boldsymbol{v}_2)^2+(\boldsymbol{u}_1\cdot\boldsymbol{v}_2+\boldsymbol{v}_1\cdot\boldsymbol{u}_2)^2\}\\ &-\boldsymbol{B}\cdot(\boldsymbol{u}_1\times\boldsymbol{v}_1+\boldsymbol{u}_2\times\boldsymbol{v}_2).\end{aligned} \tag{4b}$$

Here we have included the Zeeman term $-\boldsymbol{B}\cdot\Sigma_{\boldsymbol{n}}\boldsymbol{S}_{\boldsymbol{n}}$ describing external magnetic field $\boldsymbol{B}$.

Assuming a uniform ground state and minimizing $\langle\hat{H}\rangle$, one arrives at the mean-field phase diagram shown in Fig. 1(a): at zero field the ferromagnetic phase with $u=v=1/\sqrt{2}$ is stable for $J_2<J_1$, and at $J_2=J_1$ one has a degenerate first-order transition into the nematic phase with $\boldsymbol{v}=0$ and parallel alignment of $\boldsymbol{u}$ (actually, $\boldsymbol{u}$ and $\boldsymbol{v}$ can be used on equal terms, and we just voluntarily choose $\boldsymbol{v}$ to be zero in the ground state). Note that vector $\boldsymbol{u}$ is in this case a *director* since $\boldsymbol{u}$ and $-\boldsymbol{u}$ correspond to the same state. In external field the system acquires finite magnetization $\langle\boldsymbol{S}\rangle=\boldsymbol{B}/[Z(J_2-J_1)]$, where Z is the coordination number of the lattice, while nematic order persists in plane perpendicular to $\boldsymbol{B}$. The magnetization increases with the field, and at $B=Z(J_2-J_1)$ the nematic undergoes a second-order phase transition into the phase with fully saturated magnetic moment.

Our next aim is to study how the above classical mean-field picture changes due to quantum or thermal fluctuations. We pass to the continuum limit in Eqs. (4a) and (4b), viewing $\boldsymbol{u}$ and $\boldsymbol{v}$ as smooth field distributions. From the mean-field solution one may assume that $v\ll u$, and from the form of the Lagrangian (4a) it is clear that $\boldsymbol{v}$ plays the role of momentum conjugate to $\boldsymbol{u}$, so that $\boldsymbol{v}$ will be eventually proportional to the time derivative of $\boldsymbol{u}$ (later this will be checked in a self-consistent way). We will thus keep only terms up to the second order in $\boldsymbol{v}$, and derivatives of $\boldsymbol{v}$ will be neglected. Doing so, one obtains the following continuum version of the Lagrangian:

$$\begin{aligned}L[\boldsymbol{u},\boldsymbol{v}]=V_0^{-1}\int d^Dr\bigg\{&-2\hbar\boldsymbol{v}\cdot\partial_t\boldsymbol{u}-2Z(J_2-J_1)\boldsymbol{u}^2\boldsymbol{v}^2\\ &+2\boldsymbol{v}\cdot(\boldsymbol{B}\times\boldsymbol{u})-(J_2/2)\sum_{\alpha=1}^{Z}[(\boldsymbol{\delta}_\alpha\cdot\boldsymbol{\nabla})\boldsymbol{u}]^2\bigg\},\end{aligned} \tag{5}$$

where V_0 is the volume of the elementary cell of the D-dimensional lattice, $\boldsymbol{\delta}_\alpha$ are vectors describing the position of Z nearest neighbors with respect to a given lattice site, and constraints $\boldsymbol{u}^2+\boldsymbol{v}^2=1$, $\boldsymbol{u}\cdot\boldsymbol{v}=0$ are implied. In what follows, we will assume for simplicity that the lattice is hypercubic, then $Z=2D$, $V_0=a^D$, and $(\boldsymbol{\delta}_k\cdot\boldsymbol{\nabla})=a\nabla_k$, $k=1\cdots D$, where a is the lattice constant.

The ''slave'' variable $\boldsymbol{v}$ under the assumption $v\ll u$ can be integrated out, yielding

$$\boldsymbol{v}=[2Z(J_2-J_1)]^{-1}\{(\boldsymbol{B}\times\boldsymbol{u})-\hbar\partial_t\boldsymbol{u}\}. \tag{6}$$

Substituting Eq. (6) back into Eq. (5) gives the following effective Lagrangian depending on $\boldsymbol{u}$ only:

$$L_{\text{eff}}=\frac{J_2}{c^2}\int\frac{d^Dr}{a^{D-2}}\left\{\left(\partial_t\boldsymbol{u}-\frac{\boldsymbol{B}\times\boldsymbol{u}}{\hbar}\right)^2-c^2\sum_{k=1}^{D}(\nabla_k\boldsymbol{u})^2\right\}, \tag{7}$$

where $c=[2ZJ_2(J_2-J_1)]^{1/2}a/\hbar$ is the characteristic limiting velocity, and $\boldsymbol{u}$ now should be considered as a unit vector, $\boldsymbol{u}^2=1$. Note that according to Eq. (6) a change of sign of $\boldsymbol{u}$ automatically means a sign change for $\boldsymbol{v}$, so that $\boldsymbol{u}$ is in this approximation completely equivalent to $-\boldsymbol{u}$. The above description is valid at the energy scales $E<E_0=2Z(J_2-J_1)$. One readily observes that Eq. (7) is nothing but the Lagrangian of the well-known nonlinear σ model used as the effective theory for antiferromagnets[1,25] (without the topological term). Even the additional terms in the second line of Eq. (7), describing the effect of the external magnetic field, are identical to those appearing in the σ model for antiferromagnets. Thus, the low-energy dynamics of model (1) in the nematic phase is similar to the dynamics of an antiferromagnet, with

the only yet *important* difference that instead of the unit vector of sublattice magnetization one now has the nematic director $\boldsymbol{u}$: the order parameter space is RP^2 instead of S^2. The σ-model formulation, in contrast to the spin-wave approach of Chubukov,[11] allows one to study full nonlinear dynamics of the problem.

At zero field, one can rewrite the Lagrangian (7) in a standard notation using dimensionless space-time variables $x=(x_0,\boldsymbol{x})$, $\boldsymbol{x}=\boldsymbol{r}/a$, $x_0=ict/a$. The effective Euclidean action takes the following compact form:

$$\frac{\mathcal{A}_{\mathrm{E}}}{\hbar}=\frac{1}{2g}\int\left(\frac{\partial\boldsymbol{u}}{\partial x_\mu}\right)^2 d^{D+1}x, \tag{8}$$

with the coupling constant g is defined as

$$g=\{Z(J_2-J_1)/2J_2\}^{1/2}. \tag{9}$$

Note that smallness of the coupling constant does not require a large-S approximation, and is controlled solely by the closeness to the ferromagnetic phase boundary.

In one dimension $(D=1)$ continuous symmetry cannot be broken, and the ground state of Eq. (8) is disordered with exponentially decaying correlations. The correlation length ξ for the usual O(3) (vector) σ model can be obtained within Polyakov's RG approach[26] as $\xi_{O(3)}\sim ae^{2\pi/g}$. In the RP^2 σ model, however, there is a rescaling in flow equations because of the change in the measure: the physical field is not $\boldsymbol{u}$, but the bilinear projector $R=\boldsymbol{u}^T\otimes\boldsymbol{u}$. The action can be rewritten as

$$\frac{\mathcal{A}_{\mathrm{E}}}{\hbar}=\frac{1}{4g}\int\langle\partial_\mu R,\partial_\mu R\rangle d^{D+1}x, \tag{10}$$

where $\langle A,B\rangle=\mathrm{tr}(A^TB)$ denotes the scalar product. The β function in the leading order is the same as for the O(3) model,[27] $\beta(\Gamma)=-(1/2\pi)\Gamma^2$, with the trivially rescaled coupling constant $\Gamma=2g$. Thus for the correlation length in the RP^2 σ model one obtains

$$\xi_{RP^2}\sim ae^{\pi/g}=ae^{\pi\sqrt{J_2/(J_2-J_1)}}, \tag{11}$$

in agreement with Chubukov's one-loop RG result[11] for interacting spin waves. The elementary excitation is a massive spin-1 triplet, and the gap $\Delta=\hbar c/\xi$ opens up exponentially slow as one moves away from the phase transition point $J_2=J_1$:

$$\Delta\sim 2[J_2(J_2-J_1)]^{1/2}e^{-\pi\sqrt{J_2/(J_2-J_1)}}. \tag{12}$$

The RP^2 and O(3) σ models are also different with respect to their topological excitations. In the O(3) model there is a localized solution with nonzero π_2 topological charge $Q=(1/8\pi)\int d^2x\varepsilon_{\mu\nu}\boldsymbol{u}\cdot(\partial_\mu\boldsymbol{u}\times\partial_\nu\boldsymbol{u})$, known as the Belavin-Polyakov instanton (BPI).[28] The simplest BPI with $Q=1$ is described by $w=(z-a)/(z-b)$, where the complex variable $w(\boldsymbol{u})=(u_1+iu_2)/(1-u_3)$ is defined as a function of the complex coordinate $z=x_1+ix_0$, and generally *any analytical function* $w(z)$ yields a solution.[28] The BPI action $\mathcal{A}_{BPI}=4\pi\hbar Q/g$ does not depend on the parameters a, b which can be interpreted as coordinates of elementary entities,

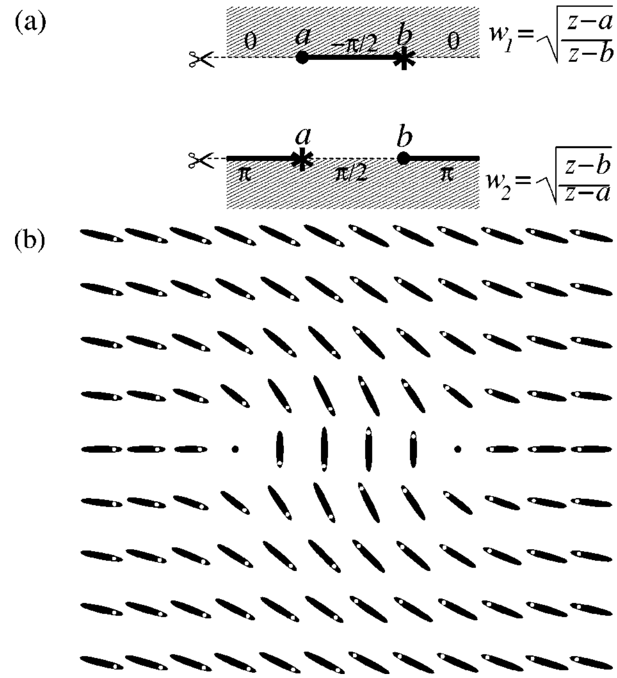

FIG. 2. Belavin-Polyakov-type soliton in a spin nematic: (a) the solution is given by $w_1(z)$ in the upper half plane (respective to the line connecting points a and b), and by $w_2(z)$ in the lower half plane, with the appropriate branch cuts shown as thick solid lines and numbers denoting the phase of w; (b) schematic view of the solution, nematic director $\boldsymbol{u}$ is shown as an ellipsoid in a projection onto the figure plane; white spot indicates the end of ellipsoid that is under the figure plane.

merons, constituting a BPI. It was speculated,[25,29] that the correlation length $\xi_{O(3)}\propto e^{\mathcal{A}_{BPI}/2\hbar}$ is related to the concentration of merons.

In the RP^2 case the director nature of the field makes possible BPI-type defects with half integer Q, whose action is exactly one-half of that for their O(3) σ model counterparts: Indeed, consider a solution of the form $w=w_1(z)=\sqrt{(z-a)/(z-b)}$. For the O(3) σ model such a solution would be invalid, because it has a branch cut. In a nematic, however, $w(\boldsymbol{u})$ and $w(-\boldsymbol{u})$ are physically identical, and the above solution can be matched with another one, $w=w_2(z)=\sqrt{(z-b)/(z-a)}$, so that $w_2(\boldsymbol{u})=w_1(-\boldsymbol{u})$ on some line. This is easily achieved by choosing the cuts as shown in Fig. 2. This solution has $Q=\pm\frac{1}{2}$, and its action is just one-half of that for the O(3) BPI. Curiously, this fact correlates with the extra factor $\frac{1}{2}$ in the correlation length exponent (11).

In the RP^2 model there is another type of topological defects, *disclinations*, characterized by a π_1 topological charge (vorticity) q. It is argued that their presence could produce the BKT transition *in the isotropic case*.[30] However, one can see that such a transition would occur above some critical value of the coupling g_{BKT} of the order of 1, and as long as $g=(1-J_1/J_2)^{1/2}\ll 1$, one may expect that the disclinations will be bound in pairs and their effect can be neglected.

Our approach easily allows one to incorporate the effect of an external magnetic field. Weak magnetic field $B<\Delta$ acts on the spectrum only in a trivial way (the Zeeman shift), but at $B=\Delta$ the gap closes and the system enters the critical phase with algebraically decaying correlations, which can be characterized as the Tomonaga-Luttinger liquid.[31] The resulting phase diagram for the one-dimensional case is shown in Fig. 1(b).

For $D=2$, at zero temperature the ground state should have long-range nematic order, in agreement with recent numerical results,[32] as long as g is small compared to some finite value g_c of the order of 1 which marks the transition into a quantum disordered phase. This latter transition is expected to be the same as a finite-temperature transition in the three-dimensional classical Lebwohl-Lasher model, which is the first order supposedly due to the effect of disclination lines.[33] At $T=0$ the phase diagram in presence of magnetic field has the mean-field form of Fig. 1(a). At $T\neq 0$ and $B=0$ nematic order is destroyed by thermal fluctuations, with the correlation length $\xi \sim a e^{2\pi J_2/T}$ (note the extra factor $\frac{1}{2}$ in the exponent, as compared to the standard result[26]).

In summary, we have shown that the low-energy dynamics of the bilinear-biquadratic $S=1$ system (1) for $\theta \gtrsim 5\pi/4$ can be effectively mapped onto the RP^2 nonlinear σ model. We have argued that in one dimension this model exhibits a disordered nematic state, supporting early proposition of Chubukov[11] and recent numerical results[24] against the commonly adopted[21–23] point of view. Using parallels with the extensively studied vector version of the σ model, one can easily extract necessary information on the properties of nematic phase. An instanton solution of the Belavin-Polyakov type with half integer topological charge is presented.

This work was supported in part by Grant No. I/75895 from the Volkswagen-Stiftung.

*Electronic address: bivanov@i.com.ua

†URL: http://www.itp.uni-hannover.de/∼kolezhuk

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