Quantum Spin Nematics, Dimerization, and Deconfined Criticality in Quasi-1D Spin-One Magnets

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(Received 19 January 2007; revised manuscript received 3 March 2007; published 13 June 2007)

We study theoretically the destruction of spin nematic order due to quantum fluctuations in quasi-one-dimensional spin-1 magnets. If the nematic ordering is disordered by condensing disclinations, then quantum Berry phase effects induce dimerization in the resulting paramagnet. We develop a theory for a Landau-forbidden second order transition between the spin nematic and dimerized states found in recent numerical calculations. Numerical tests of the theory are suggested.

DOI: 10.1103/PhysRevLett.98.247202 PACS numbers: 75.10.Jm, 71.27.+a, 75.30.Kz

In this Letter, we study various theoretical phenomena in spin $S = 1$ quantum magnets with $SU(2)$ invariant nearest neighbor interactions. Specifically, we focus on spin nematic order in such quantum magnets and its destruction by quantum fluctuations.

A general Hamiltonian describing such spin $S = 1$ quantum magnets takes the form

$$H = \sum_{\langle ij\rangle} J_{ij}\vec{S}_i \cdot \vec{S}_j - K_{ij}(\vec{S}_i \cdot \vec{S}_j)^2. \tag{1}$$

In real materials, the ratio K/J is probably small; however, it has been proposed that arbitrary values of K/J can be engineered in ultracold atomic Bose gases with spin in optical lattices [1]. We will focus exclusively on a rectangular lattice where the couplings J, K on vertical bonds are a factor of λ smaller than those on the horizontal bonds. This model was studied numerically recently (for $K > 0$) in an interesting paper by Harada *et al.* [2]. In the isotropic limit $\lambda = 1$, they found that there is a first order phase transition from a collinear Néel state to a spin nematic state (along the line $J = 0$) with order parameter

$$Q_{\alpha\beta} = \left\langle \frac{S_\alpha S_\beta + S_\beta S_\alpha}{2} - \frac{2}{3}\delta_{\alpha\beta} \right\rangle \neq 0 \tag{2}$$

even though there is no ordered moment $\langle \vec{S} \rangle = 0$. This spin nematic state corresponds to the development of a spontaneous hard axis anisotropy in the ground state. When λ is decreased from 1 to make the lattice rectangular, quantum fluctuations are enhanced. The Néel and spin nematic phases then undergo quantum phase transitions to quantum paramagnets. Interestingly, it is found that the spin nematic phase gives way to a dimerized quantum paramagnet where neighboring spin-1 moments form strong singlets along every other bond in the horizontal direction. Further, the quantum phase transition itself appears to be second order in violation of naive expectations based on Landau theory but similar to the situations studied in Ref. [3,4] for other phase transitions in quantum magnets.

In this Letter, we provide an understanding of these phenomena. First, we provide general arguments relating the spontaneous dimerization with one route to killing spin nematic order by quantum fluctuations. When applied to one dimension, our arguments explain the absence in numerical calculations [5] of the featureless quantum disordered spin nematic proposed by Chubukov [6] for spin-1 chains. Further, we show that a putative direct second order quantum phase transition between the spin nematic and dimerized phases is described by a continuum field theory with the action

$$S = \int d^3x |(\partial_\mu - iA_\mu)\vec{D}|^2 + r|\vec{D}|^2 + u(|\vec{D}|^2)^2 - v(\vec{D})^2(\vec{D}^*)^2 + \frac{1}{e^2}(\epsilon_{\mu\nu\lambda}\partial_\nu A_\lambda)^2. \tag{3}$$

Here, $\vec{D}$ is a complex three component vector, and A_μ is a noncompact $U(1)$ gauge field. The nematic phase occurs when $\vec{D}$ condenses while $\vec{D}$ is gapped in the dimerized paramagnet. This theory is an anisotropic version of the noncompact CP^2 model ($NCCP^2$). The two component version—the anisotropic $NCCP^1$ model—describes Néel-VBS transitions of easy plane spin-1/2 magnets on the square lattice [3]. A second order nematic-dimer transition on the rectangular lattice is possible if (a) this field theory has a second order transition associated with ordering of $\vec{D}$ and (b) *doubled* instantons in the gauge field A_μ are irrelevant at the corresponding critical fixed point. These instantons are relevant at the paramagnetic fixed point of Eq. (3). This leads to confinement of the $\vec{D}$ fields and to dimer order. Indeed, the dimer order parameter is simply the single instanton operator [7]. A direct second order nematic-dimer transition is thus accompanied by the dangerous irrelevance of doubled instantons and the associated two diverging length or time scales.

We will provide two different arguments to justify our results. First, we address the quantum disordering of the nematic based on general effective field theory considerations that focus on the properties of topological defects of the nematic order parameter. Second, we provide a more microscopic argument based on an exact slave "triplon" representation [8] of the $S = 1$ operators.

The order parameter manifold for the spin nematic state may be taken to be the possible orientations of the spontaneous hard axis $\hat{d}$ (the "director") and thus is S^2/Z_2. The Z_2 simply reflects the fact that $\hat{d}$ and $-\hat{d}$ are the same state. The spin nematic state allows for Z_2 point vortex defects ("disclinations") in two space dimensions. The director $\hat{d}$ winds by π on encircling such a disclination. As discussed by Lammert *et al.* [9], for classical nematics, the fate of the disclinations crucially determines the nature of the "isotropic" phase obtained when the nematic is disordered by fluctuations. If the transition out of the nematic occurs without condensing the disclinations, then a novel topologically ordered phase—interpreted in the present context as a quantum spin liquid—obtains. However, the nematic may also be disordered in a more conventional way by condensing the disclinations. In the present context, we argue that nontrivial quantum Berry phases associated with the disclinations lead to broken translational symmetry in this quantum paramagnet. Furthermore, this transition may be second order as described below (unlike the classical nematic-isotropic transition).

Following Lammert *et al.* [9], we consider the quantum phase transition out of the nematic using an effective model in terms of the director $\hat{d}$. The $\hat{d}$, $-\hat{d}$ identification requires that the $\hat{d}$ vector is coupled to a Z_2 gauge field. Thus, we consider the following action on a three dimensional spacetime lattice:

$$S = -\sum_{\langle r, r+\mu\rangle} t_\mu^d \sigma_\mu(r) \hat{d}_r \cdot \hat{d}_{r+\mu} + S_B \tag{4}$$

Here, r represent the sites of a cubic spacetime lattice, $\mu = (x, y, \tau)$, $\sigma_\mu(r) = \pm 1$ is a Z_2 gauge field on the link between r and $r + \mu$. The term S_B is the Berry phase to be elaborated below.

The Berry phases arise from the nontrivial quantum dynamics of the $\hat{d}$ vector and can be understood very simply by considering a single quantum spin $S = 1$ with a time varying hard axis $\hat{d}(\tau)$ that represents the fluctuating local director field:

$$\mathcal{H} = [\hat{d}(\tau) \cdot \vec{S}]^2 \tag{5}$$

For a *time independent* $\hat{d}$, the ground state is simply the state where the projection $\vec{S} \cdot \hat{d} = 0$. The Berry phase is obtained by considering a slow time varying closed path of $\hat{d}$ in the adiabatic approximation. There are two kinds of such closed paths that are topologically distinct. First, there are paths for which $\hat{d}$ returns to itself. For such paths, it is easy to see that the Berry phase factor is 1. Then, there are closed paths where $\hat{d}$ returns to $-\hat{d}$. In the adiabatic approximation with $S = 1$, it is easy to see that the wave function acquires a phase of π for such a path. Thus, there is a Berry phase of -1 for closed paths where $\hat{d}$ returns to $-\hat{d}$.

The phase factor of -1 for nontrivial closed time evolutions of $\hat{d}$ at a spatial site may be naturally incorporated into the effective lattice model of Eq. (4) above. First, we note that a closed loop in time where $\hat{d}$ winds by π corresponds to a configuration with Z_2 gauge flux -1 through the loop. The Berry phase is thus simply

$$e^{-S_B} = \prod_r \sigma_\tau(r). \tag{6}$$

At each space point, the product over the timelike bonds measures the flux of the Z_2 gauge field through the closed time loop at that point. Precisely, this Berry phase factor arises in Z_2 gauge theoretic formulations of a number of different strong correlation problems [10], and the theory is known as the odd Z_2 gauge theory. Thus, an appropriate effective model for disordering the $S = 1$ spin nematic state is a theory of $\hat{d}$ coupled to an odd Z_2 gauge theory [11].

The spin nematic ordered phase corresponds to a condensate of $\hat{d}$. In this phase, the Z_2 disclinations are simply associated with Z_2 flux configurations of the gauge field. Thus, the Berry phase term associated with the gauge field directly affects the dynamics of the disclinations. Disordered phases where $\hat{d}$ has short-ranged correlations may be discussed by integrating out the $\hat{d}$ field. The result is pure odd Z_2 gauge theory on a spatial lattice with rectangular symmetry. This theory is well understood. It is conveniently analyzed by a duality transformation to a stacked fully frustrated Ising model [12] followed by a soft-spin Landau-Ginzburg analysis [13]. This leads to a mapping to an XY model with fourfold anisotropy:

$$S_v = -t_v \sum_{\langle RR'\rangle} \cos(\phi_R - \phi_{R'}) - \kappa \sum_R \cos(4\phi_R). \tag{7}$$

Here, R, R' are sites of the dual cubic lattice. The real and imaginary parts of the field $e^{i\phi_R}$ correspond to Fourier components of the Z_2 vortex near two different wave vectors at which the quadratic part of the Landau-Ginzburg action has minima. The anisotropy is fourfold on the rectangular spatial lattice as opposed to the eightfold anisotropy that obtains with square symmetry [13]. There is a disordered phase where the Z_2 vortex has short-ranged correlations: this corresponds to the topologically ordered quantum spin liquid in the original spin model. In addition there are ordered phases associated with condensation of the $e^{i\phi_R}$. These phases break translation symmetry. For the rectangular lattice of interest, the natural symmetry breaking pattern is dimerization along the chain direction.

We thus see that Berry phases associated with the quantum dynamics of the director $\hat{d}$ lead to dimerization when the nematic order is disordered by condensing the Z_2 disclinations. This analysis can be easily repeated in one spatial dimension. Then, the Z_2 disclinations are point defects in spacetime. These are described by the odd Z_2 gauge theory in $1+1$ dimensions which is always confined and which has a dimerized ground state [14]. In particular, this argument shows that for $S=1$ chains, a featureless disordered spin nematic state will not exist.

Returning to two dimensions, we may now write down a field theory for the nematic-dimer transition. The Berry phases on the disclinations are encapsulated in Eq. (7). We now need to couple these back to the $\hat{d}$ vector. The main interaction between $\hat{d}$ and $e^{i\phi_R}$ is the long ranged statistical one: on going around, a particle created by $e^{i\phi}$ the vector $\hat{d}$ acquires a minus sign.

We proceed by first ignoring the κ term in Eq. (7) and using a Villain representation [15] to let

$$S_v = \sum_{\langle RR'\rangle} U j_{RR'}^2 \tag{8}$$

where $U = 1/(2t_v)$ and $j_{RR'}$ are integer valued currents of the $e^{i\phi}$ that satisfy $\vec{\nabla}\cdot\vec{j}=0$ and $(-1)^j = \prod_P \sigma$. Here, the symbol $\prod_P$ refers to a product over the four bonds of the direct lattice pierced by $\langle RR'\rangle$. This term ensures that an $e^{i\phi}$ particle acts as π flux for the $\hat{d}$ field. Substituting $\vec{j} = \vec{\nabla}\times\vec{A}$ (with A_μ integer), we get

$$(-1)^{\vec{\nabla}\times\vec{A}} = \prod_P \sigma. \tag{9}$$

Now write $A = 2a + s$ with a an integer and $s = 0, 1$ so that $\prod_P(-1)^s = \prod_P\sigma$ which can be solved by choosing $(-1)^s = \sigma$. The integer constraint on A may be implemented softly by including a term

$$-t_\theta\cos(2\pi a) = -t_\theta\sigma_{rr'}\cos(\pi A_{rr'}). \tag{10}$$

We now separate out the longitudinal part of A by letting $\vec{A}\to\vec{A}+\frac{1}{\pi}\vec{\nabla}\theta$. After a further rescaling $A\to\frac{A}{\pi}$, we finally get the action

$$S = S_d + S_\theta + S_A \tag{11}$$

$$S_\theta = -t_\theta\sum_{\langle rr'\rangle}\sigma_{rr'}\cos(\theta_r-\theta_{r'}+A_{rr'}) \tag{12}$$

$$S_A = U\sum_P(\vec{\nabla}\times\vec{A})^2 \tag{13}$$

with S_d given in Eq. (4). Summing over σ and keeping the lowest order cross term between t^d and t_θ, we get

$$S = -\sum_{\langle rr'\rangle} t_\mu\cos(\theta_r-\theta_{r'}+A_{rr'})\hat{d}_r\cdot\hat{d}_{r'} + U\sum_P(\vec{\nabla}\times\vec{A})^2 \tag{14}$$

with $t_\mu \sim t_\mu^d t_\theta$. It is instructive to introduce the complex vector $\vec{D}_r = e^{i\theta_r}\hat{d}_r$ that satisfies $|\vec{D}|^2 = 1$, $\vec{D}\times\vec{D}^* = 0$. The second condition may be imposed softly by including a term

$$v|\vec{D}\times\vec{D}^*|^2 = -v[(\vec{D})^2(\vec{D}^*)^2 - 1] \tag{15}$$

with $v > 0$. Thus we arrive at the model

$$S = S_D + S_A \tag{16}$$

$$S_D = -t\sum_{\langle rr'\rangle} e^{iA_{rr'}}\vec{D}_r^*\cdot\vec{D}_{r'} + \text{c.c.} - v(\vec{D})^2(\vec{D}^*)^2 \tag{17}$$

with $|\vec{D}|^2 = 1$. Here the v term breaks the global $SU(3)$ symmetry associated with rotations of the $\vec{D}$ down to $SO(3)$. Equation (3) is precisely a soft-spin continuum version of the lattice action above.

We now consider the role of the fourfold anisotropy on the disclination field $e^{i\phi}$ (the κ term in Eq. (7)). Without this term, the number conjugate to ϕ is conserved. In the dual description, this translates into conservation of the magnetic flux of the $U(1)$ gauge field $\vec{A}$. Thus, at $\kappa = 0$, the gauge field is noncompact. The κ term however destroys this conservation law—indeed four disclinations can be created or destroyed together. In the effective model of Eq. (3), a disclination in $\vec{D}$ corresponds to a configuration where the gauge flux is equal to π. Thus, the κ term may be interpreted as a doubled "instanton" operator that changes the gauge flux by 4π.

The nematic order parameter is simply related to the $\vec{D}$ fields:

$$Q_{\alpha\beta} = \left(\frac{D_\alpha^* D_\beta + \text{c.c.}}{2} - \frac{\delta_{\alpha\beta}}{3}\right) \tag{18}$$

Thus, when $\vec{D}$ condenses, nematic order develops. The paramagnetic phase occurs when $\vec{D}$ is gapped. In the absence of instantons, the low energy theory of this phase has a free propagating massless photon. Instantons however gap out the photon and confine the $\vec{D}$ fields. The dimer order parameter $e^{i\phi}$ is the single instanton operator and gets pinned in this phase. A direct second order transition between the nematic and dimerized states can thus occur if doubled instantons are irrelevant at the critical fixed point of the anisotropic $NCCP^2$ action associated with the condensation of $\vec{D}$.

A different more microscopic argument can also be used to justify Eq. (3) and provides further insight. Consider the following exact representation [8] of a spin-1 operator at a site i in terms of a "slave" triplon operator $\vec{w}_i$:

$$\vec{S}_i = -i\vec{w}_i^\dagger\times\vec{w}_i \tag{19}$$

together with the constraint $\vec{w}_i^\dagger\cdot\vec{w}_i = 1$. The $\vec{w}_i$ satisfy usual boson commutation relations. The nematic order parameter is readily seen to simply be

$$Q_{\alpha\beta} = \left\langle\frac{\delta_{\alpha\beta}}{3} - \frac{w_\alpha^\dagger w_\beta + \text{c.c.}}{2}\right\rangle. \tag{20}$$

As with other slave particles, this representation leads to a $U(1)$ gauge redundancy associated with letting $\vec{w}_i\to e^{i\alpha_i}\vec{w}_i$

at each lattice site. It is convenient to first consider the special point $J_{ij} = 0$ where the Hamiltonian in Eq. (1) is known to have extra $SU(3)$ symmetry. Then, H may be rewritten (up to an overall additive constant)

$$H = -\sum_{\langle ij\rangle} K_{ij}(\vec{w}_i^\dagger \cdot \vec{w}_j^\dagger)(\vec{w}_i \cdot \vec{w}_j). \qquad (21)$$

This is invariant under a global multiplication of $\vec{w}_i$ by an $SU(3)$ matrix U on one sublattice and by U^* on the other. Such magnets were studied in detail in Ref. [7], and we can take over many of their results. A standard mean field approximation with $\langle \vec{w}_i \cdot \vec{w}_j\rangle \neq 0$ yields a paramagnetic phase with gapped $\vec{w}$ particles in the $d = 1$ limit while in two dimensions, the $\vec{w}$ condense thereby breaking the $SU(3)$ symmetry. The theory of fluctuations beyond mean field includes a compact $U(1)$ gauge field. In the paramagnetic phase instanton fluctuations of this gauge field confine the $\vec{w}$ particles and their Berry phases lead to dimerization on the rectangular lattice. The results of Ref. [7] now imply that the transition associated with $\vec{w}$ condensation is described by an $NCCP^2$ model with doubled instantons; i.e., it is precisely of the form of Eq. (3) but with $v = 0$. The triplon $\vec{w}_i$ on the A sublattice $\sim\vec{D}$ while on the other sublattice $\vec{w}_i \sim \vec{D}^*$. Thus, we see that the Néel vector $\vec{N}$ is simply related to $\vec{D}$ through

$$\vec{N} \sim -i\vec{D}^* \times \vec{D} \qquad (22)$$

For the $SU(3)$ symmetric Hamiltonian all eight components of the tensor $D^*_\alpha D_\beta - |D|^2\delta_{\alpha\beta}/3$ have the same correlators. The symmetric part of this tensor is the nematic order parameter and the antisymmetric part is the Néel vector.

If now a small $J < 0$ is turned on the $SU(3)$ symmetry is explicitly broken down to $SO(3)$. This sign of J disfavors Néel ordering so that nematic ordering wins in the two dimensional limit. The $NCCP^2$ field theory of the transition to the dimer state must then be supplemented with an anisotropy term $v|\vec{N}|^2$ with $v > 0$ which due to Eq. (22) is precisely the anisotropy term of Eq. (3).

What may we say about the $NCCP^2$ field theory? While this may be studied numerically here we restrict ourselves to some simple observations. First if this theory has a critical point where $\vec{D}$ orders, the dynamical critical exponent $z = 1$. Next, we note that the instanton scaling dimension is expected to be bigger for $NCCP^2$ as compared to $NCCP^1$. In the isotropic case, existing estimates [4] give 0.63 for the single instanton scaling dimension. In a naive RPA treatment of the gauge fluctuations, the instanton scaling dimension scales like m^2N where m is the instanton charge and N is the number of boson components. Thus, within this approximation, we estimate the doubled instanton scaling dimension in $NCCP^2$ as $\frac{3}{2}(2)^2 \times (0.63) \approx 3.78$. This admittedly crude estimate nevertheless suggests that doubled instantons may be irrelevant for $NCCP^2$.

The possible irrelevance of the doubled instantons has dramatic consequences for the phenomena at the nematic-dimer transition. It implies that the critical fixed point has enlarged $U(1)$ symmetry associated with conservation of the gauge flux exactly like in Ref. [3]. This enlarged symmetry implies that the $(\pi, 0)$ columnar dimer order parameter may be rotated into the $(0, \pi)$ columnar dimer or into plaquette order parameters at $(0, \pi)$, $(\pi, 0)$. Thus right at the critical point all these different VBS orders will have the same power law correlations. It will be an interesting check of the theory of this Letter to look for this in future numerical calculations.

In summary we have studied the destruction of spin nematic order by quantum fluctuations in quasi-one-dimensional spin-1 magnets. We showed that Berry phases associated with disclinations lead to dimerization if the nematic is disordered by their condensation. We presented a continuum field theory for a putative Landau-forbidden second order transition between nematic and dimerized phases. Future numerical work or cold atoms experiments may be able to explore the physics described in this Letter.

T. S. gratefully acknowledges support from the DAE-SRC Outstanding Investigator Program in India.

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