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Chiral, nematic, and dimer states in quantum spin chains

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A phase diagram of the one-dimensional $S=\frac{1}{2}$ frustrated ferromagnetic Heisenberg model in a magnetic field is studied via a bosonization technique. Besides the ferromagnetic phase, two different nematiclike phases with additional symmetry breaking of reflections about a bond or about a site are mapped out. The prediction is made of possible fourfold degeneracy of a ground state at $H=0$ for sufficiently strong second-neighbor coupling.

The Lieb-Shultz-Mattis (LSM) theorem[1] claims that the ground state of any $S=\frac{1}{2}$ chain with translationally and rotationally invariant interaction either has a zero gap for excitations or is degenerate. While gapless behavior is peculiar for a well studied $S=\frac{1}{2}$ Heisenberg antiferromagnet,[2] a degenerate ground state with a gap exists in some frustrated models with antiferromagnetic second-neighbor (i.e., next-nearest neighbor) interaction. Thus, for the Heisenberg nearest-neighbor *antiferromagnet*, the increase of second-neighbor coupling β produces a transition to a dimerized state constructed from singlet configurations of nearest neighbors.[3,4] All the excitations in this phase have a finite gap, but the ground state is twofold degenerate since the Z_2 symmetry of translations by one site is spontaneously broken. It is a purpose of this paper to show that *different* states with broken discrete symmetry appear for *ferromagnetic* nearest-neighbor coupling.

The model I will consider reads

$$H=\sum_n -\mathbf{S}_n\cdot\mathbf{S}_{n+1}+\beta\mathbf{S}_n\cdot\mathbf{S}_{n+2}\,. \qquad (1)$$

For classical spins, it describes ferromagnetic and helical (with $\cos\theta=1/4\beta$) structures depending on whether or not β exceeds $\frac{1}{4}$. The ferromagnetic ground state clearly survives the presence of quantum fluctuations while the helical one ceases to be even a local minimum in one dimension (1D) since the classically broken SO(3) symmetry is expected to be restored by quantum fluctuations.[5] The LSM theorem thus forces us to look for other phases with presumably some discrete symmetry broken.

For the antiferromagnetic model, a search for a dimerized ground state was initiated by the observation[4] that the simple mean-field configuration constructed from noncorrelated dimers with a total spin $S=0$ is an exact ground state for a particular choice of $\beta=\frac{1}{2}$. Unfortunately, no exact solutions are known for a ferromagnetic version of the problem. However, exact ground states can be found for the anisotropic version of (1), when $\mathbf{S}_i\cdot\mathbf{S}_j$ is substituted by $S_i^\perp S_j^\perp+\Delta S_i^z S_j^z$. Namely, for $\Delta=0$ and $\beta=\frac{1}{2}$, the exact ground state is again constructed from noninteracting dimers but now the wave function of a separate dimer is $\{i,j\}=(\uparrow\downarrow+\downarrow\uparrow)/\sqrt{2}$, i.e., each dimer has $S=1$ as opposed to $S=0$ in a conventional dimerization. This exact ground-state wave function can be trivially obtained by making a rotation by π about the Z axis on the spins on even sites only from the corresponding antiferromagnetic model, where the exact ground state constructed from noninteracting dimers with $S=0$ survives also for the XY model (and more generally, for all $\Delta>-\frac{1}{2}$).[6] Rewriting each of the pair wave functions as $\{i,j\}=|0\rangle$ where $|i\rangle$ is a single-site wave function for $S=1$ and $S_z=i$ ($i=0,\pm1$), I conclude that besides a dimerization this ground state corresponds to a well-known $S=1$ XY spin-nematic phase.[7] The exact nematiclike ground state can also be found, for $\beta=\frac{1}{2}$, in the opposite case of easy-axis anisotropy: in the Ising limit it separates ferromagnetic and up-up-down-down spin configurations.

In view of the above arguments, one can expect that close to $\beta=\frac{1}{2}$ the ground state of the isotropic model (1) will also resemble a spin-nematic state, at least at relatively short spatial scales. Of course, the isotropic limit is highly nontrivial in one dimension because of the strong zero-point fluctuations. However, the formation of a nematiclike state can be checked by studying the instabilities of a well-defined ferromagnetic configuration. Really, the nematic state requires spontaneous time-reversal symmetry to be unbroken. This is not the case if the ferromagnetic instability is associated with single-particle condensation but is exactly the case if it is induced by even-particle bound-state condensation. For $S=\frac{1}{2}$, the excitations above the ferromagnetic state are created by hard-core bosons. Since only pair interactions appear in the Heisenberg model, it seems reasonable to suppose[6] that only two-particle collective excitations are important in the problem.

For the isotropic model of (1), the instability of a ferromagnetic state occurs at $\beta=\frac{1}{4}$ and involves simultaneous softening of both one- and two-particle excitations. An interest in the situation at larger β compels us to search for a region of ferromagnetic phase also for $\beta>\frac{1}{4}$. A way to get it, and also to separate single-particle and collective instabilities, is to consider the anisotropic (easy axis) version of (1) or to apply a nonzero magnetic field $H=H_z$. The results discussed below were proved to be equivalent in both cases and for definiteness I will focus on the situation in nonzero field. Classically, the field produces a canted uncollinear spin structure with helical ordering restricted to the XY plane. The XY spin components disappear at

$$H=H_c=\frac{(4\beta-1)^2}{8\beta}, \tag{2}$$

which is indeed also a condition for one-particle instability to occur while approaching this second-order spin-flip transition from the ferromagnetic phase. It is important, however, that at nonzero H this instability occurs at finite $k=k_0$, where $\cos k_0=1/4\beta$. In this case, the attractive interaction between bosons associated with the ferromagnetic sign of nearest-neighbor coupling does not go to zero at the momentum of a single-particle instability and in one and two dimensions one should expect bound states to exist below the ground state of a system of noninteracting particles.[8] In agreement with this, the exact solution of a two-particle problem for a ferromagnet shows that two-particle bound-state excitations undergo softening at *higher* fields than H_c, thus favoring unconventional ordering to arise by lowering H.

The two-particle bound-state spectrum was calculated by using a bosonization procedure based on the Dyson-Maleev transformation[9] and by solving an integral equation resulting from a summation of a ladder sequence of diagrams. I will not present the details of calculations, they are standard though cumbersome, and instead will focus on the results.

For β close to the zero-field transition value, $\beta=\frac{1}{4}$, the earliest instability of a ferromagnetic state occurs at

$$H_{\rm cr}\approx H_c+\tfrac{16}{9}(4\beta-1)^3, \tag{3}$$

against bound-state condensation with *nonzero* total momentum of a pair, $|k|\approx 2k_0$.

When β increases, $|k|$ and the gap between $H_{\rm cr}$ and H_c also grow, but at the same time the bound-state spectrum acquires a rotonlike minimum at $|k|=\pi$.[10] The roton gap diminishes with the increase of β and finally, at $\beta=\beta_c\approx 0.38$, the momentum of the earliest instability jumps from $k\approx 2k_0$ to $k=\pi$. At larger β, the earliest instability at

$$H=H_{\rm cr}^{\pi}=\frac{4\beta^2+2\beta-1}{2(1+\beta)} \tag{4}$$

is against bound-state condensation with a total momentum $|k|=\pi$.

Now I would like to discuss the spin configurations below the instability. For a moment I will neglect the role of quantum fluctuations.

First of all, the absence of a single-particle condensation ensures that the time-reversal symmetry is unbroken for the XY spin components, i.e., the expectation values $\langle S_x\rangle$ and $\langle S_y\rangle$ are equal to zero below the instability (T symmetry is explicitly broken for S_z due to nonzero external field). So, independently of the value of β (at $\beta>\frac{1}{4}$), the XY spin ordering should be of a nematic type, i.e., one should imagine that below the instability line the ground state is filled by bound pairs of $S=\frac{1}{2}$ spins which form new local objects, "molecules." Meanwhile, the character of nematiclike ordering is different for $\beta<\beta_c$ and for $\beta>\beta_c$. In the first case, the condensation occurs at $k\approx 2k_0$ and leads to a nonzero expectation value of

$$\langle S_n^{\dagger}S_{n+\lambda}^{\dagger}\rangle\propto \exp ik\left(n+\frac{\lambda}{2}\right)\frac{1}{N}\sum_q\langle a_{q+k/2}^{\dagger}a_{-q+k/2}^{\dagger}\rangle\cos q\lambda \tag{5}$$

(a and $a^{\dagger}$ are bosonic operators introduced above a ferromagnetic state).

This term breaks down a rotational T_1 symmetry and produces massless excitations. The $\exp(ikn)$ factor in (5) indicates that the "molecules" form a uniform twist restricted by the field to the XY plane, i.e., the nematic is biaxial. Of course, a picture of locally bound pairs of $S=\frac{1}{2}$ spins (i.e., of local "molecules") is highly tentative for small k. Nevertheless, I will adopt this picture to get a qualitative description of the low-k phase.

The order parameter describing a system of twisted molecules is given by a mutually orthogonal nematic director (i.e., vector with opposite points identified) and pseudovector $\mathbf{A}_k$ ($\mathbf{A}_{-k}=-\mathbf{A}_k$) measuring a twist.[11] Nonzero field selects two possible orientations of $\mathbf{A}$ depending on the sign of k (i.e., on chirality) thus producing an additional twofold degeneracy of a ground state.[12] Thus, for a system of nematics, the total order-parameter space is isomorphic to $T_1\times Z_2$ which, as usual, differs in Z_2 degree of freedom from the order parameter space, $S_1\times Z_2$, for conventional canted uncollinear magnets.[13] An important point, however, is that the "missing" Z_2 degree of freedom is actually present in the system. This symmetry is associated with the fact that at *nonzero* k the "molecules" formed by $S=\frac{1}{2}$ spins are *chiral*: for any particular "molecule" formed by the spins at the sites n and $n+\lambda$ one can write down an n-independent quantity

$$M_{\lambda}^{z}=\langle[\mathbf{S}_n\times\mathbf{S}_{n+\lambda}]_z\rangle=\langle S_n^xS_{n+\lambda}^y-S_n^yS_{n+\lambda}^x\rangle\propto\sin\frac{k\lambda}{2}\frac{1}{N}\sum_q|\langle a_{q+k/2}^{\dagger}a_{-q+k/2}^{\dagger}\rangle|^2\cos q\lambda, \tag{6}$$

which changes the sign under the reflection about the bond, $\lambda\rightarrow-\lambda$, i.e., under the permutation of spins. This chiral symmetry does not exist if one describes the ground-state configuration in terms of nematic directors and in this respect can be viewed as an internal degree of freedom for the local objects of the $S=1$ spin nematic, which keeps a memory of the underlying $S=\frac{1}{2}$ spins. Hereafter I will refer to this state as a *chiral biaxial spin nematic*.

The condensation of bound-state excitations with $|k|=\pi$ leads to a different type of a nematiclike ordering. Now

$$\langle S_n^{\dagger}S_{n+\lambda}^{\dagger}\rangle\propto(-1)^n\sum_q\langle a_{q+\pi/2}^{\dagger}a_{-q+\pi/2}^{\dagger}\rangle\exp i\left(q+\frac{\pi}{2}\right)\lambda, \tag{7}$$

yielding a *uniaxial nematic ordering in the XY* plane with a period of two lattice spacings. Since for $k=\pi$ chiral transformation $k\rightarrow-k$ does not produce a new physical state, the order-parameter space for a system of directors is now isomorphic to T_1 which again differs in the Z_2 degree of freedom from the corresponding order-parameter space for conventional canted *collinear* magnets. Moreover, the parity-breaking order parameter of Eq. (6) turns out to be zero for $|k|=\pi$. This follows from a solution of a two-particle problem which yields the following form of the vertex function along a $|k|=\pi$ instability line

$$\Phi(q_1,q_2,k,\Omega) \propto v_{q_1} v_{q_2} \Psi(\Omega,k)\,, \tag{8}$$

where $v_q = \cos q$ in 1D and Ψ has a pole at a total momentum of a pair, $|k|=\pi$ and at zero total frequency, Ω. Hence, $\langle a^\dagger_{q+\pi/2} a^\dagger_{-q+\pi/2}\rangle \propto v_q/\mathcal{J}^\pi_q$, and since the energy of a two-particle continuum

$$\mathcal{J}^k_q = \tfrac{1}{2}(\varepsilon_{q+k/2}+\varepsilon_{-q+k/2}) = H^\pi_{\rm cr} - H_c + \frac{1+8\beta^2}{2\beta} - v_{k/2}v_q + \beta v_k v_{2q} \tag{9}$$

is an *even* function of $\cos q$ for $|k|=\pi$, the same also turns out to be true for a density of particles $\langle a^\dagger_{q+\pi/2} a_{q+\pi/2}\rangle \propto |\langle a^\dagger_{q+\pi/2} a^\dagger_{-q+\pi/2}\rangle|^2$. The absence of a chiral symmetry breaking now follows from the observation that the integral in the right-hand side of Eq. (6) is zero for all odd λ (measured in lattice units), while for even λ one trivially has $\sin\lambda k/2 = 0$.

However, the "missing" Z_2 degree of freedom is again present in the system, but in the case of $|k|=\pi$ it is associated with the possibility of two boson *umklapp* processes with a momentum transfer 2π. A condensation with nonzero $\langle a_{q+\eta\pi/2} a_{-q+\eta\pi/2}\rangle$ with $\eta = A(-1)^n$ $(A=\pm 1)$ for a given choice of nonzero $\langle a^\dagger_{q+\gamma\pi/2} a^\dagger_{-q+\gamma\pi/2}\rangle$ with, say, $\gamma=1$, produces a nonzero expectation value of

$$\langle S^z_n S^z_{n+1} - S^z_n S^z_{n-1}\rangle \propto \mathrm{sgn}A(-1)^n |\langle S^\dagger_n S^\dagger_{n+1}\rangle|^2\,, \tag{10}$$

which changes the sign under the reflection about the site. This is nothing but a well-known *dimerization*.[14] Correspondingly, a picture of *locally* paired $S=\frac{1}{2}$ spins acquires a literal meaning.

The fact that the instability is induced by a simultaneous flip of neighboring spins means that the dimers thus obtained have a total spin $S=1$ as opposed to $S=0$ in a conventional dimerization. Consequently, besides dimerization the state obtained is exactly $S=1$ uniaxial spin nematic (with interatomic distance of two lattice units) placed into an external magnetic field.[15,16] I will refer to this structure as a *dimerized uniaxial spin nematic*. The corresponding ground-state wave function can be written in a mean-field approximation as

$$\Psi_\delta = \prod_{n=2l} \{n,n+\delta\},\{i,j\} = (\uparrow\uparrow + \xi\downarrow\downarrow)/(1+|\xi|^2)^{1/2} \Longrightarrow (|1\rangle + \xi|-1\rangle)/(1+|\xi|^2)^{1/2}\,, \tag{11}$$

where ξ grows from zero as the field decreases from $H^\pi_{\rm cr}$, and $\delta=\pm 1$ ensuring twofold degeneracy of the nematic ground state due to dimerization.

In a preceding discussion I neglected the role of quantum fluctuations. In 1D they are known to restore any continuous symmetry. However, for high enough fields fluctuations do not destroy chiral and dimerized nematic phases since massless behavior is known to survive the restoration of a T_1 symmetry. The proposed phase diagram for moderate fields is presented in Fig. 1. The transition between chiral and dimerized nematic phases is predicted

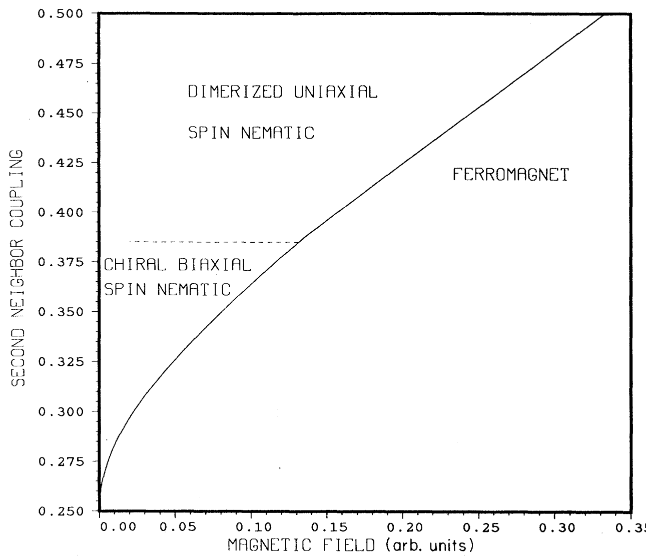

FIG. 1. Phase diagram of a frustrated $S=\frac{1}{2}$ Heisenberg magnet with ferromagnetic nearest-neighbor coupling $(=1)$ and antiferromagnetic second-neighbor coupling. The solid line corresponds to a two-particle instability which occurs at higher fields than a single-particle one and leads to a dimerized uniaxial nematic phase or to a chiral biaxial nematic phase depending on whether or not second-neighbor coupling exceeds a critical value of 0.38. The dashed line is a first-order transition line between different nematic phases. At low fields, the phase diagram will be different due to strong zero-point fluctuations.

to be of the first order since they have different discrete symmetries broken.

At zero field, fluctuations are believed to restore the symmetry completely and to produce a gap for all would-be massless excitations. The situation with a discrete symmetry is less clear, but the arguments presented above point out that both chiral and dimerized spin nematics have discrete symmetries (of reflection about a bond or about a site) which are internal symmetries for the description in terms of nematic directors. Though at this moment I enter into a speculative region, it seems reasonable to suppose that the decoupling between internal degrees of freedom and the nematic ones will preserve at $H=0$ as well, and the breakdown of internal Z_2 symmetry will survive the presence of quantum fluctuations in agreement with the LSM theorem. Note that the proposed liquid state of a chiral nematic at $H=0$ differs from a chiral spin liquid state currently topical in two dimensions[17] in that the spontaneously broken P symmetry is not combined with the T symmetry which seems to be unbroken at zero field.

Another possibility for a breakdown of a discrete symmetry at $H=0$ exists already within the description of the uniaxial phase in terms of a nematic director. The point is that in a $S=1$ bilinear-biquadratic model, the $S=1$ nematic state at $H=0$ is known to be substituted, in the presence of 1D fluctuations, not by a paramagnetic state but by a dimerized state constructed from singlet configurations of $S=1$ neighboring spins.[18,19] One can expect that the same effect will happen here, i.e., besides "internal" dimerization there will be an additional breaking of the Z_2 symmetry of translations by one site of a doubled lattice. At present, I do not know whether the whole region of a "quasiclassical" uniaxial nematic phase will be doubly dimerized, or there will be two regions with twofold (internal) and fourfold degeneracy.[20]

As an argument in favor of fourfold degeneracy at large β, the bosonic approach similar to that in Ref. 19 shows that at least in the "spin-wave" approximation the unique ground state of second-neighbor $S=\frac{1}{2}$ Heisenberg antiferromagnet becomes unstable against period-four dimerization for arbitrarily small ferromagnetic nearest-neighbor coupling.

In conclusion, I considered the phase diagram of the $S=\frac{1}{2}$ frustrated 1D Heisenberg ferromagnet. Besides the ferromagnetic phase, two different phases of biaxial and uniaxial spin nematic are mapped out. In both nematiclike phases there is an additional symmetry breaking of reflections about a bond or about a site, respectively.

The prediction is made about possible fourfold degeneracy of a ground state at $H=0$ for sufficiently strong second-neighbor coupling.

The nematiclike states were intensively searched for in two dimensions with most of the efforts focused on the antiferromagnetic J_1,J_2,J_3 model[21] in a region of parameters where quantum fluctuations restore a continuous symmetry.[22] The present analysis points out that nontrivial ground states in the 2D case can also exist near the ferromagnetic instability line, since in two dimensions an earliest instability in a magnetic field also comes from a condensation of *collective* excitations. The difference, however, is that in the 2D case a classical ground state is not destroyed by quantum fluctuations at $T=0$ (or, to be more exact, quantum corrections do not diverge) and one thus has to compare the energies of a conventional ground state and those induced by a condensation of collective excitations.

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