Incommensurate Spin Correlations in Spin-1/2 Frustrated Two-Leg Heisenberg Ladders

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We develop a low-energy effective theory for spin-1/2 frustrated two-leg Heisenberg spin ladders. We obtain a new type of interchain coupling that breaks parity symmetry. In the presence of an *XXZ*-type anisotropy, this interaction gives rise to a novel ground state, characterized by incommensurate correlations. In the case of a single ladder, this state corresponds to a spin nematic phase. For a frustrated quasi-one-dimensional system of infinitely many weakly coupled chains, this state develops true three-dimensional spiral order. We apply our theory to recent neutron scattering experiments on Cs_2CuCl_4. [S0031-9007(98)06682-4]

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Quantum spin chains have for a long time attracted the attention of both theorists and experimentalists. One of the main reasons for this continuing fascination is the dominant role played by quantum fluctuations in these systems, which lead to a rich variety of observed physical phenomena. In recent neutron scattering experiments [1] on the quasi-one-dimensional frustrated Heisenberg antiferromagnet Cs_2CuCl_4, an intriguing type of spiral order was observed and analyzed in the framework of semiclassical mean-field theory. However, on the quantum level, the very existence of such spiral order, which is an *incommensurate* structure, is rather puzzling. According to the standard lore, three-dimensional ordering of quasi-1D systems results from stabilization of the dominant spin correlations in the underlying 1D constituents. Therefore, 3D spiral order would require strong incommensurate 1D spin correlations. This is in contradiction with the known properties of simple antiferromagnetic Heisenberg spin-1/2 chains and ladders, where the only known mechanisms for generating incommensurabilities are via external magnetic fields or Dzyaloshinskii-Moria interaction.

In the present Letter we propose a novel mechanism that naturally gives rise to incommensurate correlations in spin ladders and quasi-1D materials in the absence of external fields. Interestingly, we find that this phenomenon occurs in a standard model of two coupled spin-1/2 zigzag Heisenberg chains, which has attracted much recent interest [2,3].

In the bulk of this Letter we shall concentrate on this simple frustrated ladder system in order to clearly exhibit the precise nature of the mechanism of incommensurate spin correlations. The application of our results to the quasi-1D case relevant for Cs_2CuCl_4 is briefly discussed at the end. In what follows we derive the low-energy effective theory for the zigzag ladder system, which we find to contain a parity-breaking interchain interaction. This "twist term," which was not considered in previous studies, is an operator of conformal spin 1 [4] and has important consequences: We will show that, although it alters the position of phase boundaries already in the spin rotationally invariant [SU(2)] case, it leads to incommensurate correlations only in the presence of an easy plane *XXZ* anisotropy.

The Hamiltonian of the anisotropic zigzag Heisenberg ladder is

$$\begin{aligned} H = J \sum_{j=1,2} \sum_n \{\mathbf{S}_{j,n} \cdot \mathbf{S}_{j,n+1} + (\Delta - 1) S^z_{j,n} S^z_{j,n+1}\} \\ + J' \sum_n \{\mathbf{S}_{1,n} + \mathbf{S}_{1,n+1}\} \cdot \mathbf{S}_{2,n} \\ + J' \sum_n (\Delta' - 1)\{S^z_{1,n} + S^z_{1,n+1}\} S^z_{2,n}, \end{aligned} \tag{1}$$

where $|J'| \ll J$ are the exchange couplings, and $|\Delta| \leq 1, |\Delta'| \leq 1$ are the anisotropy parameters.

In order to derive the low-energy effective field theory for (1) we use standard bosonization techniques [5]. In the continuum limit the spin operators decompose as $\mathbf{S}_{j,n} \to a_0[\mathbf{J}_j(x) + (-1)^n \mathbf{n}_j(x)]$, where a_0 is the lattice spacing and $x = na_0$. Here $\mathbf{J}_j(x)$ and $\mathbf{n}_j(x)$ are the smooth and staggered components of the magnetization operator. In the framework of the bosonization method these quantities are expressed in terms of canonical Bose fields $\Phi_j(x)$ and their dual counterparts $\Theta_j(x)$, where $[\Theta_j(t,x), \Phi_j(t,x')] = -i\theta(x - x')$. Changing to symmetric/antisymmetric combinations $\Phi_\pm = (\Phi_1 \pm \Phi_2)/\sqrt{2}$, the Hamiltonian density consists of several terms. The "free" part is

$$\mathcal{H}_0 = \sum_{\sigma=\pm} \frac{v_\sigma}{2} [(\partial_x \Theta_\sigma)^2 + (\partial_x \Phi_\sigma)^2], \tag{2}$$

where $v_\sigma \propto Ja_0$ are the spin velocities. In addition, there is an in-chain current-current perturbation

$$\mathcal{H}_{JJ} = g_1 \cos\sqrt{4\pi}\,\Phi_+ \cos\sqrt{4\pi}\,\Phi_- + g_2 \sum_{\sigma=\pm} [(\partial_x \Theta_\sigma)^2 - (\partial_x \Phi_\sigma)^2]. \quad (3)$$

The interchain interaction gives rise to two perturbations which we denote by $\mathcal{H}_{CC}$ and $\mathcal{H}_{PB}$, respectively,

$$\mathcal{H}_{CC} = g_3 \cos\sqrt{4\pi}\,\Phi_+ \cos\sqrt{4\pi}\,\Theta_- - g_4 \sum_{\sigma=\pm} \sigma[(\partial_x \Theta_\sigma)^2 - (\partial_x \Phi_\sigma)^2], \quad (4)$$

$$\mathcal{H}_{PB} = g_5(-\partial_x \Phi_- \sin\sqrt{4\pi}\,\Phi_+ + \partial_x \Phi_+ \sin\sqrt{4\pi}\,\Phi_-) + g_6 \partial_x \Theta_+ \sin\sqrt{4\pi}\,\Theta_- . \quad (5)$$

The perturbation $\mathcal{H}_{CC}$ is the well-known current-current interaction [2,3], which promotes dimerization and leads to the formation of a spectral gap. The perturbation $\mathcal{H}_{PB}$ is the novel parity-breaking term, which in terms of the staggered magnetization $\mathbf{n}_{1,2}(x)$ reads

$$\mathcal{H}_{PB} \sim \mathbf{n}_1 \cdot \partial_x \mathbf{n}_2 - \mathbf{n}_2 \cdot \partial_x \mathbf{n}_1 + (\Delta' - 1)[n_1^z \partial_x n_2^z - n_2^z \partial_x n_1^z]. \quad (6)$$

The in-chain coupling constants $g_{1,2}$ are determined by J and Δ, whereas $g_3, \ldots, g_6$ are functions of J', Δ'.

Close to the SU(2) symmetric point $\Delta = \Delta' = 1$, the bosonized Hamiltonian can be expressed in terms of four Majorana fermions [3,5]. The Hamiltonian of two decoupled chains simply becomes $\mathcal{H}_0 = -i\frac{v_s}{2}\sum_{j=0}^{3}(\xi_R^j \partial_x \xi_R^j - \xi_L^j \partial_x \xi_L^j)$. The perturbation $H' = \mathcal{H}_{JJ} + \mathcal{H}_{CC} + \mathcal{H}_{PB}$ is of the form

$$H' = \sum_{j=1}^{3} \alpha_j A_j + \sum_{j=1}^{4} \beta_j B_j , \quad (7)$$

where the operators A_j and B_j are given by

$$\begin{aligned}
A_1 &= \xi_R^0 \xi_L^1 \xi_L^2 \xi_L^3 + (R \to L), \\
A_2 &= \xi_R^0 \xi_R^1 \xi_R^2 \xi_L^3 + (R \to L), \\
A_3 &= \xi_R^0 (\xi_R^1 \xi_L^2 + \xi_L^1 \xi_R^2) \xi_R^3 + (R \to L), \\
B_1 &= \xi_R^0 \xi_L^0 (\xi_R^1 \xi_L^1 + \xi_R^2 \xi_L^2), \\
B_2 &= \xi_R^0 \xi_L^0 \xi_R^3 \xi_L^3 , \\
B_3 &= \xi_R^1 \xi_L^1 \xi_R^2 \xi_L^2 , \\
B_4 &= (\xi_R^1 \xi_L^1 + \xi_R^2 \xi_L^2) \xi_R^3 \xi_L^3 .
\end{aligned} \quad (8)$$

We note that in the above formulas we have neglected terns that lead to a renormalization of the spin velocities [3]. The couplings α_j, β_k are easily expressed in terms of the g_i. The operators A_j originate from $\mathcal{H}_{PB}$, whereas the B_k's stem from $\mathcal{H}_{CC}$ and $\mathcal{H}_{JJ}$.

All operators are marginal, but while the B_k have conformal spin 0, the A_j have conformal spin 1. We derived the renormalization-group flow for the perturbation $\mathcal{H}_{\rm pert}$ from the operator product expansion for the perturbing operators (see, e.g., [4])

$$\begin{aligned}
\dot\alpha_1 &= 2\alpha_2\beta_2 + 4\alpha_3\beta_1 , \\
\dot\alpha_2 &= 2\alpha_1\beta_2 + 4\alpha_3\beta_4 , \\
\dot\alpha_3 &= 2\alpha_1\beta_1 + 2\alpha_2\beta_4 + 2\alpha_3\beta_3 , \\
\dot\beta_1 &= -4\alpha_2\alpha_3 + 2\beta_1\beta_3 + 2\beta_2\beta_4 , \\
\dot\beta_2 &= -4\alpha_3^2 + 4\beta_1\beta_4 , \\
\dot\beta_3 &= -4\alpha_1\alpha_2 + 2\beta_1^2 + 2\beta_4^2 , \\
\dot\beta_4 &= -4\alpha_1\alpha_3 + 2\beta_1\beta_2 + 2\beta_3\beta_4 .
\end{aligned} \quad (9)$$

Here a dot denotes the derivative with respect to the RG logarithm const $\times \ln(\Lambda v_s/|\omega|)$, where Λ is a momentum cutoff [6]. The RG flow determined by (9) is clearly complicated. Therefore we performed a numerical analysis of (9). Our findings are the following.

(a) At the SU(2) symmetric point, the current-current interactions reach the strong coupling regime first (in the cases where the flow is towards strong coupling). This corresponds to a dimerized phase [3,7]. A new feature caused by the twist operators is that the tendency towards dimerization extends into part of the region of ferromagnetic current-current interchain interactions (see Fig. 1).

(b) Away from the SU(2) symmetric point *both* twist and current-current couplings generally (but not always) flow towards strong coupling. However, it is now possible for the twist terms to reach the strong coupling regime first (see Fig. 2). We take this as evidence for the existence of a novel phase, the physics of which is determined by the twist terms.

In order to elucidate the physics of this new phase we now turn to a mean-field analysis of the perturbations. The situation is particularly simple in the limit of very strong anisotropy, $|\Delta|, |\Delta'| \approx 0$, corresponding to two

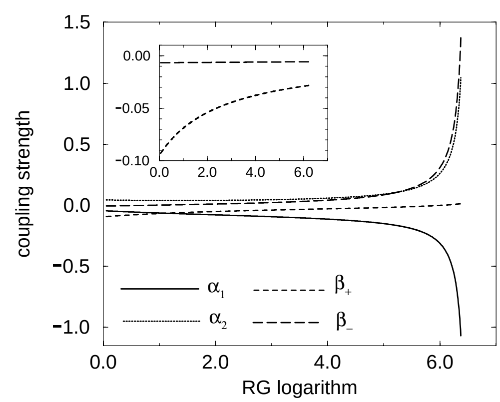

FIG. 1. RG flow in the SU(2) symmetric case. There are only 2 independent couplings for twist ($\alpha_{1,2}$) and current-current operators [$\beta_\pm = (\beta_3 \pm \beta_1)/2$], respectively. The initial conditions are chosen such that the couplings $\beta_\pm(0) < 0$ and in the absence of the twist operators would flow to zero coupling (see inset of figure).

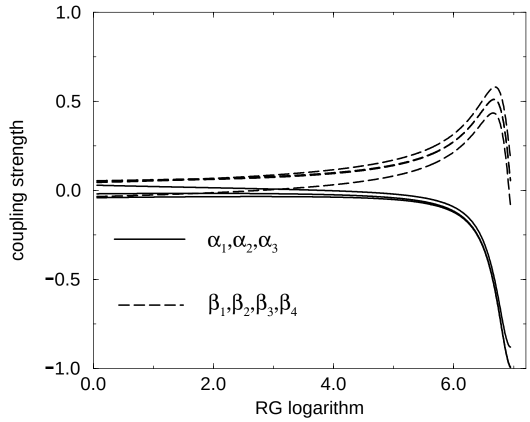

FIG. 2. Example of an RG flow where the twist couplings reach strong coupling first. The structure of Eqs. (9) is such that the twist couplings cannot grow without "help" of the current-current interaction.

coupled XX chains. Using the bosonization formulas for the XX point [4] and retaining only the relevant part of the perturbing operator we arrive at

$$\mathcal{H} = \mathcal{H}_0 + \gamma \partial_x \Theta_+ \sin\sqrt{2\pi}\,\Theta_- \,, \tag{10}$$

where $\mathcal{H}_0$ is given by (2).

In order to analyze (10) we use a self-consistent mean-field approach. Assuming that the ground state of the system is found in the sector with a nonzero topological spin current $\partial_x\Theta_+$, we arrive at the following mean-field Hamiltonian

$$\mathcal{H}_{MF} = \mathcal{H}_0 + \kappa \partial_x \Theta_+ - \mu\Lambda \sin\sqrt{2\pi}\,\Theta_- \,, \tag{11}$$

where $\kappa = \gamma\langle \sin\sqrt{2\pi}\,\Theta_-\rangle$ and $\mu\Lambda = -\gamma\langle\partial_x\Theta_+\rangle$.

Thus $\mathcal{H}_{MF}$ decomposes into two commuting parts, $\mathcal{H}_+ + \mathcal{H}_-$, with

$$\mathcal{H}_- = \frac{v_s}{2}\left[(\partial_x\Phi_-)^2 + (\partial_x\Theta_-)^2\right] - \mu\Lambda\sin\sqrt{2\pi}\,\Theta_- \,,$$

$$\mathcal{H}_+ = \frac{v_s}{2}\left[(\partial_x\Phi_+)^2 + (\partial_x\Theta_+)^2 + \frac{2\kappa}{v_s}\,\partial_x\Theta_+\right]. \tag{12}$$

The "+" channel is solved by eliminating the $\partial_x\Theta_+$ term through a field redefinition: $\Theta_+(x) \to \Theta_+(x) - \kappa x/v_s$. The average value of $\partial_x\Theta_+$ is then given by $\langle\partial_x\Theta_+\rangle = -\kappa/v_s$. The "−" channel is a sine-Gordon model for the dual field and can be solved exactly, the expectation value of the mass being $\langle\sin\sqrt{2\pi}\,\Theta_-\rangle = c(|\mu|/\Lambda v_s)^{1/3}\,\mathrm{sgn}\,\mu$, where the constant c can be calculated [8]. The self-consistency conditions then lead to the solution

$$\mu = \pm\Lambda v_s z_0^3 c^{3/2}, \qquad \kappa = \pm\Lambda v_s z_0^2 c^{3/2}, \tag{13}$$

where $z_0 = \gamma/\Lambda v_s$ is a dimensionless coupling constant. The expectation value of Θ_- is determined by the position of the minima of the sine-Gordon potential; $\langle\Theta_-\rangle = \sqrt{\pi/8}\,\mathrm{sgn}\,\mu(\mathrm{mod}\sqrt{2\pi}\,)$. This allows us to express the dual fields in chains 1 and 2 as

$$\Theta_{1,2}(x) = \frac{1}{\sqrt{2}}\,\Theta_+^0(x) - \frac{\kappa x}{\sqrt{2}\,v_s} \pm \frac{\sqrt{\pi}}{4}\,, \tag{14}$$

where $\Theta_+^0(x)$ as well as its derivative have zero expectation value. Using this together with the bosonization table at the XX point, we find the following asymptotic behavior for spin-spin correlation functions in the strong-coupling phase

$$\langle S_1^+(x)S_j^-(0)\rangle \sim \frac{(-1)^{x/a_0}}{|x|^{1/4}}\exp[-i\sqrt{\pi/2}\,(\kappa x/v_s)]\,, \tag{15}$$

where $j = 1, 2$. The transverse spin correlations still fall off with a power law, but their decay is much slower than for an isolated XX chain where $\langle n^+(x)n^-(0)\rangle \sim |x|^{-1/2}$. Furthermore, the correlations are *incommensurate*. The characteristic momentum of the magnetic spiral is $q_0 = \pi/a_0 - \sqrt{\pi/2}\,(\kappa/v_s)$. The deviation from the antiferromagnetic wave vector π/a_0 is very small for a weak interchain coupling, which is in qualitative agreement with [1]. We have performed a stability analysis of the above mean-field solution and found only convergent corrections, e.g., to the exponent $1/4$ in (15).

The solution of the XX zigzag ladder (10) describes a *spin nematic* ground state of the model. This phase, with unbroken time reversal symmetry [9] is characterized by nonzero local spin currents polarized along the anisotropy (z) axis. The longitudinal (in-chain) component of the total spin current is given by $J_{\parallel}^z(x) = -\sqrt{2/\pi}\,v_s\partial_x\Theta_+(x)$. Using equations of motion for the spin densities, one easily finds the transverse (interchain) part of the current, originating from the twist term in (10): $J_{\perp}^z(x) = -\sqrt{2/\pi}\,\gamma\sin\sqrt{2\pi}\,\Theta_-$. From the above analysis we obtain the important result that $\langle J_{\parallel}^z\rangle = -\langle J_{\perp}^z\rangle = \pm\sqrt{2/\pi}\,\gamma$. Thus, in the ground state the longitudinal and transverse spin currents are equal in magnitude but propagate in opposite directions. The resulting picture shown in Fig. 3 demonstrates local currents circulating around the triangular plaquettes in an alternating way, with the *total* spin current of the system being zero.

The spin nematic phase preserves the spin U(1) symmetry but spontaneously breaks a Z_2 symmetry of the model. Indeed, the twist term (6) is invariant under a tensor product of the site-parity and link-parity transformations [10] on the two chains, $\mathcal{P}_{12} = P_1^S \otimes P_2^L$ (though it breaks $P_1^{S(L)} \otimes P_2^{S(L)}$).

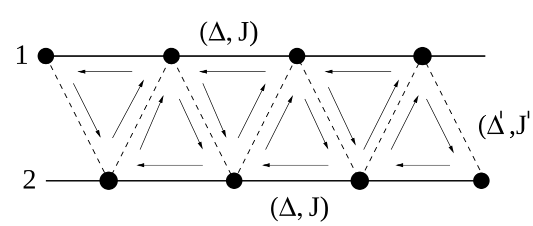

FIG. 3. Structure of the spin currents in the spin nematic phase.

In the XX case (10), this transformation reverses the signs of all currents, reflecting the Z_2 degeneracy of the ground state. The spectrum of the system contains gapless excitations in the $+$ channel, massive quantum solitons, and their bound states (breathers), as well as kinks carrying fractional topological charge.

Moving in parameter space from $\Delta, \Delta' = 0$ (XX point) to $\Delta, \Delta' = 1$ (XXX point) in the general XXZ case, we found the following.

(a) The spin-nematic phase occupies the whole region $g_4 \leq g_2$ beyond which a gap appears in the $+$ channel as well, and the spin correlations become short ranged (although they remain incommensurate).

(b) In the fully gapped phase, the spin currents and the incommensurate wave vector q_0 are reduced and continuously vanish as the SU(2) symmetric point is approached.

In light of the experimental results [1] it is important to investigate the effects of an external magnetic field. At the XX point we find that a longitudinal field has essentially only trivial effects, whereas a transverse field leads to the formation of a gap in the $+$ channel and completely destroys the spiral phase (above a critical field). Indeed, the magnetic field oriented along the x axis in spin space enters the Hamiltonian with the term [11]

$$\mathcal{H}_{\rm mag} = h \sum_{j=1,2} \sin\sqrt{4\pi}\,\Phi_j \cos\sqrt{\pi}\,\Theta_j\,,$$

where h is proportional to the applied field. This perturbation again has conformal spin 1 and, together with the twist term (10), leads to a complicated RG flow, where an effective XY anisotropy, described by the following conformal spin zero operator, is generated [11]: $\mathcal{O}_{XY} \sim h^2 \cos\sqrt{2\pi}\,\Theta_+ \cos\sqrt{2\pi}\,\Theta_-$. This strongly relevant operator locks the fields $\Theta_\pm$ at the vacuum values $\Theta_+ = \sqrt{\pi/2}$, $\Theta_- = 0$, or vice versa, and gives rise to a commensurate Néel ordering of the spins along the y axis, characterized by a nonzero average staggered magnetization $\langle n_1^y + n_2^y\rangle \sim \langle \sin\sqrt{\pi/2}\,\Theta_+\rangle\langle\cos\sqrt{\pi/2}\,\Theta_-\rangle$.

Let us now turn to the case relevant for the experiments [1], where we have two-dimensional arrays of weakly coupled chains. We illustrate our findings for the simpler XX case. The perturbation to the free part of the multichain Hamiltonian chain is

$$\mathcal{H}' = \gamma \sum_j \partial_x(\Theta_j + \Theta_{j+1}) \sin[\sqrt{\pi}\,(\Theta_j - \Theta_{j+1})]\,. \tag{16}$$

We perform a mean-field analysis in a way similar to the two-chain case above. Assuming that the following averages $\gamma\langle \sin\sqrt{\pi}\,(\Theta_j - \Theta_{j+1})\rangle = \kappa$, $\gamma\langle\partial_x(\Theta_j + \Theta_{j+1})\rangle = 2\mu$ are nonzero and redefining the fields as $\Theta_j = -2\kappa x + j\sqrt{\pi}/2 + \bar\Theta_j$, with $\langle\bar\Theta_j\rangle = 0$ we obtain a self-consistent mean-field Hamiltonian

$$\mathcal{H}_{MF} = \mathcal{H}_0[\bar\Theta_j] - 2\mu \sum_j \cos\sqrt{\pi}\,(\bar\Theta_j - \bar\Theta_{j+1})\,. \tag{17}$$

The Hamiltonian (17) can be viewed as describing coupled Josephson-junction arrays and leads to the pinning of the fields $\bar\Theta_j$. The resulting average staggered magnetization is given by

$$\langle n^\pm(x)\rangle = \exp(\pm i\pi j/2 \pm 2\sqrt{\pi}\,\kappa x)\,. \tag{18}$$

This corresponds to incommensurate spiral order along the chains with a 90° rotation of the average staggered magnetization in the transverse direction. This is in qualitative agreement with experiment [1]. Details of the above calculations as well as a more quantitative comparison to experiment will be presented in a separate publication [12].

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