Interchain Coupling Effects and Solitons in CuGeO₃

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The effects of interchain coupling on solitons and soliton lattice structures in CuGeO₃ are explored. It is shown that interchain coupling substantially increases the soliton width and changes the soliton lattice structures in the incommensurate phase. It is proposed that the experimentally observed large soliton width in CuGeO₃ is mainly due to interchain coupling effects.

The inorganic spin-Peierls (SP) system, CuGeO₃, has attracted much attention recently. Pure CuGeO₃ has a SP transition at \( T_{sp} \approx 14.3\, K \). Below \( T_{sp} \), the system is in a dimerized spin singlet state, and the gap to spin triplet excitations is \( \Delta \approx 24.5\, K \). It is known that the interchain coupling in CuGeO₃ is mainly due to interchain coupling effects.

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Jordan-Wigner transformation, and the fermionic model is bosonized. The resulting continuum Hamiltonian is
\[
\mathcal{H} = \frac{\tilde{v}}{2\pi K_\sigma} \int dx[\mathcal{K}_\sigma^2((\partial_0 \phi)^2 + (\partial_x \phi)^2) + \int dx \frac{K}{2J}u^2(x) + \frac{g_x}{2a^2} \int dx \cos(4\phi) - \frac{\beta}{a} \int dxu(x) \sin(2\phi) + \frac{\gamma^2 Z}{a^2} \int dxh(x) \cos(2\phi) + \int dx \frac{\gamma Z}{a^2} h^2(x),
\]

where \(a\) is the short distance cutoff, \(u(x) = (-1)^i u_i/a\) and \(h(x) = (-1)^i h_i/a\) are slowly varying variables. The bare value of the Umklapp term is \(g_3 = 1 - 3a_0\) and we shall assume that the renormalized \(g_3\) has approximately the same \(a_0\)-dependence.

Here \(\tilde{v}\) is the spin wave velocity and \(K_\sigma\) is a critical exponent. For the unfrustrated AFM Heisenberg spin chain, the following renormalized values should be used\[8\]: \(\tilde{v} = \pi/2\) and \(K_\sigma = 1/2\). However, the values of \(\tilde{v}\) and \(K_\sigma\) in the frustrated Heisenberg model is dependent on \(a_0\). With increase of frustration, the spin wave velocity decreases. In nonlinear sigma model\[8\], \(\tilde{v} = 0\sqrt{1 - 4a_0}\) for small \(a_0\). In a recent numerical calculation, it is shown that the variation of \(\tilde{v}\) with \(a_0\) is approximately\[8\]: \(\rho_v = 2\tilde{v}/\pi \approx (1 - 1.12a_0)\). Although we don’t know \(K_\sigma\) at finite \(a_0\) precisely, it is known\[8\] that \(K_\sigma \geq 1/2\) at small frustration \(a_0 < a_0^* \approx 0.3\). Define \(\rho_K = 2K_\rho - 1\), then \(\rho_K \ll 1\) and \(\rho_v \lesssim 1\).

For the ground state, \(u(x) = u_0\), \(h(x) = h_0\), and \(Z = Z\). If there is no Umklapp interaction \(g_3\), the model\[3\] is exactly solvable by Bethe Ansatz. Due to the \(g_3\)-term, an approximation has to be employed. We use the self-consistent Gaussian approximation, which was previously shown to be reliable for the SP chains. To this end, we write \(\phi(x) = \phi_s(x) + \tilde{\phi}(x)\), where \(\phi_s\) is the semiclassical solution and \(\tilde{\phi}\) is the fluctuation around \(\phi_s\). We retain \(\phi\) to quadratic order in the action. The first order term vanishes at the saddle point. Then,
\[
\frac{\partial^2}{\partial x^2}(4\phi_s) + \frac{1}{\xi^2} \sin(4\phi_s) = 0
\]

where
\[
\frac{1}{\xi^2} = \frac{1}{\xi_0^2} - 4\gamma Z^2 \sigma^2,
\]

and
\[
\frac{1}{\xi_0^2} = \frac{4\beta^2 J}{a^2 K} \sigma^2 - \frac{8g_3}{a^2} \sigma^4.
\]
The quantity \(\sigma\) is given by
\[
\sigma = e^{-2\langle \phi^2 \rangle}.
\]

\(\sigma\) describes the renormalization of \(g_1\) and \(g_3\) due to fluctuations of \(\phi\) around \(\phi_s\). Note the derivation is appropriate for systems with a finite gap, otherwise, \(\sigma\) has infrared divergence. In deriving these equations, we have used the self-consistent equations
\[
u(x) = (\beta J/K)\sigma \sin(2\phi_s),
\]
\[
h(x) = (\tilde{Z}/Z) \sigma \cos(2\phi_s).
\]

The “uniform” ground state (i.e. \(u_i = (-1)^i u_0a\) and \(h_i = (-1)^i h_0a\)) calculated from Eq.\[3\] corresponds to \(\sin(4\phi_s) = 0\). Therefore, either \(\phi_s = 0\) or \(\pi/4\). When \(\phi_s = 0\), \(u(x) = 0\), \(h_0 \neq 0\), the system has long range AFM order; when \(\phi_s = \pi/4\), \(h(x) = 0\), \(u_0 \neq 0\), the system is dimerized. The spin-lattice coupling and inter-chain coupling strengths dictate the solution that has the lowest energy. It is clear that on symmetry grounds these two homogeneous solutions are mutually exclusive.

The calculation of ground state energy and excitation spectrum in the self-consistent Gaussian approximation is straightforward and can be read off from Ref.\[3\], so we will just state the results. The excitation spectrum corresponding to uniform \(\phi_s\) is
\[
\omega_\phi = J\tilde{v} \sqrt{q^2 + q_0^2}
\]

In the dimerized phase \(\phi_s = \pi/4\) and \(\phi_0 = 0\), and it can be easily shown that \(q_0 = 1/\xi_0\). From Eq.\[3\], the spin triplet excitation gap is \(\Delta = J\tilde{v} q_0\). The scaling of the spin triplet excitation gap is
\[
\frac{\Delta}{2\pi J\tilde{v}} \propto \delta^{(2-2\rho_K)/(3-\rho_k)}.
\]

where \(\delta = \beta u\) is the bond alternation induced by lattice dimerization. For the unfrustrated SP chain, \(\rho_K = 1/2\), \(\rho_k = 0\), and we obtain the correct scaling relation\[8\]: \(\Delta \propto \delta^{2/3}\).

Comparing the ground state energies between dimerized phase \(\phi_s = \pi/4\) and AFM phase \(\phi_s = 0\), we get, for \(\rho_K \ll 1\), that the crossover from \(\phi_s = 0\) to \(\phi_s = \pi/4\) is determined by
\[
C_K = \frac{J\gamma Z}{\delta} \frac{\Delta}{\Delta^3} \frac{\rho_k}{\rho_v} \rho_k^{\rho_k} = 1.
\]

If \(C_K < 1\) then \(\phi_s = \pi/4\), \(\delta = \beta u\), \(h = 0\), and the system is dimerized; otherwise, \(\delta = \gamma Zh\), \(u = 0\), and the ground state has long range AFM order. A similar critical value of the interchain coupling for the unfrustrated SP model was derived by Inagaki and Fukuyama\[4\]. Using \(\Delta \approx 245K\) and \(J \approx 120K\), we find that \(C_K \approx 0.98\rho_v(0.021/\rho_v)^{\rho_k} < 1\), which is consistent with the fact that CuGeO\(_3\) is dimerized at zero temperature. Since \(\rho_v\) (\(\rho_K\)), which is less (greater) than 1(0), decreases (increases) with increase of frustration, the frustration pushes the SP-Néel transition to stronger interchain coupling. If \(\rho_v \gtrless 1\) and \(\rho_K \ll 1\), the interchain coupling is close to the critical value for the long range AFM order to be realized. This is probably significant, as materials with only 3% Zn exhibit long range AFM order.
Consider the nonuniform solutions of Eq. (3), which correspond to the solitonic excitations of the dimerized phase. In zero magnetic field, the soliton solution has lower energy than the spin-triplet excitation with the gap $\Delta$. In this case, we can continue to assume that $\bar{Z}/Z$ is a constant, and the soliton solution from Eq. (3) is

$$ u(x) \propto \sin(2\phi_s) = \pm \tanh \frac{x}{\xi} $$

with the half-width

$$ \xi = \frac{J_{a\bar{w}}}{\Delta} / \sqrt{1 - (\bar{Z}/Z)^2 C_K}. $$

The corresponding magnetization, $M(x)$, is

$$ M(x) = \cosh^{-1}(x/\xi) / (2\pi \xi) $$

and the staggered magnetization, $N(x)$, is

$$ N(x) = (-)^x \sqrt{\frac{qa}{2\pi}} \cosh^{-1}(x/\xi). $$

From Eq. (13), we can see that the soliton width is increased by interchain coupling, while the effects of frustration $\alpha_0 = J_2/J$ appear only in $\Delta$ and $\bar{w}$.

Without interchain coupling, the soliton width is $\xi_0 = J_{a\pi \rho_0}/(2\Delta) \lesssim 8a$ for CuGeO$_3$. With $\bar{Z} = Z$, $\langle S_{i,j}^z \rangle = -\langle \bar{S}_{i,j}^z \rangle$, the soliton excitation described by Eq. (12) is an array of antiferromagnetically coupled solitons in a direction perpendicular to the SP chains. As discussed in the introduction, the spins are antiferromagnetically ordered inside the soliton, therefore increased soliton size will lead to a gain in the interchain coupling energy. This is the physical origin of the increased soliton width in the presence of interchain coupling. When the interchain coupling is so strong that the soliton width diverges, i.e. $C_K = 1$, the system crosses over to the long range antiferromagnetically ordered phase. This criterion $C_K = 1$, derived from consideration of the soliton size, is the same as that derived from Eq. (13) for small $\rho_k$.

If the solitons are excited locally without forming a regular array, $\langle S_{i,j}^{z+\mu} \rangle \neq -\langle S_{i,j}^{z-\mu} \rangle$, and $\bar{Z}/Z$ is smaller than unity. The soliton size will still be increased with the increased interchain coupling $\gamma$, and AFM domains will form and increase in size. We propose that for the solitonic excitations due to magnetic or non-magnetic impurities similar AFM domains will form. The percolation of these AFM domains must be relevant to impurity induced AFM ordering in the doped CuGeO$_3$ system.

In a high magnetic field, there will be a transition from the zero field commensurate dimerized phase to the incommensurate soliton lattice phase. The ground state of this soliton lattice phase corresponds to the self-consistent periodic solutions of the coupled nonlinear equations similar to Eq. (3). Here, we consider only the qualitative aspects of the effect of the interchain coupling in the soliton lattice phase. To this end, we assume a constant $\xi$ in Eq. (3) for each chain. The effect of the interchain coupling is to renormalize $\xi$, as in Eq. (13). The periodic solution of Eq. (3) is:

$$ u(x) \propto \sin \left( \frac{x}{k \xi} \right), $$

$$ M(x) = \frac{1}{2\pi k \xi} \sin \left( \frac{x}{k \xi} \right), $$

$$ N(x) = (-)^x \sqrt{\frac{qa}{2\pi}} \cosh \left( \frac{x}{k \xi} \right), $$

where $\xi$ is the soliton width defined in Eq. (13), and $sn$, $dn$, and $cn$ are the Jacobi elliptic functions. The inter-soliton distance is $2K(k)\xi$ [see Fig. (1)], where the modulus $k$ of the elliptic integral $K$ is related to the total magnetization induced by the external magnetic field that can be derived from the minimization of the energy. These equations are the same as those of the soliton lattice without interchain coupling.

In the experiment of Kiryukhin et al. the value of $\xi$ is measured in the soliton lattice phase. The measured value of $\xi$ is $\xi = (13.6 \pm 0.3)a$, which is substantially larger than the value $\xi_0 \sim 8a$ without interchain coupling. If we use an average $\bar{Z}/Z$, from $\xi = (13.6 \pm 0.3)a$ we estimate $\bar{Z}/Z \sim 0.8$ at $\alpha_0 = 0$. With finite $\alpha_0$, the estimated $\bar{Z}/Z$ will be larger. In these experiments the inter-soliton distance is $40 \sim 70a$, so $k \sim 0.7 \sim 0.9$. The magnetization $M(x)$ and staggered magnetization $N(x)$ are shown in Fig. (1) for $k = 0.8$. The ratio $\langle M(x) \rangle / \sqrt{\langle N^2(x) \rangle}$ is 0.1, which is the right order of magnitude for the effective $\bar{Z}/Z \sim 0.8 \sim 1.0$. In the NMR experiment, the maximal value of the effective local spin is measured to be $S_{max} \sim 0.065$, which is smaller than the value corresponding to a single chain given by $\sqrt{\Delta/(J^{2} \rho_{0})}$ $\gtrsim 0.14$. However, because the solitons in the neighboring chains are antiferromagnetically coupled, the effective local magnetization at each site is reduced by the interchain effects; a reduction factor of the order of $2 \sim 3$ of $S_{max}$ is quite reasonable.

In conclusion, we have studied the combined effects of the frustration and interchain coupling on solitons and soliton-lattice excitations in CuGeO$_3$. We find that the interchain coupling can substantially increase the soliton size, while the NNN frustration will decrease it. When the interchain coupling strength is close to the SP-Néel transition, the size of the soliton diverges. The analysis of the soliton structure presented here is consistent with the experimental observations.
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24 Note that our expressions of soliton lattice solutions for $M(x)$ and $N(x)$ are slightly different from those of Fujita and Machida, but the nature of these solutions are the same as shown in Fig. 1.
25 The relation between $\langle M(x) \rangle / \sqrt{\langle N^2(x) \rangle}$ and $\tilde{Z}/Z$ is subtle, since $\langle S_i^{\perp} \rangle / \langle S_i^{\parallel} \rangle$ oscillates between $1 - \epsilon \sim 1 + \epsilon$. 

FIG. 1. The lattice distortion and magnetizations in the soliton lattice phase with $\xi = 13.6$, $k = 0.8$. The scale of $u(x)$ is arbitrary.