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## MAGNETIC STRUCTURE IN SPIN-PEIERLS SYSTEMS

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**Abstract.** - We study theoretically the magnetic structure in the incommensurate phase of spin-Peierls systems under high magnetic fields, utilizing the analytic soliton lattice solution of the mean-field Pytte Hamiltonian. The temperature and field dependence of the magnetic components of the modulated magnetization and staggered spin configuration are calculated.

### 1. Introduction

Spin-Peierls (SP) system [1] is a quasi-one-dimensional Heisenberg antiferromagnetic (AF) chain which is coupled to the spin-lattice distortion. In this system, the spin chain undergoes a second order transition to a dimerized state at a critical temperature  $T_{sp}$ . The SP transition can be regarded as the magnetic analogue of the electronic Peierls transition in low dimensional systems with the correspondence between the applied magnetic field in the SP system and the chemical potential in the Peierls system. Applying fields  $T_{sp}$  is lowered because of the reduction of the energy gain on the dimerization. Due to the commensurability, however, the dimerized phase persists up to a critical field  $B_c$ . Above  $B_c$ , it is predicted that the commensurate-incommensurate (C-IC) transition occurs and spin-lattice distortion becomes IC with the underlying lattice periodicity.

Based on the mean-field Hamiltonian developed by Pytte [2] and utilizing the mathematical equivalence to the Peierls Hamiltonian where the exact analytical solution of the soliton lattice is known, we studied the thermodynamic properties at none-zero temperatures under fields and calculated various quantities such as the magnetization, susceptibility and specific heat [3], and showed the satisfactory agreement with the experiments on the TTF-AuBDT [4]. Recently Hijmans *et al.* [5] perform the NMR and ESR experiments on the high-field phase of TTF-AuBDT which probe the local magnetic field distribution and show the evidence for an IC state. They argue that the staggered structure of the spin configuration, which is originated from the inherent AF nature, is important to explain their data, in addition to the modulated magnetization which is induced by the Zeeman energy gain and is associated with each kink giving rise to the spin 1/2 net moment. The purposes of this paper are to investigate the temperature and field dependence of the spatial variation of the magnetization associated with the soliton lattice solution in the IC phase under high fields in order to facilitate detailed analysis of the NMR and ESR experiments.

### 2. Formulation

The spin Hamiltonian for the SP system is described by

$$H = \sum_i J(i, i+1) \left( \mathbf{S}_i \cdot \mathbf{S}_{i+1} - \frac{1}{4} \right) - g\mu_B H_{ex} \sum_i S_i^z + \sum_{\mathbf{q}} \omega_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}} \quad (1)$$

where  $J(i, i+1)$  is a function of the lattice spacing,  $\mathbf{S}_i (b_{\mathbf{q}}^\dagger)$  is the spin (phonon) creation operator and  $H_{ex}$  is an external field. According to Pytte [2], we obtain the following Hamiltonian described in terms of the spinless fermion operator  $c_k$  via the Jordan-Wigner transformation:

$$H = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_{kq} g c_k^\dagger c_{k-q} (b_q + b_{-q}^\dagger) + \sum_{\mathbf{q}} \omega_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}}, \quad (2)$$

where  $\varepsilon_k = pJ \cos ka - g\mu_B H_{ex}$ .

By applying the mean-field approximation to the fermion-phonon coupling term and writing the fermion operator as  $\psi(x) = ue^{i\pi x/2a} - ive^{-i\pi x/2a}$  where  $u$  and  $v$  are slowly varying functions, the problem can be reduced to solving the so-called Bogoliubov-de Gennes equation:

$$\left[ -ihv_F \sigma_3 \frac{d}{dx} - \Delta(x) \sigma_1 - g\mu_B H \right] \begin{bmatrix} u \\ v \end{bmatrix} = \varepsilon \begin{bmatrix} u \\ v \end{bmatrix} \quad (3)$$

with  $\Delta(x) = -\frac{2g^2 a}{\omega} \langle u^* v + v^* u \rangle$  where  $\sigma_i$  is the Pauli matrix. The order parameter  $\Delta(x)$  describes the envelope of the spatial variation of the lattice distortion. It has been proved that the snoidal form

$$\Delta(x) = (1 - k') \delta \text{sn}((1 + k')\delta x, (1 - k') / (1 + k')),$$

with  $k' = \sqrt{1 - k^2}$  is the exact self-consistent solution at  $T = 0$  and also valid at finite temperatures. The two parameters  $k$  and  $\delta$  are obtained by the minimization conditions of the thermodynamic potential.

The spin polarization at  $n$ -th site

$$S_z^n(x) = \langle \psi^\dagger(x) \psi(x) \rangle - 1/2$$

is composed of the non-staggered part

$$M(x) = \langle |u|^2 + |v|^2 \rangle - 1/2$$

and the staggered part  $S(x) = i(v^* u - u^* v)$ , that is,

$$S_z^n(x) = M(x) + (-1)^n S(x).$$

Using the expression of the eigenfunctions  $u$  and  $v$ , we finally obtain [6]

$$M(x) = \rho_0 + \frac{h}{\pi} - \rho_1 (k\delta)^2 \left\{ \text{sn}^2(\delta x, k) + \text{sn}^2(\delta x + K(k), k) \right\} \quad (4)$$

$$S(x) = \rho_1 (k\delta)^2 \left\{ \text{sn}^2(\delta x, k) - \text{sn}^2(\delta x + K(k), k) \right\} \quad (5)$$

with

$$\rho_0 = \frac{1}{\pi} \int_0^\infty [f(-\varepsilon - h) + f(\varepsilon + h)] \times \\ \times \left\{ \theta((\varepsilon^2 - \delta^2)(\varepsilon^2 - (k\delta)^2)) \sqrt{\frac{\varepsilon^2 - \delta^2}{\varepsilon^2 - (k\delta)^2}} - 1 \right\} d\varepsilon \\ \rho_1 = \frac{1}{2\pi} \int_0^\infty [f(-\varepsilon - h) + f(\varepsilon + h)] \times \\ \times \left\{ \theta((k\delta)^2 - \varepsilon^2) - \theta(\varepsilon^2 - \delta^2) \right\} \frac{1}{\sqrt{(\varepsilon^2 - \delta^2)(\varepsilon^2 - (k\delta)^2)}} d\varepsilon$$

where  $f(\varepsilon)$  is the Fermi distribution function,  $K(k)$  is the complete elliptic integral of the first kind and  $h$  is the Zeeman energy normalized by  $\delta_0$  which is the gap at  $t (= T/T_{sp}) = 0$  in the C phase.

### 3. Results

We show the schematic figure of the spin polarization on each site, the curves of  $M(x)$  and  $S(x)$  and the order parameter  $\Delta(x)$  which represents the lattice distortion in figure 1. The non-staggered part  $M(x)$  is the magnetization induced by an applied field and thermal excitations across the energy gap. In the IC phase each kink carries a net spin of one-half so as to gain the Zeeman energy in compensation for the dimerization energy. The staggered part  $S(x)$  is originated from inherent AF coupling in the SP system. Its amplitude takes the maximum value at the kink site. The period of  $S(x)$  is as same as the one of  $\Delta(x)$ , on the other hand the period of  $M(x)$  is half of the one of  $\Delta(x)$ .

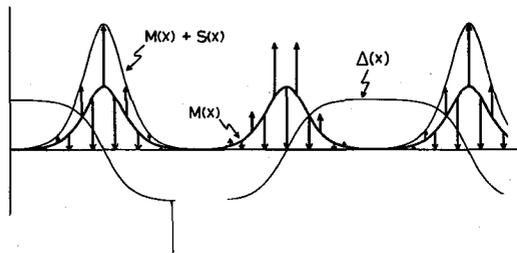


Fig. 1. - Schematic figure of spin polarization  $S_z^n$  (represented by the arrows), the curves of the non-staggered part  $M(x)$  and the staggered part  $S(x)$  and the order parameter  $\Delta(x)$ .

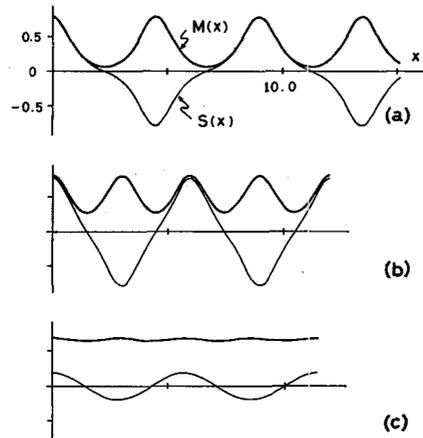


Fig. 2. - Spatial variation of  $M(x)$  and  $S(x)$  when  $h = 0.64$ (a) and  $0.68$ (b) at  $t = 0$  and  $h = 0.68$  at  $t = 0.4$ (c). The vertical axis is normalized by  $\chi_p (= 1/\pi)$ .

The spatial variations of  $M(x)$  and  $S(x)$  at some selected points in the IC phase are shown in figure 2 when  $h = 0.64$ (a) and  $0.68$ (b) at  $t = 0$  and  $h = 0.68$  at  $t = 0.4$ (c). As the field increases the period of the soliton lattice becomes short, the solitons overlap each other and the magnetization  $M$  increases. The amplitudes of  $M(x)$  and  $S(x)$  is of the same order near the C-IC transition, but  $M(x)$  tends to be uniform as  $h$  increases. The temperature dependence of the magnetic structure is important to examine the experimental data. We can calculate the magnetic structure at any points in the  $h - t$  plane. The temperature dependence of  $\rho_1 (k\delta)^2$ , which is the amplitude of the spatial modulation of  $S(x)$  is  $\sqrt{T_{sp} - T}$  near  $T_{sp}$  same as that of  $\Delta(x)$ . On the other hand the amplitude of modulated part in  $M(x)$  decreases more rapidly and behaves as  $T_{sp} - T$  in spite that  $S(x)$  still remains. The staggered component  $S(x)$  should have significant influence upon the microscopic measurements of the IC phase, which probe local fields in SP systems.

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