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MAGNETIC PROPERTIES OF THE TWO-LEG ZIG-ZAG LADDER IN QUANTUM SPIN SYSTEM NH_4CuCl_3

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ABSTRACT

MAGNETIC PROPERTIES OF THE TWO-LEG ZIG-ZAG LADDER IN QUANTUM SPIN SYSTEM NH_4CuCl_3. Numerical analysis of the two-leg zig-zag ladder as a single chain with next-nearest neighbour interactions has been formulated by Cabra (1999) with the following Hamiltonian:

$$H = J' \sum_{X=1}^{L} \{\Delta S_X^Z . S_{X+1}^Z + \frac{1}{2}(S_X^+ . S_{X+2}^- + S_X^+ . S_{X+2}^-)\} + J \sum_{X=1}^{L} \{\Delta S_X^Z . S_{X+1}^Z + \frac{1}{2}(S_X^+ . S_{X+2}^- + S_X^+ . S_{X+2}^-)\} - h \sum_{X=1}^{L} S_X^Z$$

Other formulation for two leg zig-zag ladder with dimmerized chains and coupling between the chains is as follow :

$$H = J \sum_{i=1}^{2} \sum_{x=1}^{L} (1 + (-1)^x \delta) \vec{S}_{i,x} . \vec{S}_{i,x+1} + J' \sum_{x=1}^{L} \{(1 + \delta') \vec{S}_{1,x} . \vec{S}_{2,x} + (1 - \delta'') \vec{S}_{1,x} . \vec{S}_{2,x+1} - h \sum_{i=1}^{2} \sum_{x=1}^{L} S_{i,x}^z$$

From these formulations, we study the closing of the gap at zero magnetization by means of the fine–tuning mechanism and disappreance of the ½ plateau (gap) at finite <M> by alternating dimerization of the chains along the rungs. We also described NH_4CuCl_3 under high magnetic fields in a two-leg system.

Key words : Two leg zig-zag ladder, NH_4CuCl_3, dimerized chain.

ABSTRAK

SIFAT MAGNET NH_4CuCl_3 DALAM SISTEM QUANTUM SPIN (TWO LEG ZIG ZAG LADDER / TANGGA DUAKAKI ZIG ZAG). Sifat magnet NH_4CuCl_3 dalam system quantum spin tangga dua kaki zig zag. Analisis numeric dari interaksi antara tangga dua kaki zig zag sebagai rantai tunggal dengan tetangga terdekatnya telah di formulasikan oleh Cabra (1999) dengan persamaan Hamilton berikut :

$$H = J' \sum_{X=1}^{L} \{\Delta S_X^Z . S_{X+1}^Z + \frac{1}{2}(S_X^+ . S_{X+2}^- + S_X^+ . S_{X+2}^-)\} + J \sum_{X=1}^{L} \{\Delta S_X^Z . S_{X+1}^Z + \frac{1}{2}(S_X^+ . S_{X+2}^- + S_X^+ . S_{X+2}^-)\} - h \sum_{X=1}^{L} S_X^Z$$

Formulasi lainnya yaitu untuk interaksi antara Tangga dua kaki zig zag dengan rantai yang telah diredupkan dan pasangan antar rantai adalah sebagai berikut :

$$H = J \sum_{i=1}^{2} \sum_{x=1}^{L} (1 + (-1)^x \delta) \vec{S}_{i,x} . \vec{S}_{i,x+1} + J' \sum_{x=1}^{L} \{(1 + \delta') \vec{S}_{1,x} . \vec{S}_{2,x} + (1 - \delta'') \vec{S}_{1,x} . \vec{S}_{2,x+1} - h \sum_{i=1}^{2} \sum_{x=1}^{L} S_{i,x}^z$$

Dari persamaan di atas dapat dipelajari penutupan jurang (*gap*) pada *Zero Magnetization* (magnetisasi nol) dengan cara mekanisme penghalusan dan hilangnya ½ dataran (*gap*) pada batas/*finite* <M> dengan cara menukar nukar peredupan rantai sepanjang tangga. Sifat Magnet NH_4CuCl_3 juga diuraikan dalam ***high magnetic fields in two leg system*** (system dua kaki di bawah medah magnet tinggi)

Kata kunci : Tangga dua kaki zig zag, NH_4CuCl_3, rantai yang diredupkan.

INTRODUCTION

The property of zig-zag ladder has received much attention from both the theoretical and experimental side. The appearance of the plateaus in magnetization curves of NH_4CuCl_3 at high field have been observed. At room temperature, the crystal structure of this material is known to be composed of double chains (two-leg ladder) with three difference nearest neighbour interactions.

The paper is the organised as follows : in section II, we explained the basic theory of antiferromagnetic system and magnetic curve at zero temperature for the antiferromagnetic Heisenberg linier curve. In section III, we described static and dynamic magnetic properties of NH_4CuCl_3 and in section IV, we discuss about magnetic properties of two-leg zigzag ladder. Finally we discuss plateaus phenomena in quantum spin system NH_4CuCl_3.

THE ANTIFERROMAGNETIC HEISENBERG LINIER CHAIN

Bethe Equations

Magnetic materials are very interesting especially antiferromagnetic materials. The properties of antiferromagnetic insulator are often discussed on the basis of Heisenberg model of exchange between neighbouring atoms. Due to difficulties to get exact solution for two and three dimension, there is some interest in examining the one dimensional case, for which a certain a mount of progress has been made to ward an exact solution.

$$H = 2J\sum_{i=1}^{N} S_i . S_{i+1} \qquad S_{N+1} \equiv S_1 \tag{1}$$

Bethe showed the eigenvalue problem for a chain of N spin- ½ atoms Hamiltonian

$$E_F = \frac{1}{2}NJ \qquad E_{AF} = NJ\left(\frac{1}{2} - 2\ln 2\right) \tag{2}$$

with J>0, corresponding to the ferro- and antiferromagnetic ground states,

$$\Psi = \sum \sum_{p=1}^{r!} \exp i\left(\sum_{j=1}^{r} kp_j n_j + \frac{1}{2}\sum_{j<l}\Phi p_j p_l\right). \Psi(n_1, n_2, n_3, n_4 .....n_r) \tag{3}$$

The eigen function discussed by Bethe are in the following form :
where the summation extends over all permutations of the integer 1,2,3...r, and p_j is the image of j under the P-th permutations. Other formulation for the anti-ferromagnetic ground state, state of minimum energy and state of maximum energy was discussed by Hulthen.

The hamiltonian in equation 1 for the lower energy bound on the minimum energy curve could be written as :

$$H = 2J\left\{\sum_{i=1}^{N}(S_i^x . S_{i+1}^x + S_i^y . S_{i+1}^y) + \sum_{i=1}^{N} S_i^z . S_{i+1}^z\right\} \tag{4}$$

with the superscript denotes the x,y,z components of the spin operators.

Magnetization And Susceptibility At Zero Temperature

Let there be a magnetic filed H along positive axis. The Zeeman energy

$$H_z = g\mu H \sum_{i=1}^{N} S_i^z \tag{5}$$

The lowest level of the chain with a given total spin S will have an energy as follow :

$$E_M(S) = E(S) - g\mu HS \qquad E(S) = 2NJ\eta(S/N) + E_{AF} \qquad g\mu H/J = 2\frac{d\eta}{d\sigma} \text{ when } \sigma = \sigma_0 \tag{6}$$

At zero temperature average magnetization per spin, M, is given by :

$$M = g\mu\sigma_0 \tag{7}$$

Grifith showed that the ratio M/H when H goes to zero as :

$$\chi = 0.0506661 g^2\mu^2/J \tag{8}$$

THE HIDDEN ANTIFERROMAGNETIC ORDER IN THE HALDANE PHASE

Haldane (1983) predicted that ground state of the integer spin chain is in a massive phase with a finite gap in the energy spectrum and exponential decay of the half integer spin chain is in massless phase with no gap in the energy spectrum and the power-law decay of the two-spin correlation functions. This prediction is surprising since it was believe that there should be a spin wave excitation without an energy gap. Many physicist do the research by analytical and numerical studies to confirm this argument and how it is believe that the conjecture is correct.

Consider the following S=1 Heisenberg Hamiltonian with uniaxial anisotropy with haldane correction :

$$H = \sum_i \left[S_i^x . S_{i+1}^x + S_i^y . S_{i+1}^y + \lambda S_i^z . S_{i+1}^z + D(S_i^z)^2\right] \tag{9}$$

this formulation could be show the energy gap in the spectrum energy.

STATIC AND DYNAMIC MAGNETICS PROPERTIES QUANTUM SPIN SYSTEM NH_4CuCl_3

The system crystal of NH_4CuCl_3 is monoclinic and space group P_2/c, the crystal structure composes double chain of the edge–sharing $CuCl_6$ octahedral along the

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a-axis . The double chain are located at the corner and the centre of the unit cell in the *bc*-plane and are separated by NH_4 ions. The double chains are described as a spin- ½ alternating Heisenberg chain consisting of J_2 and J_3 interaction with the next neighbour interactions J_1.

The susceptibility shows a board maximum at 4 K, when temperature is lowered, but no anomaly indicative of three dimensional ordering is observed down to 1.7 K. High field magnetization result at 0.5 K reveals that nature of the ground state is magnetic at zero field and that in contrast the previously theoretical calculation two wide plateau at one-quarter and three quarter of the saturation magnetization are observed when magnetic is increased.

Experiment result show that ESR data reveals that the frequency versus field diagram for H//a and H//b coincide, when normalized by the g-factors and that magnetic properties of the sample are isotropic both statically and dynamically. Low temperature specific heat and magnetization measurement show that the present undergoes three dimensional ordering at T=1.3 K small entropy S_m= 0.03 R In 2 indicates that the phase transition takes place under the condition of well-developed spin correlation.

MAGNETIC PROPERTIES OF THE TWO-LEG ZIG-ZAG LADDER

Numerical Analysis Of Two-Leg Zig-Zag Ladder With And Without Dimmer

Cabra described Hamiltonian without dimmer (δ=0) as :

$$H = J'\sum_{x=1}^{L}\left\{\Delta S_x^z.S_{x+1}^z + \frac{1}{2}\left(S_x^+.S_{x+1}^- + S_x^-.S_{x+1}^+\right)\right\} + \sum_{x=1}^{L}\left\{\Delta S_x^z.S_{x+2}^z + \frac{1}{2}\left(S_x^+.S_{x+2}^- + S_x^-.S_{x+2}^+\right)\right\} - h\sum_{x=1}^{L} S_x^z$$

Cabra use fourier transforms to simplify the determination of the spectrum when h=0, the isotropic point Δ = 1 and normalization J + [J'] =1. For these approximation we know that :

- J' = 0 corresponds to decouple chain
- J' = 1 corresponds to a single antiferromagnetic chain
- J' = -1 corresponds to a single ferromagnetics chains

Burshill also stated that for h=0, a study of the static structure factor exhibited a transition to commensurate behaviour at $J'/J \approx 1.92025$.

The antiferromagnetic when J'>0, here spin flips one after the other, from the interpolation by Cabra we know that at :

- 0< J' < 4J, the ground state momentum are in general incommensurate
- J' > 4J, all ground state momentum are commensurate and convergent with system size is good
- 2J ≥ J' ≥J, a gap existence in the region but a part from these is no evidence for any non-trivial plateaux.
- 0>J'≥-3J/2, spin flip in pairs
- J' = -3J, number of spins that flips simultaneously in a finite –site varies between 1 and 3
- J' = -4J a transition completely ferromagnetic takes place

The numerical diagonalization determines the critical field associated to the transition from two flipped spins to one flipped spins.

$$\begin{aligned} &J' \neq 4J \\ &h_{uc} - h \approx \left(1 - \langle M \rangle\right)^2 \\ &J = 4J \\ &h_{uc} - h \approx \left(1 - \langle M \rangle\right)^4 \end{aligned} \tag{11}$$

When <m> →1, this phenomena can be explained by the bond structure.

Hamiltonian with dimmer for two-leg zig-zag ladder (δ≠0) and coupling between chains is :

$$\begin{aligned} H &= J\sum_{i=1}^{2}\sum_{x=1}^{L}(1 + (-1)^x\delta)\vec{S}_{i,x}.\vec{S}_{i,x+1} \\ &+ J'\sum_{x=1}^{L}\{(1+\delta')\vec{S}_{1,x}.\vec{S}_{2,x} + (1-\delta'')\vec{S}_{1,x}.\vec{S}_{2,x+1} \\ &- h\sum_{i=1}^{2}\sum_{x=1}^{L} S_{i,x}^z \end{aligned}$$

We assume that $J'(1 \pm \delta')$, $J(1-i) \ll J(1+i)$. The coupling between the two chain is J(1-δ) with an effective XXZ anisotropy Δ_{eff} = ½. The coupling between the two chain is not only dimmerized but also has an alternating XXZ anisotropy. Other formulation by Cabra in bosonized action can be interpreted as the gap is closed when <M> =0 in all term commensurate and relevant. The critical line is given by :

$$\frac{J'}{J} \propto \delta^2 \tag{12}$$

The interesting phenomena can be observed when the plateau is ½ of the saturation value to appearance of the radiative correction. In the case of normal dimmerization, we can find that :

$$\gamma = \delta j'\langle M \rangle \tag{13}$$

It was also understood that the difference in a sort of strong coupling limit δ→1. It can be readily checked that the normal dimmerization display an <M> = ½ for all h when (2J,4J) with J'=J, while no plateau in staggered array.

HIGH FIELD MAGNETIZATION PROCESS MEASUREMENT

The experiment were done by increasing and decreasing external field, some remarkable result were obtained from high field magnetization process measurement. At 0.5 K these phase transition show that the best distinction thus assign the transition field at H_{c1}=5.0 T, H_{c2}=12.8 T, H_{c3}=17.9 T, H_{c4}=24.7 T, and H_s=29.1 T. The saturation magnetization is M_s=1.09 μ_B/Cu^{+2}.

DISCUSSION

The two-leg ladder with dimmerized coupling along the chains have not only plateaus at <M>=0 and <M>= ½ but also at <M> = ¼ and <M> = ¾. This must be relevant to magnetization experiment on NH_4CuCl_3. Kolezhuk did study to a spin system consisting strongly and weakly couple dimmer. In strongly couple dimmer, the plateaus appear at 1/3 and 2/3 of the saturation magnetization. For three dimensional lattice structure of the $KCuCl_3$ family, the plateau appear at ¼ and ¾ of saturation From these phenomena, all plateaus of magnetization curve of NH_4CuCl_3 appear in the two leg zig-zag ladder with dimmerized chains and couplings at low temperature.

CONCLUSION

Magnetic properties of the Two-Leg Zig-Zag Ladder in Quantum Spin System NH4CuCl3 have been studied. Wxperimentally, we found that the plateaus appear at one-quarter and three-quarters of saturation magnetization. The Cabra result showed that the closing of the gap at zero magnetization was caused by means of the fine-tuning mechanism and disappreance of the 1/2 plateau (gap) at finite <M> is caused by alternating dimerization of the chains along the rungs. Other formulation by Cabra in bosonized action can be interpreted as the gap is closed when <M>=0 in all term of commensurate.

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