



# Studies on effects from a Dzyaloshinskii-Moriya interaction

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Himalayas Peak  
Higher  
dimensions  
DMRG?

## Collaborators

J.Z. Zhao: ITP, CAS  
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Lu Yu: ITP & ICTS, CAS  
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# Outlines

- **Brief introduction on the Dzyaloshinskii-Moriya interaction**
- **Studies on copper Benzoate**
  - Experimental findings
  - Models and conformal field analysis
  - Density matrix renormalization group studies **PRL. 90, 207204(2003)**
  - Summary
- **Half integer vs. integer spin chains** **to be submitted**
  - Mid-gap state
- **Multiple leg ladders** **in preparation**
  - $1d \rightarrow 2d$
- **CuCl<sub>2</sub> (dimethylsulfoxide)**
  - Experimental findings
  - Model calculations **in progress**
- **Discussions**



## (1) Brief introduction

### ➤ Dzyaloshinskii-Moriya interaction

- For many magnetic or strongly correlated materials, the Heisenberg interaction:

$$H_H = J \sum_{i=1}^L S_i^z S_{i+1}^z + \frac{1}{2} (S_i^+ S_{i+1}^- + \text{h.c.})$$

is a basic one.

- some interactions: an order smaller in magnitude, and even also nearest neighbor, e.g. Dzyaloshinskii-Moriya interaction

$$H_{DM} = \sum_{i=1}^L (-1)^i D \cdot (S_i \times S_{i+1})$$

Dzyaloshinskii (1958)

Moriya (1960)

- existing in some materials, especially for 1D systems since later of 60's, but nothing significant found.



## (1) Brief introduction

### ➤ “Irrelevance” of DM interaction

- For  $D/J \ll 1$ , take a local unitary transform

$$S_{2i}^+ = S_{2i}^+ e^{i\alpha/2}, \quad S_{2i+1}^+ = S_{2i+1}^+ e^{-i\alpha/2}$$

$$\alpha = \tan^{-1} D / J$$

rotating spin around  $D$  alternatively

- Transformed into the standard xxz-Heisenberg model

$$H = \sum_i \left[ J S_i^z S_{i+1}^z + \frac{|J|}{2} (S_i^+ S_{i+1}^- + \text{h.c.}) \right]$$

with  $\mathbf{J} = J + i |\mathbf{D}|$  and  $\mathbf{D}$  is assumed along z-direction.

—— naturally to imagine nothing dramatically changed

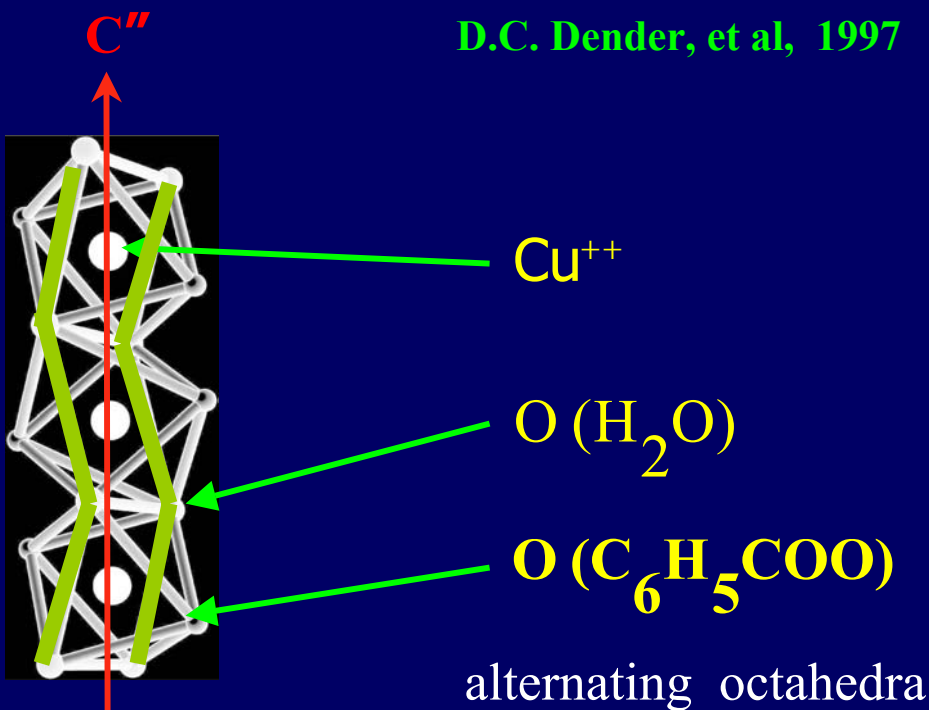


## (2) Studies on Copper Benzoate

➤ **Copper Benzoate**  
 $\text{Cu}(\text{C}_6\text{H}_5\text{COO})_2 \cdot 3\text{H}_2\text{O}$

M. Date et al, 1963

D.C. Dender, et al, 1997



$\text{Cu}^{++}$  form a spin 1/2 chain

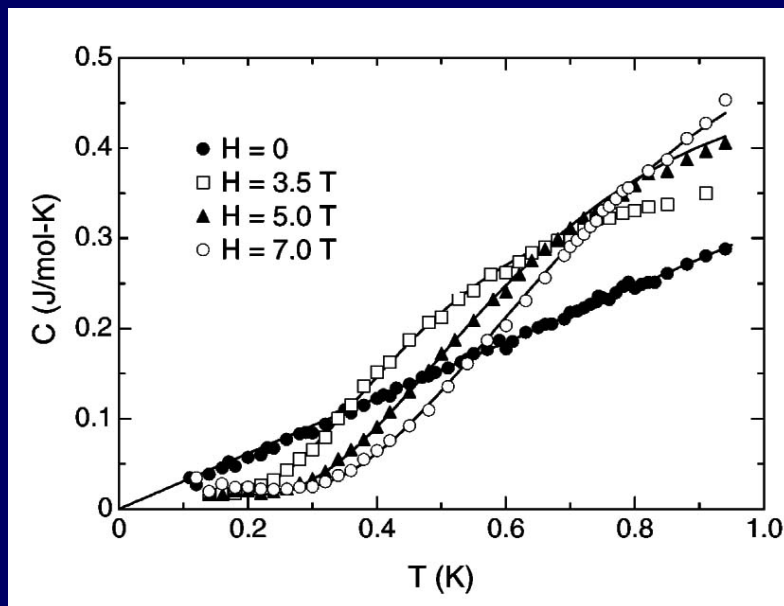


## (2) Studies on Copper Benzoate

### ➤ Experimental findings

D.C. Dender, et al, 1997

### Specific heat



— At low temperature:

$C_V$  proportional to  $T$ , at  $H=0$ ; → 1D nature.

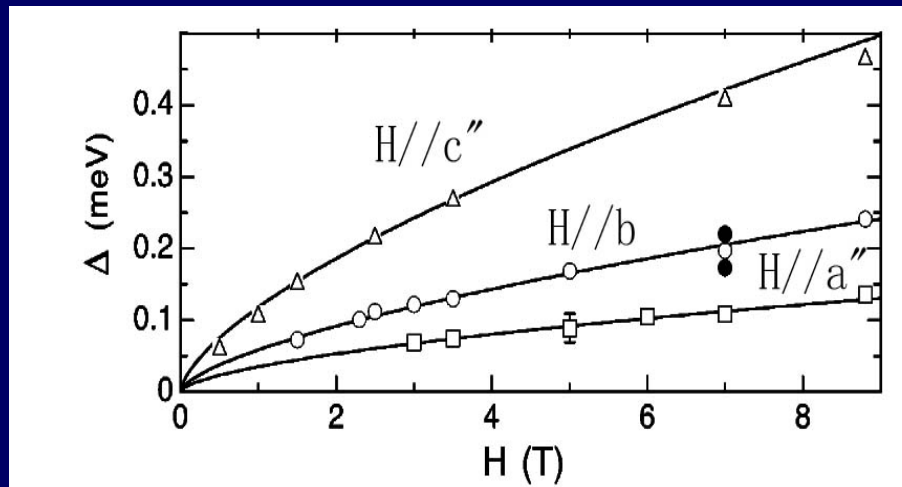
$C_V \sim T^{3/2} \exp(-\Delta/T)$ , for  $H>0$ ; → gap exists.



## (2) Studies on Copper Benzoate

$\Delta$  depending on orientations of H

D.C. Dender, et al, 1997



— For small magnetic fields:

$$\Delta_{\alpha} \sim H^{2/3} \text{ for small } H \ (\alpha=a'', b, c'');$$

$$\Delta_{a''} : \Delta_b : \Delta_{c''} = 0.55 : 1.0 : 2.0 .$$



## (2) Studies on Copper Benzoate

### ➤ Model Hamiltonian

$$\begin{aligned} H = & J \sum_{i=1}^L \mathbf{S}_i \cdot \mathbf{S}_{i+1} \\ & + \sum_{i=1}^L (-1)^i \mathbf{D} \cdot (\mathbf{S}_i \times \mathbf{S}_{i+1}) \\ & + \sum_{i=1}^L \mu_B H^a \left[ g_{a\beta}^u + (-1)^i g_{a\beta}^s \right] S_i^\beta \end{aligned}$$

Heisenberg exchange term

Dzyaloshinskii-Moriya term

Zeeman splitting term

$$g^u = \begin{pmatrix} 2.1150 & 0 & 0.0906 \\ 0 & 2.0590 & 0 \\ 0.0906 & 0 & 2.3160 \end{pmatrix} \quad g^s = \begin{pmatrix} 0 & 0.0190 & 0 \\ 0.0190 & 0 & 0.0495 \\ 0 & 0.0495 & 0 \end{pmatrix}$$

Oshima, et al 1963

**J=1.57mev**

**D=(0.13,0.0,0.02)J?**

**Date et al, 1970**

**Oshikaw and Affleck, 1997**



## (2) Studies on Copper Benzoate

### ➤ Conformal field analysis

- as did before for  $D/J \ll 1$ , rotating spin around  $D$

$$S_{2i}^+ = S_{2i}^+ e^{i\alpha/2}, \quad S_{2i+1}^+ = S_{2i+1}^+ e^{-i\alpha/2}$$

$$\alpha = \tan^{-1} D/J$$

- DM-term eliminated, while contributing to the staggered term

$$\mathbf{H}^s = \mathbf{g}^s \cdot \mathbf{H} + \frac{1}{2J} \mathbf{D} \times \mathbf{g}^u \cdot \mathbf{H}$$

- neglecting a small anisotropic term, an effective Hamiltonian

$$\hat{H}_{\text{eff}} = \sum_i^L JS_i \cdot S_{i+1} - HS_i^z - (-1)^i h S_i^x$$

Lou, Qin, Chen, Su & Yu, 2002



## (2) Studies on Copper Benzoate

- In the small  $\hbar$  limit,  $H$  just modifies the Fermi energy

$$\hat{H}_{\text{eff}} = \sum_i^L JS_i \cdot S_{i+1} - (-1)^i \hbar S_i^x$$

- Using Abelian bosonization technique, the low energy behavior described by a sine Gordon model:

$$\mathbf{L} = \frac{1}{2}(\partial_\mu \varphi)^2 + \text{const} \times \hbar \cos(2\pi R \varphi)$$

- Oshikawa and Affleck predicted (1997)

$$\Delta \propto (\hbar / J)^{2/3} |\ln(\hbar / J)|^{1/6}$$

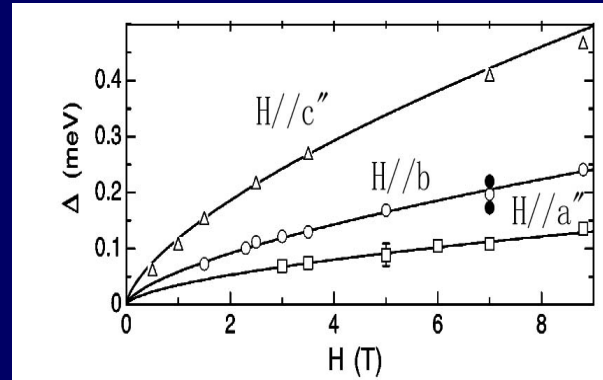
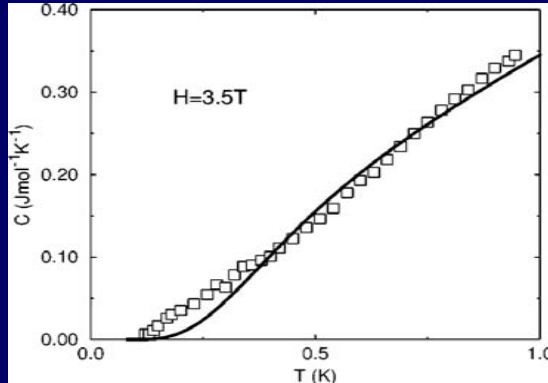
——consistent with experimental finding



## (2) Studies on Copper Benzoate

### Interpretation of experimental data

- They believed gap to be zero for  $H//a''$  according to  $C_V$



- i.e. assuming  $H^S = 0$   $H//a$ , then for  $H//b$  and  $H//c''$ , using

$$\Delta_b : \Delta_{c''} = 1.0 : 2.0,$$

- they obtained the Dzyaloshinskii-Moriya vector coupling:

$$\mathbf{D} = (0.13, 0.0, 0.02) J$$

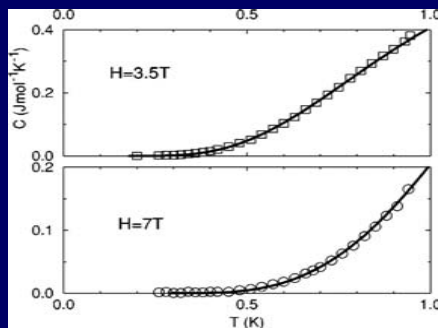


## (2) Studies on Copper Benzoate

### Detailed studies on specific heat

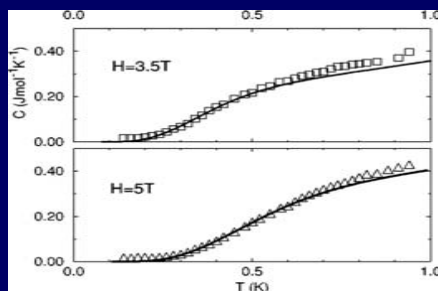
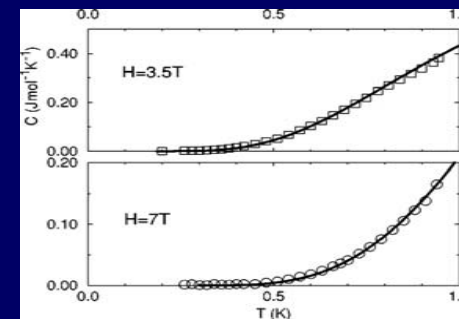
Essler, 1999

- solving the sine-Gorden model with Bethe ansatz
- considering contributions from the antisoliton and 1<sup>st</sup> breather

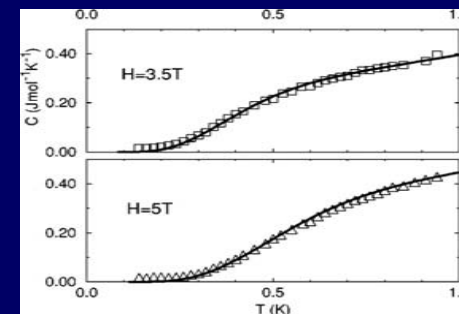


$H // c''$

80%  $v_s$



$H // b$

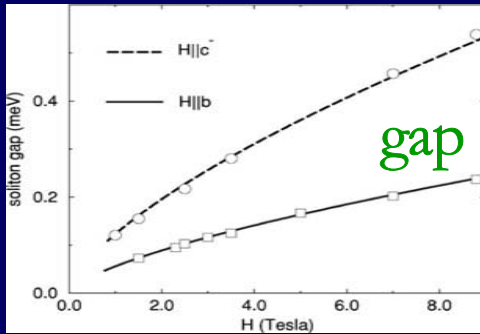




## (2) Studies on Copper Benzoate

obtaining the vector  $D$

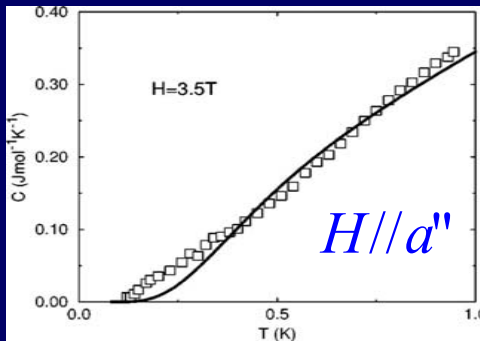
Essler, 1999



$$\Delta_b : \Delta_{c''} = 1.0 : 2.0$$



$$D = (0.12, 0.0, 0.02)J$$



Mechanisms:

- (1) Experimental results unreliable?
- (2) Effective model not sufficient?
- (3) Interchain coupling response?

$$H_{ani} = -\gamma \sum_i S_i^x S_{i+1}^x$$

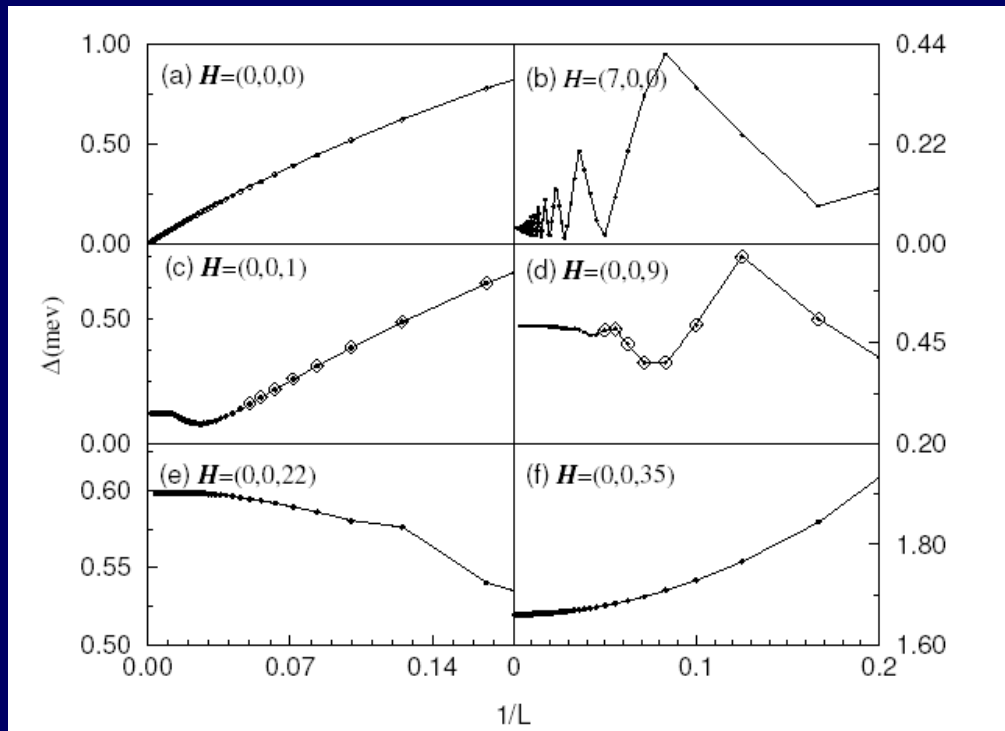
——full studies on original model



## (2) Studies on Copper Benzoate

### ➤ Density matrix renormalization group studies

gap



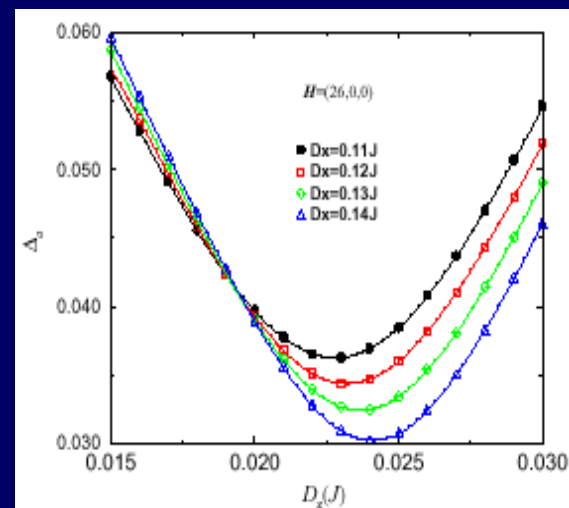
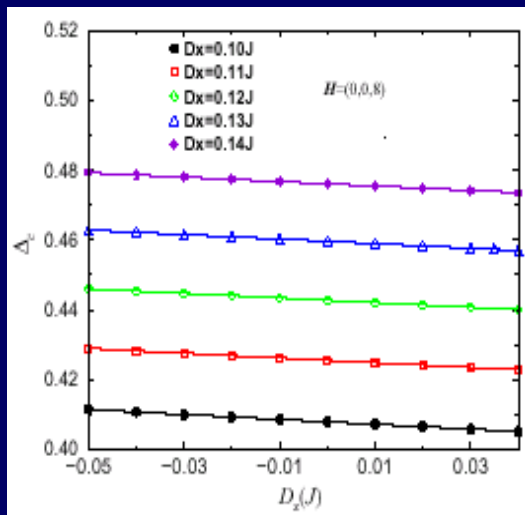
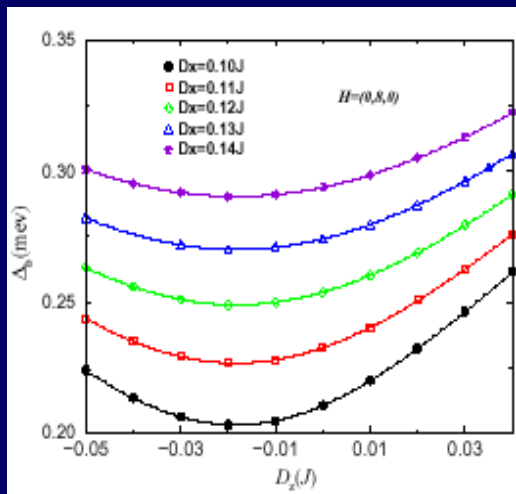
non-monotonic scaling behavior

—— Only is DMRG method a proper tool!



## (2) Studies on Copper Benzoate

➤ Numerical results: 1) fits experimental data

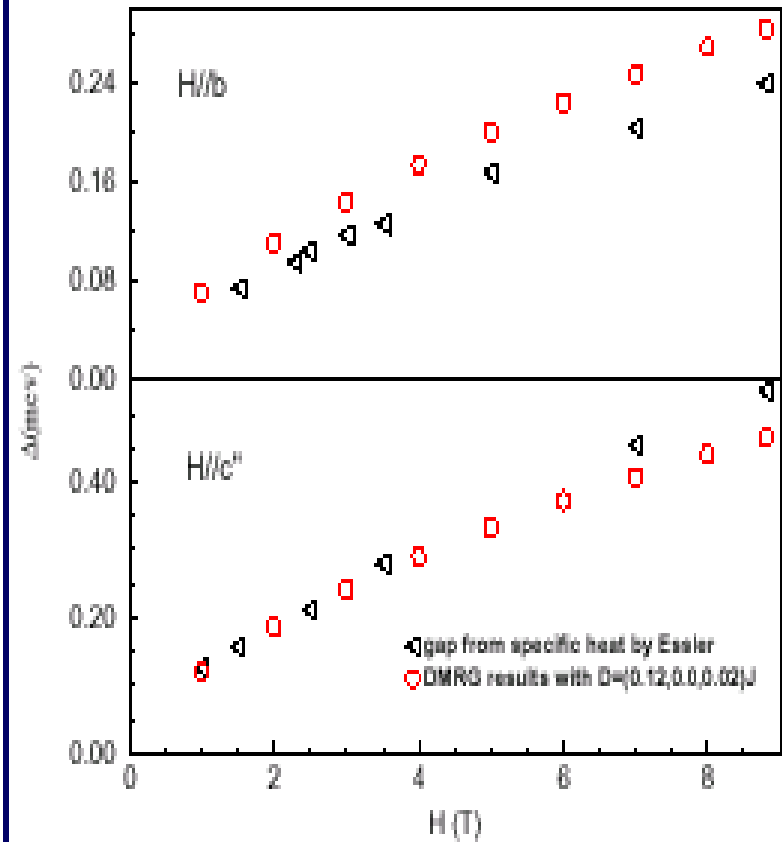
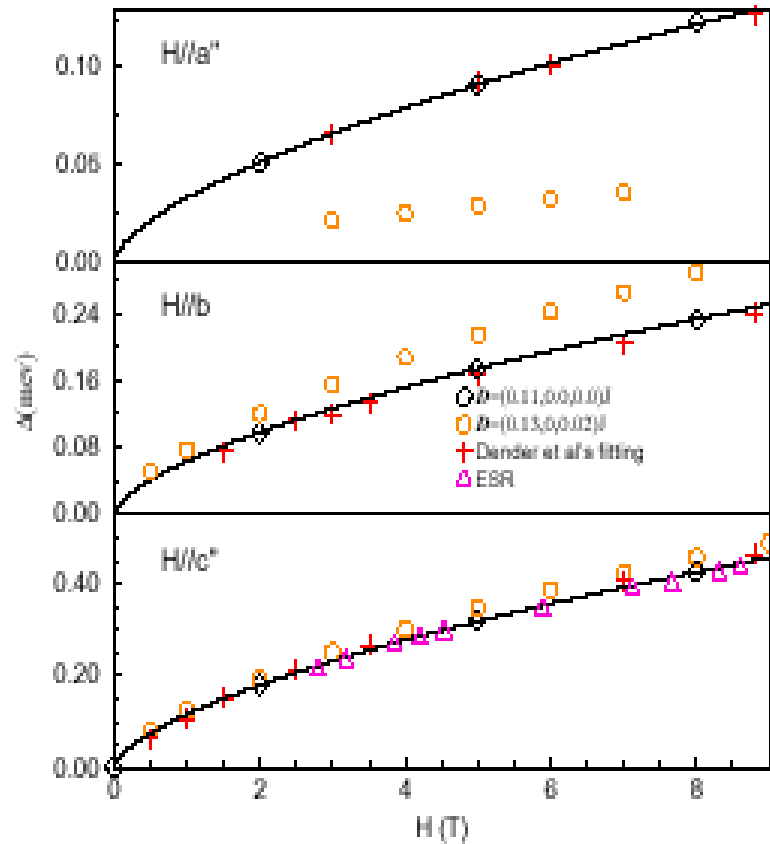


— we obtained  $D=(0.11, 0.0, 0.0)J$



## (2) Studies on Copper Benzoate

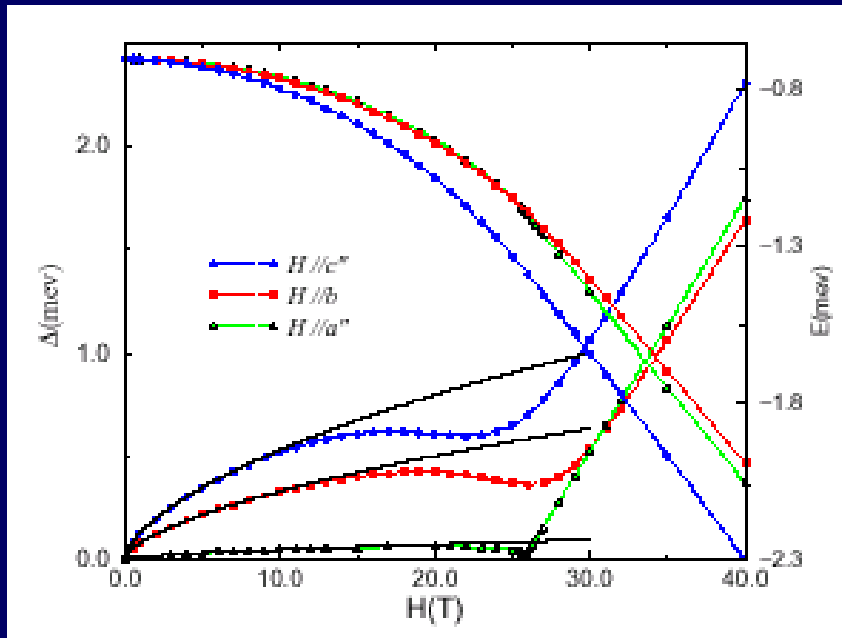
### 1) fits experimental data (continued)





## (2) Studies on Copper Benzoate

### 2) a crossover for gap



crossover originates from the competition between  $H^S$  and  $H^U$  terms.

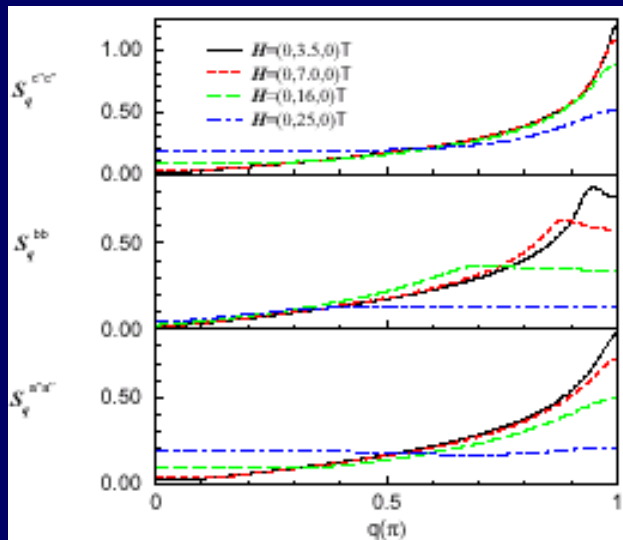
For small  $H$ :  $\Delta \propto H^{2/3} |\ln(H^S \mu_B / J)|^{1/6}$  confirming analytical prediction

For large  $H$ :  $\Delta \propto g_{\alpha\alpha} H$



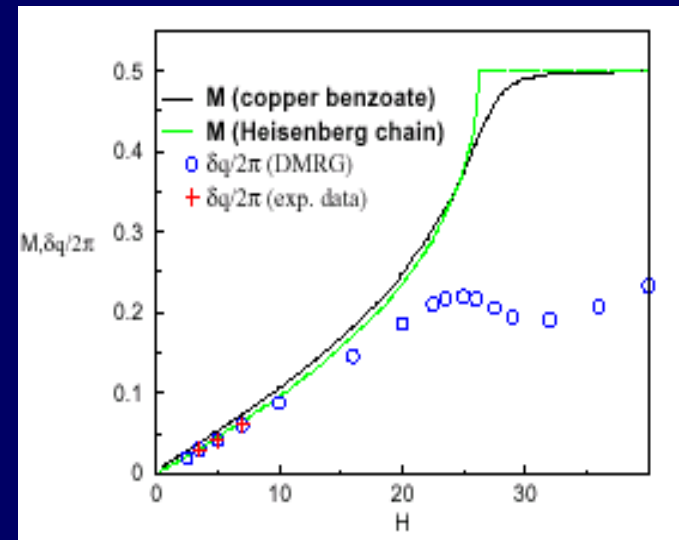
## (2) Studies on Copper Benzoate

### 3) incommensurate antiferromagnetism and uniform magnetization



$H//b$

$$\mathbf{H}^s = \mathbf{g}^s \cdot \mathbf{H} + \frac{1}{2J} \mathbf{D} \times \mathbf{g}^u \cdot \mathbf{H}$$



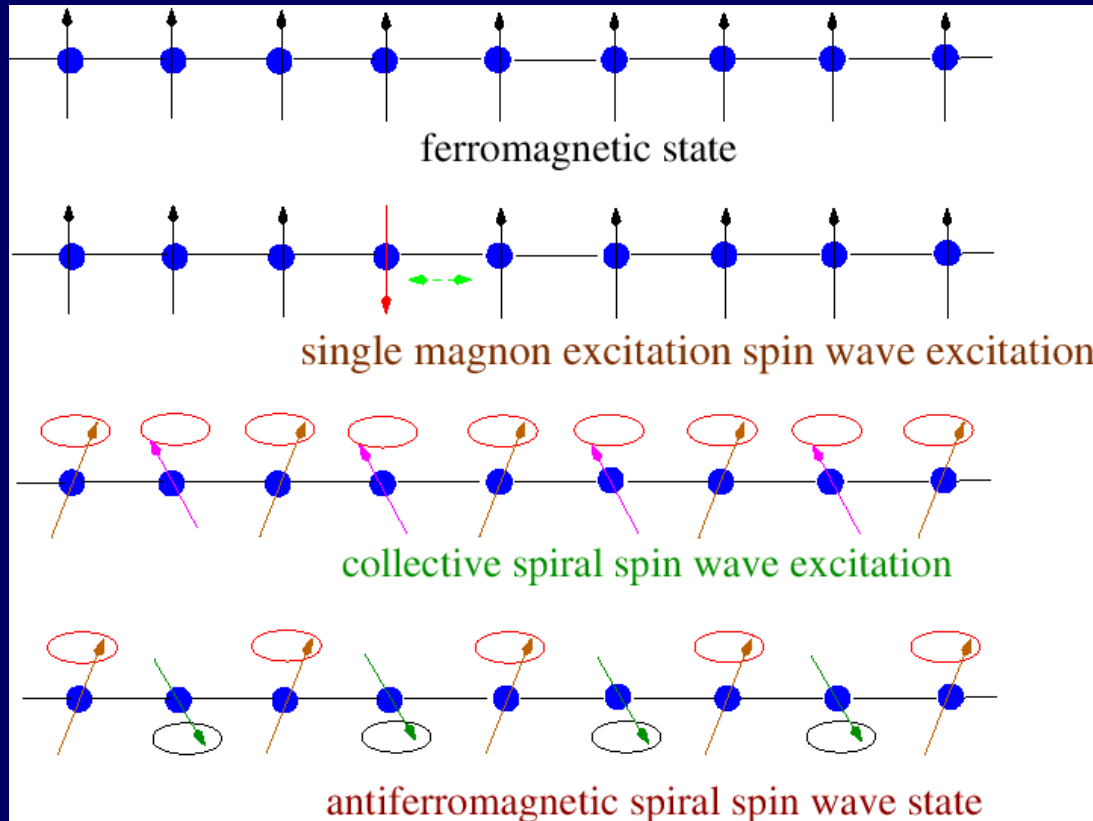
two consequences from DM int.

- ✓  $M \neq \delta q/2\pi$
- ✓  $M$  is not singular at  $H_C$



## (2) Studies on Copper Benzoate

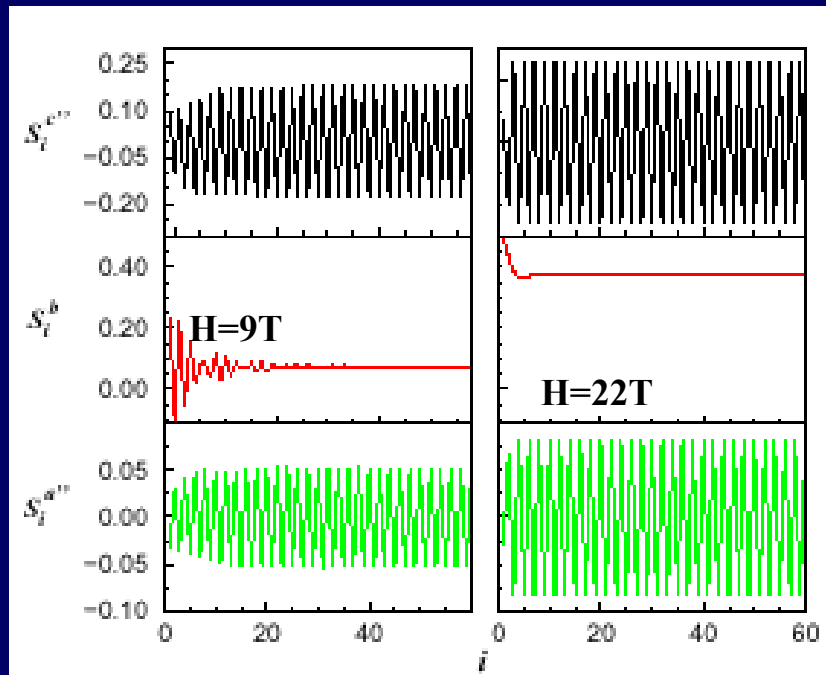
collective excitation instead of single magnon one





## (2) Studies on Copper Benzoate

### 4) simultaneously (anti-)ferromagnetically magnetized



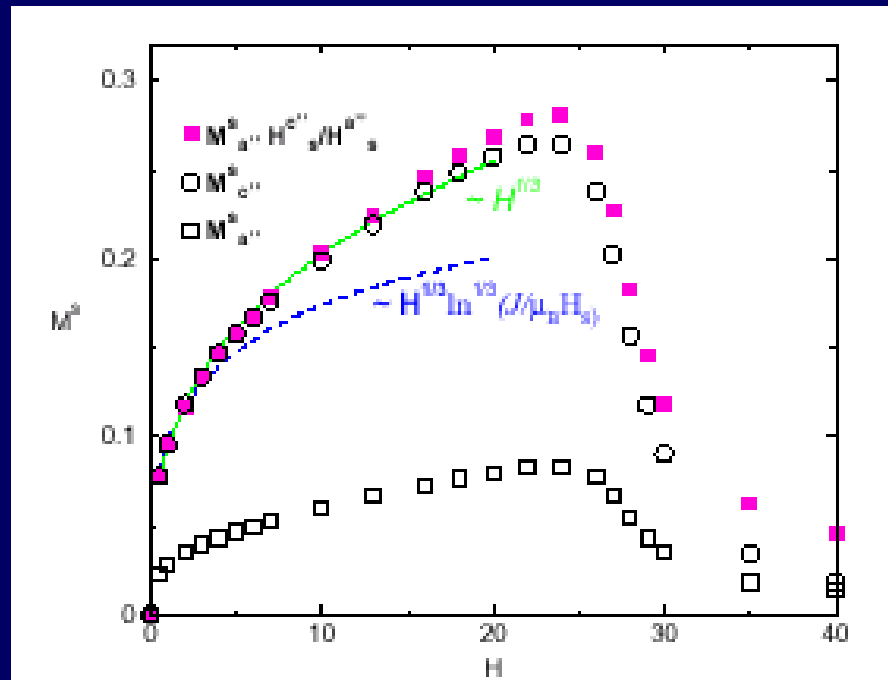
external field  
applied along  
the  $b$  direction

$$\mathbf{H}^s = \mathbf{g}^s \cdot \mathbf{H} + \frac{1}{2J} \mathbf{D} \times \mathbf{g}^u \cdot \mathbf{H}$$



## (2) Studies on Copper Benzoate

### 5) Staggered magnetization



— for small  $H^S$  but wide range:

$$M^S \propto H^{1/3} \text{ rather than } H^{1/3} \ln^{1/3}(J/H^S \mu_B)$$



## (2) Studies on Copper Benzoate

### ➤ Summary

a) Copper benzoate is an ideal one-dimensional magnetic system  
interchain interaction irrelevant for experimental findings

b) DMRG method is so far only a way to handle this problem

We found that

- (1)  $D=(0.11,0,0)$  for Copper Benzoate
- (2) full gap behavior  $\rightarrow$  crossover
- (3) co-existence of (anti-)ferromagnetic moments
- (4) magnetizations

In IMS of Japan, and NHML of USA, H. Nojiri and N. Takano's groups are carrying higher magnetic field measurements.



### (3) Integer vs half-integer chains with $H^S$

➤ Studying the effective model:

$$\hat{H}_{\text{eff}} = \sum_i^L J \mathbf{S}_i \cdot \mathbf{S}_{i+1} - (-1)^i h_S S_i^x$$

with  $S=1/2, 1,$  and  $3/2$ .

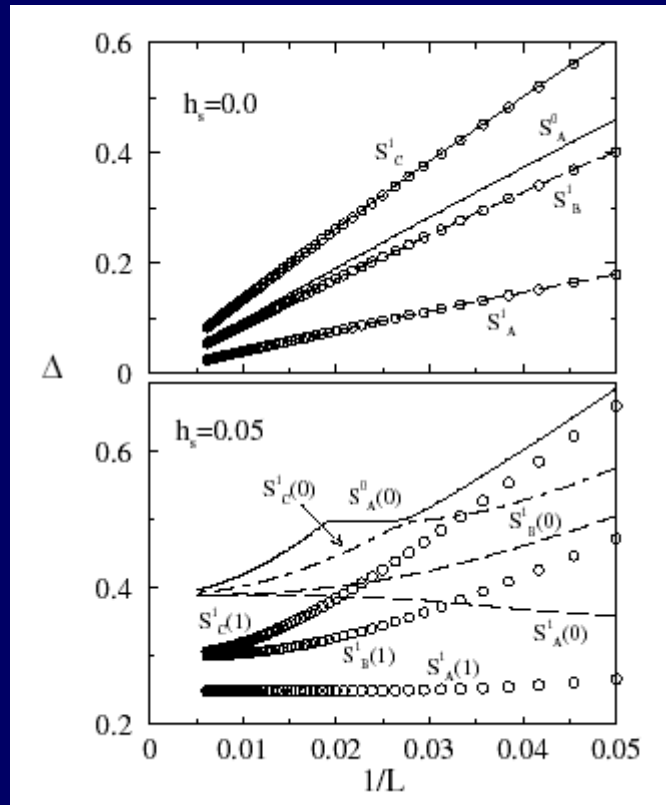
➤ We found

- 1) the spectra are split into transverse and longitudinal branch.
- 2) midgap states exist inside the gap for open chains which are inherent to real materials.
- 3) the low-field scaling behavior is different for different cases.
- 4) whether the low energy of about model can fully be described by quantum sine Gordon model.



### (3) Integer vs half-integer chains with $H^S$

➤  $S=1/2$  case: splitting of spectra

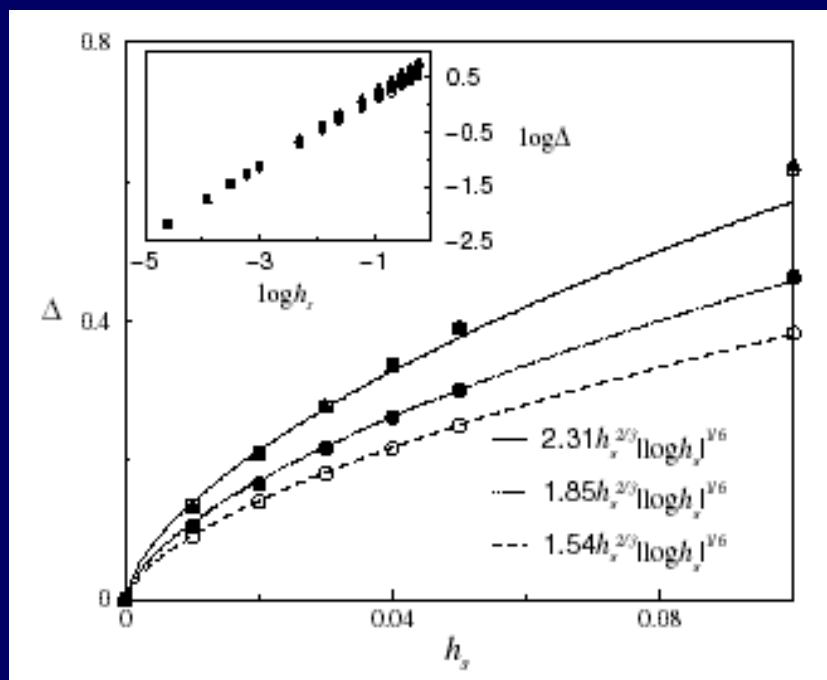


Small staggered field splits the spectra into transverse ranch and longitudinal branch



### (3) Integer vs half-integer chains with $H^S$

➤  $S=1/2$  case: low-field behavior

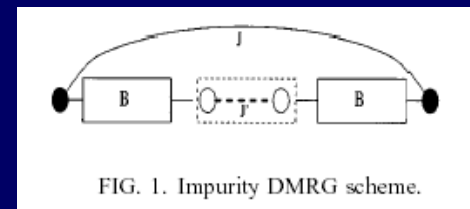
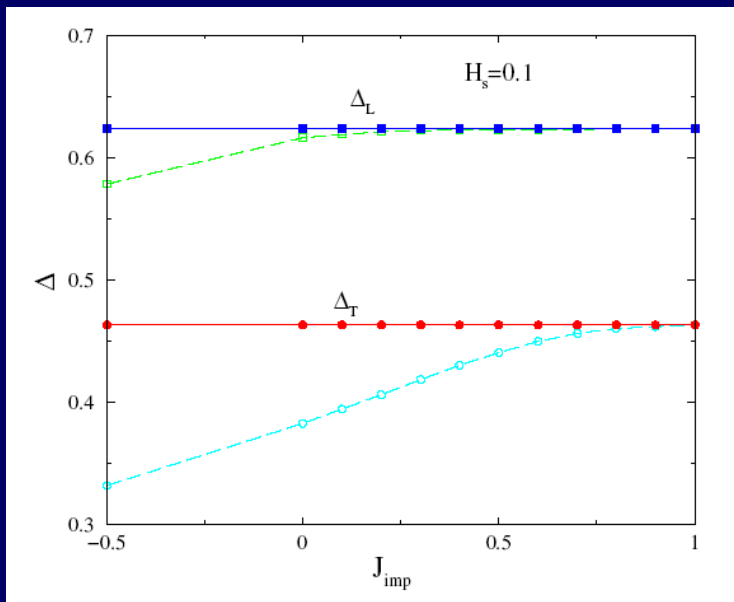


—— transverse branch fits the field theory results



### (3) Integer vs half-integer chains with $H^S$

➤  $S=1/2$  case: origin of the midgap states



- common topological edge effects
- midgaps just explicitly give the evidence

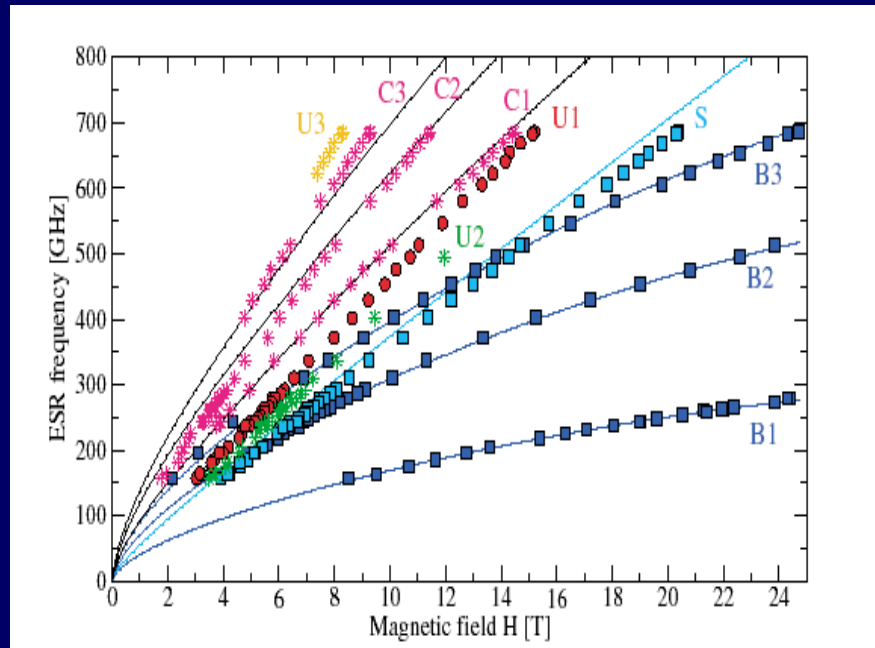
Ng, 1986



### (3) Integer vs half-integer chains with $H^S$

- $S=1/2$  case: most recent experiment supports our findings

$[\text{PM-Cu}(\text{NO}_3)_2(\text{H}_2\text{O})_2]_n$   
PM=pyrimidine



— Excitation Hierarchy of the Quantum sine Gordon  
Zvyagin, et al, PRL, 93, 027201(2004)

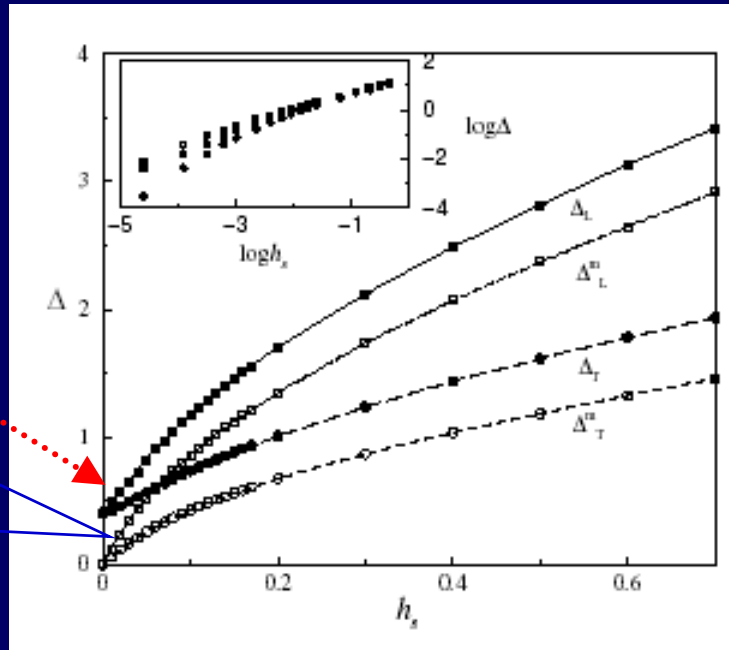


### (3) Integer vs half-integer chains with $H^S$

➤  $S=1$  case: low-field behavior

$\sim h_S^2$

Far from  $h_S^{2/3} |\ln h_S|^{1/6}$  for q-sine Gordon model

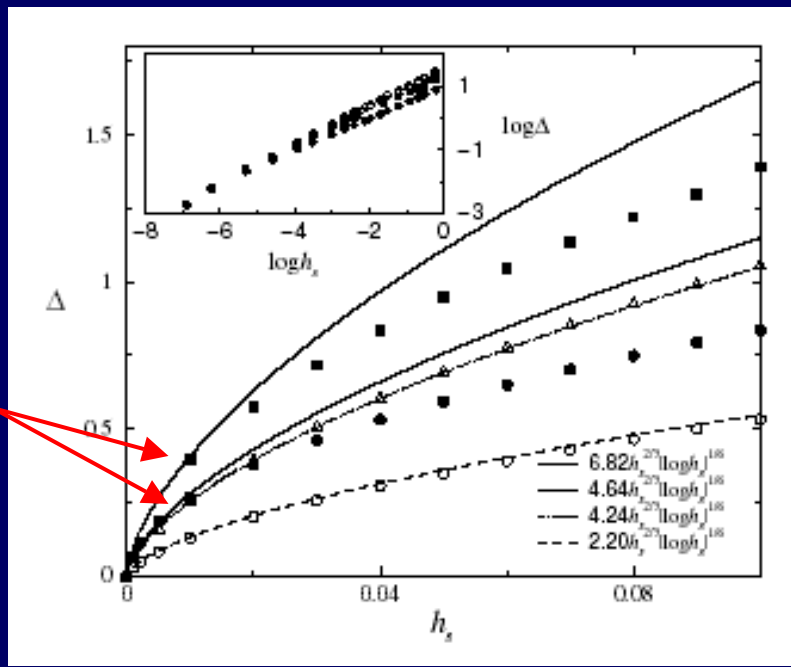


— existing low-field theory not applicable



### (3) Integer vs half-integer chains with $H^S$

➤  $S=3/2$  case: low-field behavior



gaps fit  $h_s^{2/3} |\ln(h_s/J)|^{1/6}$  for very small  $h_s$

— midgaps follows up  $h_s^{2/3} |\ln(h_s/J)|^{1/6}$  very well



## (4) Multiple leg ladders: 1d $\rightarrow$ 2d

- Studying the effective model:

$$\hat{H}_{eff} = \sum_{i,k}^{L,N} J S_{i,k} \cdot S_{i+1,k} - (-1)^{i+k} h^S S_{i,k}^x$$

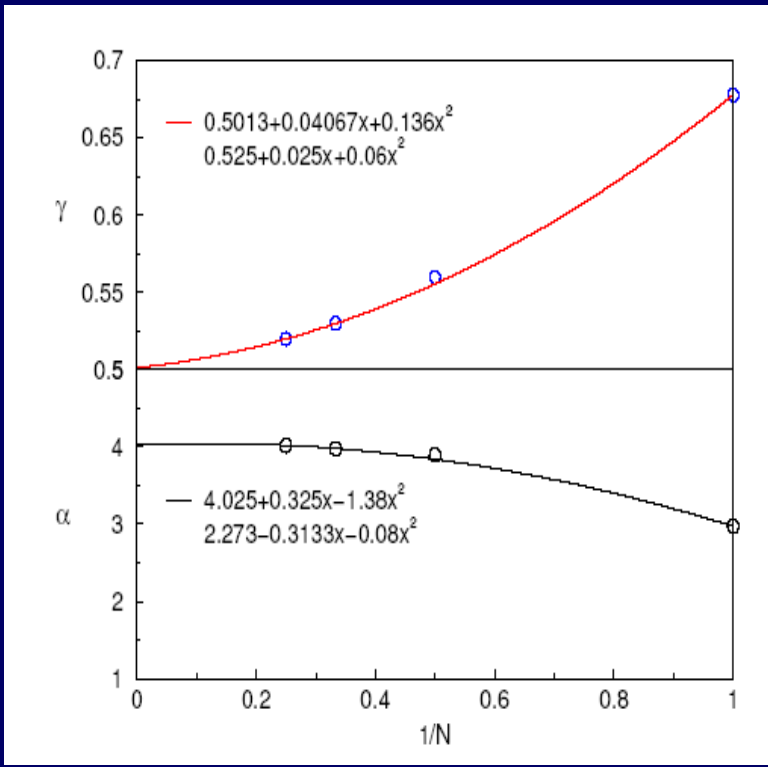
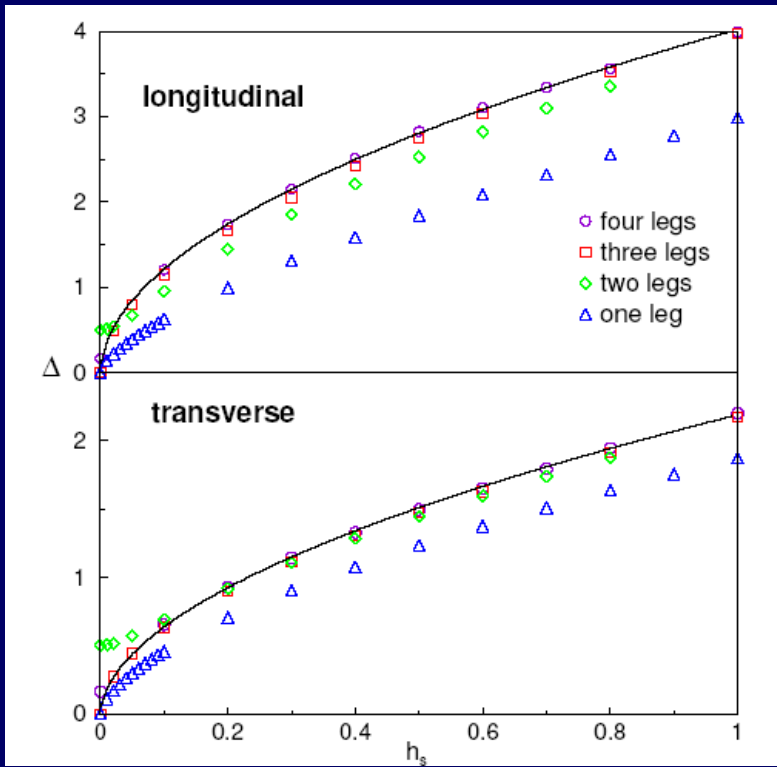
where  $L$  is the length of the ladder, and  $N$  is the number of legs.

- We are interested in whether those features survive for ladders and for two dimensional case.

Here we just show you some features related to the critical behavior in two dimensions.



# (4) Multiple leg ladders: 1d $\rightarrow$ 2d

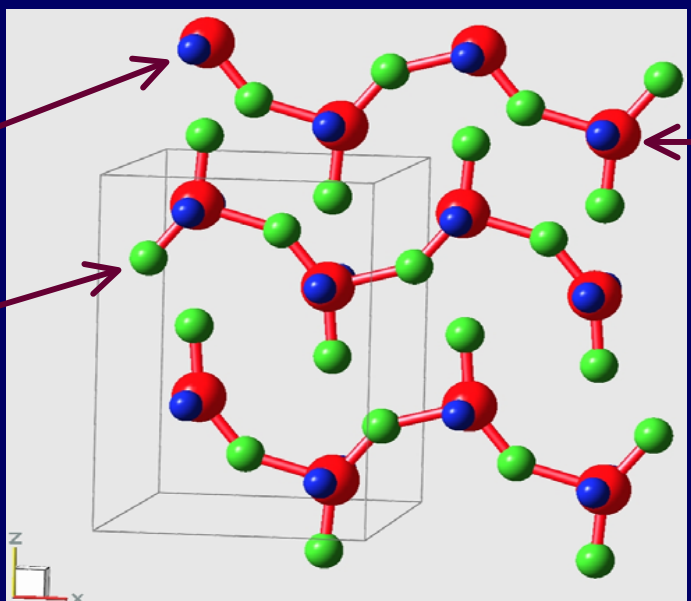


$\Delta \propto h_s^{1/2}$  in two dimensions



(5)  $\{(\text{CH}_3)_2\text{SO}\}_2 \text{CuCl}_2$

*Landee et al. (1986)*



$(\text{CH}_3)_2\text{SO}$

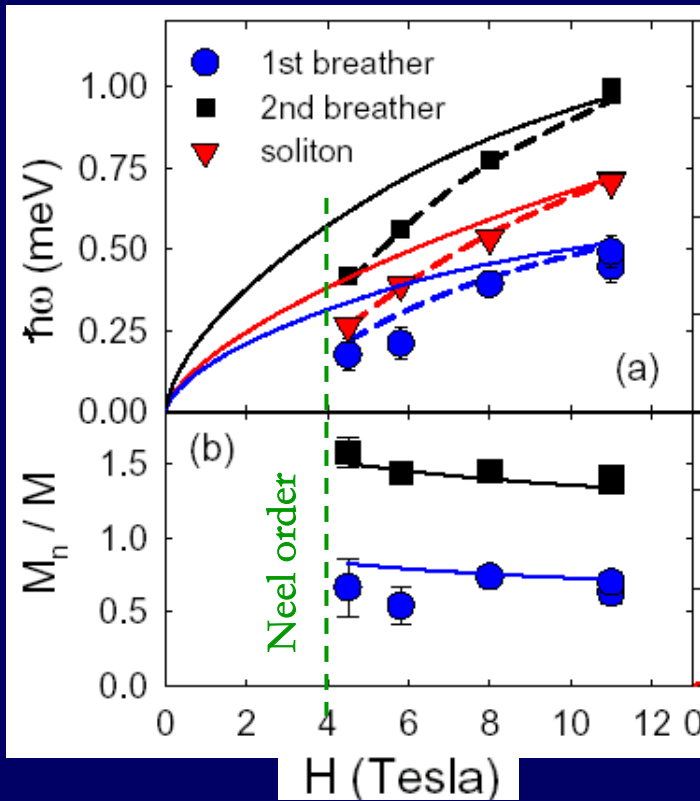
Cl

Cu

Spin- $\frac{1}{2}$  chain with two spins per chain unit

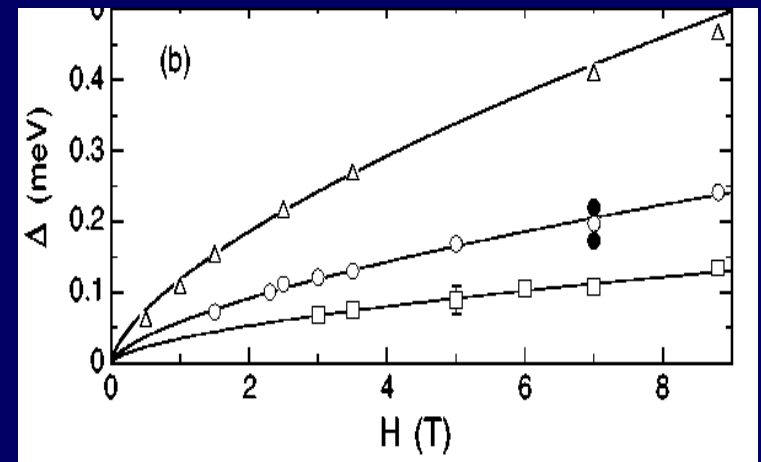


(5)  $\{(\text{CH}_3)_2\text{SO}\}_2 \text{CuCl}_2$



*Kenzelmann et al. PRL, July, 2004*

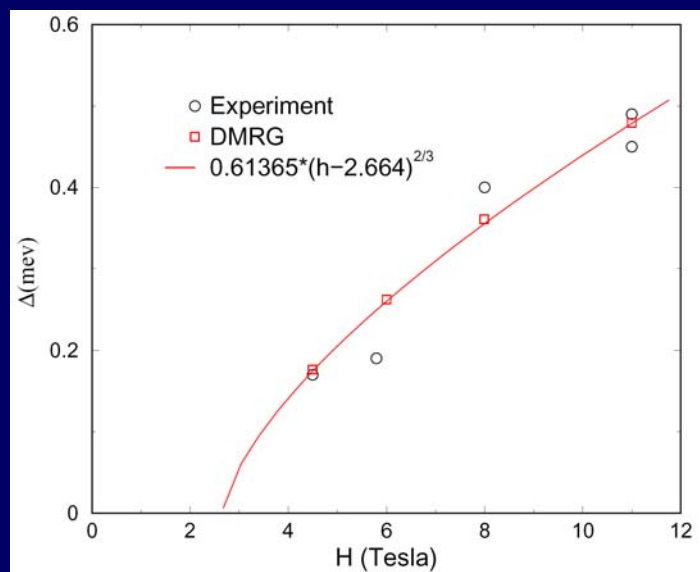
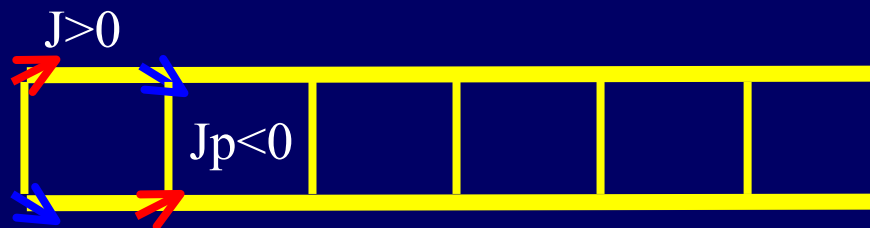
*Landee et al. (1986)*



*Cu Benzoate, Dender et al, PRL, 97*



# (5) $\{(\text{CH}_3)_2\text{SO}\}_2 \text{CuCl}_2$





## (6) Discussions

- a) Present work shows again that DMRG method is very efficient tool for interpretation and prediction of rich physics properties of new materials.
- b) Copper benzoate is well described by the Heisenberg-Dzyaloshinskii-Moriya interactions with  $d=1$ .
- c) It remains to be further investigated whether the low-energy properties of the Heisenberg-Dzyaloshinskii-Moriya interaction systems can be sufficiently described by quantum sine-Gordon model.
- d) The midgap states should be shown in the experimental measurements, but how experimentists can identify them.
- e) Although  $|D|/J \sim 0.1$ , but involves rich physics, once  $H \neq 0$ . More importantly, it widely exists in materials, e.g.  $\text{Yb}_4\text{As}_3$ ,  $\text{BaCu}_2\text{Si}_2\text{O}_7$ ,  $\{(\text{CH}_3)_2\text{SO}\}_2\text{CuCl}_2$ , etc. For metallic materials, it could affect differently the transport properties of electrons which has different spin.





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谢谢大家

Thank you!