

Lieb-Shultz-Mattis Theorem

1次元ハイゼンベルグ系、半奇数スピン

--- 基底状態に縮退がなければ励起ギャップは存在しない。

高次元系にも適用可能？

励起ギャップが生じる場合：次近接相互作用

$$H = J_1 \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \sum_i \vec{S}_i \cdot \vec{S}_{i+2}$$

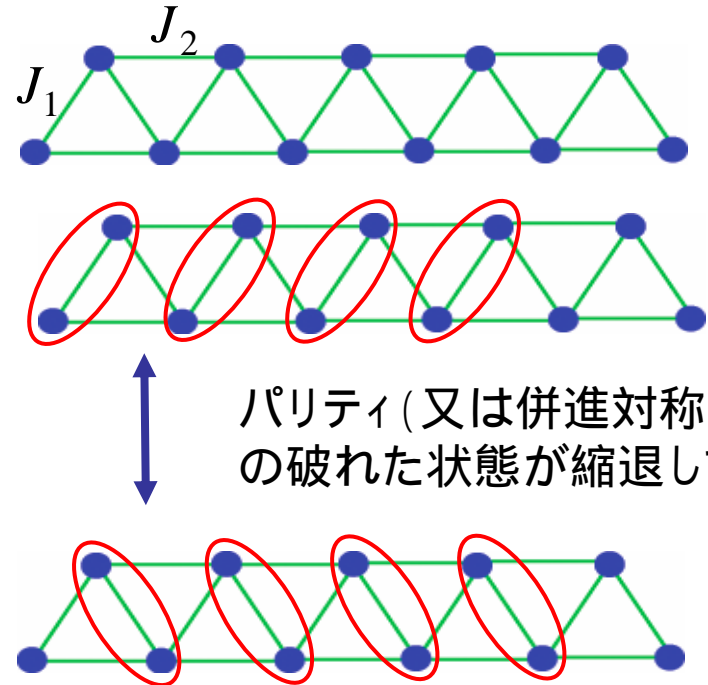
Majumdar-Ghosh模型：

$J_1 = \frac{J_2}{2}$ のとき、基底状態は厳密に

$$\Psi_g = \otimes_{j=\text{odd}} |S_j\rangle, \quad |S_j\rangle = \frac{1}{\sqrt{2}} (|\uparrow_j \downarrow_{j+1}\rangle - |\downarrow_j \uparrow_{j+1}\rangle)$$

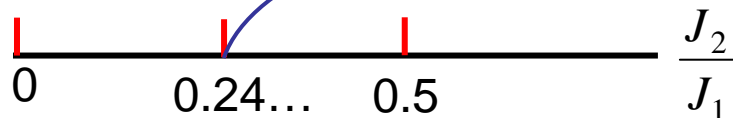
$$P = \frac{1}{3} (\vec{S}_i + \vec{S}_{i+1} + \vec{S}_{i+2})^2 - \frac{1}{4}$$

合成スピン3/2に対する射影演算子



↑ ↓
パリティ(又は併進対称性)の破れた状態が縮退している。

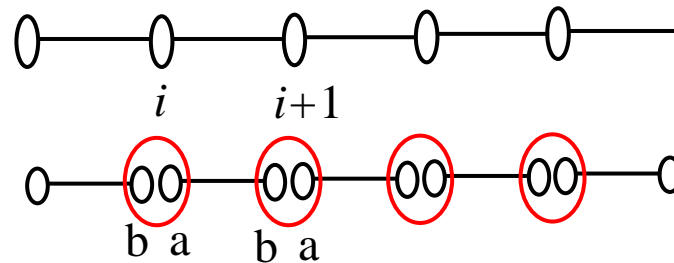
エネルギー・ギャップ



併進対称性を破らない例:

S=1、最近接ハイゼンベルグ系におけるハルデイン・ギャップ

$$H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$



Ni²⁺: NENP, NDMAP
V³⁺: AgVP₂S₆

各サイトのスピン1を2個のスピン1/2の合成と考える。

Valence Bond Solid 状態:

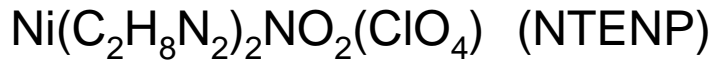
$$\Psi_{\text{preVBS}} = \bigoplus_i \left\{ \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_{i,a} |\downarrow\rangle_{i+1,b} - |\downarrow\rangle_{i,a} |\uparrow\rangle_{i+1,b} \right) \right\}$$

$$\Psi_{\text{VBS}} = S \Psi_{\text{preVBS}} \quad \text{同一サイトの2個のスピンa,bについて対称化}$$

$$\Psi_{\text{VBS}} \quad \text{は、} \quad H = J \sum_i \left\{ \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3} (\vec{S}_i \cdot \vec{S}_{i+1})^2 \right\} \quad \text{に対する厳密な基底状態。}$$

$$P = \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3} (\vec{S}_i \cdot \vec{S}_{i+1})^2 + \frac{2}{3} \quad \text{は全スピン2に対する射影演算子}$$

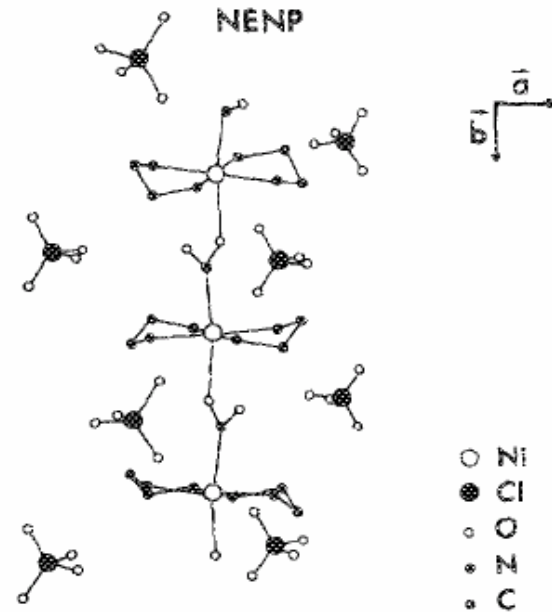
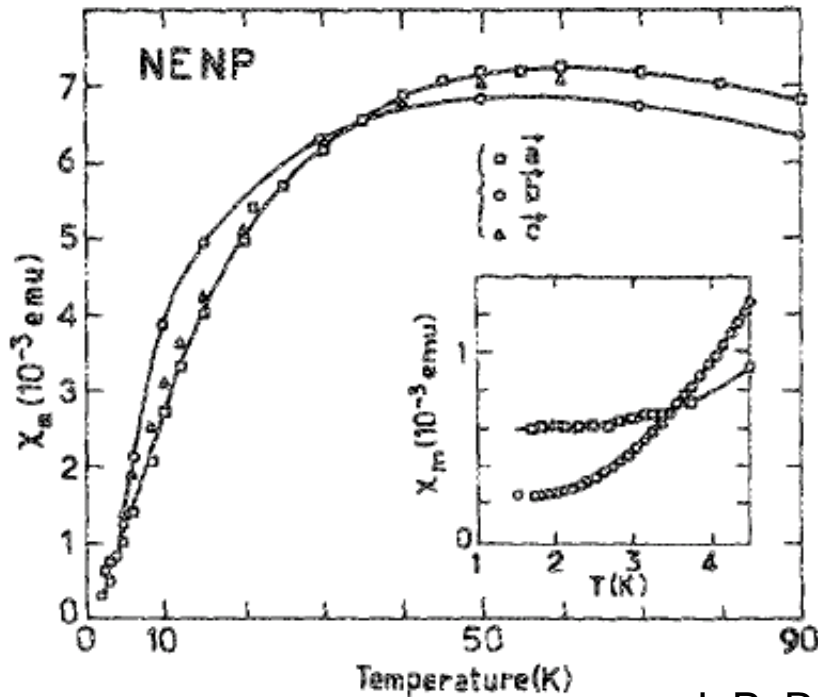
ハルデイン・ギャップの例



結晶構造: Orthorhombic ($Pnma$)

b方向に1次元鎖。
鎖同士は ClO_4 によって隔離されている。

$$J'/J \approx 10^{-4}$$



低温で磁化率が指数関数的に減少。

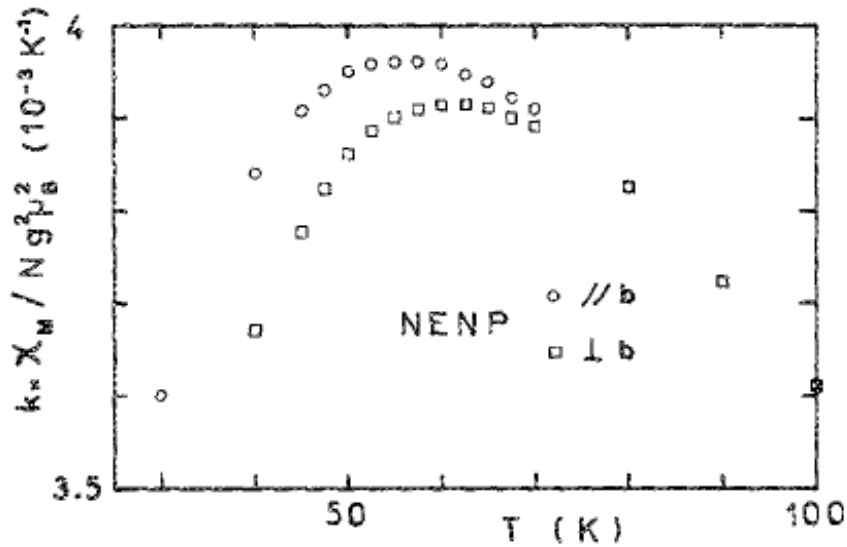
$$\chi(T) = \chi(0) + C \exp(-E_g/kT),$$

$$E_g/k_B = 11 \quad (H // b), \quad E_g/k_B = 17 \quad (H \perp b)$$

$$\frac{J}{k_B} = 47$$

磁化率の異方性 - - - 1イオン異方性

$$H_D = DS_z^2 + E(S_x^2 - S_y^2), \quad z // b$$



1イオン異方性エネルギー

$$D = (\lambda/2)(g^{\parallel} - g^{\perp}),$$

$$g_a = 2.23$$

$$g_b = 2.15$$

$$g_c = 2.21$$

$$D/k_B = 12$$

最近のより正確な値:

$$J/k_B = 44$$

$$D/k_B = 8$$

$$E/k_B = 0.4$$

中性子散乱

エネルギー・ギャップの直接観測

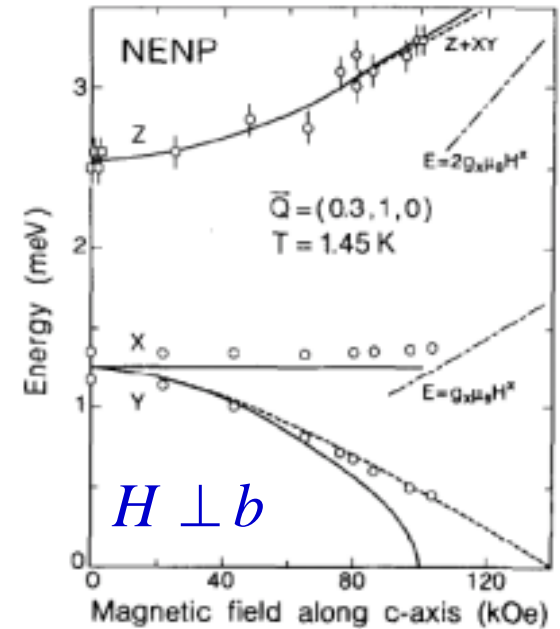
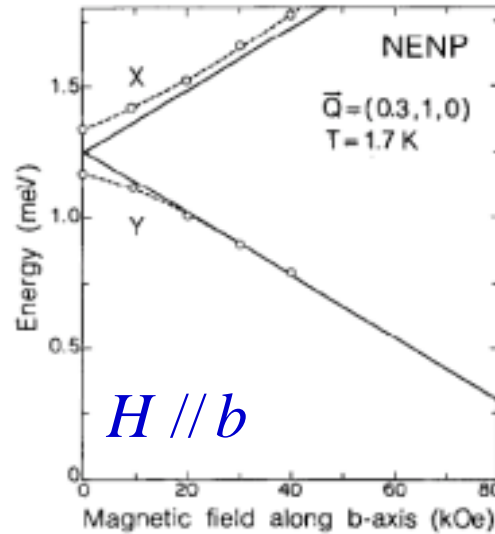
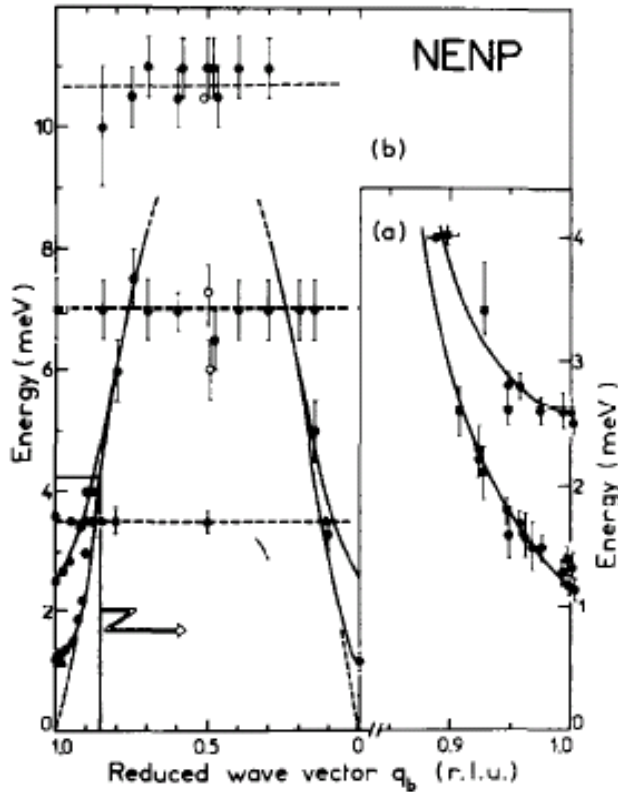
$$E_G^{x,y} / k_B = 30$$

$$E_G^z / k_B = 15$$

$$E_G^z - E_G^{x,y} = 1.8D$$

励起エネルギーの磁場依存性

L. P. Regnault *et al.*, Physica B180-181 (1992) 188.



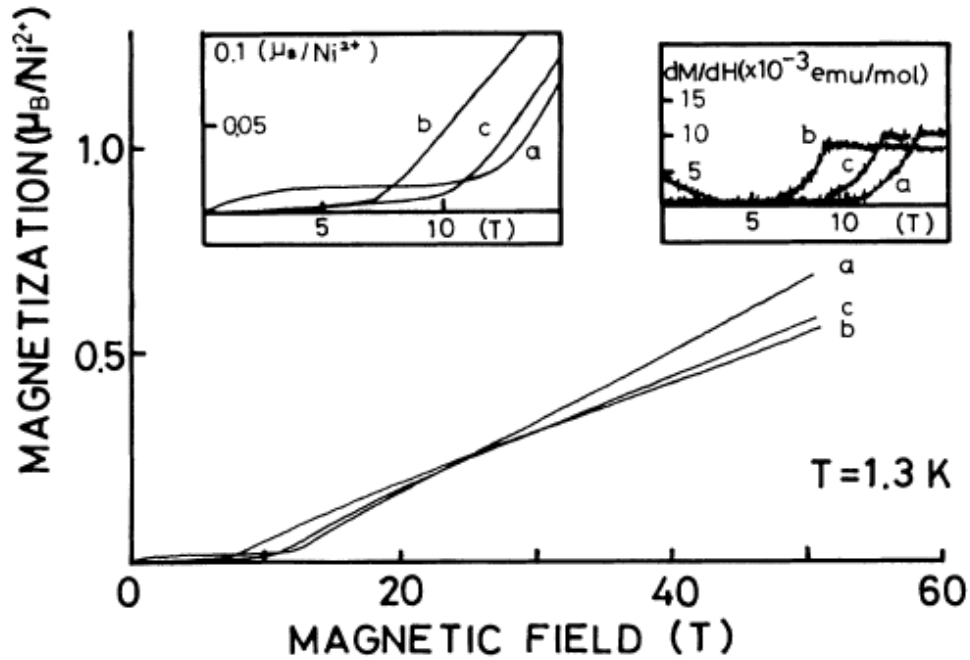
$$E_G^{x,y}(H_z) = E_G^{x,y} \pm g_z \mu_B H_z$$

$$E_G^z(H_z) = E_G^z$$

J. P. Renard *et al.*,
J. de Phys. Colloque. 49 (1988) C8-1425.

強磁場磁化過程

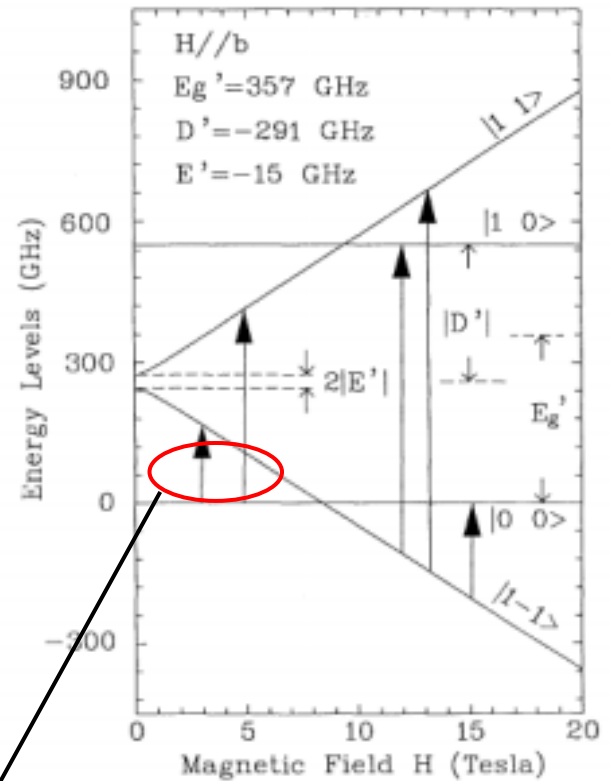
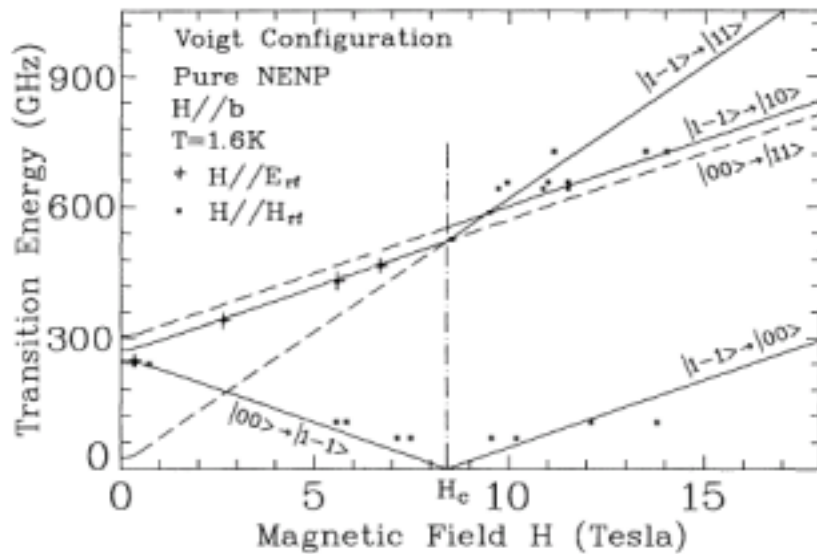
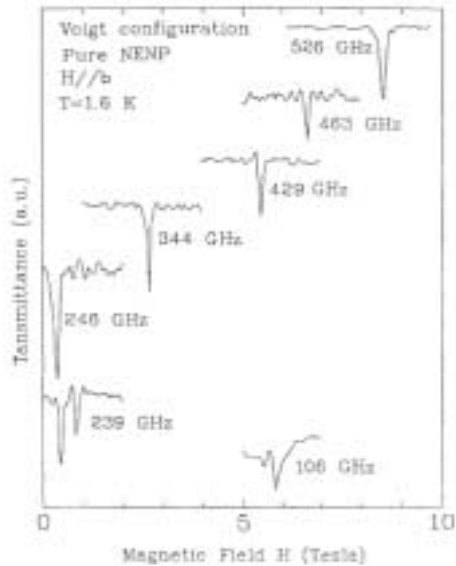
K. Katsumata et al., Phys. Rev. Lett. 63 (1989) 86.



電子スピン共鳴

W. Lu et al.,
Phys. Rev. Lett. 67 (1991) 3716.

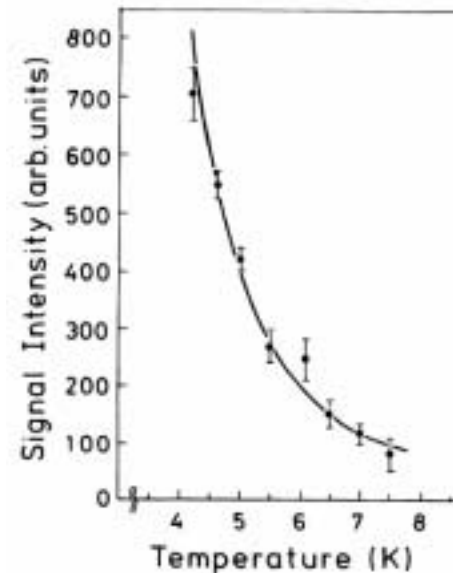
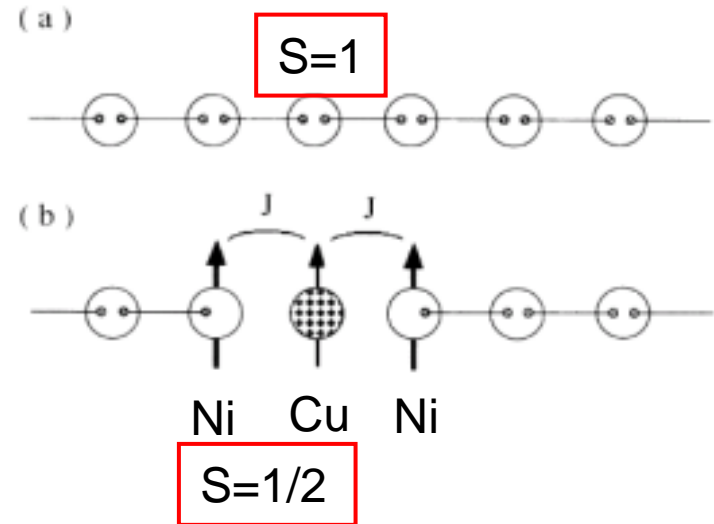
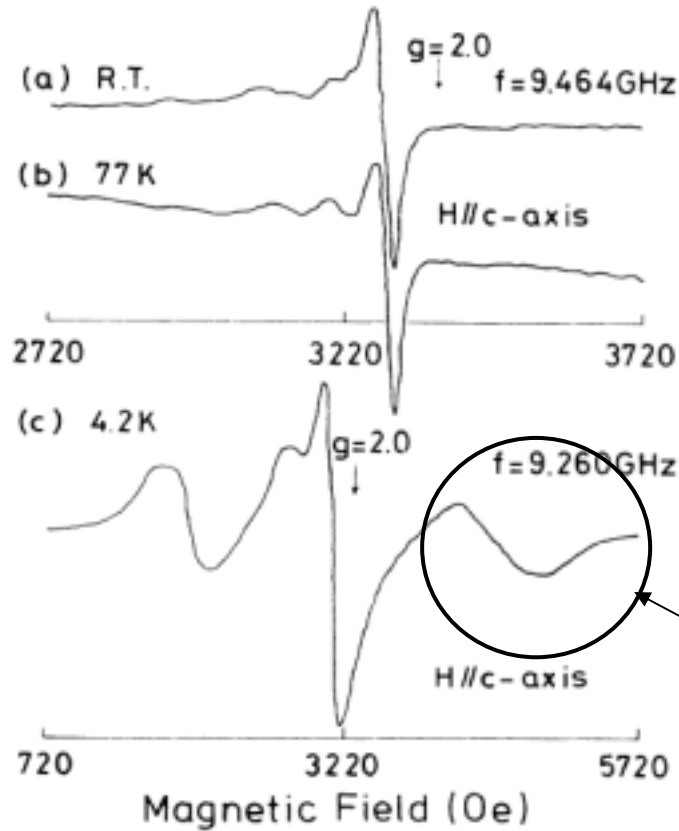
$$\mathcal{H} = \sum_i \left\{ -JS_i \cdot S_{i+1} + \mu_B S_{z_i} g_b H + D \left[S_{z_i}^2 - \frac{S(S+1)}{3} \right] + E(S_{x_i}^2 - S_{y_i}^2) \right\}.$$

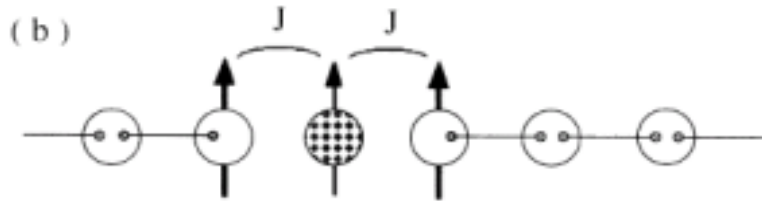


本来は禁制遷移
何故観測できるのか？

Valence Bond Solid 状態の実験的検証 (不純物誘起スピンのESR)

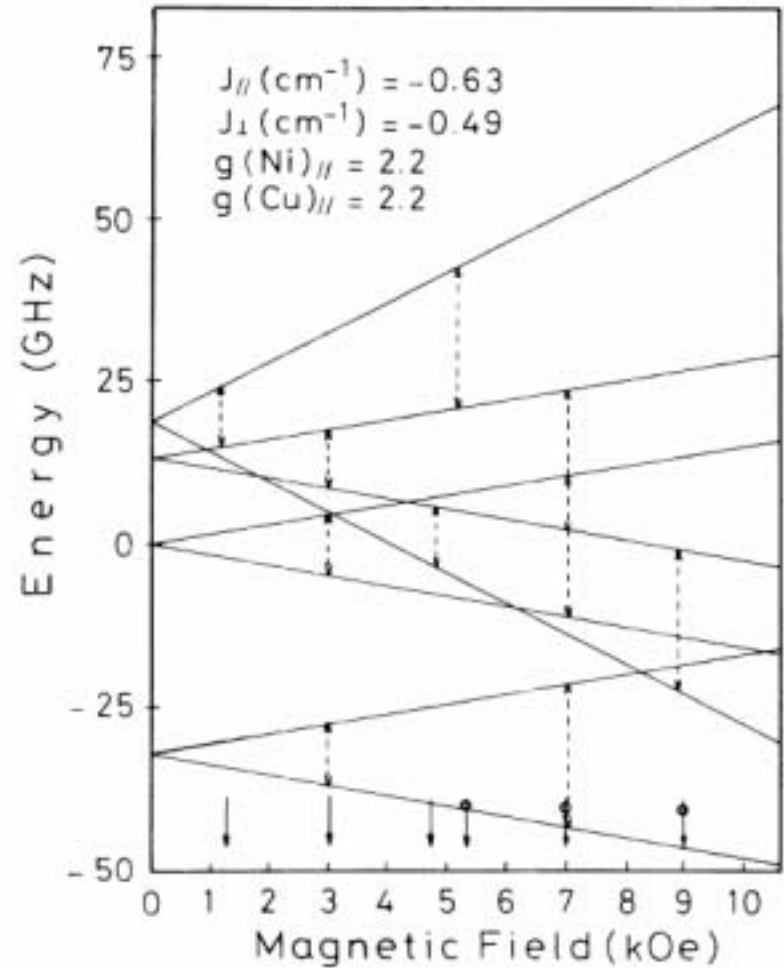
Hagiwara *et al.*, Phys. Rev. Lett. **65** (1990) 3181.





$$\begin{aligned}
 H = & -2J_{\parallel} (S_1^z + S_2^z) s^z \\
 & -2J_{\perp} \left\{ (S_1^x + S_2^x) s^x + (S_1^y + S_2^y) s^y \right\} \\
 & + G_{\parallel} \mu_B H (S_1^z + S_2^z) + g_{\parallel} \mu_B H s^z
 \end{aligned}$$

3個の1/2スピン
 (1イオン異方性エネルギーなし)



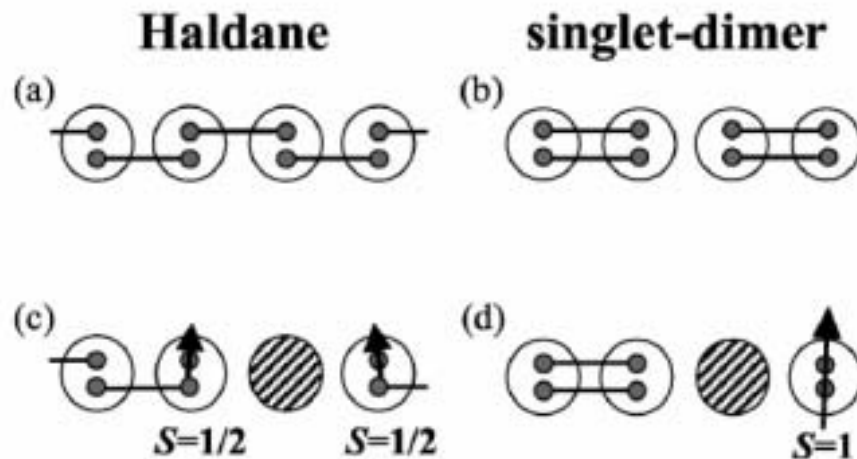
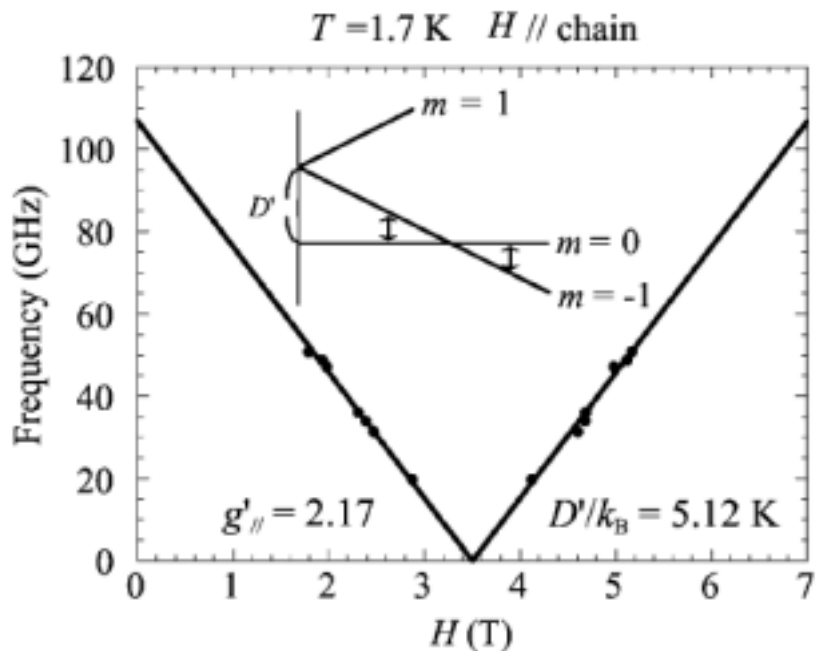
ボンド交替があるS=1ハイゼンベルグ鎖

ボンド交替比が大きい場合はVBS相より
シングレットダイマー相が安定となる。

不純物誘起スピンのESR

Hagiwara et al., Phys. Rev. Lett. **86** (2001) 324.

NTENP



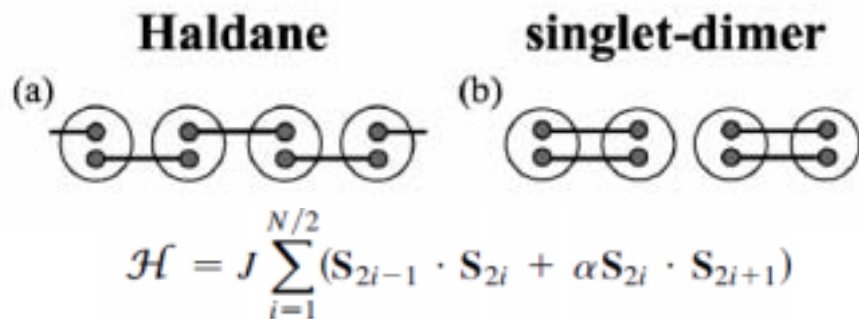
$$\mathcal{H}_{\text{chain}} = J \sum_{i=1}^{L/2} (S_{2i-1} \cdot S_{2i} + \alpha S_{2i} \cdot S_{2i+1}) + \sum_{i=1}^L D(S_i^z)^2 - \sum_{i=1}^L \mu_B S_i \tilde{g} H,$$

$D=13.6\text{K}$

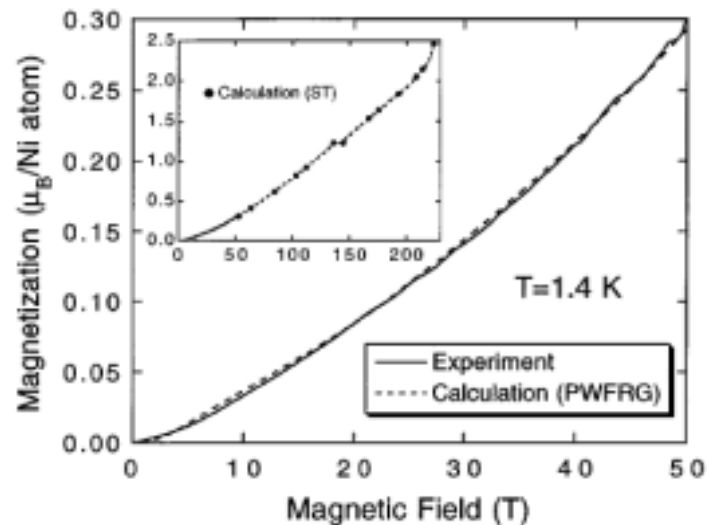
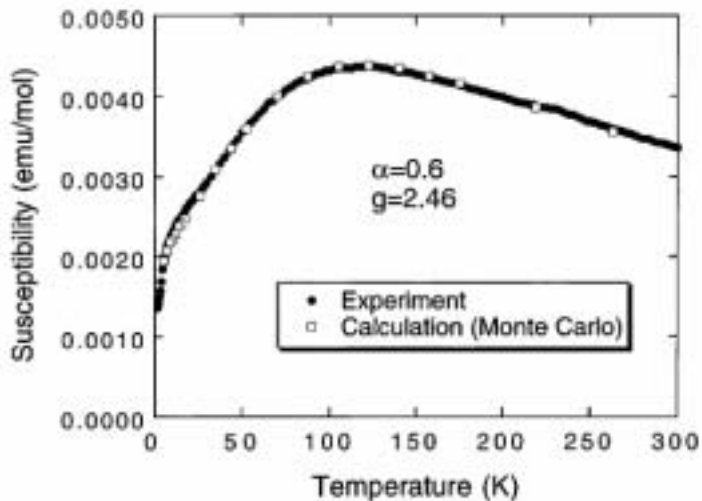
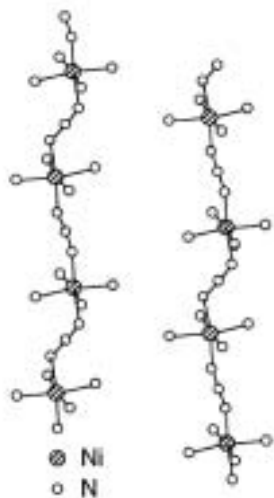
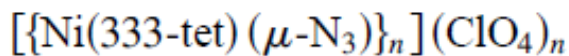
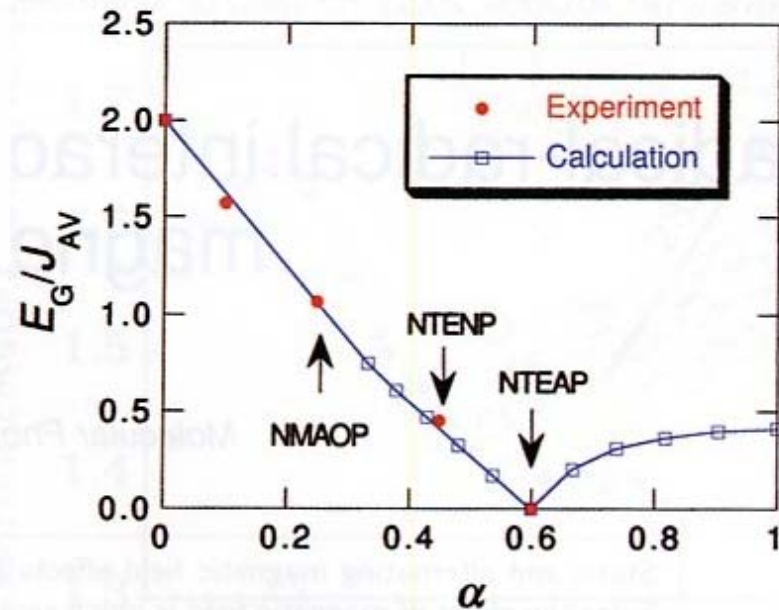
$$\mathcal{H}_{\text{edge}} = D'(s^z)^2 - \mu_B s \tilde{g}' H$$

$D'=5.1\text{K}$

S=1 Bond Alternating Chainにおける量子相転移



ボンド交替比を変えるるとダイマー・シングレット相からハルデン相への量子相転移が起こる。



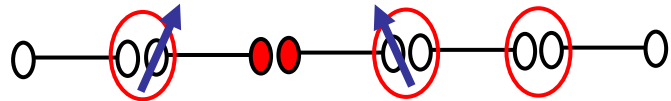
2-1: Impurity effects in spin chains

In highly correlated spin system, local impurities may disturb the spin correlation over a large distance. Response to non-magnetic defects reflects the nature of the ground state.

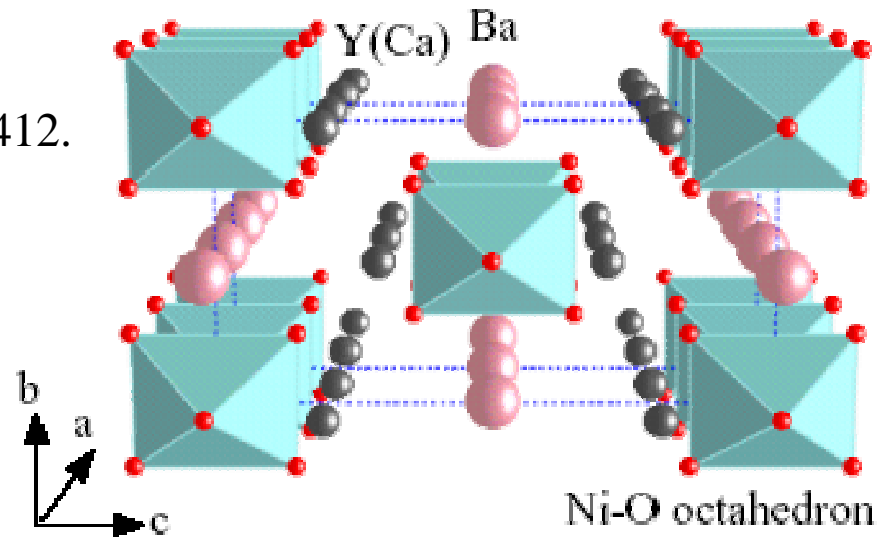
Example 1. End-spins in S=1 Haldane chains

^{89}Y NMR in $\text{YBa}_2\text{Ni}_{1-x}\text{Mg}_x\text{O}$

Tedoldi, Santachiara, Horvatic, PRL83 (1999) 412.



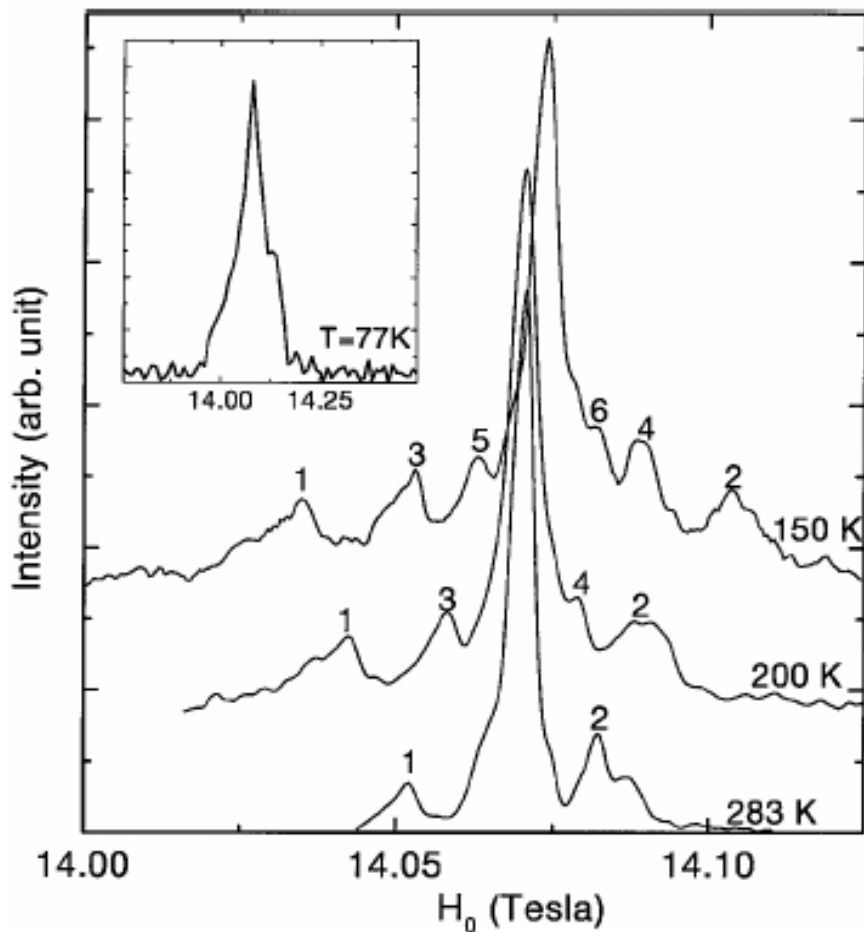
$$J = 280\text{K} \quad \left| \frac{J'}{J} \right| \leq 5 \times 10^{-4}$$



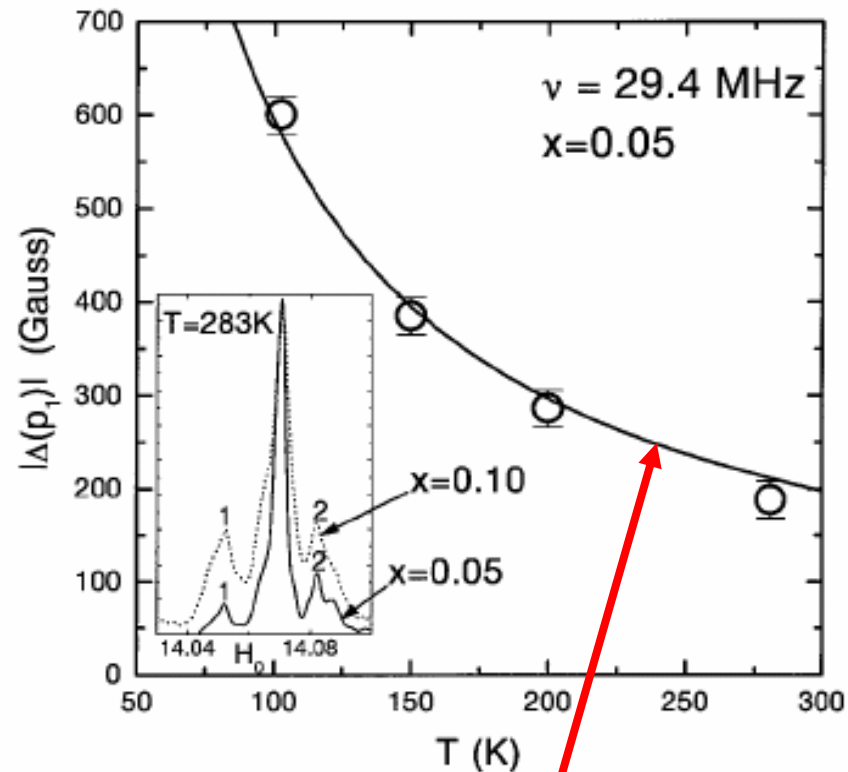
Each Y nucleus couples to two Ni spins on adjacent chains.

$$\vec{H}_{\text{hf}} = A(\vec{S}_1 + \vec{S}_2) \quad A = 0.13 \text{ T}$$

^{89}Y NMR spectra for $x=0.05$



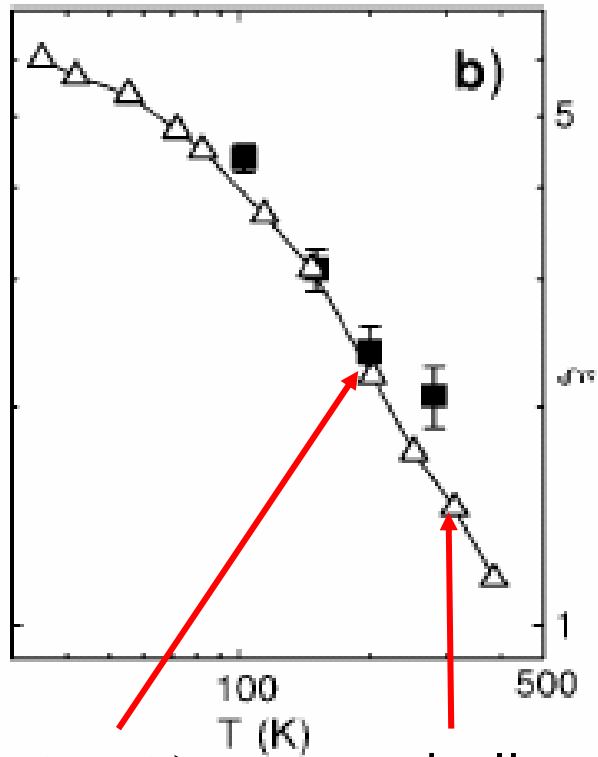
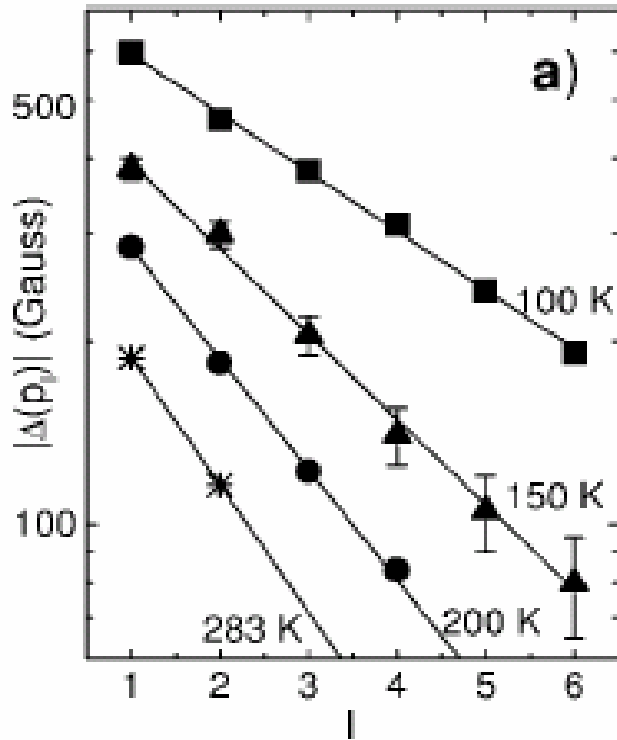
Shift of the 1st satellite line.



$$\Delta(p_1) = A \frac{g\mu_B S(S+1)}{3kT} H_0 \quad \left(S = \frac{1}{2} \right)$$

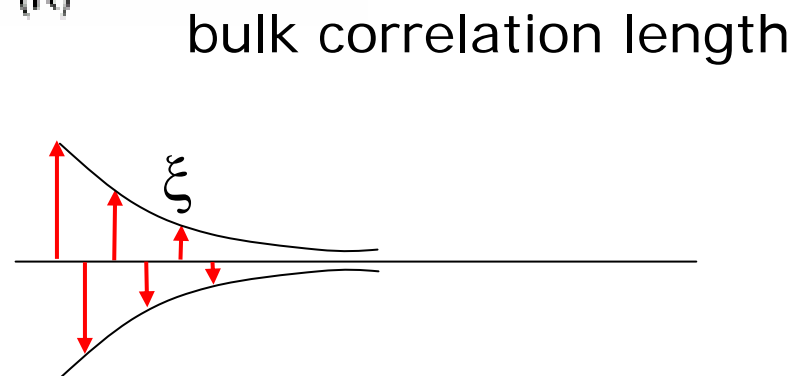
Free spin 1/2

Site dependence of the shift



Exponential decay of the staggered magnetization with the **bulk** correlation length.

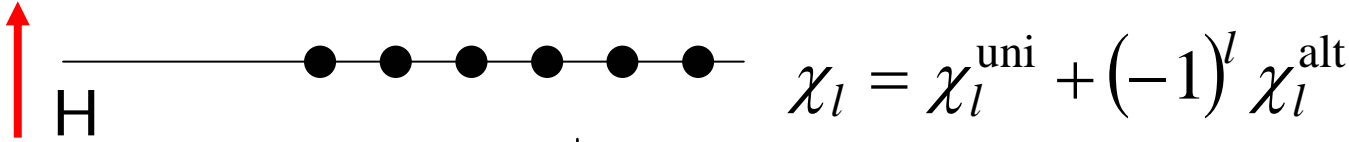
$$\Delta(p_l)(T) = \Delta(p_1) \exp\left(-\frac{(l-1)}{\xi(T)}\right)$$



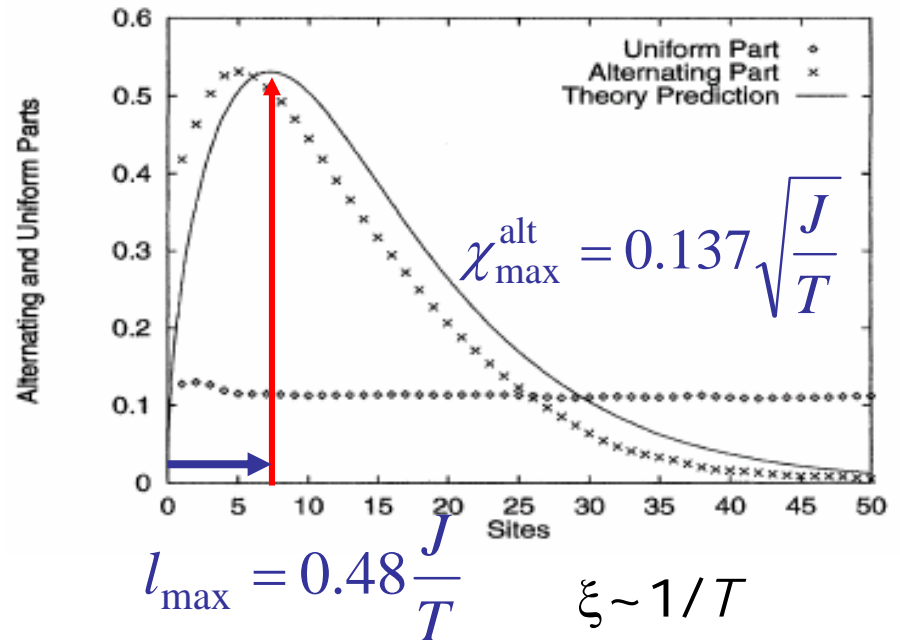
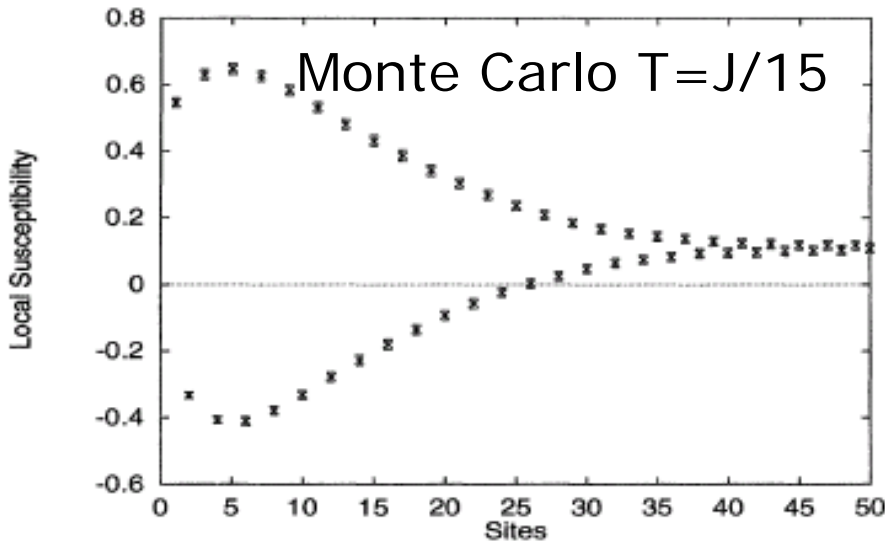
Example 2: field-induced staggered magnetization for $s=1/2$ chains

Eggert and Affleck, PRL75 (1995) 934.

A uniform field induces oscillating magnetization near chain ends.



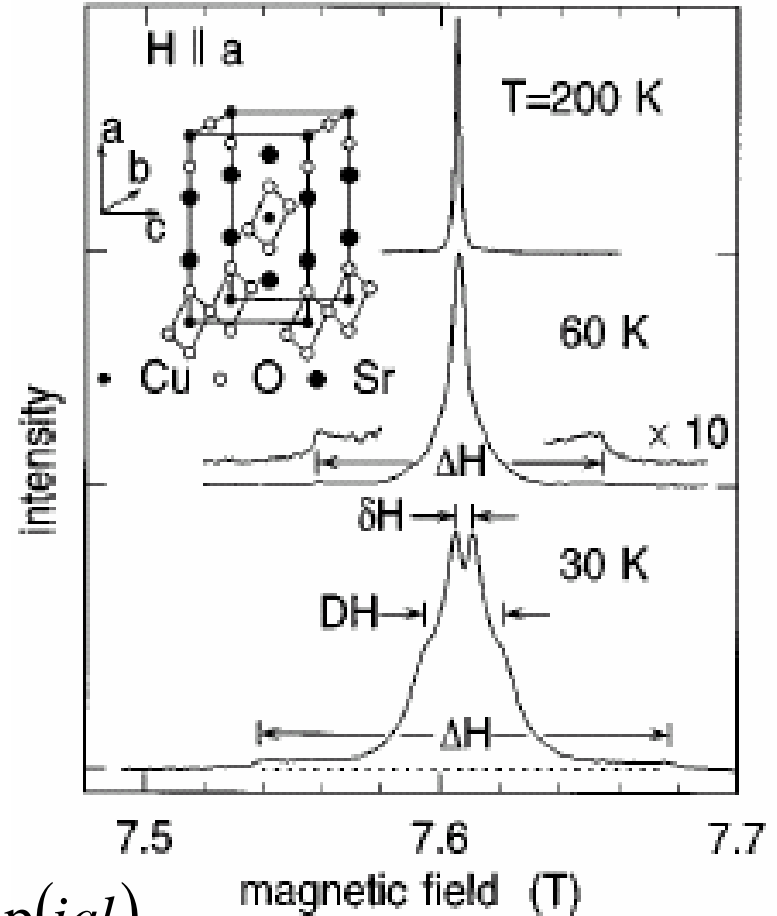
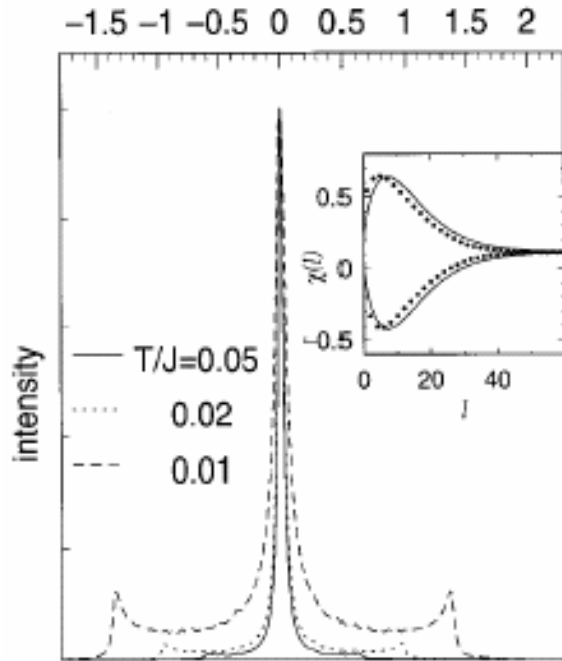
$$\chi_l(T) = \frac{\partial}{\partial H} \left\langle S_l^z \right\rangle \Big|_{H=0} \quad \chi_l^{\text{alt}} = \frac{2a}{\pi J} \frac{l}{\sqrt{\left(\frac{J}{2T}\right) \sinh\left(\frac{4lT}{J}\right)}}, \quad a = 0.58$$



^{63}Cu NMR spectrum in Sr_2CuO_3

Takigawa et al., PRB55 (1997) 14129.

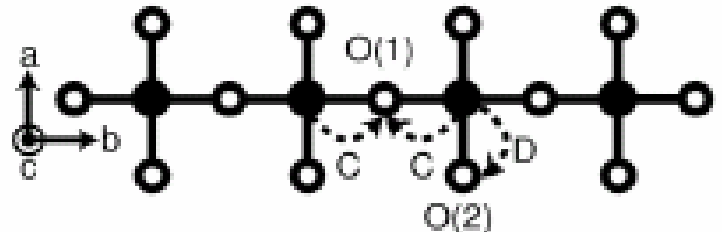
Simulation
up to $l=450$

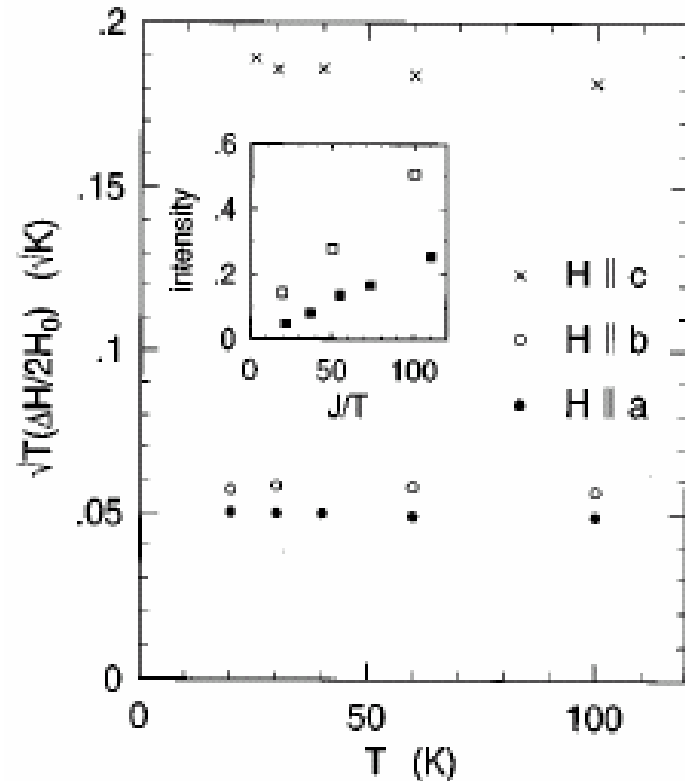
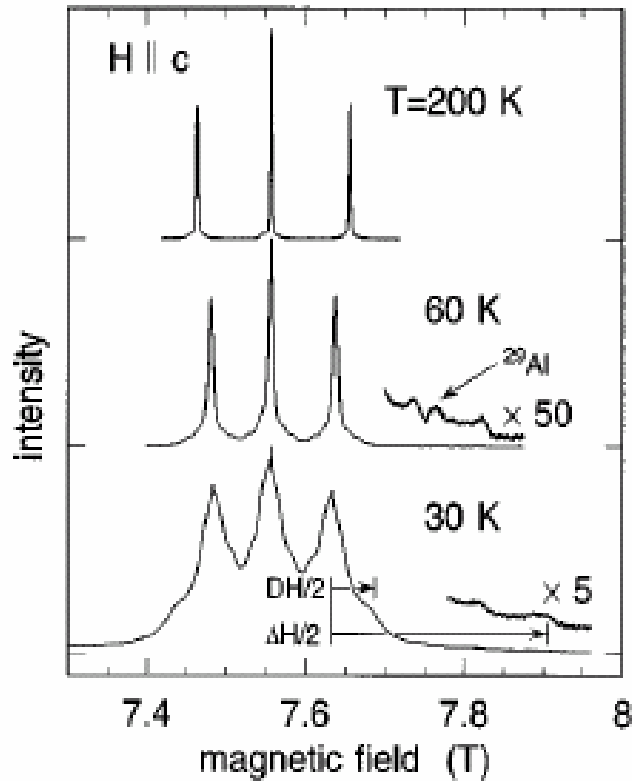


Hyperfine form factor

$$H_{\text{hf}}^{\alpha}(i) = I_i^{\alpha} \sum_l A_{i-l}^{\alpha} S_l^{\alpha}, \quad A(q) = \sum_l A_l \exp(iql)$$

$$K(i) = A^z(0)\chi^{\text{uni}} + A^z(\pi)\chi^{\text{alt}}(i)$$





ΔH is proportional to $\frac{1}{\sqrt{T}}$ and anisotropic.

$$\Delta H_a : \Delta H_b : \Delta H_c = 1 : 1.2 : 3.7$$

$$|A^a(\pi)| : |A^b(\pi)| : |A^c(\pi)| = 1 : 1.1 : 3.3$$

$$\left(\frac{1}{T_1}\right)_a \propto A^b(\pi)^2 + A^c(\pi)^2, \text{ etc.}$$

Average chain length ~ 1800 .

Origin of the defects ?