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SUMMER SCHOOL
on
LOW-DIMENSIONAL QUANTUM SYSTEMS:
Theory and Experiment
(16 - 27 JULY 2001)

PLUS

PRE-TUTORIAL SESSIONS
(11 - 13 JULY 2001)

PLATEAUX IN MAGNETIZATION CURVES OF ONE-DIMENSIONAL QUANTUM ANTIFERROMAGNETS

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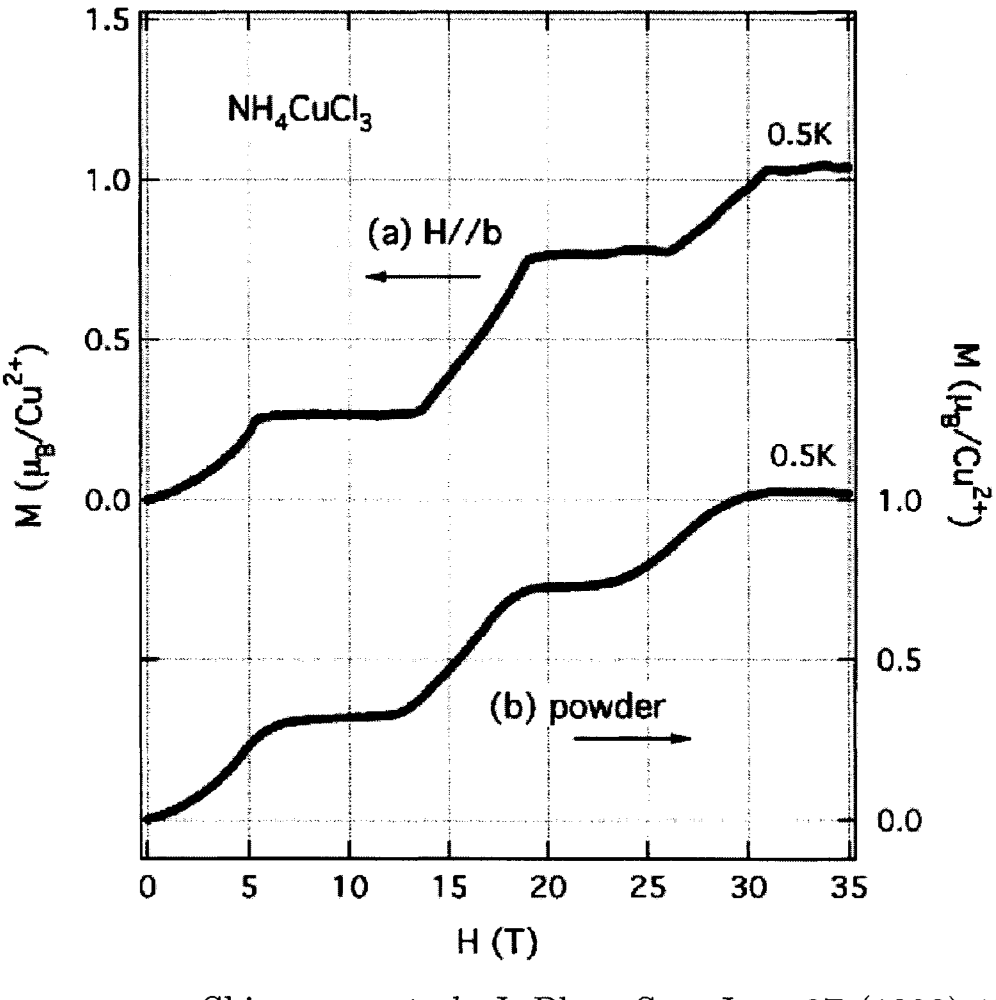
Festkörper-Theorie

Plateaux in magnetization curves of one-dimensional quantum antiferromagnets

abdus salam ictp, Trieste, 25.07.2001

Andreas Honecker

TU Braunschweig, Germany



Shiramura *et al.*, J. Phys. Soc. Jpn. **67** (1998) 1548

Plateaux (spin gap) $\leftrightarrow$ macroscopic quantum effects

Analogy: Fractional quantum Hall effect

Short review: **Cabra**, Grynberg, A.H., **Pujol**, cond-mat/0010376

Quantization condition in 1D

Plateaux obey the quantization condition

$$VS(1 - \langle M \rangle) \in \mathbb{Z}\,. \qquad (\star)$$

V : Volume of translational unit cell in the groundstate. Translational invariance of the Hamiltonian can be broken spontaneously ! (Many frustrated systems: Period ≥ 2).

S : Local spin, e.g. $S = 1/2$.

$\langle M \rangle$: Magnetization (normalized to ± 1).

... and a generalized Lieb-Schultz-Mattis theorem

Oshikawa, Yamanaka, Affleck, Phys. Rev. Lett. **78** (1997) 1984

Either the condition $(\star)$ is satisfied *or* the spectrum is gapless *or* the groundstate is degenerate.

Sketch of the proof:

Let

- $|\,\psi_0\,\rangle$ be the groundstate (wolg. unique),
- $U_k = \mathrm{e}^{-ik \sum_{x=1}^{L} x \sum_{\vec{x} \in \mathcal{U}_x} S^z_{\vec{x}}}$, $(|\mathcal{U}_x| = V)$
- $|\,\psi_k\,\rangle := U_k |\,\psi_0\,\rangle\,.$

Step 1: Show $|\,\psi_k\,\rangle \perp |\,\psi_0\,\rangle$ for suitable k unless $(\star)$ is satisfied

Step 2: Check that

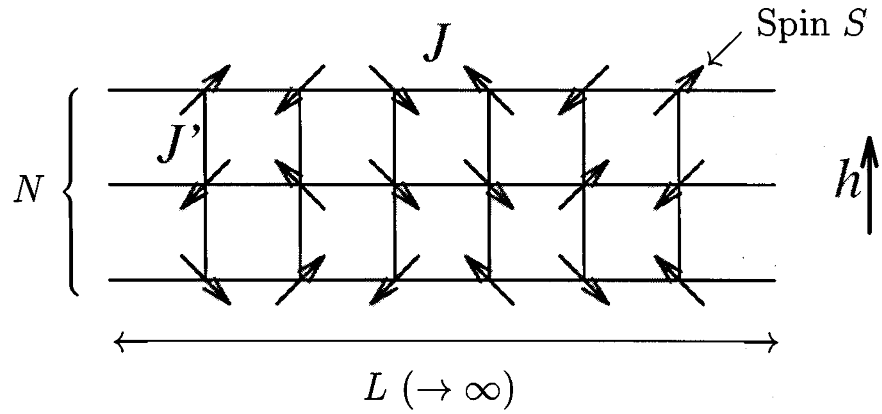
$$\langle\,\psi_{\frac{2\pi}{L}}\,|\mathcal{H}|\,\psi_{\frac{2\pi}{L}}\,\rangle - \langle\,\psi_0\,|\mathcal{H}|\,\psi_0\,\rangle = \mathcal{O}\left(\frac{1}{L}\right)\,.$$

Problems:

- Existence of a gap if $(\star)$ is satisfied not shown.
- Excitation $|\,\psi_k\,\rangle$ is non-magnetic
  $\Rightarrow$ Complementary arguments needed to link magnetic and non-magnetic excitations.

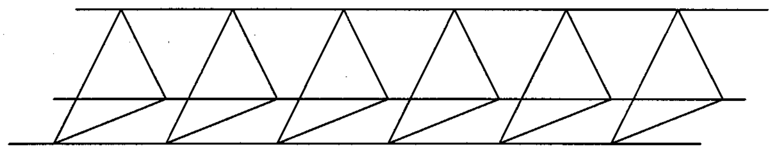
Spin ladders

($N = 3$, open boundary conditions (OBC))



realized e.g. in $Sr_2Cu_3O_5$

(or periodic boundary conditions (PBC), $N = 3$)



Hamilton operator:

$$\begin{aligned}
\mathcal{H}^{(N)} &= J \sum_{i=1}^{N} \sum_{x=1}^{L} \left\{ \Delta S^z_{i,x} S^z_{i,x+1} + \frac{1}{2} \left(S^+_{i,x} S^-_{i,x+1} + S^-_{i,x} S^+_{i,x+1} \right) \right\} \\
&+ J' \sum_{i,j} \sum_{x=1}^{L} \vec{S}_{i,x} \vec{S}_{j,x} \\
&- h \sum_{i,x} S^z_{i,x}
\end{aligned}$$

Magnetization:

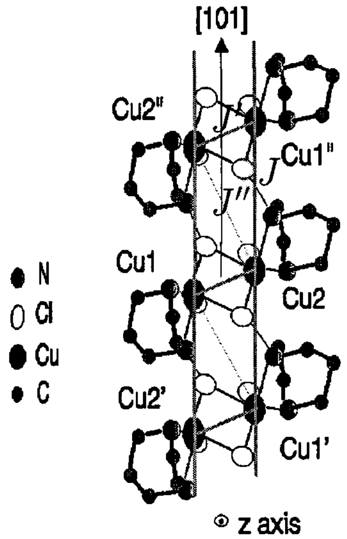
$$\langle M \rangle = \frac{1}{SLN} \left\langle \sum_{i,x} S^z_{i,x} \right\rangle$$

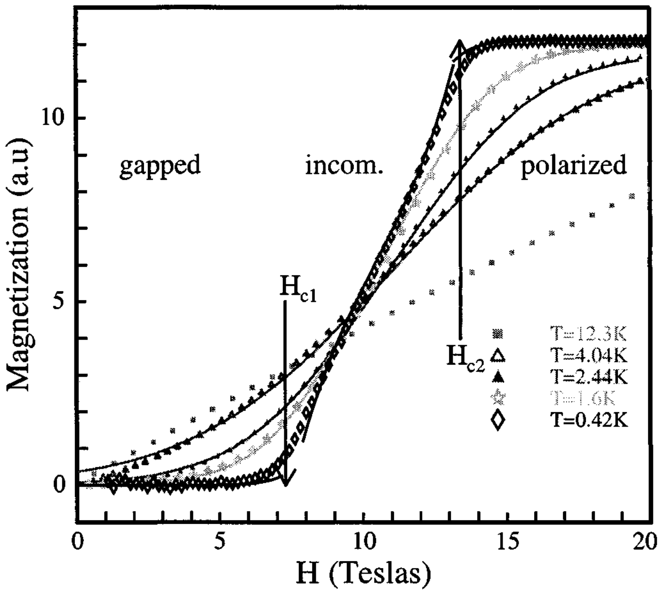
Technical remark:

M conserved $\Rightarrow$
Behaviour at $h \neq 0$ $\Leftrightarrow$ behaviour at $h = 0$ and fixed $\langle M \rangle$

Magnetization curves of $S = 1/2$, $N = 2$-leg ladder materials

a) $J'/J \approx 5$:



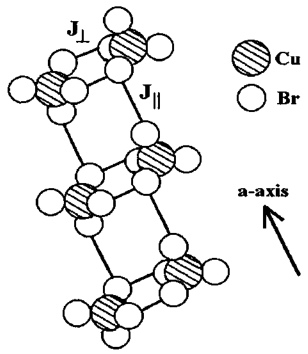


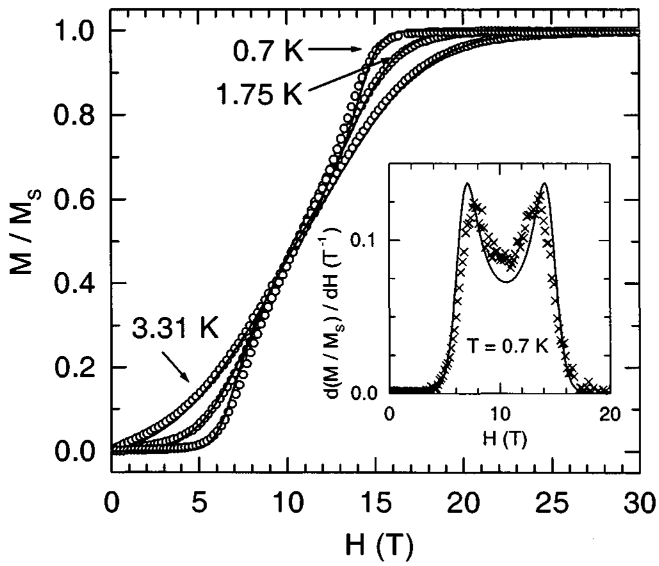
Structure of $Cu_2(C_5H_{12}N_2)_2Cl_4$, High-field magnetization curves.

Chaboussant *et al.*, Phys. Rev. **B55** (1997) 3046;
Eur. Phys. J. **B6** (1998) 167

STOP Recent inelastic neutron scattering measurements
$\Rightarrow$ Cu_2(1,4-diazacycloheptane)$_2Cl_4$ not a spin ladder
Stone *et al.*, cond-mat/0103023

b) $J'/J \approx 3.5$:



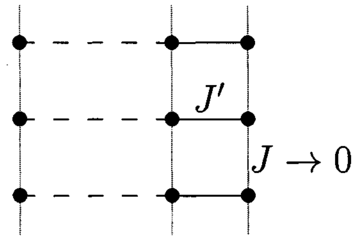


Structure of $(C_5H_{12}N)_2CuBr_4$, High-field magnetization curves.

Watson *et al.*, Phys. Rev. Lett. **86** (2001) 5168

Strong-coupling limit

Consider the limit $J' \gg J$



In zeroth order ($J = 0$), rungs are decoupled:

$$\mathcal{H}_{\text{eff.}} = J' \sum_{i=1}^{N(-1)} \vec{S}_i \vec{S}_{i+1} - h \sum_{i=1}^{N} S_i^z \,.$$

N spin-1/2 spins $\Rightarrow$ only possible values of magnetization:

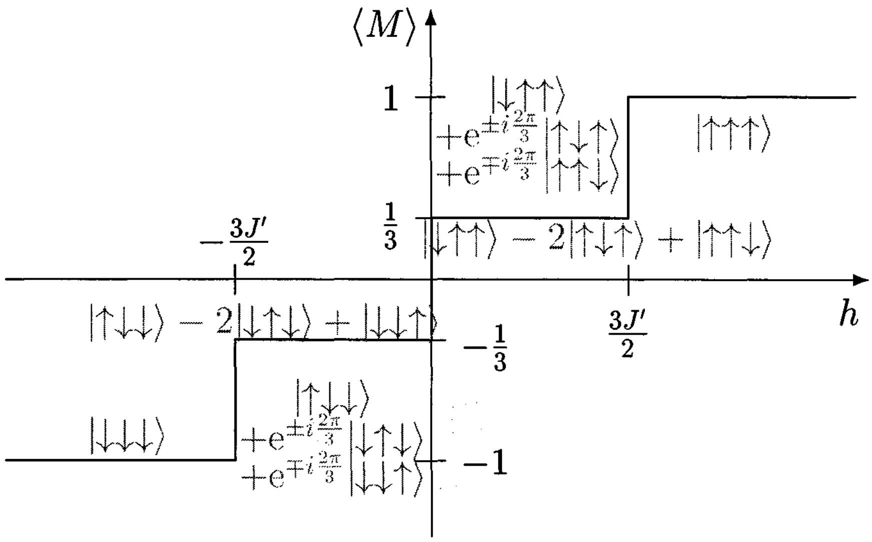
$$\langle M \rangle \in \left\{ -1, -1 + \frac{2}{N}, \ldots, 1 - \frac{2}{N}, 1 \right\}$$

$\Rightarrow$ plateaux with magnetization m/N !

(These are precisely the solutions of ($\star$) with $V = N$, $S = 1/2$).

Example: $N = 3$

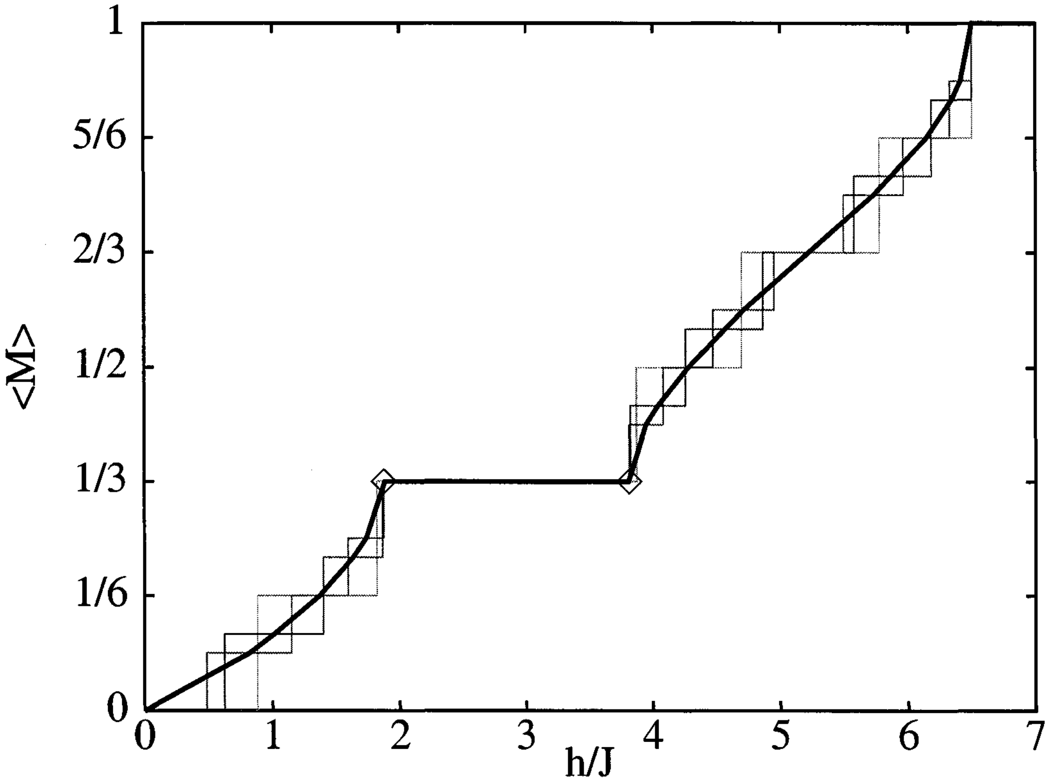
$J' > 0$, $J = 0$:



Both OBC and PBC: Plateau with $\langle M \rangle = 1/3$.

$J', J > 0$: Transitions soften, but plateaux survive:

Magnetization curve of the OBC $N = 3$-leg ladder
$(J'/J = 3)$



$L = 8$, $L = 6$, $L = 4$, **extrapolation**
Diamonds: 4th-order series results for boundaries of plateau

Remarks:

- First order in J: transitions between plateaux can be described by effective Hamiltonians.
  Quite often, one finds an XXZ chain.
  Totsuka, Chaboussant *et al.*, Mila, Wessel & Haas, ...
  $\Delta_{\text{eff.}} > 1 \Rightarrow$ Translational invariance spontaneously broken.
- The strong-coupling argument is essentially independent of the model ! One only needs a limit where the system decouples into clusters of V spins.

Abelian bosonization

following Schulz, Affleck *et al.*, Totsuka

(Convenient way to study the weak-coupling regime ($J' \ll J$) in the thermodynamic limit)

$J' = 0$: Spin-1/2 XXZ-Heisenberg chain in a magnetic field

$$H_{XXZ} = J \sum_{x=1}^{L} \left\{ \Delta S^z_x S^z_{x+1} + \frac{1}{2} \left(S^+_x S^-_{x+1} + S^-_x S^+_{x+1} \right) \right\} - h \sum_{x=1}^{L} S^z_x$$

can be described by a $c = 1$ one-boson CFT:

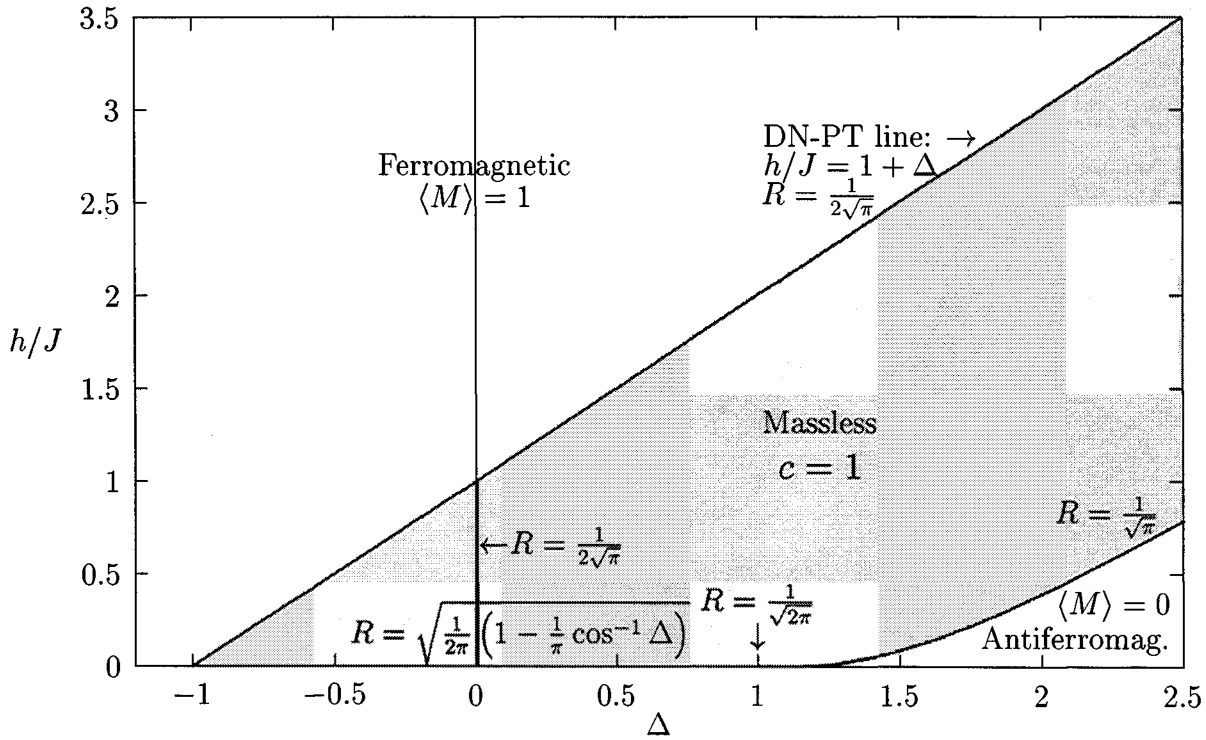
$$\bar{H}_{XXZ} \sim \int \mathrm{d}x \frac{\pi}{2} \left\{ \frac{1}{(4R(\langle M \rangle, \Delta))^2} \Pi^2(x) + R^2(\langle M \rangle, \Delta) \left(\partial_x \phi(x)\right)^2 \right\}$$

with $\Pi = \frac{1}{\pi} \partial_x \tilde{\phi}$, and $\phi = \phi_L + \phi_R$, $\tilde{\phi} = \phi_L - \phi_R$.

Woynarovich, Eckle, Truong, J. Phys. A: Math. Gen. **22** (1989) 4027

Bogoliubov, Izergin, Korepin, Nucl. Phys. **B275** (1986) 687

Magnetic field h & XXZ-anisotropy Δ enter only through radius of compactification $R(\langle M \rangle, \Delta)$ – can be computed exactly from Bethe-ansatz solution of the XXZ-chain:



http://www.tu-bs.de/~honecker/roc.html

... for spin-1/2 ladders

Use:

- field theory Hamiltonian for single chain
- bosonized expressions for the spin operators:

$$S^z_{i,x} \approx \frac{1}{\sqrt{2\pi}}\frac{\partial \phi_i}{\partial x} + const. : \cos(2k^i_F x + \sqrt{4\pi}\phi_i) : + \frac{\langle M_i \rangle}{2}$$
$$S^\pm_{i,x} \approx \; : \mathrm{e}^{\pm i\sqrt{\pi}\tilde{\phi}_i}(1 + const. \cos(2k^i_F x + \sqrt{4\pi}\phi_i)) :$$

  with Fermi momenta $k^i_F = \pi(1 - \langle M_i \rangle)/2$.

⇒ interaction terms (assume now complete symmetry, *i.e.* PBC):

- $: \cos\left(2x(k^i_F + k^j_F) + \sqrt{4\pi}(\phi_i + \phi_j)\right) :$
  commensurate only for $\langle M \rangle = 0, \pm 1$
- $: \cos\left(2x(k^i_F - k^j_F) + \sqrt{4\pi}(\phi_i - \phi_j)\right) : , \quad : \cos\left(\sqrt{\pi}(\tilde{\phi}_i - \tilde{\phi}_j)\right) :$
  relevant interactions; give a mass to relative degrees of freedom.

⇒ a single bosonic field $\psi_D = \frac{1}{\sqrt{N}}\sum_{i=1}^{N}\phi_i$ remains massless so far.

plateau $\longleftrightarrow$ ψ_D acquires a mass

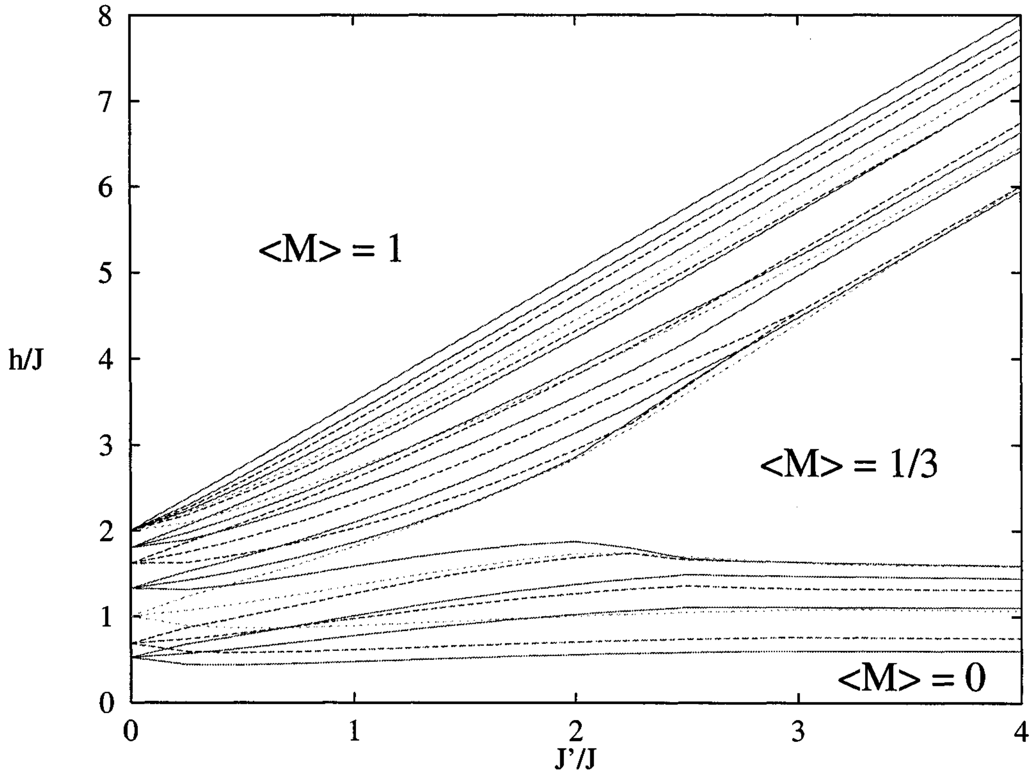
radiatively, we can generate the following interaction term

$$J'^N \cos\left(2x\sum_{i=1}^{N} k^i_F + \sqrt{4\pi}\sum_{i=1}^{N}\phi_i\right) = J'^N \cos\left(2x\sum_{i=1}^{N} k^i_F + \sqrt{4\pi N}\psi_D\right) .$$

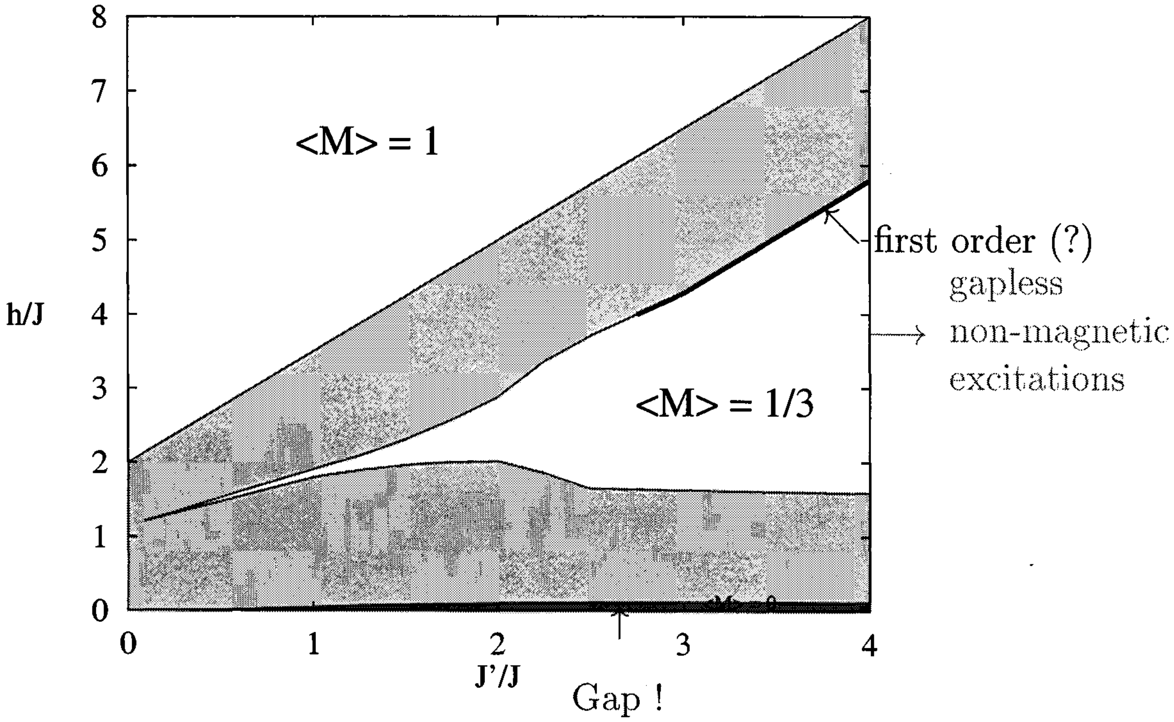
1. is commensurate only if
$$\frac{N}{2}(1 - \langle M \rangle) \in \mathbb{Z}$$
2. provides a mass for ψ_D if it is relevant, *i.e.* its zero-loop scaling dimension
$$\dim\left(\cos\left(\sqrt{4\pi N}\psi_D\right)\right) = \frac{N}{4\left(\pi R^2 + \frac{N-1}{\pi}\frac{J'}{J}\right)}$$
   should be less than 2.

Magnetic phase diagram for $N = 3$ (PBC)

Lanczos: $L = 8$, $L = 6$, $L = 4$



Schematic:



(c.f. Kawano, Takahashi, J. Phys. Soc. Jpn. **66** (1997) 4001)

... and for p-merized spin-1/2 chains

Cabra, Grynberg, Phys. Rev. **B59** (1999) 119

modulated coupling constants

$$J(x) = \begin{cases} J' & \text{if } x \text{ a multiple of } p \\ J & \text{otherwise} \end{cases}$$

$\delta = J - J'$ small

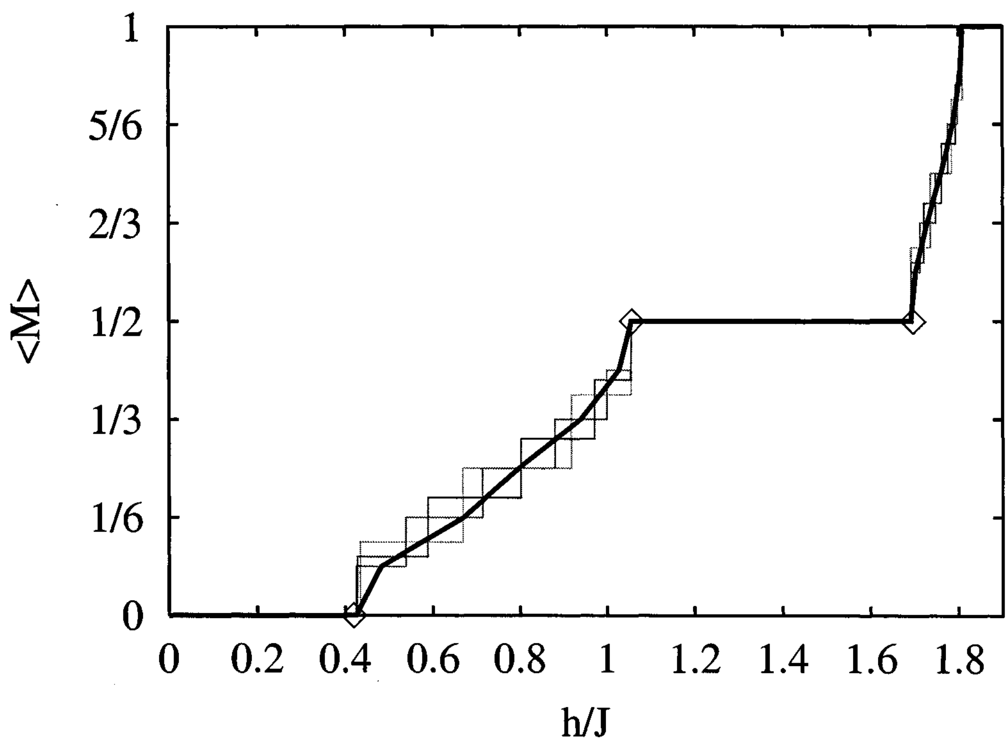
$\Rightarrow$ perturbing operator $\qquad \cos\left(2pk_F x + \sqrt{4\pi}\phi\right)$

1. is commensurate if
$$\frac{p}{2}(1 - \langle M \rangle) \in \mathbb{Z}$$
2. scaling dimension
$$\dim\left(\cos\left(\sqrt{4\pi}\phi\right)\right) = \frac{1}{4\pi R^2}$$

$$R \geq \frac{1}{2\sqrt{\pi}} \text{ for } \Delta \geq 0 \quad \Rightarrow \quad \dim\left(\cos\left(\sqrt{4\pi}\phi\right)\right) \leq 1$$

relevant $\Rightarrow$ plateau always present for $J' \neq J$

Quadrumerized chain ($J' = J/2$)

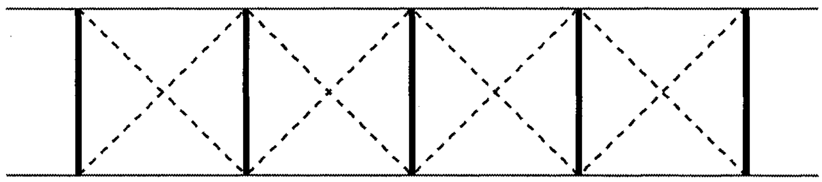


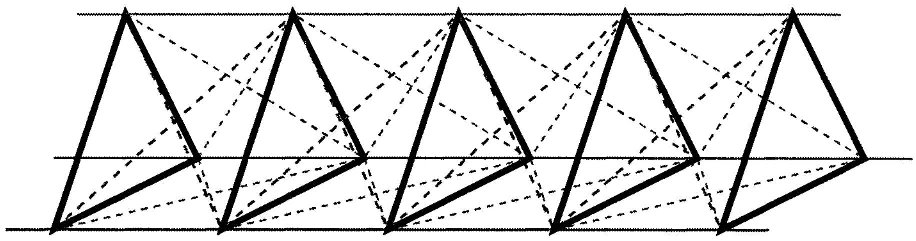
$L = 24$, $L = 20$, $L = 16$, **extrapolation**

Diamonds: 2nd-order series results for boundaries of plateaux

Models with local conservation laws

with Mila, Troyer





$J_\times = J \Rightarrow$ Total spin on each rung

$$\vec{T}_x = \sum_{i=1}^{N} \vec{S}_{i,x}$$

is conserved

$\Rightarrow$ Diagonalize family of Hamiltonians $H(\{T_x\})$

$$H(\{T_x\}) = J \sum_{x=1}^{L} \vec{T}_x \cdot \vec{T}_{x+1} + J' \sum_{x=1}^{L} \frac{1}{2}\left(\vec{T}_x^2 - \frac{3N}{4}\right) - h \sum_{x=1}^{L} T_x^z .$$

with $\vec{T}_x^2 = T_x(T_x+1)$, $T_x = N/2, N/2-1, \ldots$

J' appears only linearly in front of a constant !

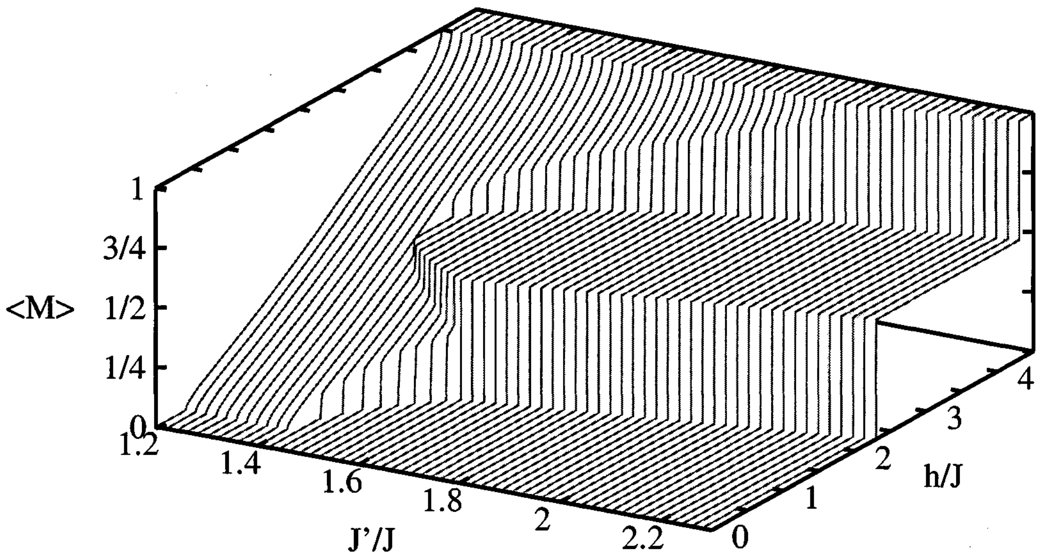
Only a few combinations $\{T_x\}$ appear as groundstates in a magnetic field – e.g.

$\underline{N=3:}$

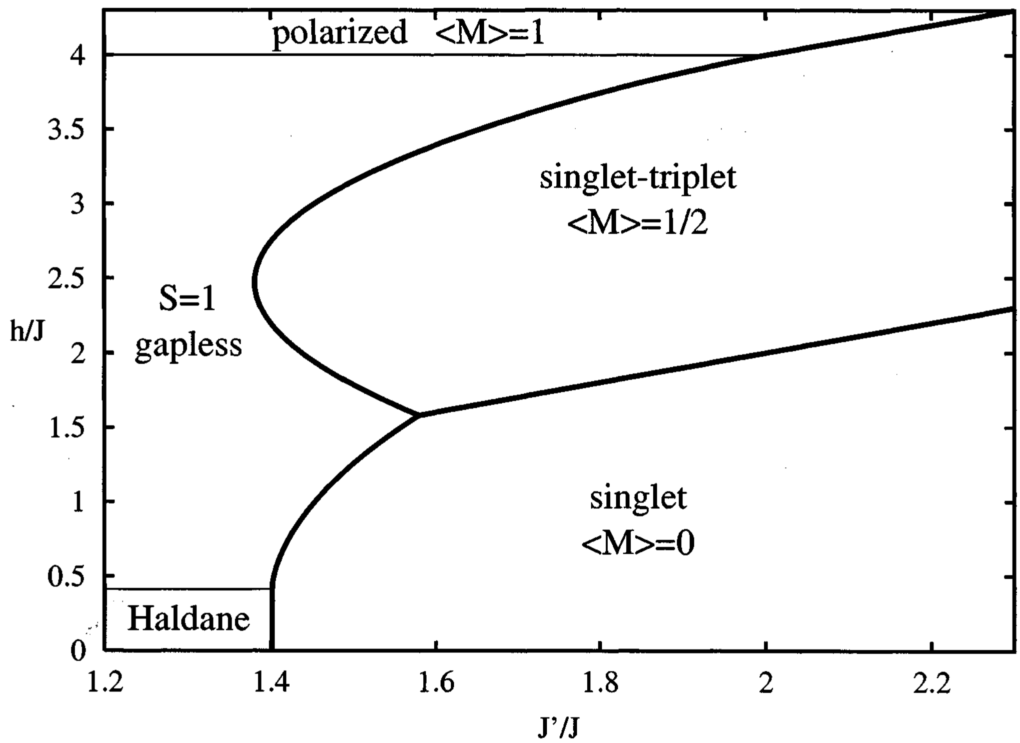
1. Spin-3/2 states on all rungs $\Leftrightarrow S = 3/2$ chain
2. Alternating spin-1/2 and -3/2 on the rungs $\Leftrightarrow S =$ 3/2-1/2 ferrimagnetic chain
3. Spin-1/2 on each rung $\Leftrightarrow S = 1/2$ chain

These chains can be diagonalized by White's DMRG (or Bethe ansatz)

Magnetization curves for $N = 2$



Groundstate phase diagram for $N = 2$

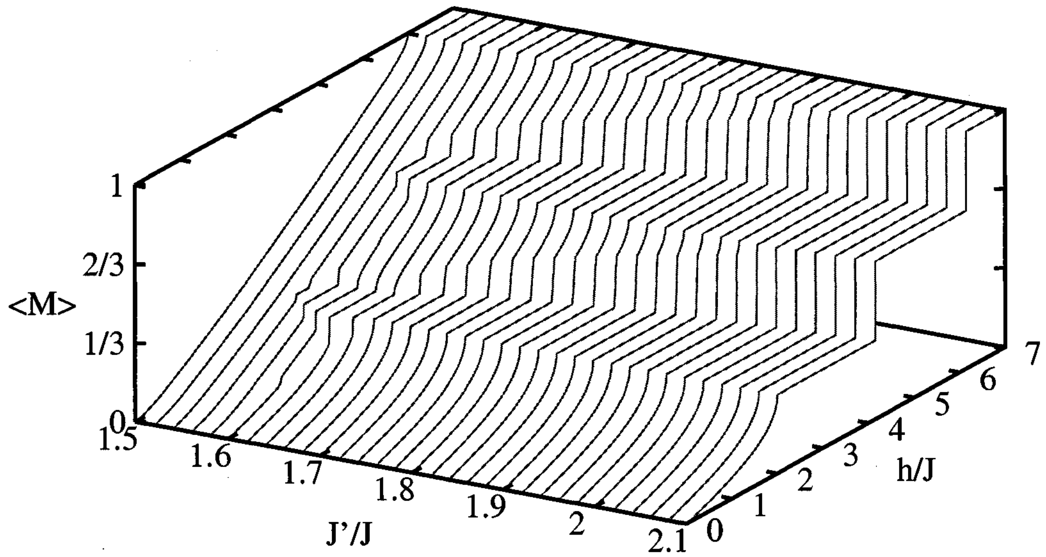


Bold lines: First order transitions
Thin lines: Second order transitions

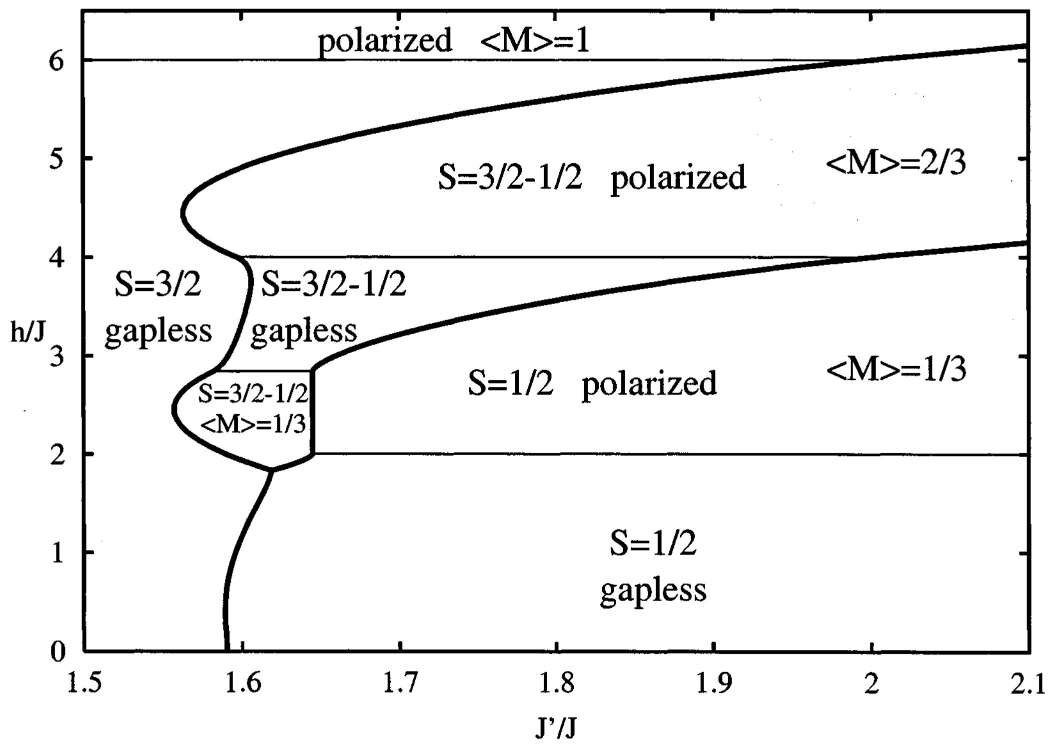
$J' > 2J$: First-order strong-coupling picture is exact

$J' \lesssim 1.381J$: $S = 1$ chain

Magnetization curves for $N = 3$



Groundstate phase diagram for $N = 3$



Bold lines: First order transitions
Thin lines: Second order transitions

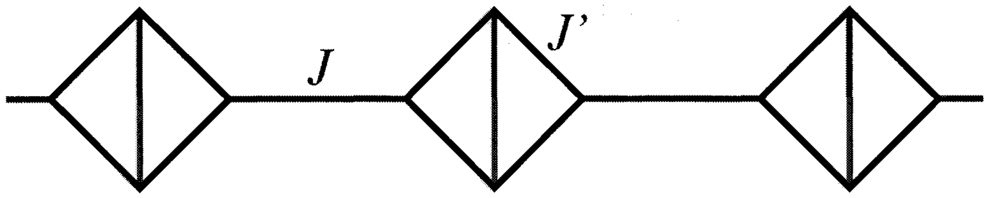
$J' > 2J$: First-order strong-coupling picture is exact

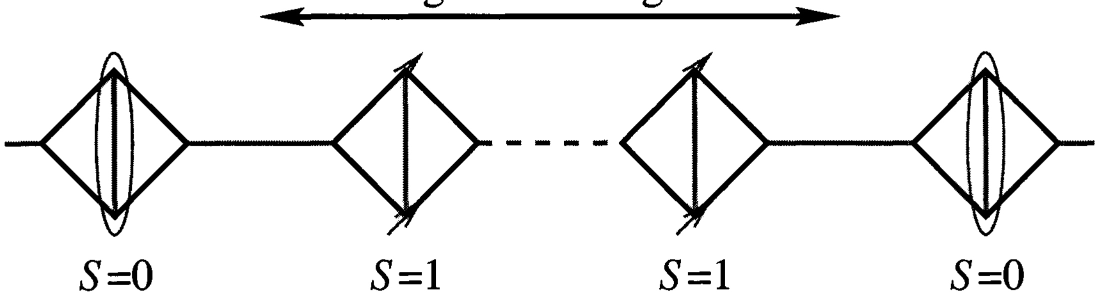
$J' \lesssim 1.557J$: $S = 3/2$ chain

Plateaux have a simple picture in this model

A model with (infinitely) many plateaux

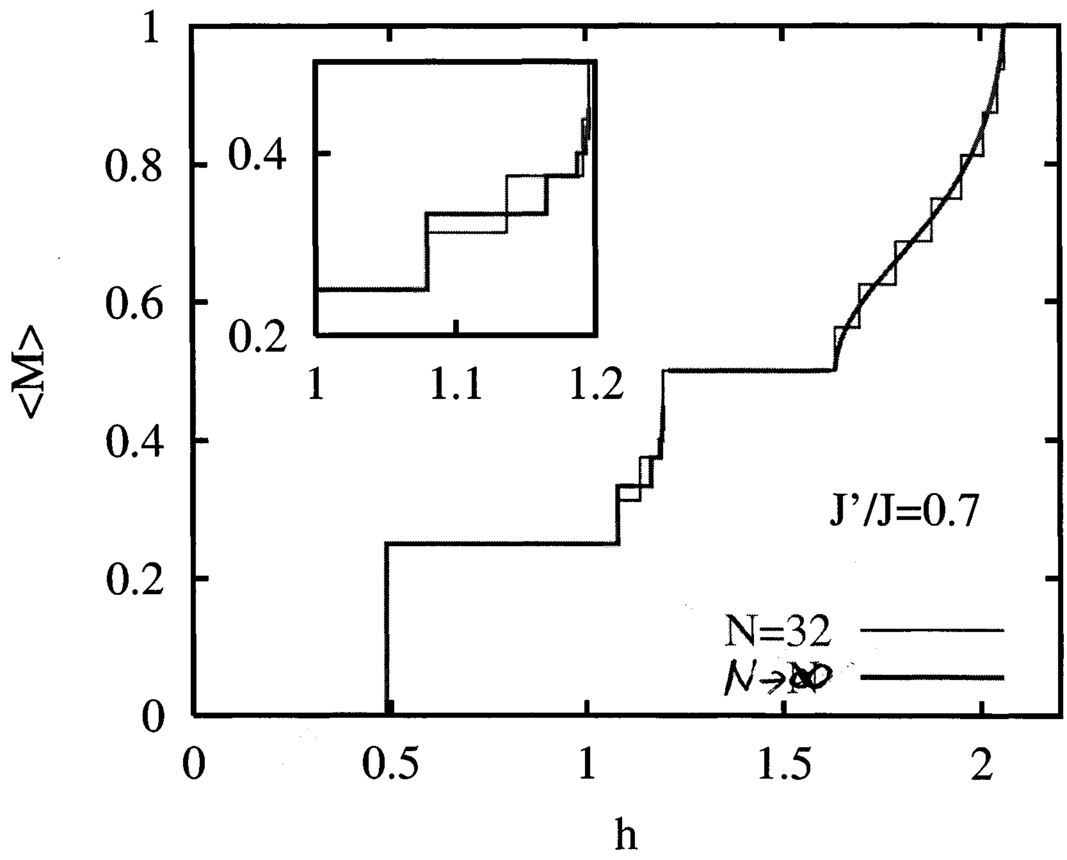
Schulenburg, Richter, cond-mat/0107137





$\Rightarrow$ Plateau with magnetization $\langle M \rangle = \dfrac{k}{2k+2}$

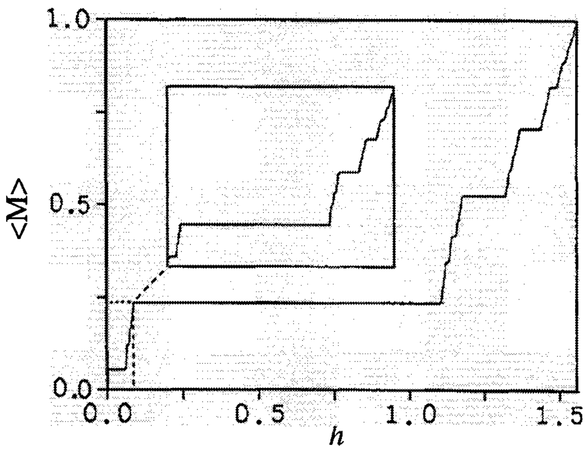
Magnetization curve ($J'/J = 0.7$)



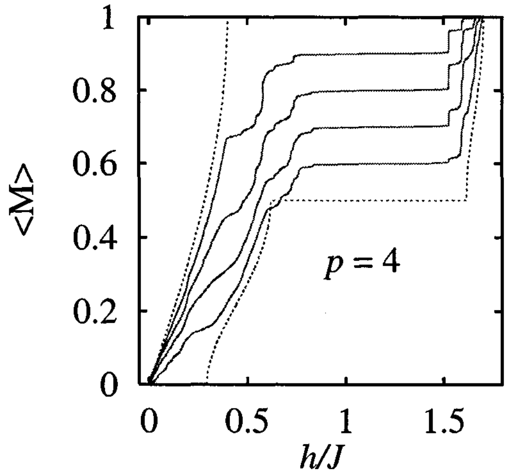
Is rationality of the magnetization fundamental ?

1. Break translational invariance completely

Hierarchical lattice
⇒ selfsimilar magnetization curve



discrete bond disorder
⇒ disorder-dependent $\langle M \rangle$ on plateau



Tokihiro, Phys. Rev. **B41** (1990) 7334

Cabra *et al.*, Phys. Rev. Lett. **85** (2000) 4791

2. Several magnetic species whose total density is fixed

⇒ plateaux can appear in the magnetization curve for irrational $\langle M \rangle$ if one species becomes commensurate and acquires a gap

doped p-merized Hubbard chains

with Cabra, **De Martino**, Pujol, **Simon**

Hamilton-Operator:

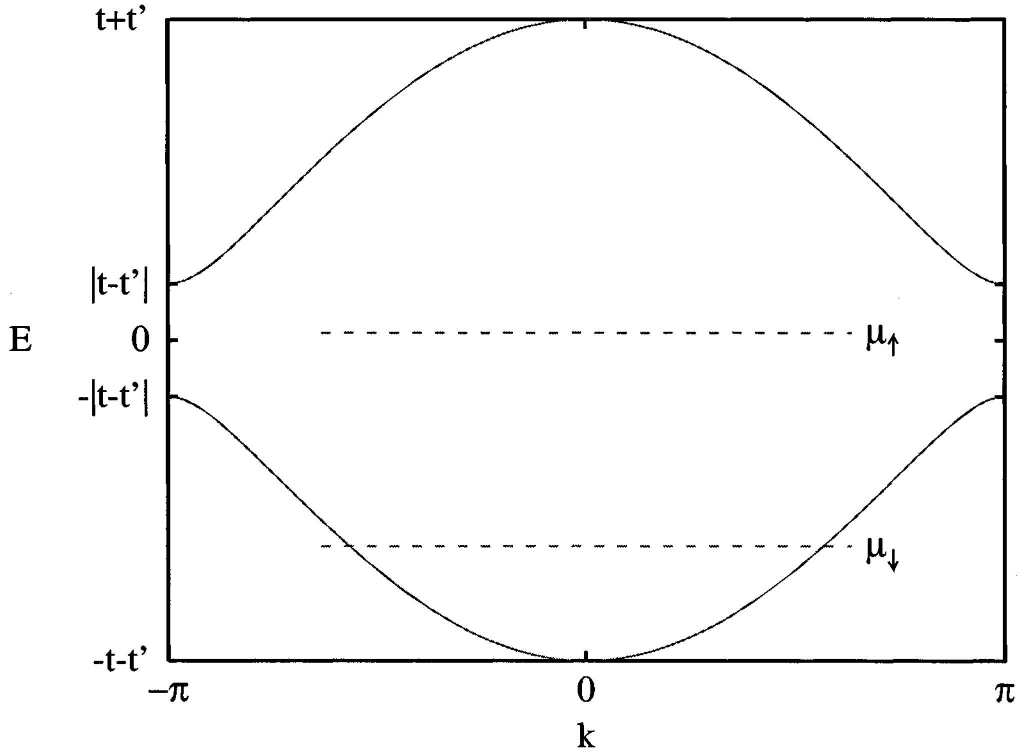
$$H = -\sum_{x=1}^{L} t(x) \sum_{\sigma} \left(c^\dagger_{x+1,\sigma} c_{x,\sigma} + c^\dagger_{x,\sigma} c_{x+1,\sigma} \right) + U \sum_{x=1}^{L} n_{x,\uparrow} n_{x,\downarrow} + \mu \sum_{x=1}^{L} (n_{x,\uparrow} + n_{x,\downarrow}) - \frac{h}{2} \sum_{x=1}^{L} (n_{x,\uparrow} - n_{x,\downarrow})$$

$c^\dagger$, c	electron creation and annihilation operators
$n_{x,\sigma} = c^\dagger_{x,\sigma} c_{x,\sigma}$	number operator
$m = n_{x,\uparrow} - n_{x,\downarrow}$	magnetization
$U > 0$	onsite repulsion
μ	chemical potential
h	dimensionless magnetic field
$t(x)$	hopping parameter ($t(x) = t'$ for x a multiple of p, $t(x) = t$ otherwise)

$\Rightarrow$ Doping-dependent magnetization plateaux (at fixed n)

$m = 1 - n$ plateau for $p = 2$

$U = 0$:



- $\mu_\uparrow = \mu - h/2$ in band gap
  $\Rightarrow n_\uparrow = 1/2$ ($\Leftrightarrow m = 1 - n$)
- h changes a little $\Rightarrow \mu_\uparrow$ changes but remains in band gap
  $\Rightarrow \mu$ must be readjusted to keep $\mu_\downarrow = \mu + h/2$ fixed because n is fixed
  $\Rightarrow$ magnetic gap = plateau
- For $U > 0$ (small): Perturbative corrections, but picture remains valid

Abelian bosonization for the Hubbard chain

1. Zero field ($h = 0$)

Hubbard chain ($t(x) = t$) with general filling (n or μ) can be written in terms of two bosonic fields

$$\bar{H}_{Hubbard} = \frac{v_c}{2}\int \mathrm{d}x \left\{(\partial_x\phi_c)^2 + \left(\partial_x\tilde{\phi}_c\right)^2\right\} + \frac{v_s}{2}\int \mathrm{d}x \left\{(\partial_x\phi_s)^2 + \left(\partial_x\tilde{\phi}_s\right)^2\right\} \qquad (\star)$$

with $\phi_c = \frac{1}{\xi}(\phi_\uparrow + \phi_\downarrow)$ and $\phi_s = \frac{1}{\sqrt{2}}(\phi_\uparrow - \phi_\downarrow)$

Parameters v_c, v_s and ξ can be determined exactly from Bethe-ansatz for any given U and μ (or n)

Frahm, Korepin, Phys. Rev. **B42** (1990) 10553;
Phys. Rev. **B43** (1991) 5653

Perturb with $\delta = t' - t$

$\Rightarrow$ interaction

$$H_I = \lambda \int \mathrm{d}x\Phi + \lambda' \int \mathrm{d}x\Phi'$$

with

$$\begin{aligned}\Phi(x) &= \sin\left(\frac{k_+}{2} + pk_+x - \sqrt{\pi}\xi\phi_c\right)\cos\left(\sqrt{2\pi}\phi_s\right)\\ \Phi'(x) &= \cos\left(k_+ + 2pk_+x - \sqrt{4\pi}\xi\phi_c\right)\end{aligned}$$

and λ, $\lambda' \sim \delta$ and $k_+ = k_{F,\uparrow} + k_{F,\downarrow} = \pi n$

- $pn \in \mathbb{Z}$ $\Rightarrow$ Φ' commensurate $\Rightarrow$ charge gap
- $pn \in 2\mathbb{Z}$ $\Rightarrow$ Φ also commensurate $\Rightarrow$ spin (& charge) gap

2. With magnetic field ($h \neq 0$)

Hamiltonian ($\star$) remains valid for Hubbard chain ($t(x) = t$), but representation of ϕ_c and ϕ_s more complicated

Penc, Sólyom, Phys. Rev. **B47** (1993) 6273

$$\begin{pmatrix}\phi_c\\ \phi_s\end{pmatrix} = \frac{1}{\det\ Z}\begin{pmatrix}Z_{ss} & Z_{ss} - Z_{cs}\\ Z_{sc} & Z_{sc} - Z_{cc}\end{pmatrix}\begin{pmatrix}\phi_\uparrow\\ \phi_\downarrow\end{pmatrix}$$

Z: 'dressed charge matrix' – can be computed from Bethe-ansatz for given h, U and μ

Switch on $\delta = t' - t$

$\Rightarrow$ interaction

$$H_I = \lambda \int \mathrm{d}x\Phi + \lambda' \int \mathrm{d}x\Phi'$$

with

$$\begin{aligned}\Phi(x) &= \sin\left(\frac{k_+}{2} + pk_+x - \sqrt{\pi}\left(Z_{cc}\phi_c - Z_{cs}\phi_s\right)\right) \\ &\quad \times \cos\left(\frac{k_-}{2} + pk_-x - \sqrt{\pi}\left((Z_{cc} - 2Z_{sc})\phi_c - (Z_{cs} - 2Z_{ss})\phi_s\right)\right) \\ \Phi'(x) &= \cos(k_+ + 2pk_+x - \sqrt{4\pi}(Z_{cc}\phi_c - Z_{cs}\phi_s))\end{aligned}$$

where now $k_- = k_{F,\uparrow} - k_{F,\downarrow} = \pi m$

A) $\quad \frac{p}{2}(n+m) \in \mathbb{Z} \quad$ and $\quad \frac{p}{2}(n-m) \in \mathbb{Z}$

$\Rightarrow$ Φ and Φ' commensurate $\Rightarrow$ spin and charge gap

B) $\quad$ only $\quad \frac{p}{2}(n+m) = l \in \mathbb{Z}$

$\Rightarrow$ switch back to $\phi_\uparrow$, $\phi_\downarrow$

$\Rightarrow$ after treatment of marginal terms, Hamiltonian can be written as

$$H = \int \mathrm{d}x \frac{v_\uparrow}{2}\left[(\partial_x\phi_\uparrow)^2 + \left(\partial_x\tilde{\phi}_\uparrow\right)^2\right] + \frac{v_\downarrow}{2}\left[(\partial_x\phi_\downarrow)^2 + \left(\partial_x\tilde{\phi}_\downarrow\right)^2\right] + \lambda \sin 2\sqrt{\pi}\phi_\uparrow$$

relevant perturbation for $\phi_\uparrow$ $\Rightarrow$ $\phi_\uparrow$ massive
integrate out $\phi_\uparrow$ $\Rightarrow$ apparently free Hamiltonian for $\phi_\downarrow$ (with effective velocity v and compactification radius R)

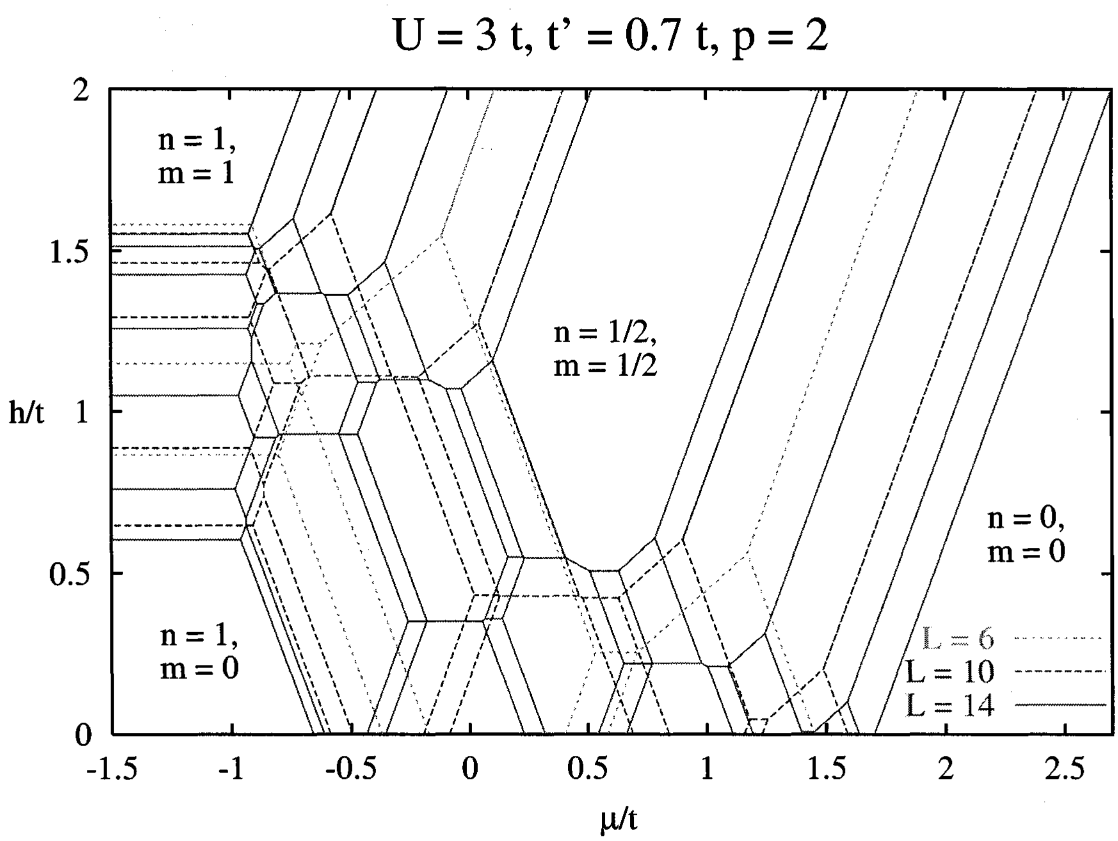
constraint: n fixed $\Rightarrow$ $\phi_\downarrow$ in topological sector $\frac{1}{\sqrt{\pi}}\phi_\downarrow|_0^L = Q$
$\Rightarrow$ susceptibility $\chi = 0$ $\Rightarrow$

Plateau in magnetization curve with magnetization m

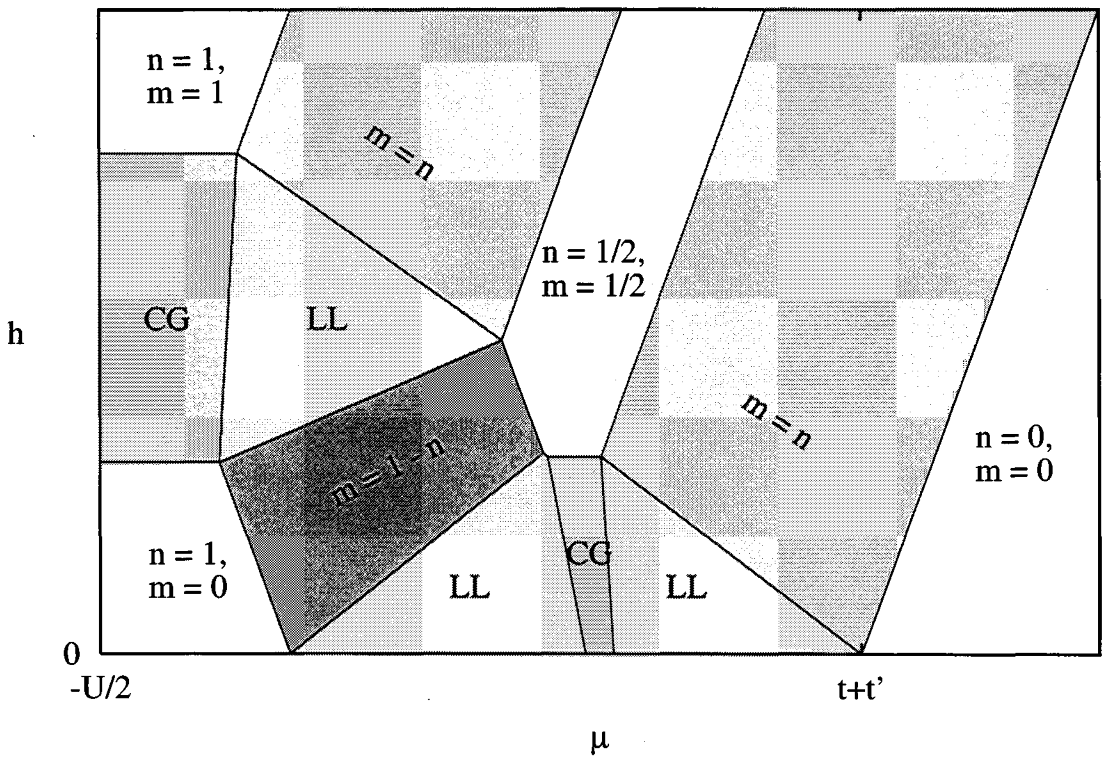
m depends on doping n through $m = 2l/p - n$

Lanczos diagonalization for the dimerized Hubbard chain

Groundstate phase diagram in the μ-h plane

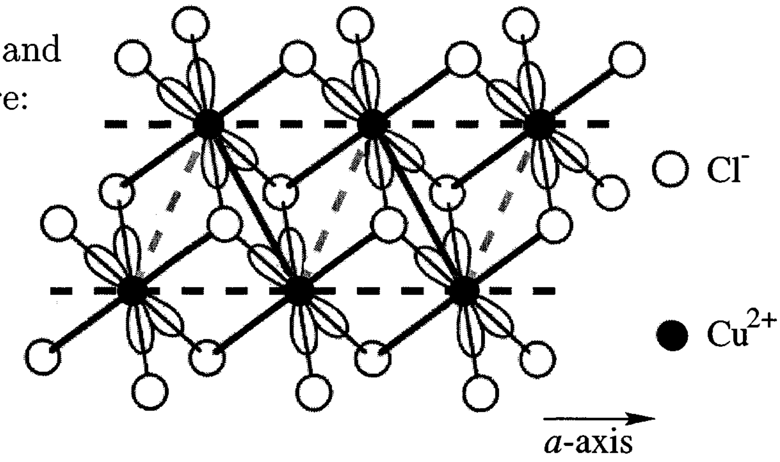


schematic

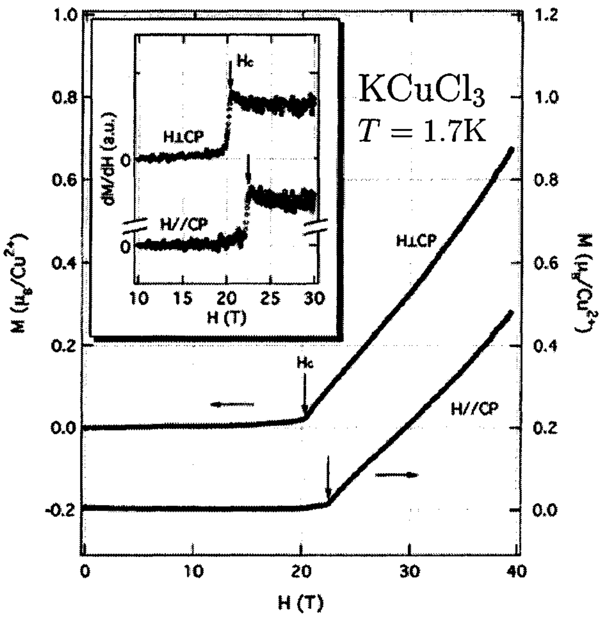


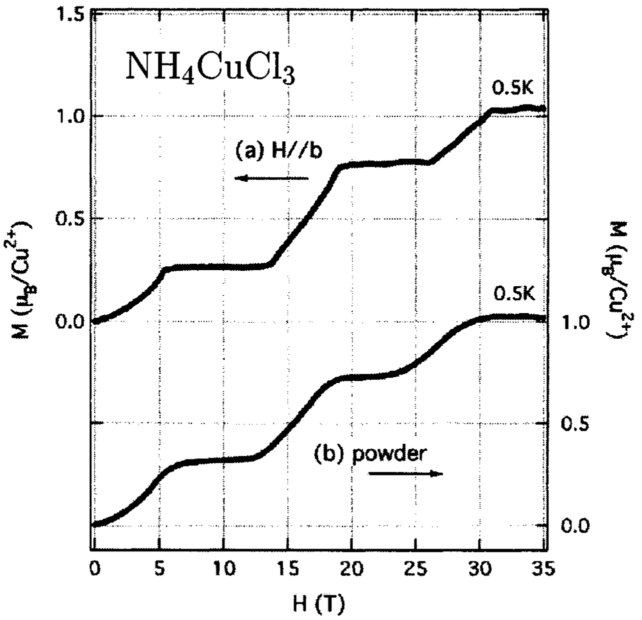
What is the model for NH_4CuCl_3 ?

Structure of $KCuCl_3$, $TlCuCl_3$ and NH_4CuCl_3 at room temperature:



Low-temperature magnetization curves





Shiramura *et.al.*, J. Phys. Soc. Jpn. **66** (1997) 1999;
J. Phys. Soc. Jpn. **67** (1998) 1548

$KCuCl_3$:

Just a spin gap, as expected from the 1D model.
But $KCuCl_3$ is actually a 3D network of weakly coupled dimers.
(Cavadini *et.al.*, Eur. Phys. J. **B7** (1999) 519)

NH_4CuCl_3:

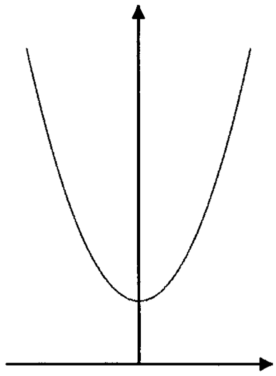
No spin gap, but $\langle M \rangle = 1/4,\ 3/4$ plateaux
$\Rightarrow$ Need $V = 8$ ($S = 1/2$)

- Why $V = 8$? (structural phase transition at about 70K)
- With $V = 8$ also plateaux with $\langle M \rangle = 0,\ 1/2$ would be permitted. Why are those absent ?

Transition to saturation

Dispersion of **magnons** usually quadratic close to minimum:

$\epsilon \equiv h$



k

magnons $\equiv$ δ-function bosons

$\Rightarrow$ mapping to low-density Bose gas

$D = 1$:

Filling: Uniform & independent of type of quasiparticles

$\epsilon \equiv h$

k

$\Rightarrow$ $k \equiv M_c - \langle M \rangle$

$\Rightarrow$ transitions at plateau-boundaries: DN-PT universality class

$$M_c - \langle M \rangle \sim \sqrt{|h_c - h|}$$

(Dzhaparidze, Nersesyan, JETP Lett. **27** (1978) 334,
Pokrovsky, Talapov, Phys. Rev. Lett. **42** (1979) 65)

Very general in $D = 1$!

Exceptions:

- Dispersion not quadratic ($\Rightarrow$ special parameters)
- First-order tansition/formation of bound states

Conclusions

- magnetization plateaux at rational fractions of saturation magnetization
- quantization condition

$$VS(1 - \langle M \rangle) \in \mathbb{Z}$$

- no upper limit on period of spontaneous breaking of translational symmetry
- also irrational magnetization values possible:
  - charge carriers (Hubbard model: $n \notin \mathbb{Q}$)
  - discrete bond disorder
- transition at plateau-boundaries: universal (Bose condensation; $D = 1$: DN-PT)
- some experimental systems (NH_4CuCl_3) remain a challenge for theory