

Metamagnetism in frustrated ferromagnetic spin chains

M. Arlego¹, F. Heidrich-Meisner², A. Honecker³, G. Rossini¹, T. Vekua⁴

¹Universidad Nacional de La Plata, ARGENTINA
Universities of ²Munich, ³Göttingen, ⁴Hannover, GERMANY

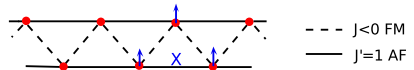
Geometrically Frustrated Magnets

IIP-Natal

December 16, 2011

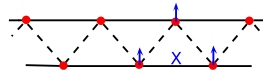
Frustrated ferromagnetic spin chain

$$H_S = \sum_{i=1}^L \left[\left(J \vec{S}_i \cdot \vec{S}_{i+1} + J' \vec{S}_i \cdot \vec{S}_{i+2} - h S_i^z \right) \right]$$



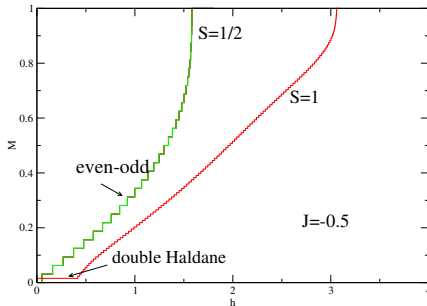
Frustrated ferromagnetic spin chain

$$H_S = \sum_{i=1}^L \left[\left(J \vec{S}_i \cdot \vec{S}_{i+1} + J' \vec{S}_i \cdot \vec{S}_{i+2} - h S_i^z \right) \right]$$



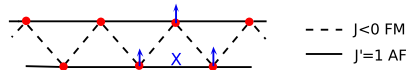
--- $J < 0$ FM
— $J' = 1$ AF

$S = 1/2$ realized in LiCuVO_4 , $\text{Li}_2\text{ZrCuO}_4$. We looked at $S = 1$:

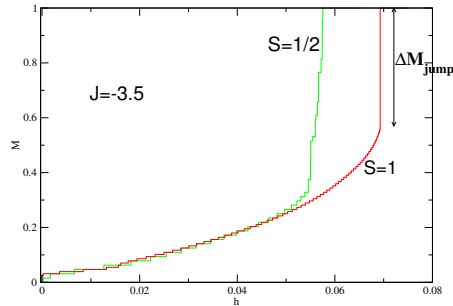
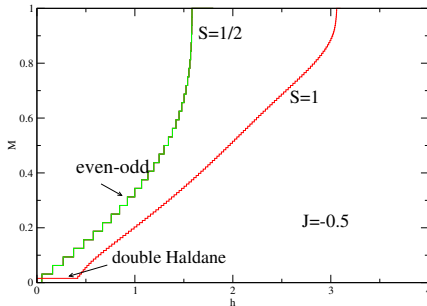


Frustrated ferromagnetic spin chain

$$H_S = \sum_{i=1}^L \left[\left(J \vec{S}_i \cdot \vec{S}_{i+1} + J' \vec{S}_i \cdot \vec{S}_{i+2} - h S_i^z \right) \right]$$



$S = 1/2$ realized in LiCuVO_4 , $\text{Li}_2\text{ZrCuO}_4$. We looked at $S = 1$:



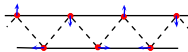
Outline

- 1 Classical picture
- 2 Two magnon problem
- 3 Multimagnon problem, $S \geq 1$
- 4 DMRG results

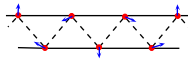
Limit $S \rightarrow \infty$

- $h = 0$: spiral order,

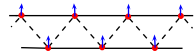
$$\theta = \arccos(-J/4)$$



$$J = 0, \theta = \pi/2$$



$$-4 < J < 0, 0 < \theta, \pi/2$$

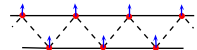
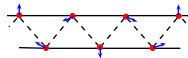
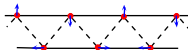


$$J \leq -4, \theta = 0$$

Limit $S \rightarrow \infty$

- $h = 0$: spiral order,

$$\theta = \arccos(-J/4)$$



$$J = 0, \theta = \pi/2$$

$$-4 < J < 0, 0 < \theta, \pi/2$$

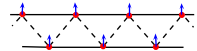
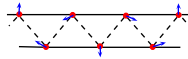
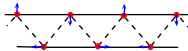
$$J \leq -4, \theta = 0$$

- $h \neq 0$: spiral in xy plane + canting towards z axis

Limit $S \rightarrow \infty$

- $h = 0$: spiral order,

$$\theta = \arccos(-J/4)$$

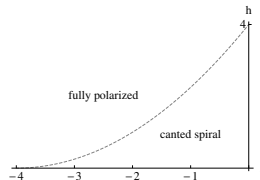


$$J = 0, \theta = \pi/2$$

$$-4 < J < 0, 0 < \theta, \pi/2$$

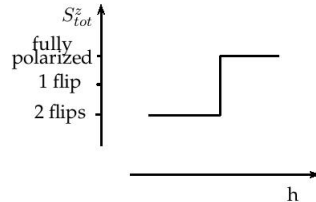
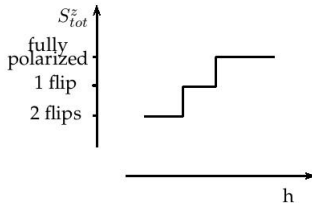
$$J \leq -4, \theta = 0$$

- $h \neq 0$: spiral in xy plane + canting towards z axis
- $h_{\text{sat}} = S/4(J+4)^2$



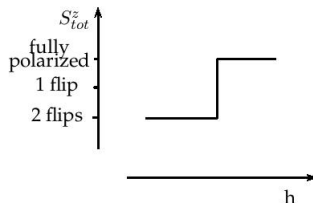
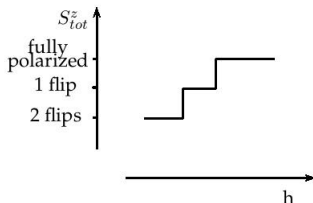
Bound states and jumps

- $H_S(h) = H_S(h=0) - hS_{tot}^z$



Bound states and jumps

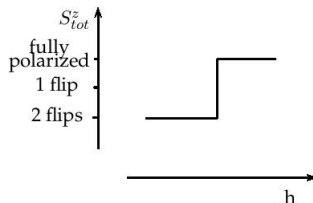
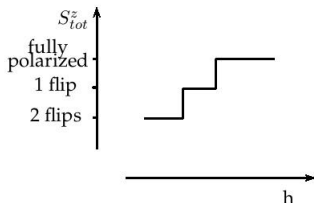
- $H_S(h) = H_S(h=0) - hS_{tot}^z$



- S^z sector with especially low energy \rightarrow hides following S^z sectors in the magnetization curve

Bound states and jumps

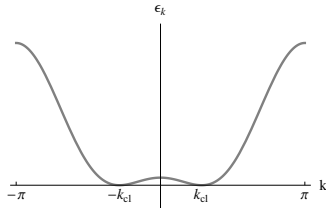
- $H_S(h) = H_S(h=0) - hS_{tot}^z$



- S^z sector with especially low energy \rightarrow hides following S^z sectors in the magnetization curve
- See jumps? \rightarrow Look for bound states

One magnon dispersion

$$\epsilon_k = \frac{1}{2} V_k - \frac{1}{2} V_{k_d} \geq 0 \quad \text{with} \quad V_k = 2J \cos(k) + 2 \cos(2k)$$



$$k_d = \arccos(-J/4), \text{ incommensurate}$$

- Two magnon states basis, with momentum K , relative coordinate r :

$$|K, r\rangle = \sum_{l=1}^L e^{iK(l+r/2)} S_l^- S_{l+r}^- | \uparrow \uparrow \cdots \uparrow \uparrow \rangle$$

- Two magnon states basis, with momentum K , relative coordinate r :

$$|K, r\rangle = \sum_{l=1}^L e^{iK(l+r/2)} S_l^- S_{l+r}^- | \uparrow \uparrow \cdots \uparrow \uparrow \rangle$$

- Two magnon states:

$$|\Psi_{2M}\rangle = \sum_r C_r |K, r\rangle$$

- Two magnon states basis, with momentum K , relative coordinate r :

$$|K, r\rangle = \sum_{l=1}^L e^{iK(l+r/2)} S_l^- S_{l+r}^- | \uparrow \uparrow \cdots \uparrow \uparrow \rangle$$

- Two magnon states:

$$|\Psi_{2M}\rangle = \sum_r C_r |K, r\rangle$$

- $S = 1/2$: $C_0 = 0$, strictly hardcore

- Two magnon states basis, with momentum K , relative coordinate r :

$$|K, r\rangle = \sum_{l=1}^L e^{iK(l+r/2)} S_l^- S_{l+r}^- | \uparrow \uparrow \cdots \uparrow \uparrow \rangle$$

- Two magnon states:

$$|\Psi_{2M}\rangle = \sum_r C_r |K, r\rangle$$

- $S = 1/2$: $C_0 = 0$, strictly hardcore
- Eigenstates:

$$H_S |\Psi_{2M}\rangle = E_{2M} |\Psi_{2M}\rangle$$

Two magnon eigenstates

Schrödinger equation ($S \geq 1$) for eigenstates with momentum K

$$\begin{aligned}\Omega_0 C_0 &= \frac{S}{\sqrt{S(2S-1)}} (\zeta_1 C_1 + \zeta_2 C_2) \\ (\Omega_0 - J) C_1 &= \frac{(2S-1)^{3/2}}{S^{3/2}} \zeta_1 C_0 + \zeta_1 C_2 + \zeta_2 (C_1 + C_3) \\ (\Omega_0 - 1) C_2 &= \frac{(2S-1)^{3/2}}{S^{3/2}} \zeta_2 C_0 + \zeta_2 C_4 + \zeta_1 (C_1 + C_3)\end{aligned}$$

and for $r \geq 3$:

$$\Omega_0 C_r = \zeta_1 (C_{r+1} + C_{r-1}) + \zeta_2 (C_{r+2} + C_{r-2})$$

where Ω_0 is the eigenvalue, $\zeta_1 = 2SJ \cos(K/2)$, $\zeta_2 = 2S \cos(K)$

Two magnon bound states

- Bound state Ansatz:

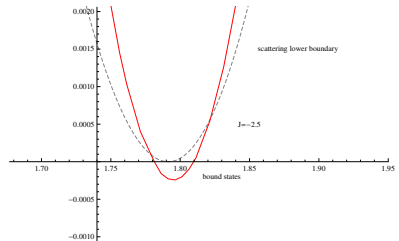
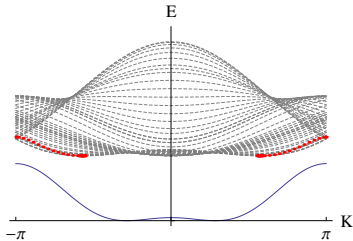
$$C_r = e^{-\kappa-r} + v e^{-\kappa+r} \quad (r \geq 1)$$

Two magnon bound states

- Bound state Ansatz:

$$C_r = e^{-\kappa - r} + v e^{-\kappa + r} \quad (r \geq 1)$$

- Provides solutions for $J < J_{cr}(S)$, with width $a_s = 1/\min\{\text{Re}[\kappa_{\pm}]\}$

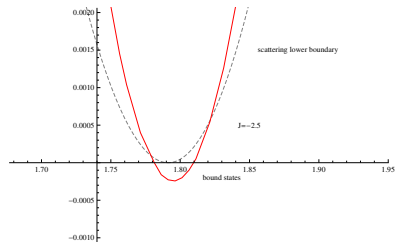
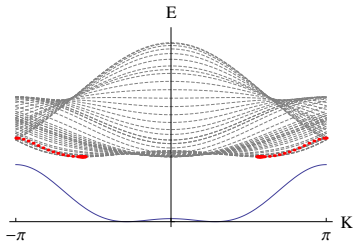


Two magnon bound states

- Bound state Ansatz:

$$C_r = e^{-\kappa - r} + v e^{-\kappa + r} \quad (r \geq 1)$$

- Provides solutions for $J < J_{cr}(S)$, with width $a_s = 1/\min\{\text{Re}[\kappa_{\pm}]\}$
- Example: $S=1$, $J=-2.5$. Bound state solutions shown in red.



- Bound states below the continuum, with negative binding energy:

$$E_b(K^*) \simeq -1/ma\xi^2$$

- Bound states below the continuum, with negative binding energy:

$$E_b(K^*) \simeq -1/ma_S^2$$

- Bound state *width*:

$$a_S = 1/\min\{\text{Re}[\kappa_{\pm}]\}$$

- Bound states below the continuum, with negative binding energy:

$$E_b(K^*) \simeq -1/ma_S^2$$

- Bound state *width*:

$$a_S = 1/\min\{\text{Re}[\kappa_{\pm}]\}$$

- $S \geq 1$: *extended* bound states in a finite window

$$-4 < J < J_{cr}(S)$$

- Bound states below the continuum, with negative binding energy:

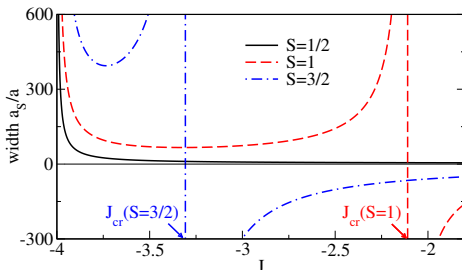
$$E_b(K^*) \simeq -1/ma_S^2$$

- Bound state *width*:

$$a_S = 1/\min\{\text{Re}[\kappa_{\pm}]\}$$

- $S \geq 1$: *extended* bound states in a finite window

$$-4 < J < J_{cr}(S)$$



S	1/2	1	3/2	2	5/2
$J_{cr}(S)$	—	-2.11	-3.31	-3.68	-3.84

- Bound states below the continuum, with negative binding energy:

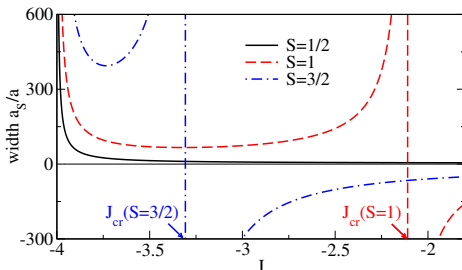
$$E_b(K^*) \simeq -1/ma_S^2$$

- Bound state *width*:

$$a_S = 1/\min\{\text{Re}[\kappa_{\pm}]\}$$

- $S \geq 1$: *extended* bound states in a finite window

$$-4 < J < J_{cr}(S)$$

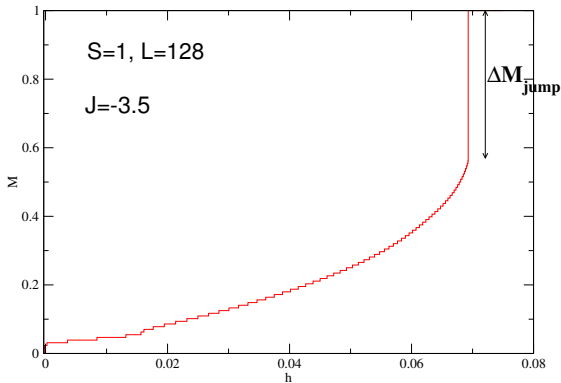


S	1/2	1	3/2	2	5/2
$J_{cr}(S)$	—	-2.11	-3.31	-3.68	-3.84

Wide bound states \rightarrow *Hard coreness of magnons plays no major role in this regime!*

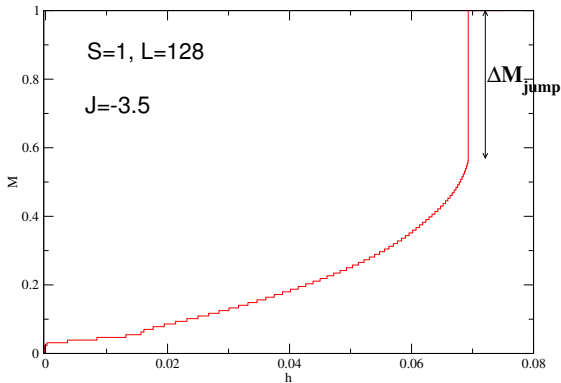
Metamagnetism

- $M = S_{Total}^z / (SL)$: normalized magnetization



Metamagnetism

- $M = S_{Total}^z / (SL)$: normalized magnetization
- Metamagnetic jump: step to saturation with finite $\Delta M \longleftrightarrow$ finite density of magnons for $L \rightarrow \infty$



Multimagnon problem

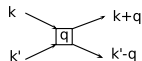
Dyson-Maleev (same results at $1/S$ using Holstein-Primakoff)

$$\begin{aligned} S_i^z &= S - a_i^\dagger a_i, \quad S_i^+ = \sqrt{2S} a_i, \\ S_i^- &= \sqrt{2S} a_i^\dagger (1 - a_i^\dagger a_i / 2S), \rightarrow \end{aligned}$$

$$\rightarrow H_S = \sum_k (2S\epsilon_k - \mu(h)) a_k^\dagger a_k + \sum_{k,k',q} \frac{\Gamma_0(q; k, k')}{2L} a_{k+q}^\dagger a_{k'-q}^\dagger a_k a_{k'}$$

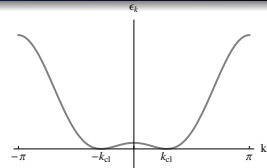
with one-magnon like dispersion $\sim 2S\epsilon_k$ close to saturation $\mu(h) = h_s^d - h \rightarrow 0^+$

and bare 4-leg vertex coupling $\Gamma_0(q; k, k') = V_q - \frac{1}{2}(V_k + V_{k'})$



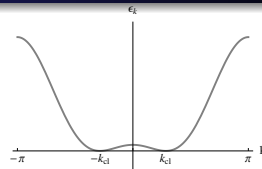
Low energy regime

$k \approx \pm k_{cl} \rightarrow$ two boson species \pm

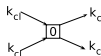


Low energy regime

$k \approx \pm k_{cl} \rightarrow$ two boson species \pm

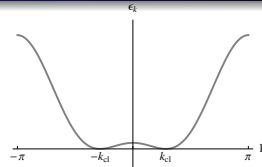


- Intra-species coupling $g_0 \sim \Gamma_0(0; k_{cl}, k_{cl}) = \Gamma_0(0; -k_{cl}, -k_{cl})$

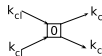


Low energy regime

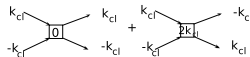
$k \approx \pm k_{cl} \rightarrow$ two boson species \pm



- Intra-species coupling $g_0 \sim \Gamma_0(0; k_{cl}, k_{cl}) = \Gamma_0(0; -k_{cl}, -k_{cl})$

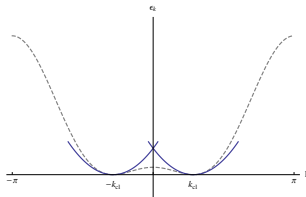


- Inter-species coupling $\tilde{g}_0 \sim \Gamma_0(0; k_{cl}, -k_{cl}) + \Gamma_0(2k_{cl}; k_{cl}, -k_{cl})$



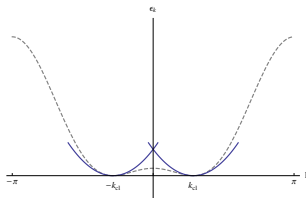
Low density, low energy effective model

- Low magnon density + wide bound states ($S \geq 1$): *we can ignore hard core constraint and curvature*



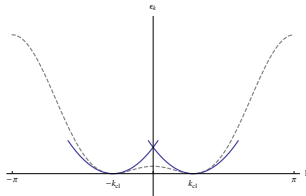
Low density, low energy effective model

- Low magnon density + wide bound states ($S \geq 1$): we can ignore hard core constraint and curvature
- Approximate boson modes around k_{cl} and $-k_{cl}$ by quadratic dispersion bosons $\psi_-(x)$, $\psi_+(x)$ with mass $m = \frac{2}{S(4-J)(4+J)}$



Low density, low energy effective model

- Low magnon density + wide bound states ($S \geq 1$): we can ignore hard core constraint and curvature
- Approximate boson modes around k_{cl} and $-k_{cl}$ by quadratic dispersion bosons $\psi_-(x)$, $\psi_+(x)$ with mass $m = \frac{2}{S(4-J)(4+J)}$



- ... getting a two component Lieb-Liniger model, with contact density-density interactions

$$\mathcal{H}_{\text{eff}} = \sum_{\alpha=\pm} -\frac{|\nabla\psi_{\alpha}|^2}{2m} + \frac{g_0}{2}(n_-^2(x) + n_+^2(x)) + \tilde{g}_0 n_-(x)n_+(x)$$

Effective coupling constants

Couplings depend on S through renormalization

$$\mathcal{H}_{\text{eff}} = \sum_{\alpha=\pm} -\frac{|\nabla\psi_{\alpha}|^2}{2m} + \frac{g_0(S)}{2}(n_-^2(x) + n_+^2(x)) + \tilde{g}_0(S) n_-(x)n_+(x)$$

Effective Coupling Regimes

- $g_0(S) > 0 (< 0)$: repulsive (attractive) intra-species interaction
- $\tilde{g}_0(S) > 0 (< 0)$: repulsive (attractive) inter-species interaction

$g_0(S)$, $\tilde{g}_0(S)$ are obtained from the renormalized $\Gamma(q; k, k')$:

$$g(S) = \Gamma(0; k_d, k_d)$$

$$\tilde{g}(S) = \Gamma(0; k_d, -k_d) + \Gamma(2k_d; k_d, -k_d)$$

Renormalization is done at the RG fixed point of a dilute, two-component Bose gas, dictated by $SU(2)$ symmetry (Kolezhuk, PRA 81 (2010))

$$\lim_{\mu \rightarrow 0} g(S) = \lim_{\mu \rightarrow 0} \tilde{g}(S) = \pi \sqrt{\mu(S)} / \sqrt{2m}$$

Then one expects

$$g(S) = \frac{g_0(S)}{1 + g_0(S) \sqrt{2m} / (\pi \sqrt{\mu(S)})}$$

$$\tilde{g}(S) = \frac{\tilde{g}_0(S)}{1 + \tilde{g}_0(S) \sqrt{2m} / (\pi \sqrt{\mu})}$$

Extract

\Rightarrow

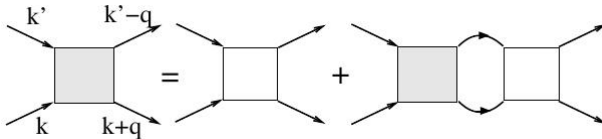
$g_0(S)$

$\tilde{g}_0(S)$

1/S vertex renormalization

Bethe-Salpeter equation

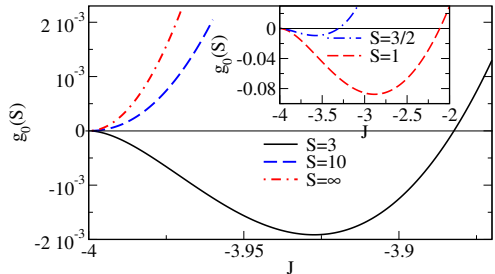
$$\Gamma(q; k, k') = \Gamma_0(q; k, k') - \frac{1}{2SL} \sum_p \frac{\Gamma_0(q - p; k + p, k' - p)}{\epsilon_{k+p} + \epsilon_{k'-p}} \Gamma(p; k, k')$$



1/S expansion makes sense here, though the model is 1D. All integrals are evaluated analytically.

Attractive regime

- $g_0(S)$ may be tuned *attractive* \leftrightarrow *repulsive*
- $\tilde{g}_0(S)$ is always repulsive for $-4 < J < 0$



Collapsed Bose gas - Metamagnetism

- Different species repulsion leads to a **chiral** phase: magnons appear with momenta close to either k_d or $-k_d$.

Collapsed Bose gas - Metamagnetism

- Different species repulsion leads to a **chiral** phase: magnons appear with momenta close to either k_d or $-k_d$.
- Same species attraction leads to a wave function **collapse**, forming a multimagnon bound state **below** the scattering continuum.
- This resembles Feschbach resonances in Bose gases

Collapsed Bose gas - Metamagnetism

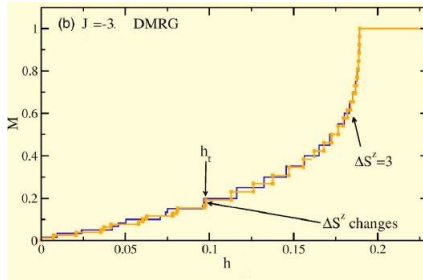
- Different species repulsion leads to a **chiral** phase: magnons appear with momenta close to either k_d or $-k_d$.
- Same species attraction leads to a wave function **collapse**, forming a multimagnon bound state **below** the scattering continuum.
- This resembles Feshbach resonances in Bose gases
- This leads to suppressed S^z states in the magnetization curves \implies **Metamagnetic jump** ΔM

Collapsed Bose gas - Metamagnetism

- Different species repulsion leads to a **chiral** phase: magnons appear with momenta close to either k_d or $-k_d$.
- Same species attraction leads to a wave function **collapse**, forming a multimagnon bound state **below** the scattering continuum.
- This resembles Feshbach resonances in Bose gases
- This leads to suppressed S^z states in the magnetization curves \implies **Metamagnetic jump** ΔM
- How large ΔM ? Increasing density will break the low density approximation.

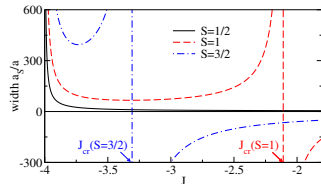
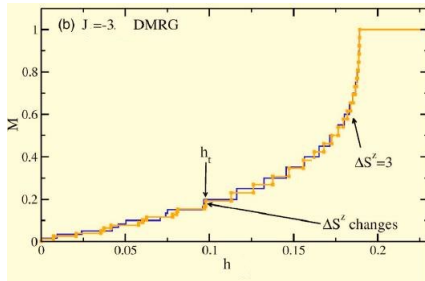
$$S = 1/2$$

Materials like LiCuVO_4 realize the spin 1/2 case



$$S = 1/2$$

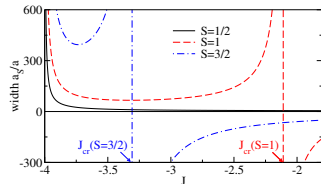
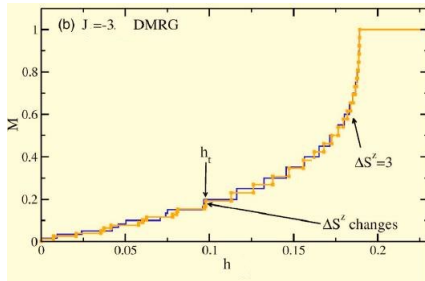
Materials like LiCuVO_4 realize the spin 1/2 case



- two magnon bound states with $k = \pi$, binding magnons in different legs
- no jump, but more than two magnon states appear close to saturation, for $J \rightarrow -4$

$$S = 1/2$$

Materials like LiCuVO_4 realize the spin 1/2 case

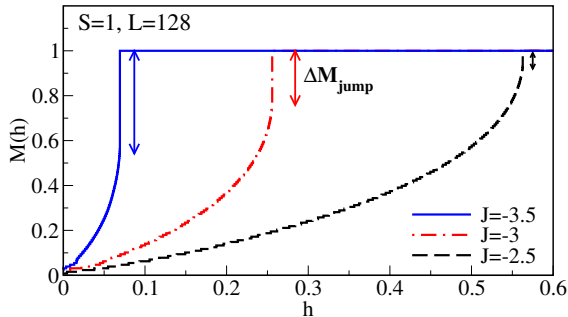


- two magnon bound states with $k = \pi$, binding magnons in different legs
- no jump, but more than two magnon states appear close to saturation, for $J \rightarrow -4$

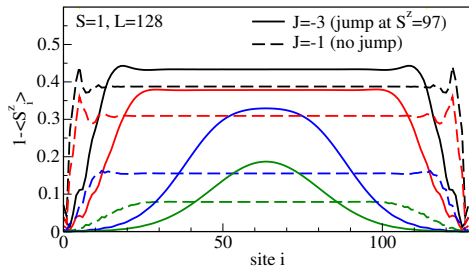
Heidrich-Meisner, Honecker, Vekua, PRB74(2006)

Sudan, Lüscher, Läuchli, PRB80(2009)

$S = 1$ magnetization curves

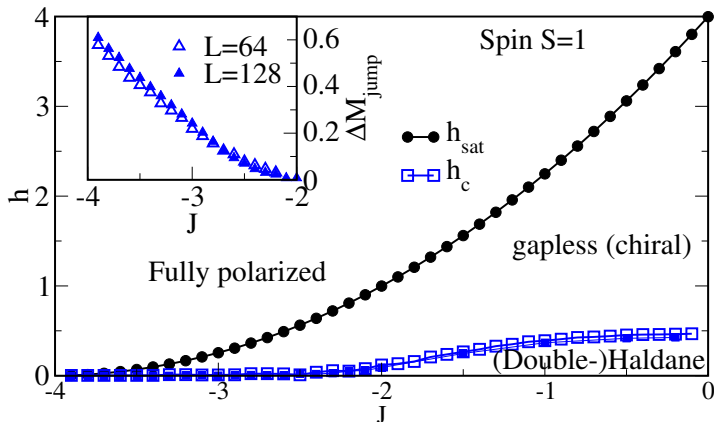


Wave function collapse

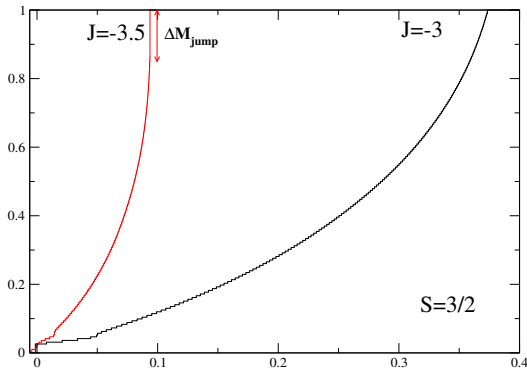


black: $S_z = 80 / 128$
red: $S_z = 90 / 128$
blue: $S_z = 110 / 128$
green: $S_z = 120 / 180$

$S = 1$ ground state phase diagram

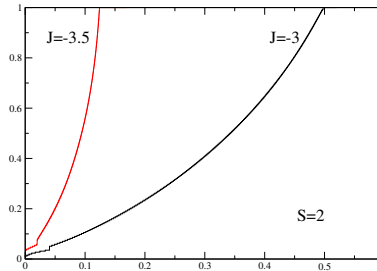


Larger S



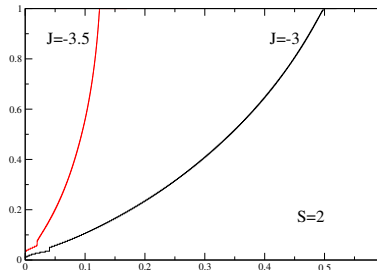
S	1/2	1	3/2	2	5/2
$J_{\alpha}(S)$	—	-2.11	-3.31	-3.68	-3.84

Larger S



S	1/2	1	3/2	2	5/2
$J_{cr}(S)$	—	-2.11	-3.31	-3.68	-3.84

Larger S



S	1/2	1	3/2	2	5/2
$J_{cr}(S)$	—	-2.11	-3.31	-3.68	-3.84

Critical S

Critical S above which metamagnetism window disappears: $S_{cr} = 5$ (Vekua, Kolezhuk, in progress)

Summary

- The ferromagnetic frustrated spin chain, close to saturation, behaves very differently for $S \geq 1$ than for $S = 1/2$

PRB 84, 224409 (2011)

Summary

- The ferromagnetic frustrated spin chain, close to saturation, behaves very differently for $S \geq 1$ than for $S = 1/2$
- Metamagnetism can be explained by the appearance of collapsed chiral multimagnon states

PRB 84, 224409 (2011)

Summary

- The ferromagnetic frustrated spin chain, close to saturation, behaves very differently for $S \geq 1$ than for $S = 1/2$
- Metamagnetism can be explained by the appearance of collapsed chiral multimagnon states
- The $1/S$ approach works fine in $1D$

PRB 84, 224409 (2011)

Summary

- The ferromagnetic frustrated spin chain, close to saturation, behaves very differently for $S \geq 1$ than for $S = 1/2$
- Metamagnetism can be explained by the appearance of collapsed chiral multimagnon states
- The $1/S$ approach works fine in $1D$
- We predict a critical value of S above which metamagnetism disappears

PRB 84, 224409 (2011)

Summary

- The ferromagnetic frustrated spin chain, close to saturation, behaves very differently for $S \geq 1$ than for $S = 1/2$
- Metamagnetism can be explained by the appearance of collapsed chiral multimagnon states
- The $1/S$ approach works fine in $1D$
- We predict a critical value of S above which metamagnetism disappears
- Metamagnetism for $S = 1/2$ still shows up in a very narrow window close to spontaneous ferromagnetism

PRB 84, 224409 (2011)

Summary

- The ferromagnetic frustrated spin chain, close to saturation, behaves very differently for $S \geq 1$ than for $S = 1/2$
- Metamagnetism can be explained by the appearance of collapsed chiral multimagnon states
- The $1/S$ approach works fine in $1D$
- We predict a critical value of S above which metamagnetism disappears
- Metamagnetism for $S = 1/2$ still shows up in a very narrow window close to spontaneous ferromagnetism
- May be some material realizes $S = 1$ ferromagnetic frustrated spin?

PRB 84, 224409 (2011)