Lanczos study of the $S = 1/2$ frustrated square-lattice antiferromagnet in a magnetic field

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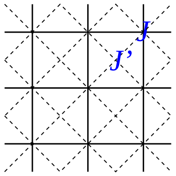
The model



Hamiltonian:

$$H = J \sum_{\substack{\text{next}\\ \text{neighbors}}} \vec{S}_{\vec{x}} \cdot \vec{S}_{\vec{y}} + J' \sum_{\substack{\text{diagonal}\\ \text{neighbors}}} \vec{S}_{\vec{x}} \cdot \vec{S}_{\vec{y}} - h \sum_{\vec{x}} S^z_{\vec{x}}$$

Magnetization:

$$\langle M \rangle = \frac{1}{SV} \left\langle \sum_{\vec{x}} S^z_{\vec{x}} \right\rangle$$

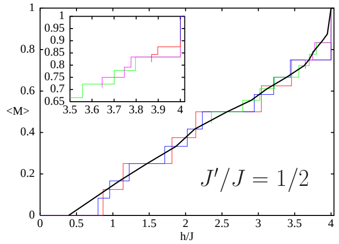
V: Number of lattice points

One-magnon dispersion above ferromagnetic state:

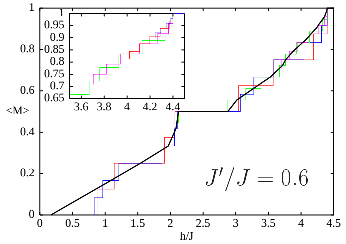
$$\mathcal{E}_{1s}(k_x, k_y) = -2(J+J') + J(\cos k_x + \cos k_y) + 2J' \cos k_x \cos k_y$$

$\Rightarrow$ Lines of minima for $J'/J = 1/2$

Magnetization curves

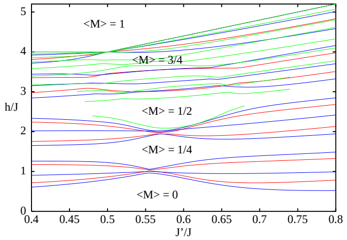


System sizes: 4×4, 6×4, 6×6, 8×6 (Insets: 8×8, 10×10)



For 4×4 lattice compare:
Lozovik, Notych, Solid State Communications **85** (1993) 873
Value of spin gap: Kotov *et.al.*, Phys. Rev. **B60** (1999) 14613

Transition lines



Sytem sizes: 4×4, 6×4, 6×6

$\Rightarrow$ Transition to saturation special at $J'/J = 1/2$:
Jump of size

$$\delta\langle M \rangle = \frac{1}{L}$$

L: length of shorter edge

$\Rightarrow \lim_{L\to\infty} \delta\langle M \rangle = 0$ (smooth transition for infinite size)

$\Rightarrow$ asymptotic form open (should follow from Bose condensation of magnons into lines of minima of single-magnon dispersion)

(Conclusion of Yang, Mütter, Z. Phys. **B104** (1997) 117: $1 - \langle M \rangle \sim \sqrt{4 - h/J}$ invalid – artifact of choice of clusters & analysis method)

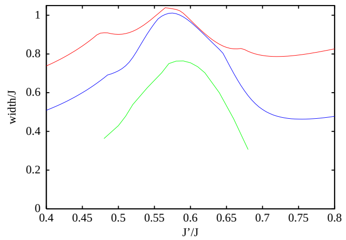
$\Rightarrow J'/J \gtrsim 1/2$: Plateau just below saturation ?
Gluzman, Phys. Rev. **B50** (1994) 6264

Candidate:

$$\langle M \rangle = 1 - \frac{1}{L}$$

vanishes as $L \to \infty$

Width of the finite-size $\langle M \rangle = 1/2$ plateau



Sytem sizes: 4×4, 6×4, 6×6

$\Rightarrow$ $\langle M \rangle = 1/2$ **plateau** for $0.5 \lesssim J'/J \lesssim 0.65$

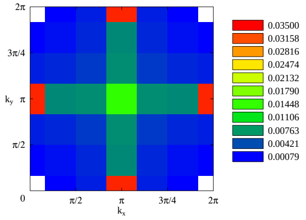
Static structure factors

$$S^{\alpha\beta}(k_x, k_y) = \frac{1}{V^2} \sum_{x,y,r,s} e^{i(k_x x + k_y y)} \left\langle S^\alpha_{r,s} S^\beta_{r+x,s+y} \right\rangle$$

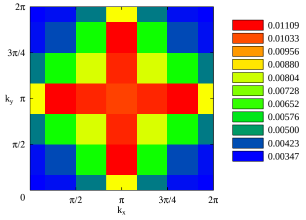
Remark: Use $\left(S^{\alpha\beta}(k_x,k_y) + S^{\alpha\beta}(k_y,k_x)\right)/2$ when cluster is not square or groundstate not symmetric under $x \leftrightarrow y$

$J'/J = 0.6$, $\langle M \rangle = 1/2$: 6×6 cluster

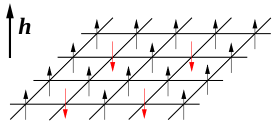
$S^{zz}(k_x, k_y)$



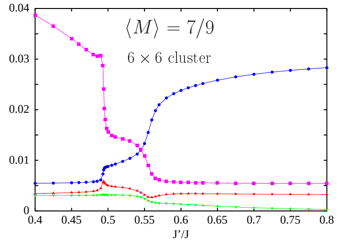
$S^{xx}(k_x, k_y)$



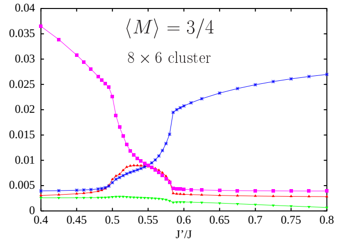
$\Rightarrow$ ordered state 'uuud':

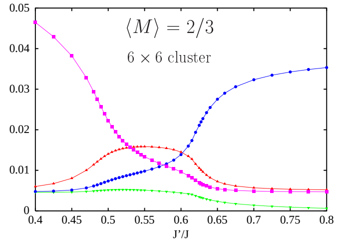


Parameter dependence of the peaks

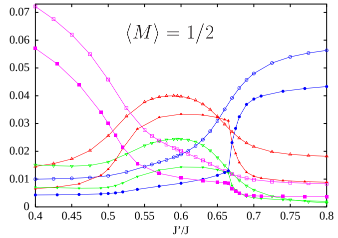


$S^{zz}(0,\pi)$, $S^{zz}(\pi,\pi)$, $S^{xx}(0,\pi)$, $S^{xx}(\pi,\pi)$





$S^{zz}(0,\pi)$, $S^{zz}(\pi,\pi)$, $S^{xx}(0,\pi)$, $S^{xx}(\pi,\pi)$



open symbols: 4×4 cluster, filled symbols: 6×6 cluster

$\Rightarrow J'$ small: Néel order in transverse components (for generic $\langle M \rangle$)

$\Rightarrow J'$ large: collinear order in transverse components (for generic $\langle M \rangle$)

$\Rightarrow 0.5 \lesssim J'/J \lesssim 0.65$, $\langle M \rangle = 1/2$: 'uuud' order in longitudinal components

Groundstate quantum numbers

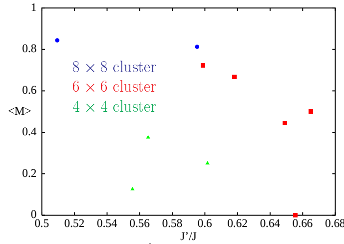
$V/2 - S^z$ = number of magnons: **odd** $\Rightarrow$ groundstate carries

- $\vec{k} = (\pi, \pi)$ for $J' \ll J$ (Néel order)
- $\vec{k} = (0, \pi)$ for $J' \gg J$ (collinear order)

$V/2 - S^z = 2n$ with n **odd** $\Rightarrow$ groundstate is

- even under diagonal reflections for $J' \ll J$ (Néel order)
- odd under diagonal reflections for $J' \gg J$ (collinear order)

Positions of unique groundstate level crossings



$\langle M \rangle = 0$ crossing on 6×6 cluster:
Schulz *et.al.*, J. Phys. I France **6** (1996) 675