Two-Dimensional Antiferromagnets in a Magnetic Field

A. Honecker, M.E. Zhitomirsky, Institut für Theoretische Physik, ETH-Hönggerberg, 8093 Zürich, Switzerland
O.A. Petrenko, ISIS facility, Department of Physics, Oxford University, England

Magnetization plateaux in the XXZ model on classical two-dimensional lattices

A. Honecker, J. Phys.: Condensed Matter **11** (1999) 4697

Hamiltonian:

$$H = J \sum_{\langle \vec{r},\vec{s} \rangle} \left\{ \Delta S^z_{\vec{r}} S^z_{\vec{s}} + \frac{1}{2} \left(S^+_{\vec{r}} S^-_{\vec{s}} + S^-_{\vec{r}} S^+_{\vec{s}} \right) \right\} - h \sum_{\vec{r}} S^z_{\vec{r}}$$

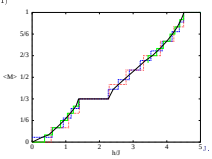
Magnetization: $\langle M \rangle = \frac{1}{SV} \left\langle \sum_{\vec{r}} S^z_{\vec{r}} \right\rangle$

V: Number of lattice points

For the $S = 1/2$ XXZ model on the three monohedral Archimedian tilings one finds:

- An $\langle M \rangle = 0$ plateau on the square and honeycomb lattice for $\Delta > 1$.
- An $\langle M \rangle = 1/3$ plateau on the triangular lattice for $\Delta \gtrsim 0.85$.

Magnetization curve of the isotropic $S = 1/2$ model on the triangular lattice: ($\Delta = 1$)



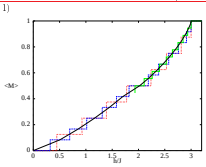
Plateau with $\langle M \rangle = 1/3$

(See also Nishimori, Miyashita, J. Phys. Soc. Jpn. **55** (1986) 4448)

System sizes: 6×3, $V = 27$, $V = 36$

Data for $|M| \leq 1/3$ and $V = 27$, $V = 36$: Taken from Bernu et.al., Phys. Rev. **B50** (1994) 10048

Magnetization curve of the isotropic $S = 1/2$ model on the honeycomb lattice: ($\Delta = 1$)



No non-trivial plateaux

System sizes: 4×4, 6×4, 6×6

Spin-1/2 systems on other Archimedian lattices:

$Sr_2Cu_2(BO_3)_2$: – a dimer system on

Experimentally observed: Magnetization plateaux at $\langle M \rangle = 1/4$ and $\langle M \rangle = 1/8$.
Kageyama et.al., Phys. Rev. Lett. **82** (1999) 3168

Proposal: This can be obtained with coupled dimers on the lattice shown above.
Miyahara, Ueda, Phys. Rev. Lett. **82** (1999) 3701

Under which general conditions do magnetization plateaux arise in two dimensions ?

Asymptotic behaviour of the magnetization curve

In two dimensions, the transition to saturation at $h_{\rm uc}$ is characterized by the following universal asymptotic behaviour of the magnetization:

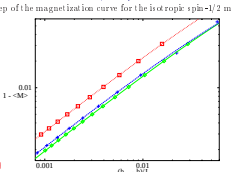
$$1 - \langle M \rangle \sim (h_{\rm uc} - h) \ln\left(\frac{b}{h_{\rm uc} - h}\right) \qquad (\star)$$

This form is supported by:

Spinwave theory for the square lattice
Zhitomirsky, Nikuni, Phys. Rev. **B57** (1998) 5013

Exact diagonalization for the square, triangular and honeycomb lattice
Honecker, J. Phys.: Condensed Matter **11** (1999) 4697

Midpoint of the last step of the magnetization curve for the isotropic spin-1/2 model ($\Delta = 1$):



Lines: best fit with $(\star)$

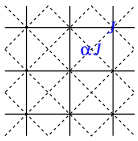
Mapping to a low-density Bose gas
Gluzman, Z. Phys. **B90** (1993) 313;
Sachdev, Senthil, Shankar, Phys. Rev. **B50** (1994) 258
Balyer, Braginskiĭ, Soviet Physics JETP **60** (1984) 781

A single relevant band of one-magnon excitations; unique minimum with (typically) quadratic dispersion. $S = 1/2$ magnons behave as a δ-function Bose gas !

The frustrated square lattice

Hamiltonian:

$$H = J \sum_{\substack{\text{nearest} \\ \text{neighbours}}} \vec{S}_{\vec{x}} \cdot \vec{S}_{\vec{y}} + \alpha J \sum_{\substack{\text{diagonal} \\ \text{neighbours}}} \vec{S}_{\vec{x}} \cdot \vec{S}_{\vec{y}} - h \sum_{\vec{x}} S^z_{\vec{x}}$$



One-magnon-dispersion above the ferromagnetic state:

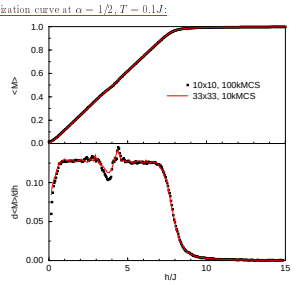
$$\mathcal{E}_{1s}(k_x, k_y)/J = -2(1+\alpha) + \cos k_x + \cos k_y + 2\alpha \cos k_x \cos k_y$$

Lines of minima for $\alpha = 1/2$!

Classical spins

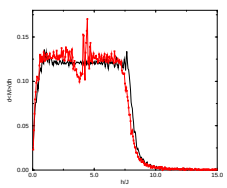
Monte Carlo simulation with a Metropolis algorithm

Magnetization curve at $\alpha = 1/2$, $T = 0.1J$:



⇒ A plateau-like feature at $\langle M \rangle = 1/2$

$\alpha = 0.54$, $\alpha = 1/2$

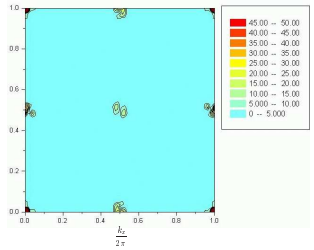


10×10 lattice, $T = 0.1J$, 100kMCS

⇒ No signal in $d\langle M \rangle/dh$ at $\langle M \rangle = 1/2$ and $\alpha = 0.54$

Static structure factor $S^{zz}(k_x, k_y)$ at $\alpha = 1/2$, $h = 4J$, $T = 0.1J$:

33×33 lattice, average over 50 frames every 5000 MCS



⇒ **Four-sublattice structure at $\langle M \rangle = 1/2$**

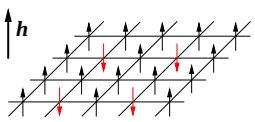
Spinwave theory

At $\alpha = 1/2$ rewrite the classical Hamiltonian with a four-sublattice structure as

$$H = \frac{J}{2}\left(\vec{S}_1 + \vec{S}_2 + \vec{S}_3 + \vec{S}_4\right)^2 - 2JS^2 - h\left(S^z_1 + S^z_2 + S^z_3 + S^z_4\right)$$

⇒ **Large groundstate degeneracies** for $T = 0$ at $\alpha = 1/2$ for all magnetic fields

For $\langle M \rangle = 1/2$ apply the Holstein-Primakoff transformation to the following spin configuration:



This spin configuration leads to a static structure factor $S^{zz}(k_x, k_y)$ with peaks at $(k_x, k_y) = (0,0), (\pi,\pi), (0,\pi), (\pi,0)$ – as observed by Monte Carlo.

Retaining only terms quadratic in the boson operators, we find the classical spinwave spectrum

$$\omega_1 = h - 4SJ + J\sqrt{\mathcal{E}}, \qquad \omega_2 = -h + 4SJ + J\sqrt{\mathcal{E}}, \qquad \omega_{3,4} = h - 2SJ \pm J\sqrt{4S^2 - \mathcal{E}}$$

with

$$\mathcal{E} = S^2 (1 - \cos k_x)(1 - \cos k_y) .$$

At $h = h_{\rm uc}/2 = 4SJ$ (to ensure $\langle M \rangle = 1/2$) there are 3 zero-energy modes: $k_x = k_y = 0$ ⇒

$$\omega_1 = \omega_2 = \omega_4 = 0$$

⇒ The above four-sublattice structure is stable.

Quantum fluctuations are expected to stabilize the collinear structure in a finite range of magnetic fields

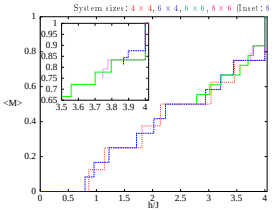
⇒ Plateau with $\langle M \rangle = 1/2$

(under investigation)

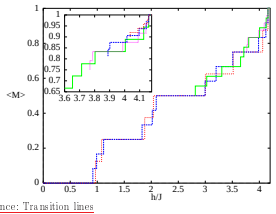
Exact diagonalization for spin 1/2

Finite-size magnetization curves:

$\alpha = 1/2$:

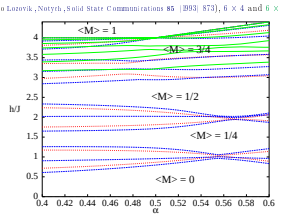


$\alpha = 0.54$:



α-dependence: Transition lines

4×4 (see also Lozovik, Notych, Solid State Communications **85** (1993) 873), 6×4 and 6×6 lattice:



⇒ A plateau with $\langle M \rangle = 1/2$ for $\alpha \approx 1/2$.

⇒ The transition to saturation at $\alpha = 1/2$ is special: A jump is observed for finite system-sizes. However, the height of the jump could scale to zero with $V \to \infty$ according to our finite-size data.
In any case, the precise functional form is unclear (the claim $1 - \langle M \rangle \sim \sqrt{4 - h/J}$ [Yang, Mütter, Z. Phys. **B104** (1997) 117] may be incorrect).

⇒ The plateau at $\langle M \rangle = 1/4$ is probably an artifact of the small system size (like the one with $\langle M \rangle = 3/4$).

⇒ It is numerically not clear if the universal form $(\star)$ holds for $\alpha > 1$ where the one-magnon dispersion does not have a unique minimum.

⇒ Gluzman [Phys. Rev. **B50** (1994) 6264] predicted a plateau just below saturation for $\alpha \geq 1/2$. There is a candidate for such a plateau at $\langle M \rangle = M(V) \approx 0.8$ whose scaling is however compatible with $M(V) \to 1$ as $V \to \infty$.

Summary

⇒ Plateau with $\langle M \rangle = 1/2$

⇒ In the classical model, this corresponds to an ordered phase for $\langle M \rangle \approx 1/2$ which arises without an ordered phase in zero magnetic field

⇒ Transition to saturation at $\alpha = 1/2$ is special

Open problems

⇒ Are there other plateaux than at $\langle M \rangle = 1/2$ (and $\langle M \rangle = 0$ – see also Kotov et.al., cond-mat/9903154 and references therein) ?
Is there in particular one just below saturation ?

⇒ What is the precise nature of the transition $\langle M \rangle \to 1$ at $\alpha = 1/2$?

⇒ Does $(\star)$ hold for $\alpha > 1/2$?