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Geometrically Frustrated Magnets at High Fields: exact low-temperature behavior

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- Introduction
- Localized spin flips near saturation field
- Scattering states of localized spin flips
- Mapping to hard-dimer (sawtooth chain) and to hard-hexagon (kagome AF) models

in collaboration with :
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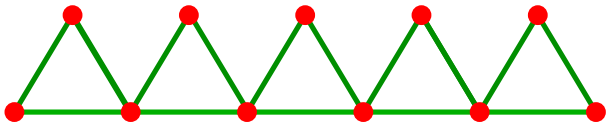
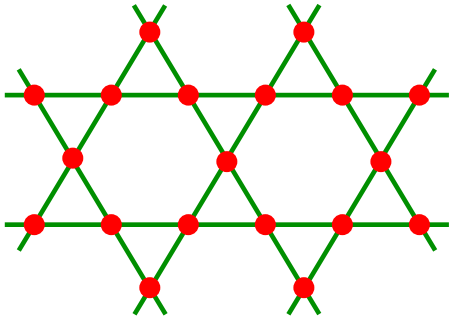
GEOMETRICALLY FRUSTRATED LATTICES

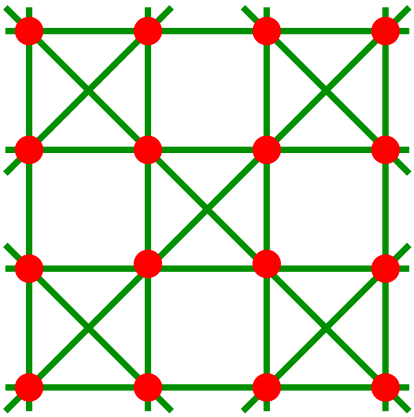
- sawtooth chain



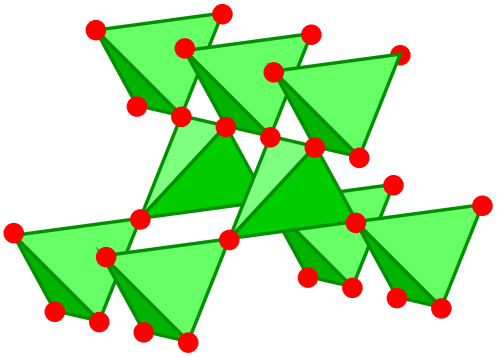
- kagome lattice



- checkerboard lattice



- pyrochlore lattice



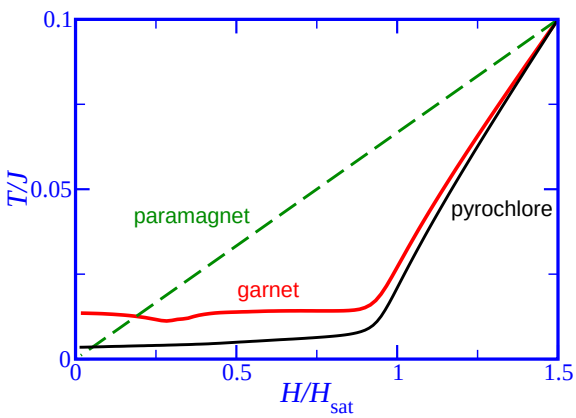
MOTIVATION

- pyrochlores, $Gd_2Ti_2O_7$, $Gd_2Sn_2O_7$, garnet (hyper-kagome), $Gd_3Ga_5O_{12}$, with small saturation fields $H_c \sim 1.5$–10 T

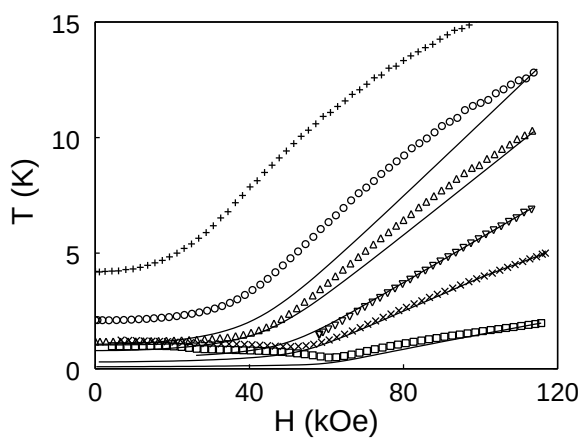
- Bose condensation of infinite # of modes

- Magnetocaloric effect:

  classical frustrated models



experiment on $Gd_2Ti_2O_7$



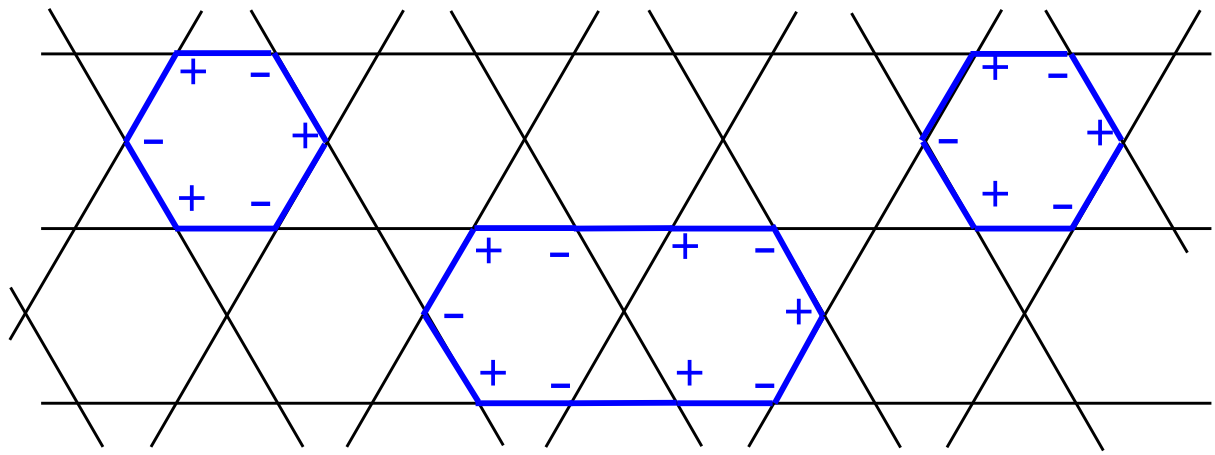
LOCALIZED MAGNONS

- Exact one-magnon states in Ferromagnetic background

$$|i\rangle = S_i^-|\mathrm{FM}\rangle \ , \qquad \sum_{i,j}\langle i|\hat{\mathcal{H}}|j\rangle e^{-i\mathbf{k}(\mathbf{r}_i-\mathbf{r}_j)} \Longrightarrow \omega_{\mathbf{k}}$$

- Kagome antiferromagnet: dispersionless branch

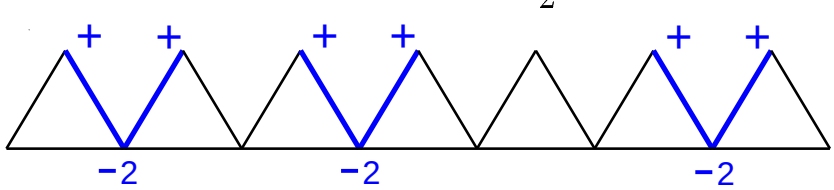
$$\omega_1 = H - 3 \ , \qquad \omega_{2,3} = H - \frac{3}{2} \pm \frac{1}{2}\sqrt{3(1+2\gamma_{\mathbf{k}})}$$



$$|\varphi_i\rangle = \frac{1}{\sqrt{6}}\sum_n (-1)^{n-1} S_{ni}^-|\mathrm{FM}\rangle, \quad N_{\max} = \frac{1}{3}N_{\mathrm{hex}} = \frac{N}{9}$$

- Sawtooth chain: dispersionless branch $(J_2 = \frac{1}{2}J_1)$

$$\omega_1 = H - 2 \ , \qquad \omega_2 = H - \frac{1}{2}(1-\cos k)$$

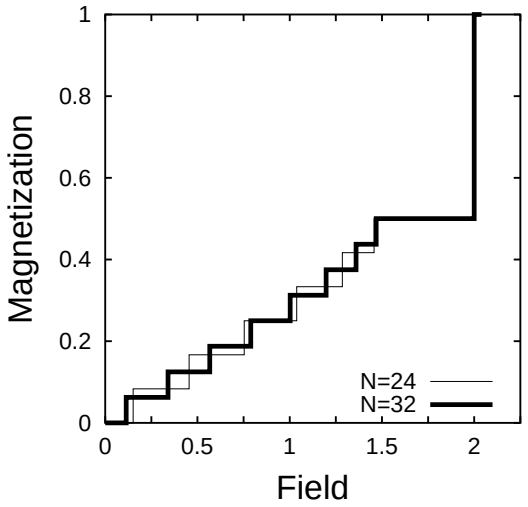


$$|\varphi_i\rangle = \frac{1}{\sqrt{6}}(S_{1i}^- - 2S_{2i}^- + S_{3i}^-)|\mathrm{FM}\rangle, \quad N_{\max} = \frac{1}{4}N$$

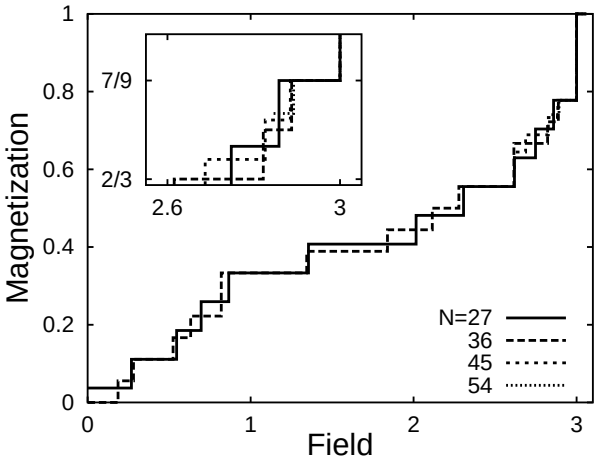
MAGNETIZATION CURVES BY EXACT DIAGONALIZATION

Schulenburg et al

- sawtooth chain



- kagome AF



LOCALIZED MAGNONS: exact multiparticle states

- Low-temperature Mapping of Independent Localized Magnons to a gas of Classical particles with an exclusion principle:

$$Z = \sum_{n=0}^{N_{\max}} w(n, N) e^{-n(H-H_c)/T}$$

- Mapping is valid provided:
  - Independent localized magnons $|n\rangle_{\rm ilm}$ are the lowest energy states in every n-magnon subsector

$$\hat{\mathcal{H}}^{zz}|n\rangle_{\rm ilm} = n(H-2)|n\rangle_{\rm ilm} \quad \hat{\mathcal{H}}^{\perp}|n\rangle_{\rm ilm} = -n|n\rangle_{\rm ilm}$$

$$\langle\hat{\mathcal{H}}^{zz}\rangle \geq n(H-2) \quad \langle\hat{\mathcal{H}}^{\perp}\rangle \geq \langle\hat{\mathcal{H}}^{\perp}\rangle_{\rm boson} = -n$$

  - No other lowest energy states or their contribution vanishes as $n \to \infty$
  - Scattering states are separated by a gap and $T \ll \Delta$

Scattering States in 2-magnon sector: sawtooth chain

- $N/2$ one-magnon states in the lowest branch $\omega_1 = H - 2$

  $\frac{(N/2)(N/2+1)}{2}$ two-magnon states, which include:

  $\frac{(N/2)(N/2-3)}{2}$ independent localized magnons and

  $\frac{N}{2} + \frac{N}{2}$ defect or scattering states:

  two localized magnons are in the same or in adjacent valleys

- Variational basis for scattering states:

$$|\psi_i\rangle \simeq |\varphi_i \varphi_{i+1}\rangle \ , \quad |\widetilde{\psi}_i\rangle \simeq |\varphi_i^2\rangle$$

$$\langle \psi_i | \psi_{i\pm 1}\rangle = 1/35 \ , \quad \langle \psi_i | \widetilde{\psi}_i\rangle = \langle \psi_i | \widetilde{\psi}_{i+1}\rangle = \sqrt{5/49}$$

- Variational ansatz: $|k\rangle = \Sigma_i \, e^{-ikr_i} |\psi_i\rangle$

$$E = \frac{\langle k|\hat{\mathcal{H}}|k\rangle}{\langle k|k\rangle} \ = \ E_{\rm FM} + 2(H-2) + \varepsilon_k$$

$$\Delta = \varepsilon_{k=0} = \frac{20}{37} \approx 0.54$$

- Improved ansatz: $|k\rangle = \Sigma_i \, e^{-ikr_i} \left(|\psi_i\rangle + c|\widetilde{\psi}_i\rangle \right)$

$$\Delta \approx 0.44 \ , \quad \text{for} \ \ c = -0.24 \ ; \quad \text{numerically} \ \ \Delta \approx 0.42$$

- Weak dispersion $\delta\varepsilon_k \simeq 0.1\Delta$, gap is determined by n.n. repulsion

Scattering States in 2-magnon sector: kagome AF

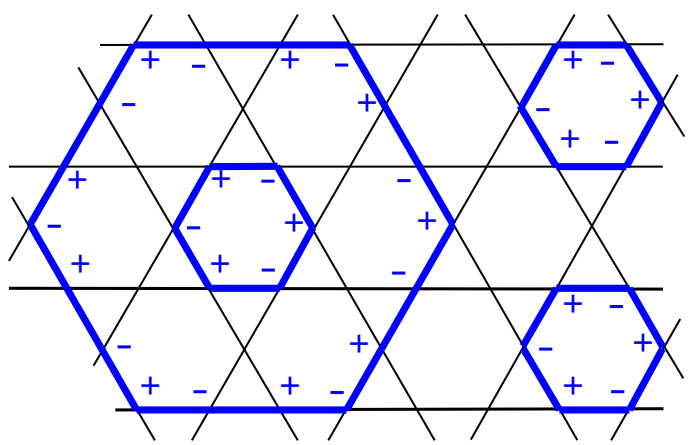
- $N/3$ one-magnon states in the lowest branch $\omega_1 = H - 3$:

$\frac{(N/3)(N/3-7)}{2}$ 'hard-hexagon' states and $N + \frac{N}{3}$ scattering states

- Variational ansatz for scattering states:

$$|\psi_{\alpha i}\rangle \simeq |\varphi_i \varphi_{i+\delta_\alpha}\rangle \ , \quad \delta_\alpha = (1,0), (\pm\tfrac{1}{2}, \tfrac{\sqrt{3}}{2})$$
$$\langle\psi_{2i}|\psi_{1i}\rangle = -\tfrac{1}{7} \ , \quad \langle\psi_{3i}|\psi_{1i}\rangle = \tfrac{1}{35}$$
$$|k\rangle = \sum_i e^{-ikr_i} \left(a|\psi_{1i}\rangle + b|\psi_{2i}\rangle + c|\psi_{3i}\rangle\right) \quad \text{yields} \quad \Delta \approx 0.24$$

- Additional low-energy states:
  - Dispersive magnon $\omega_{3k} \approx H - 3 + \frac{1}{8}k^2$
    renormalizes due to multiple scattering on localized magnons
    and acquires a gap $\Delta_3 \simeq 12n/N$
  - Extra localized magnons:



Superposition of localized magnons in adjacent valleys
their # is smaller than # of hard-hexagon states by $1/N$,
disappear completely for $3n/N > 0.1$

Hard Classical dimers on a chain

- Partition function:

$$Z = \sum_{\{\sigma\}} \exp\left[-\frac{\varepsilon}{T}\sum_i \sigma_i\right] \prod_{\langle ij\rangle} (1-\sigma_i\sigma_j)\ , \quad \varepsilon = (H - H_c)\ , \quad \sigma_i = 0, 1$$

$$Z = \mathrm{Tr}\mathcal{T}^L\ , \qquad \mathcal{T}(\sigma,\sigma') = \begin{pmatrix} 1 & \mathrm{e}^{-\varepsilon/2T} \\ \mathrm{e}^{-\varepsilon/2T} & 0 \end{pmatrix} \simeq \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

- Thermodynamic potential:

$$\begin{aligned} F/L &= -T\ln\lambda_1 = -T\ln\left(\frac{1}{2} + \sqrt{\frac{1}{4} + \mathrm{e}^{-\varepsilon/T}}\right), \\ S/L &= \ln\left(\frac{1}{2} + \sqrt{\frac{1}{4} + \mathrm{e}^{-\varepsilon/T}}\right) + \frac{\varepsilon}{4T}\left(2 - \frac{1}{\sqrt{\frac{1}{4} + \mathrm{e}^{-\varepsilon/T}}}\right). \\ M/L &= \frac{1}{2} + \frac{1}{4\sqrt{\frac{1}{4} + \mathrm{e}^{-\varepsilon/T}}} \end{aligned}$$

- Universal values at the saturation: $H = H_c\ (\varepsilon = 0)$

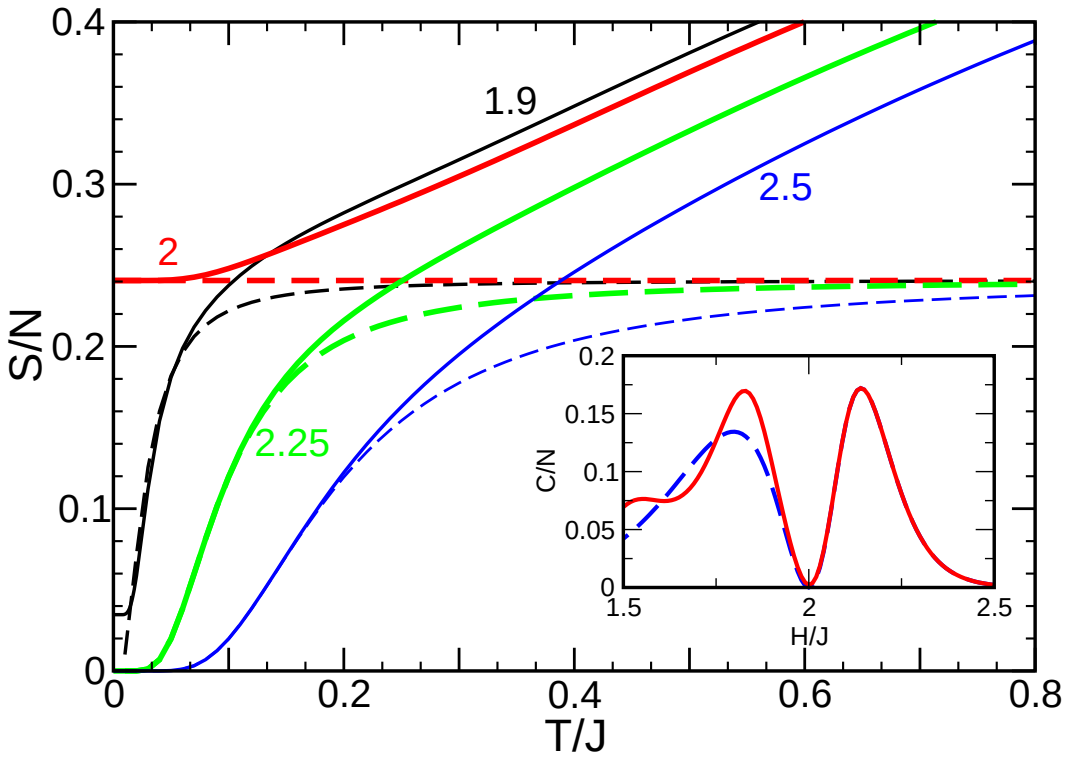
$$\begin{aligned} S/L &= \ln\left(\frac{1+\sqrt{5}}{2}\right) \approx 0.481212 \\ M/L &= \frac{1+\sqrt{5}}{2\sqrt{5}} \approx 0.723607 \end{aligned}$$

- Correlation length: $\xi^{-1} = \ln|\lambda_1/\lambda_2| = \varepsilon/T + 2\ln\lambda_1$

$$\xi \approx T/(H - H_c), \quad (\varepsilon \gg T)\ , \quad \xi \approx e^{(H_c - H)/T}, \quad (|\varepsilon| \gg T)\ ,$$

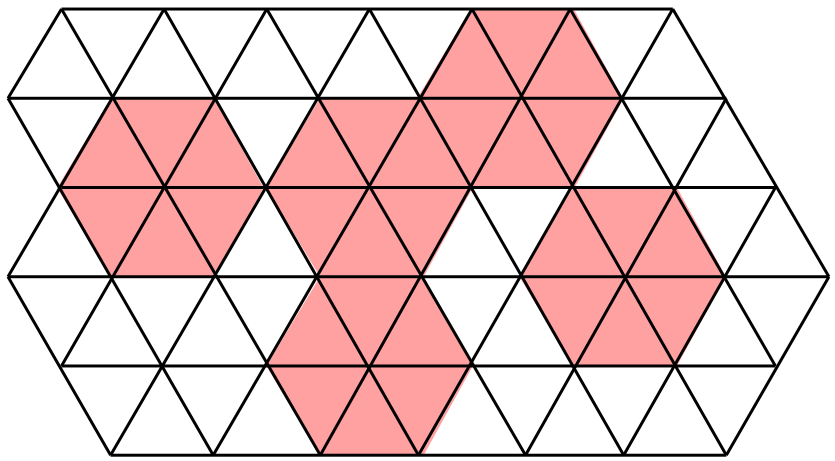
Sawtooth chain: comparison to numerical results

exact diagonalization data by A. Honecker for $N = 24$



Hard Hexagons on a Triangular Lattice

Baxter '81



- Thermodynamic functions:

$$Z = \sum_{n=0}^{N/3} z^n w(n,N)\,, \quad z = e^{-(H-H_c)/T}\,, \quad F = -T\ln\kappa\,, \quad \kappa = Z^{1/N}$$

- At the saturation field, $H = H_c$ ($z = 1$):

$$S = 0.33324\,,\ \rho = 0.16243 \quad \Longrightarrow \quad S_{\rm kag} = \tfrac{1}{3}S_{\rm hex} = 0.11108$$

- Phase transition at $H = H^*$:

$$z_c = \tfrac{1}{3}(11+5\sqrt{5}) = 11.0902 \quad \Longrightarrow \quad H^*(T) = H_c - T\ln z_c = 3 - 2.406T$$

$$\rho_c = \tfrac{1}{10}(5-\sqrt{5}) = 0.2764 \quad \Longrightarrow \quad M_{\rm kag} = M_{\rm sat} - \tfrac{1}{3}\rho_c = 0.4079$$

critical exponents of 2D three-state Potts model:

$$\alpha = \tfrac{1}{3},\ \beta = \tfrac{1}{9},\ \nu = \tfrac{5}{6}$$

- Magnetocaloric Effect:

$$S = f[(H-H_c)/T] \quad \Longrightarrow \quad T = T_i\,\frac{H-H_c}{H_i-H_c}$$

fast temperature drop as $H \to H_c$!

Baxter's solution for the thermodynamic potential

- High fields: $H > H^*, \;\; 0 < z < z_c, \quad -1 < x < 0$

$$z = -x\frac{H^5(x)}{G^5(x)}\ , \quad H(x) = \prod_{n=1}^{\infty}[(1-x^{5n-4})(1-x^{5n-1})]^{-1},$$

$$G(x) = \prod_{n=1}^{\infty}[(1-x^{5n-3})(1-x^{5n-2})]^{-1}, \quad Q(x) = \prod_{n=1}^{\infty}(1-x^n)\ ,$$

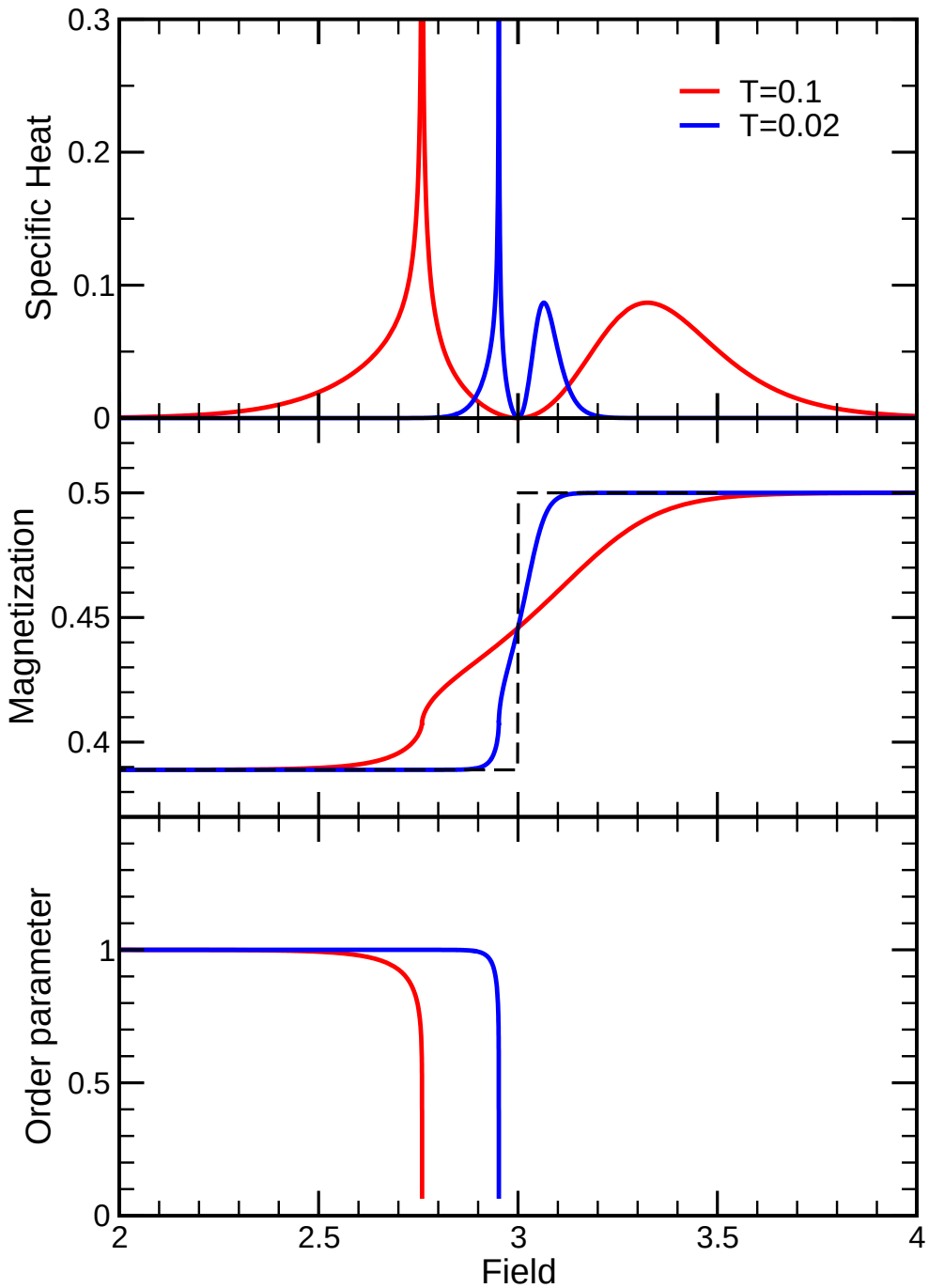
$$\kappa = \frac{H^3(x)Q^2(x^5)}{G^2(x)}\prod_{n=1}^{\infty}\frac{(1-x^{6n-4})(1-x^{6n-3})^2(1-x^{6n-2})}{(1-x^{6n-5})(1-x^{6n-1})(1-x^{6n})^2}$$

- Low fields: $H < H^*, \;\; z_c < z < \infty, \;\; 0 < x < 1$

$$z = x^{-1}\frac{G^5(x)}{H^5(x)}\ , \quad R(x) = \frac{Q(x)Q(x^5)}{Q^2(x^3)}\ ,$$

$$\kappa = \frac{x^{-1/3}G^3(x)Q^2(x^5)}{H^2(x)}\prod_{n=1}^{\infty}\frac{(1-x^{3n-2})(1-x^{3n-1})}{(1-x^{3n})^2}$$

Thermodynamics of Kagome AF from the exact solution



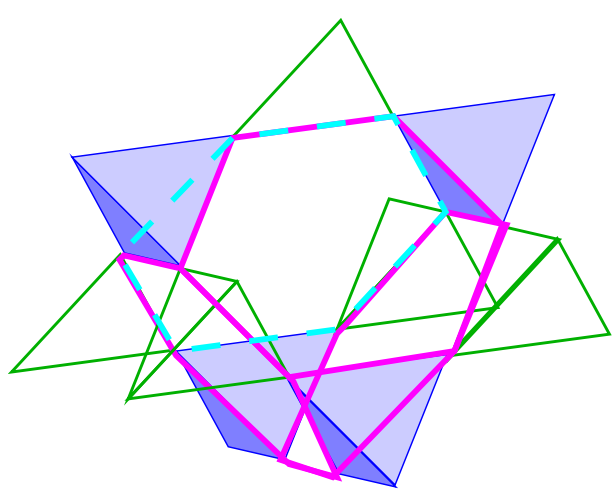
When There is No Exact Solution...

• spin-1/2 Heisenberg AF on a checkerboard lattice is mapped to a hard-square model: lattice gas on a square lattice with nearest and next-nearest neighbor exclusion

• Antiferromagnetic Ising models at the transition into a saturated state. Single spin flips one neighboring sites loose energy $\Delta E \sim J$. At low temperatures $T \ll J$ nearest-neighbor exclusion.

Frustrated quantum Heisenberg model near saturation	$\Longrightarrow$	Statistical model of classical particles with an exclusion principle	$\Longleftarrow$	Ising model near saturation

MC simulations on equivalent Ising model yield:

$$S_{\text{checker}} = 0.162 > S_{\text{kag}} \qquad \text{at } H = H_c$$

• Pyrochlore lattice—an open problem: localized magnons become linear dependent