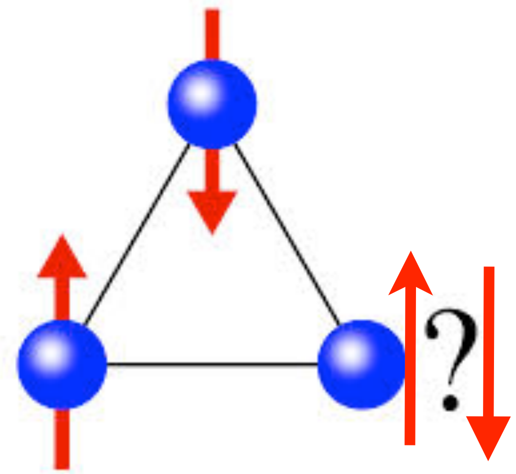
Frustrated magnetism via bold diagrammatic Monte Carlo

Oleg Starykh, University of Utah



collaborators: S. A. Kulagin, N. Prokof'ev, B. Svistunov, and C. N. Varney
(U Mass, Amherst)

*International Workshop on the Sign Problem in QCD and beyond,
GSI, Darmstadt, February 18 - 21, 2014*

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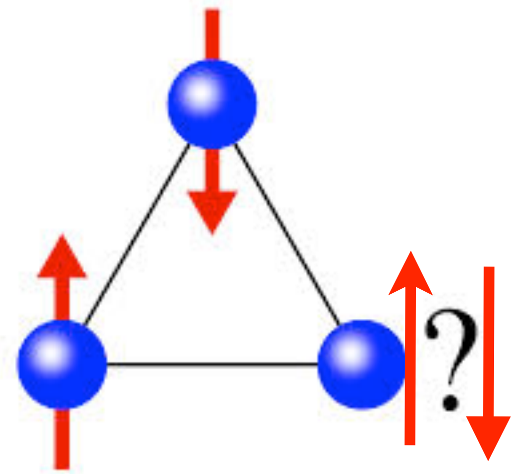

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Outline

- Geometrically frustrated magnets
  - experiments
  - Field theory vs numerics at finite T
- Popov-Fedotov fermions and bold diagrammatic Monte Carlo
- Quantum-classical correspondence (at intermediate T)
- Physical insight into prolonged “high-T” behavior
- Conclusions

Triangular lattice Ising antiferromagnet

PHYSICAL REVIEW VOLUME 79, NUMBER 2 JULY 15, 1950

Antiferromagnetism. The Triangular Ising Net

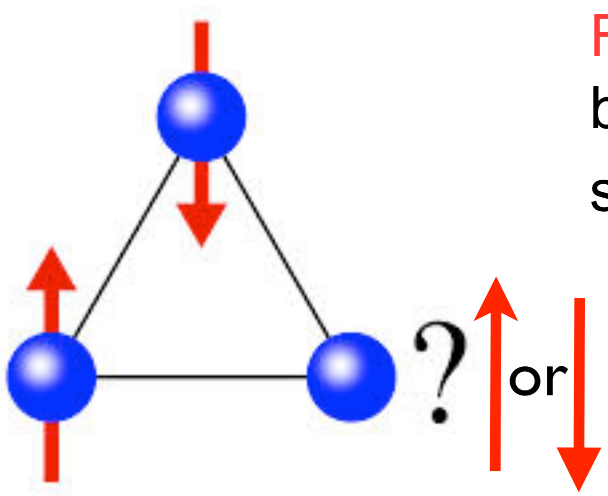
G. H. WANNIER
Bell Telephone Laboratories, Murray Hill, New Jersey

(Received February 11, 1950)

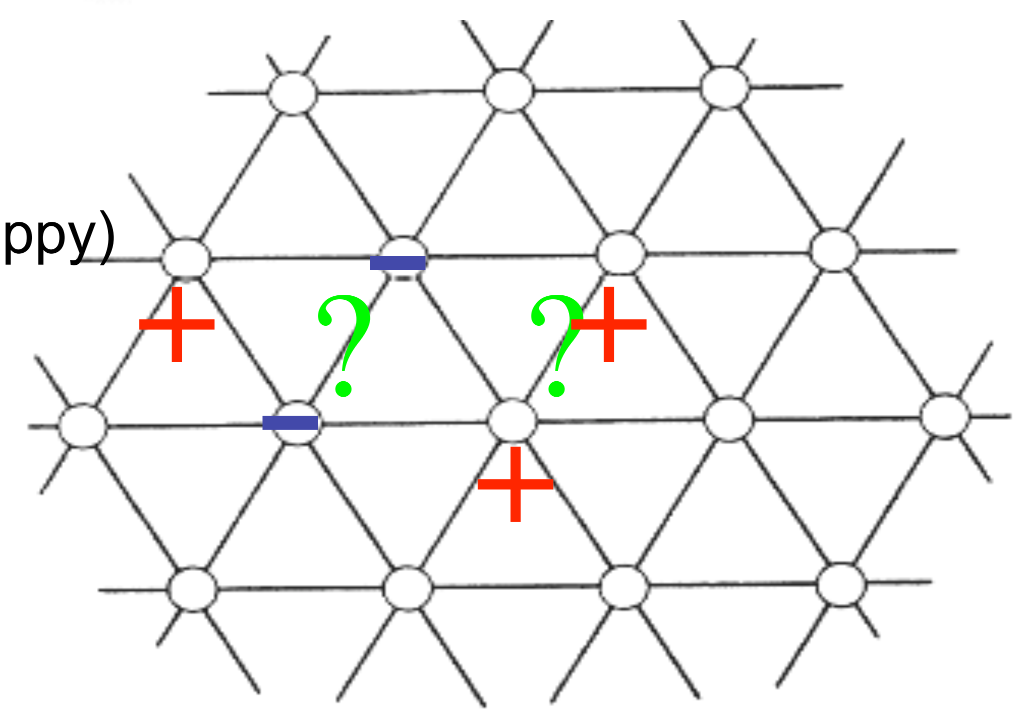
In this paper the statistical mechanics of a two-dimensionally infinite set of Ising spins is worked out for the case in which they form either a triangular or a honeycomb arrangement. Results for the honeycomb and the ferromagnetic triangular net differ little from the published ones for the square net (Curie point with logarithmically infinite specific heat). The triangular net with antiferromagnetic interaction is a sample case of antiferromagnetism in a non-fitting lattice. The binding energy comes out to be only one-third of what it is in the ferromagnetic case. The entropy at absolute zero is finite; it equals

$$S(0)=R\frac{2}{\pi}\int_0^{\pi/3}\ln(2\cos\omega)d\omega=0.3383R.$$

The system is disordered at all temperatures and possesses no Curie point.



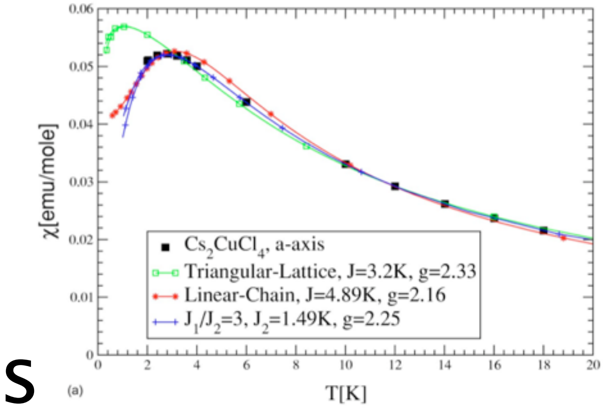
Frustration: pairwise interactions between spins cannot be minimized simultaneously (1/3 of bonds are unhappy)



Ising spins S_r= +1 or -1 only

Experimental indications

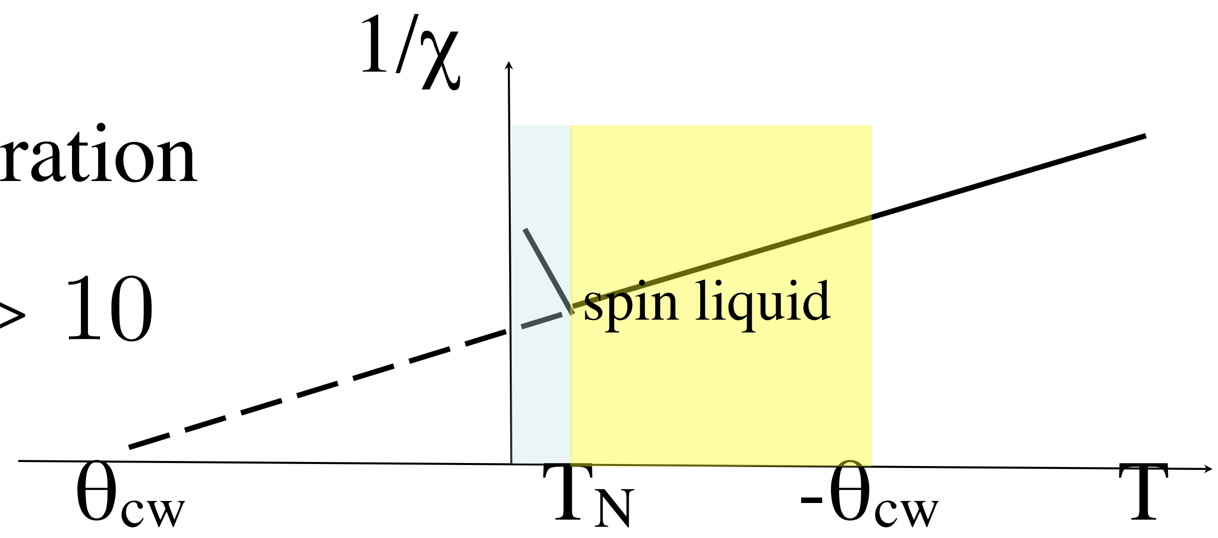
A. Ramirez (Annu.Rev.Mater.Sci. 1994)

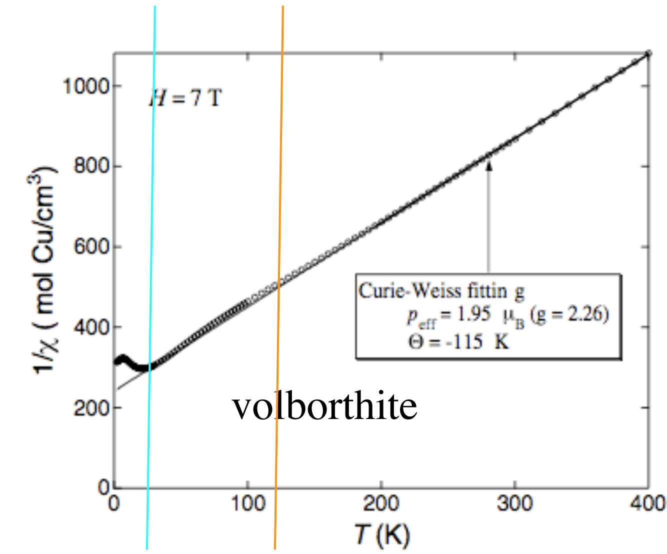


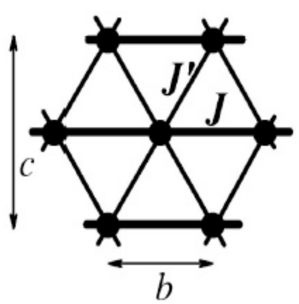
- spin liquid: no broken symmetries, strong correlations

strong frustration

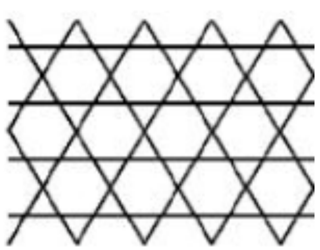
$$f = \frac{\theta_{\mathrm{cw}}}{T_{\mathrm{N}}} > 10$$



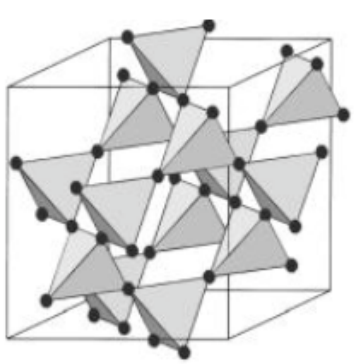




triangular



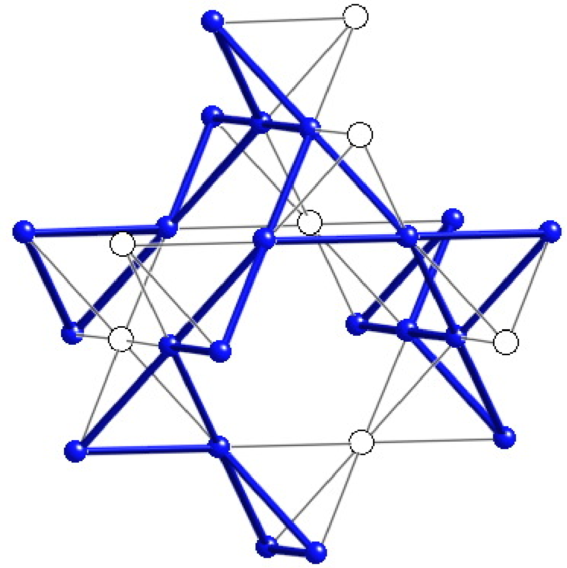
kagome



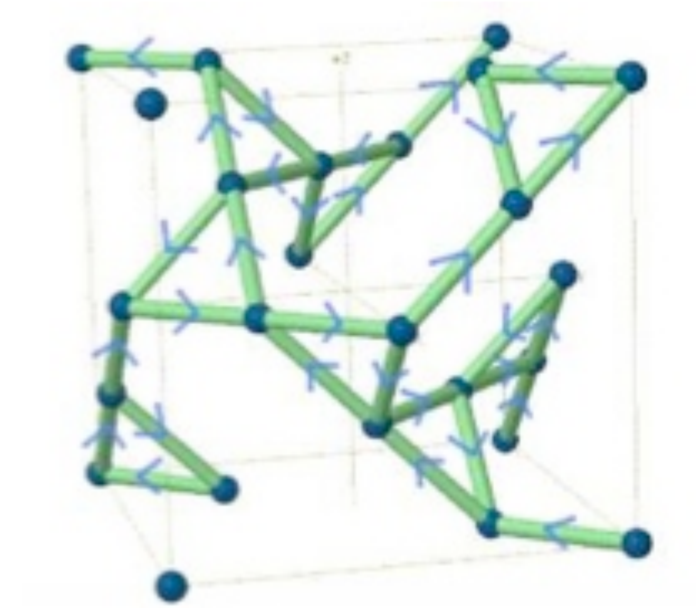
pyrochlore

Compound	Magnetic lattice	$-\theta_{cw}$ (K)	T_c (K)	f	Ordered state	Electronic configuration
wo-dimensional magnets						
VCl_2	triangular	437	36	12	AF	$3d^3$
$NaTiO_2$	triangular	1000	<2	>500	—	$3d^1$
$LiCrO_2$	triangular	490	15	33	AF	$3d^3$
$Gd_{0.8}La_{0.2}CuO_2$	triangular	12.5	0.7	16	SG	$4f^7$
$SrCr_8Ga_4O_{19}$	kagome	515	3.5	150	SG	$3d^3$
$KCr_3(OH)_6(SO_4)_2$	kagome	70	1.8	39	AF	$3d^3$
hree-dimensional magnets						
$ZnCr_2O_4$	B-spinel	390	16	24	AF	$3d^3$
K_2IrCl_6	FCC	321	3.1	10	AF	$5d^5$
FeF_3	B-spinel	240	15	16	AF	$3d^5$
$CsNiFeF_5$	B-spinel	210	4.4	48	SG	$3d^8$, $3d^5$
$MnIn_2Te_4$	zinc blende	100	4	25	SG	$3d^5$
$Gd_3Ga_5O_{12}$	garnet	2.3	<0.03	>100	—	$4f^7$
Sr_2NbFeO_6	perovskite	840	28	30	SG	$3d^4$
Ba_2NbVO_6	perovskite	450	15	30	SG	$3d^3$

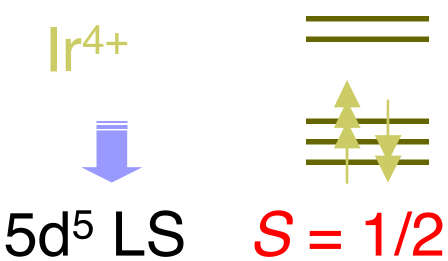
Hyper-Kagome $Na_4Ir_3O_8$: 3D lattice of corner-sharing triangles



decimated pyrochlore lattice



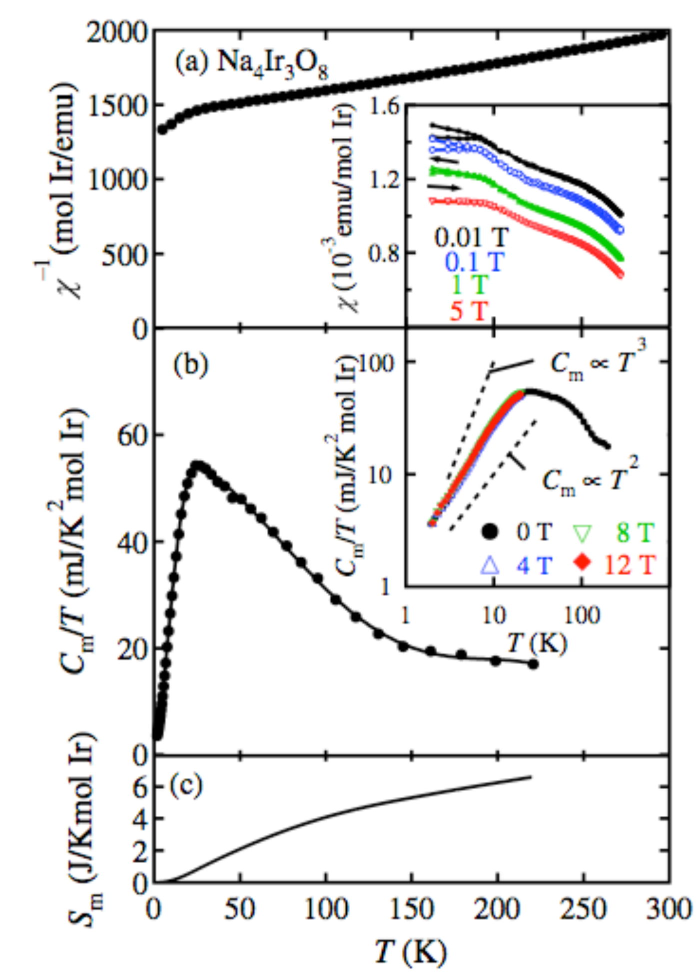
Takagi et al, 2007



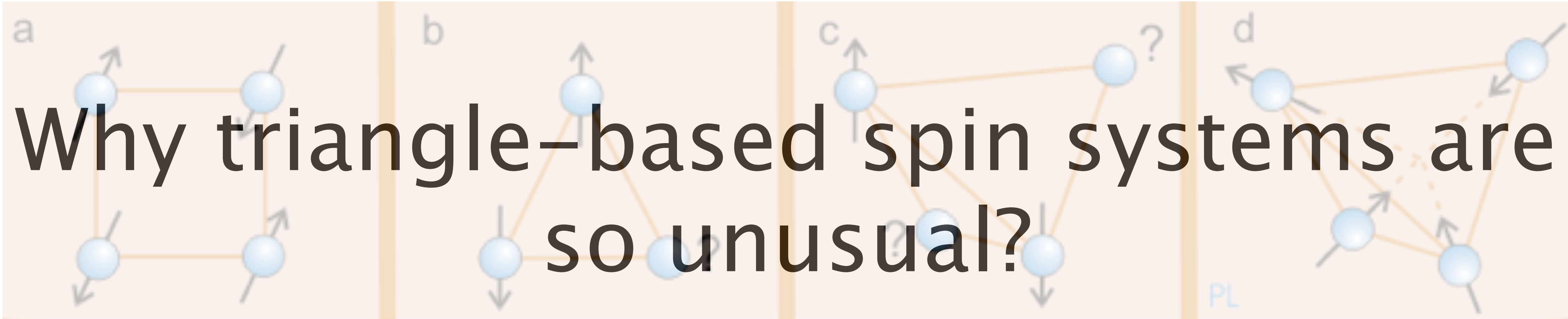
$$\theta_{cw} = -650\ \mathrm{K},\ T_N < 2\ \mathrm{K}$$

Experimentally very relevant issue:
temperature interval from T ~ J to
T << J is often **the only accessible** regime.

And yet we do not have good description of it.

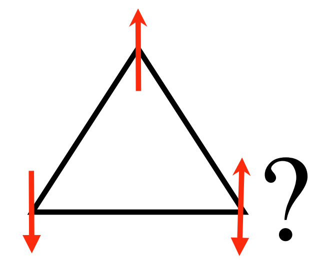


Why triangle-based spin systems are so unusual?



- Classically – strongly frustrated

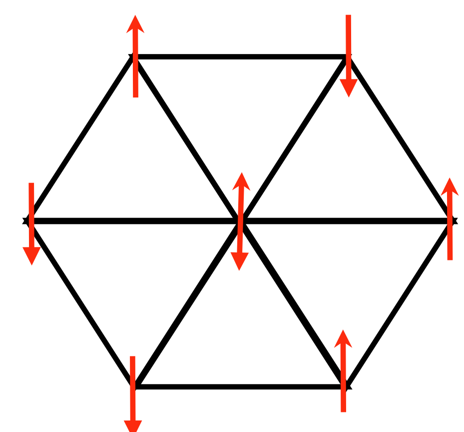
(unable to satisfy all pairwise interactions simultaneously; finite entropy at T=0)

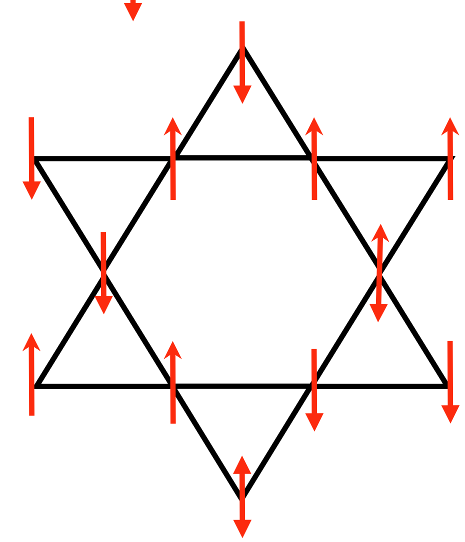


$$E = J \sum_{i,j} S_i S_j$$

J > 0, S = + 1 or -1

- Number of classical (Ising) ground states (**N** sites):
  - ✳triangular lattice = $e^{0.323\ N}$
  - ✳kagome lattice = $e^{0.502\ N}$





- Frustration leads to classical degeneracy
- Quantum fluctuations: can stabilize spin liquid via sampling of all classical degenerate states?

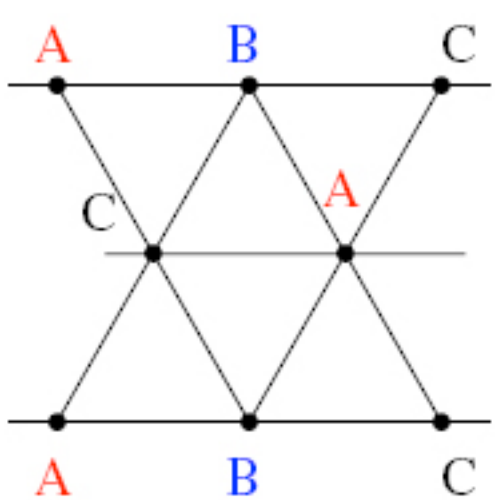
Z_2 spin liquid in kagome and J_1-J_2 models [Huse, White 2011]

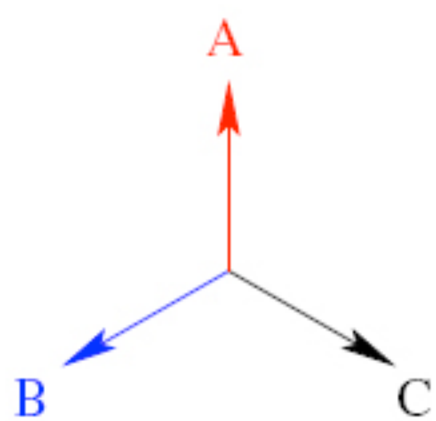
Heisenberg (vector) spins relieve frustration

Classical vector spins: three-sublattice 120^o structure

Spiral magnetic order: co-planar , non-collinear

$$H = J \sum_{i,j} \vec{S}_i \cdot \vec{S}_j = \frac{J}{2} \sum_{\triangle} \Big(\sum_{i \in \triangle} \vec{S}_i \Big)^2 + \text{const}$$





$$\vec{S}_A + \vec{S}_B + \vec{S}_C = 0$$

Relieve frustration by sharing it with the neighbors: Energy per bond = $S^2 \cos(120^o) = -0.5\, S^2$

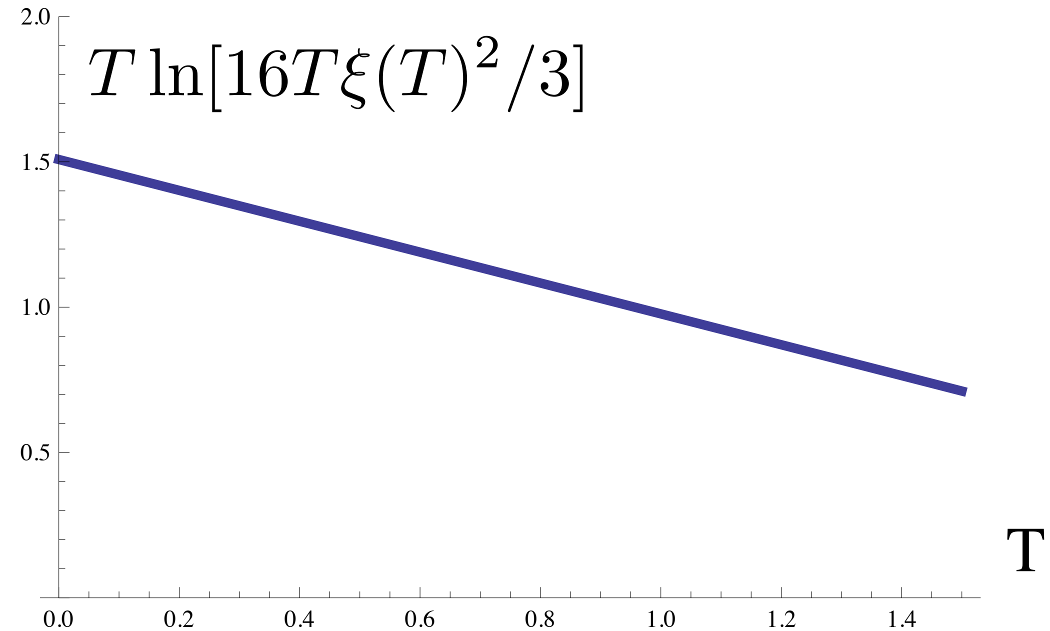
Does it hold for quantum S=1/2 spins? **YES**

Numerical results: classical 120^o structure survives
(Singh, Huse 1992 … Chernyshev, White 2007)

Finite T expectations (field theory = nonlinear sigma model)

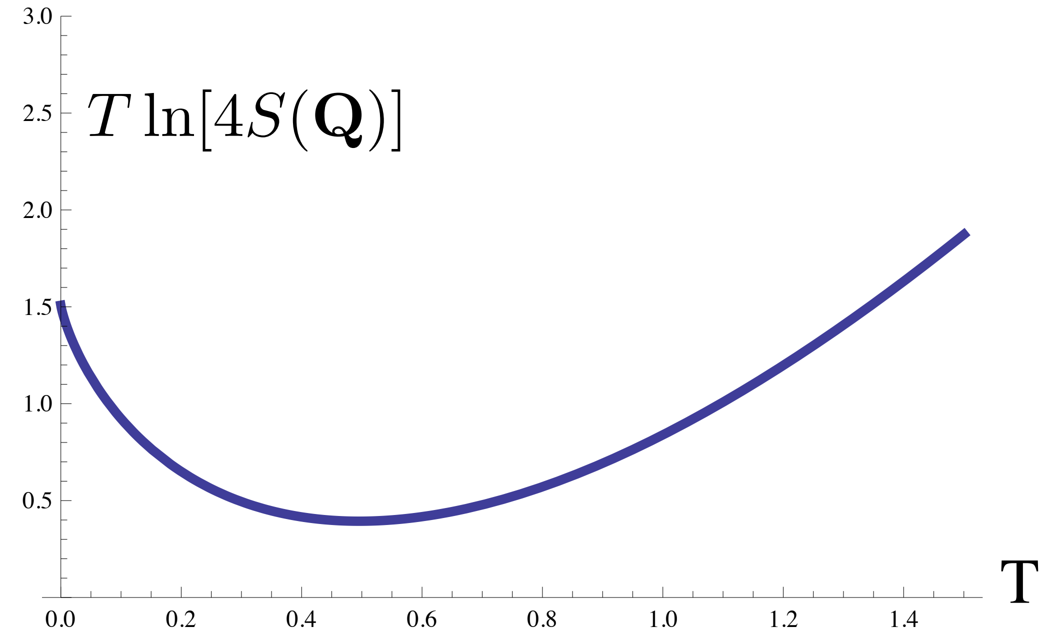
- d=2 and SU(2) symmetric spin system is characterized by exponentially large spin correlation length

$$\xi(T) = 0.021\left(\frac{c}{\rho_s}\right)\left(\frac{4\pi\rho_s}{T}\right)^{1/2}\exp\left(\frac{4\pi\rho_s}{T}\right)$$



- Static structure factor

$$S(Q) \simeq 0.85\left(\frac{T}{4\pi\rho_s}\right)^4 \xi(T)^2,$$



Finite T: classical triangular AFM

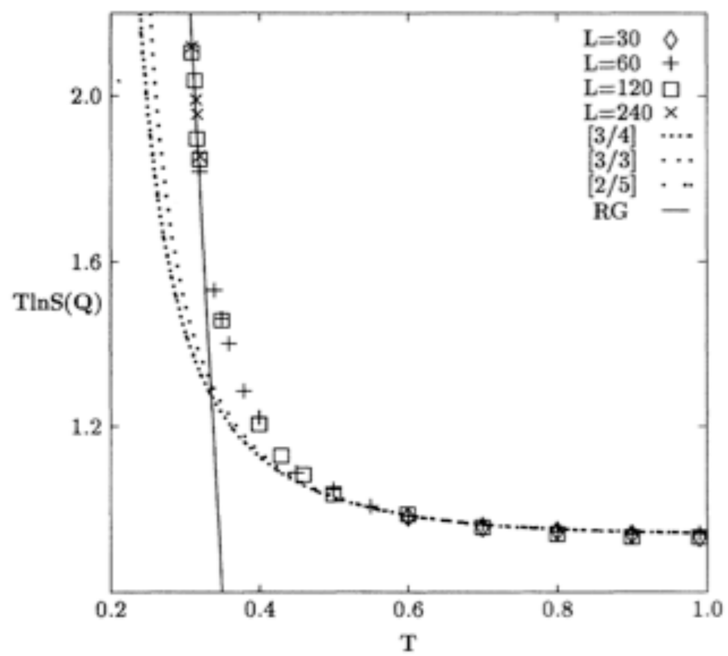


FIG. 3. $T \ln S(\mathbf{Q})$ as a function of temperature T. The Monte Carlo data for different system sizes are indicated by the symbols. The solid line is a fit to the low-T RG predictions (Ref. 3) and the dotted lines represent Padé approximants to the function using the high-temperature series coefficients in the table. $[N/M]$ denotes the ratio of a polynomial of order N in the numerator to one of order M in the denominator.

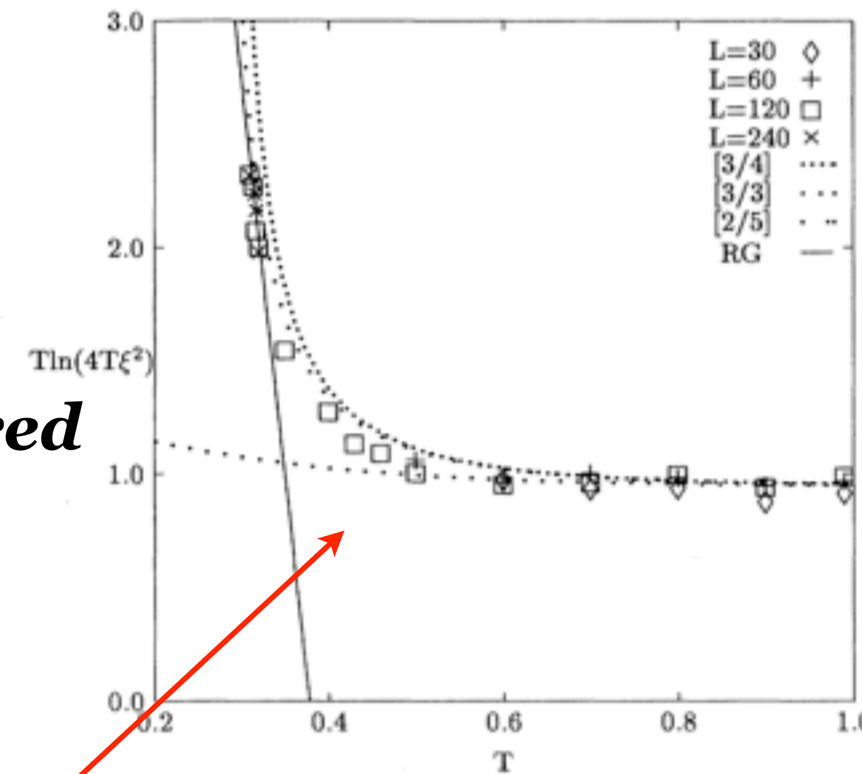


FIG. 4. $T \ln(4T\xi^2)$ as a function of temperature T. The notation is the same as that in Fig. 3.

ordered

Southern, Young 1993

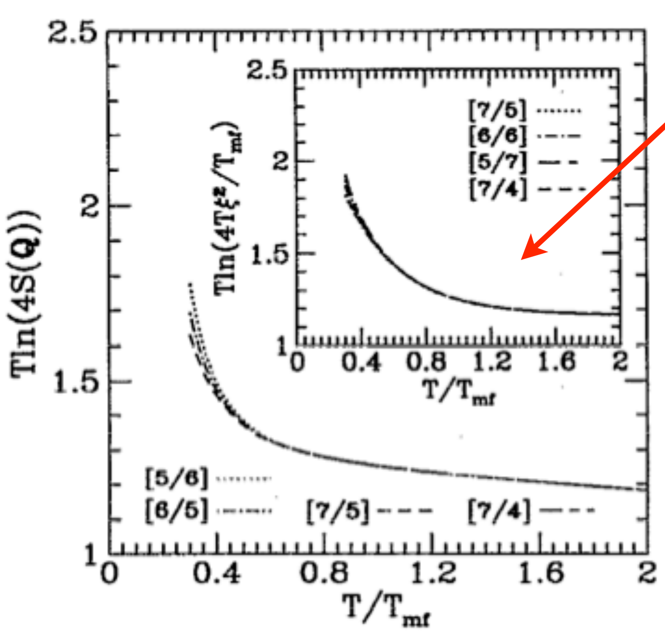
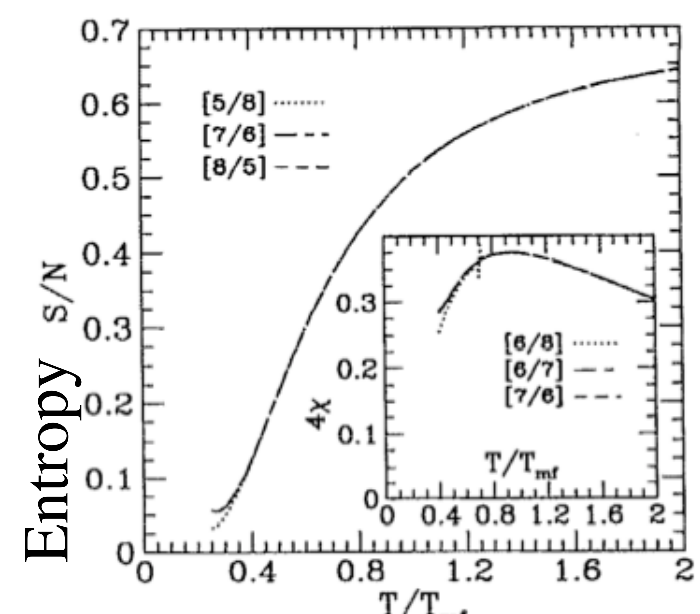


FIG. 2. Square lattice: $T \ln[4S(\mathbf{Q})]$ and $T \ln(4T\xi^2/T_{\rm mf})$ (on the insert) vs $T/T_{\rm mf}$; $u = 1/(T+0.2)$.

ordered



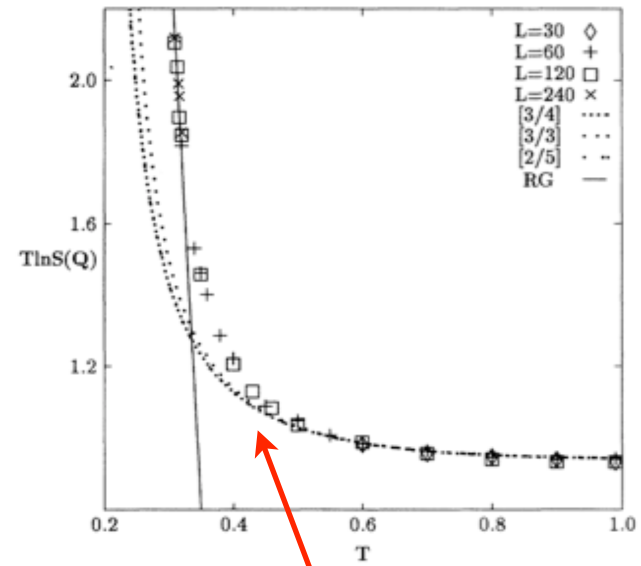
low entropy

FIG. 4. Square lattice: entropy S/N and susceptibility 4χ vs $T/T_{\rm mf}$; $u = 1/(T+0.2)$.

spin-½ square AFM

Elstner, Singh, Young 1994. High-T series expansion

Finite T: triangular AFM $S = \infty$ vs $S = 1/2$



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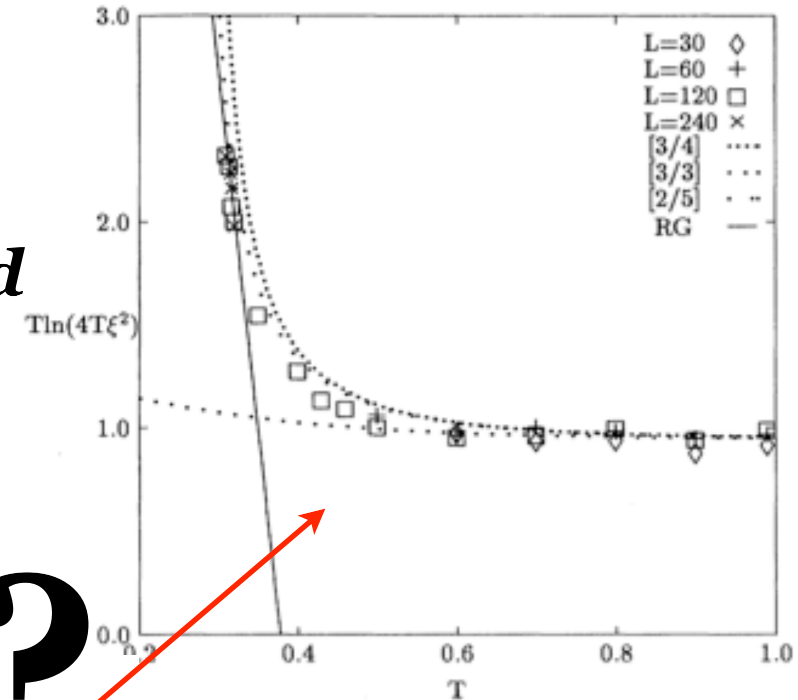
ordered

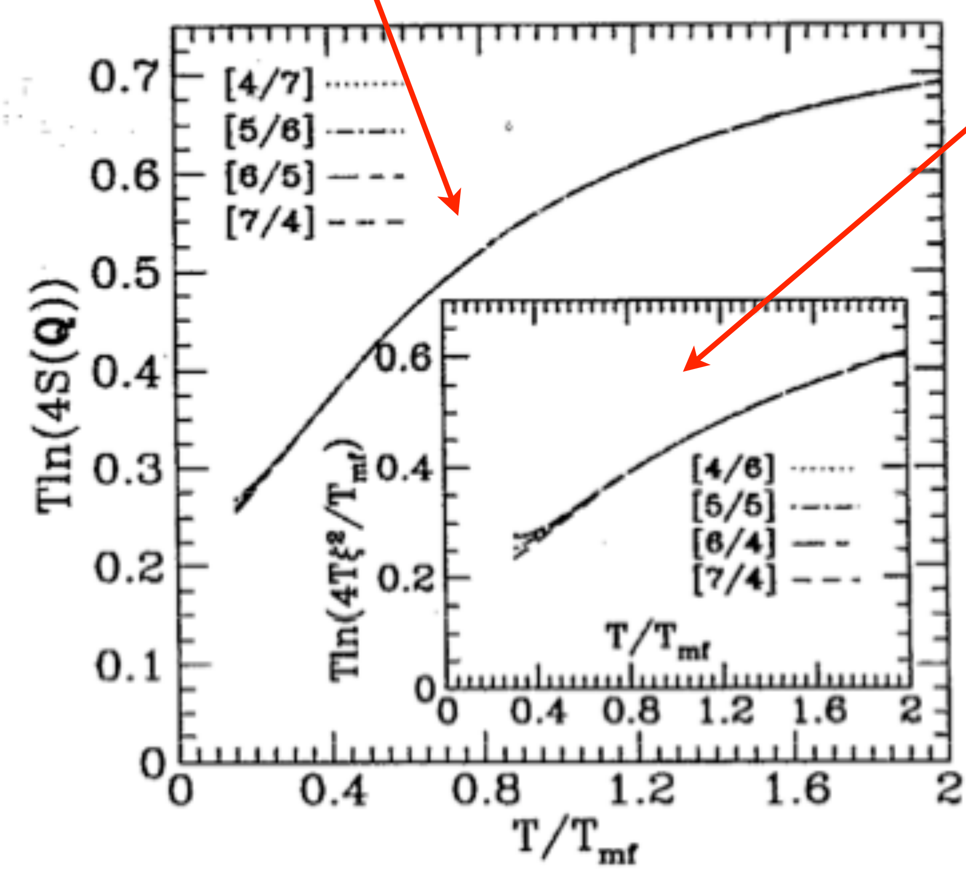


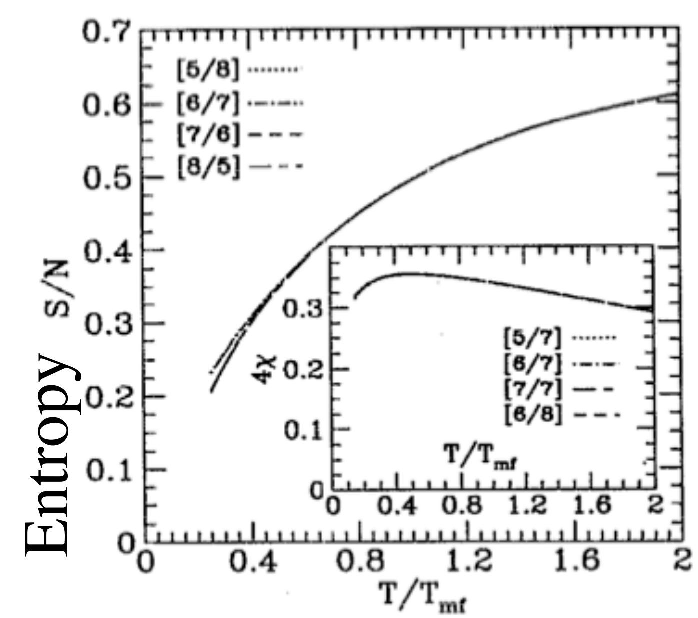
$T \ln(4T\xi^2)$ as a function of temperature T. The the same as that in Fig. 3.

$S = \infty$

Southern, Young 1993

?





high entropy

FIG. 3. Triangular lattice: entropy S/N vs T/T_{mf}; $u = 1/(T+0.2)$; on the insert: susceptibility 4χ vs T/T_{mf}; $u = 1/(T+0.08)$.

$S = 1/2$

spin-½ triangular AFM

Elstner, Singh, Young 1994. High-T series expansion

FIG. 1. Triangular lattice: $T \ln[4S(\mathbf{Q})]$ vs T/T_{mf}. The plots represent $[L, M]$ Padés in the Euler transformed variable $u = 1/(T+0.08)$. The insert shows results for the correlation length. $T \ln[4T\xi^2/T_{mf}]$ vs T/T_{mf}; $u = 1/(T+0.2)$.

Popov Fedotov fermions (JETP 1988)

$$H = J \sum_{\langle R,R' \rangle} \vec{S}_R \cdot \vec{S}_{R'} = \frac{J}{4} \sum_{\langle R,R' \rangle} c^\dagger_{R,\alpha} \vec{\sigma}_{\alpha\beta} c_{R,\beta} \cdot c^\dagger_{R',\gamma} \vec{\sigma}_{\gamma\delta} c_{R',\delta}$$

Spin states $|\text{phys}\rangle = |\uparrow\rangle, |\downarrow\rangle$

Fermion states $|\uparrow\rangle, |\downarrow\rangle, \underbrace{\boxed{|0\rangle, |2 = \uparrow,\downarrow\rangle}}_{|\text{unphys}\rangle}$ $\quad \vec{S}_R |\text{unphys}\rangle = 0$

At any finite T, contribution of **unphysical** states can be *removed exactly* with the help of single **complex chemical potential** μ

$$H \to H_{\text{PF}} = H + \frac{i\pi}{2\beta} \sum_{s=\uparrow,\downarrow} c^\dagger_{R,s} c_{R,s}$$

$$\mu = -\frac{i\pi}{2\beta}$$

Popov Fedotov fermions (JETP 1988)

$$\mathrm{Tr}\ e^{-\beta H_{\mathrm{PF}}} \to \mathrm{Tr}_{\text{the rest}}\left(\mathrm{Tr}_{R,\text{phys}}\ e^{-\beta H_{\mathrm{PF}}} + \mathrm{Tr}_{R,\text{unphys}}\ e^{-\beta H_{\mathrm{PF}}}\right)$$

$$\mathrm{Tr}_{R,\text{unphys}}\ e^{-\beta H_{\mathrm{PF}}} = \ e^{-\beta H_{\mathrm{PF},\neq \mathrm{R}}}\{\langle 0|e^{-i\frac{\pi}{2}\hat{N}_R}|0\rangle + \langle 2|e^{-i\frac{\pi}{2}\hat{N}_R}|2\rangle\}$$
$$\to \{1 + (-1)\} = 0.$$

Obtained standard diagram technique for PF fermions, but with **shifted** Matsubara frequency

$$G = \frac{1}{i\omega_n + \mu} = \frac{1}{i\omega_n - \frac{i\pi}{2\beta}} \quad \text{with} \quad \omega_n - \frac{\pi}{2\beta} = \frac{2\pi}{\beta}(n + \frac{1}{4})$$

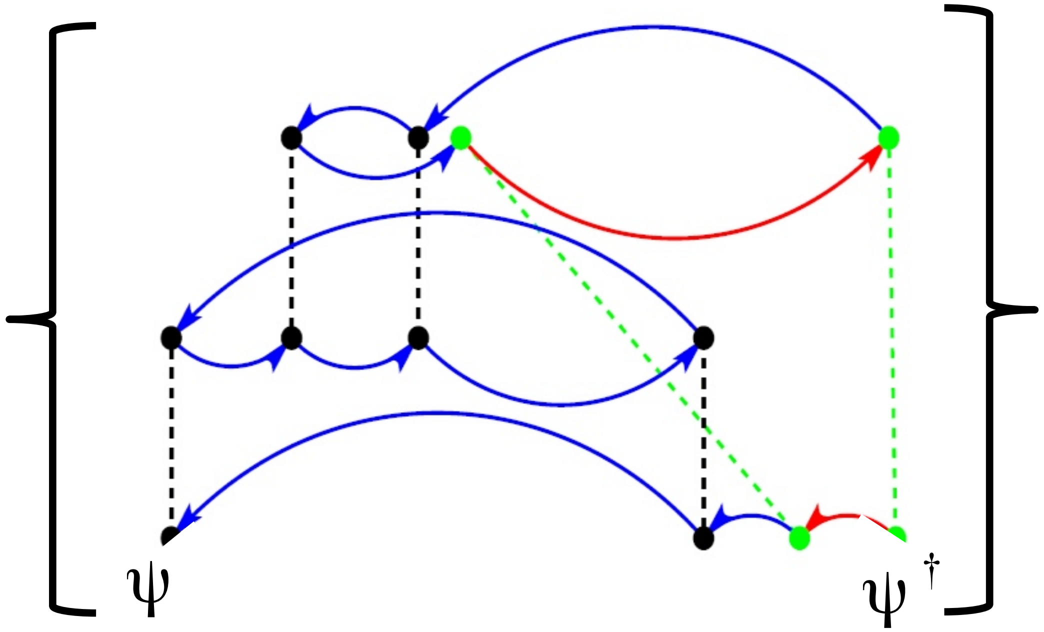
Alternatively, fermions with **semionic** boundary conditions in 'time'

$$\psi_R(\beta) = i\psi_R(0),$$
$$\psi_R^\dagger(\beta) = -i\psi_R^\dagger(0)$$

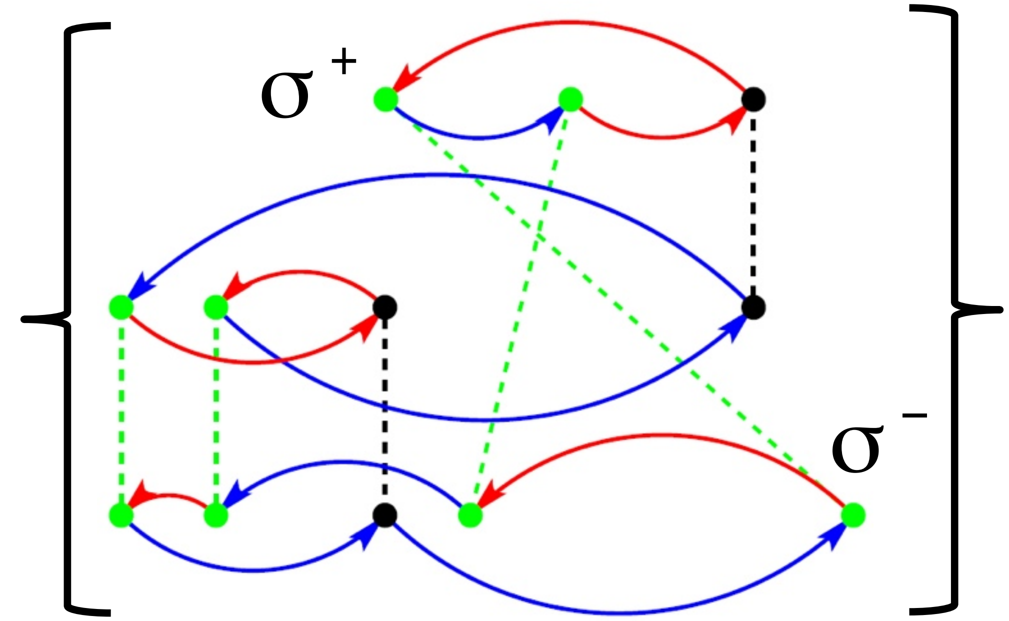
More arguments in Prokof'ev, Svistunov PRB 2011

Standard diagrammatics for interacting fermions starting from the flat band.

$\Sigma =$



$\Pi =$



$$G_\sigma = G_\sigma^{(0)} + G_\sigma^{(0)} \Sigma_\sigma G_\sigma$$

$$U = J - J \Pi U$$

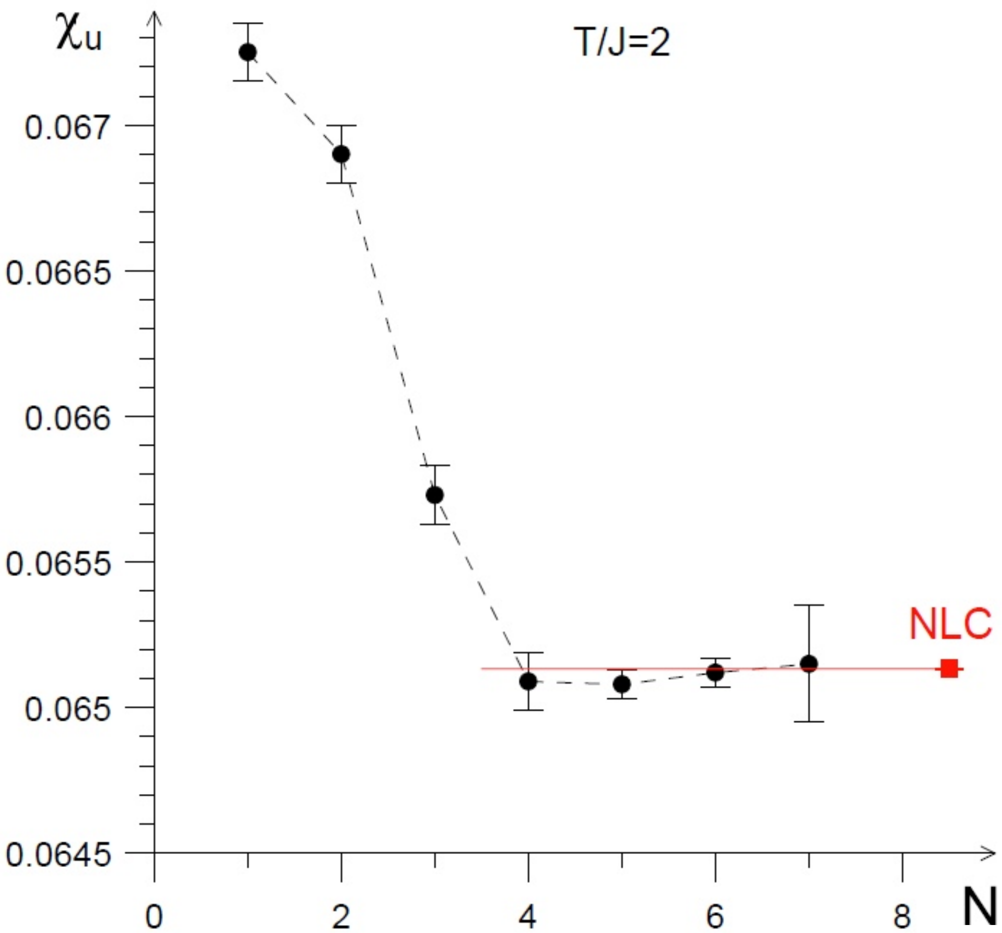
Main quantity of interest is magnetic susceptibility

$$\chi = \left\langle S_0^z(0) S_j^z(\tau) \right\rangle_\omega = \frac{\Pi}{1 - J\Pi}$$

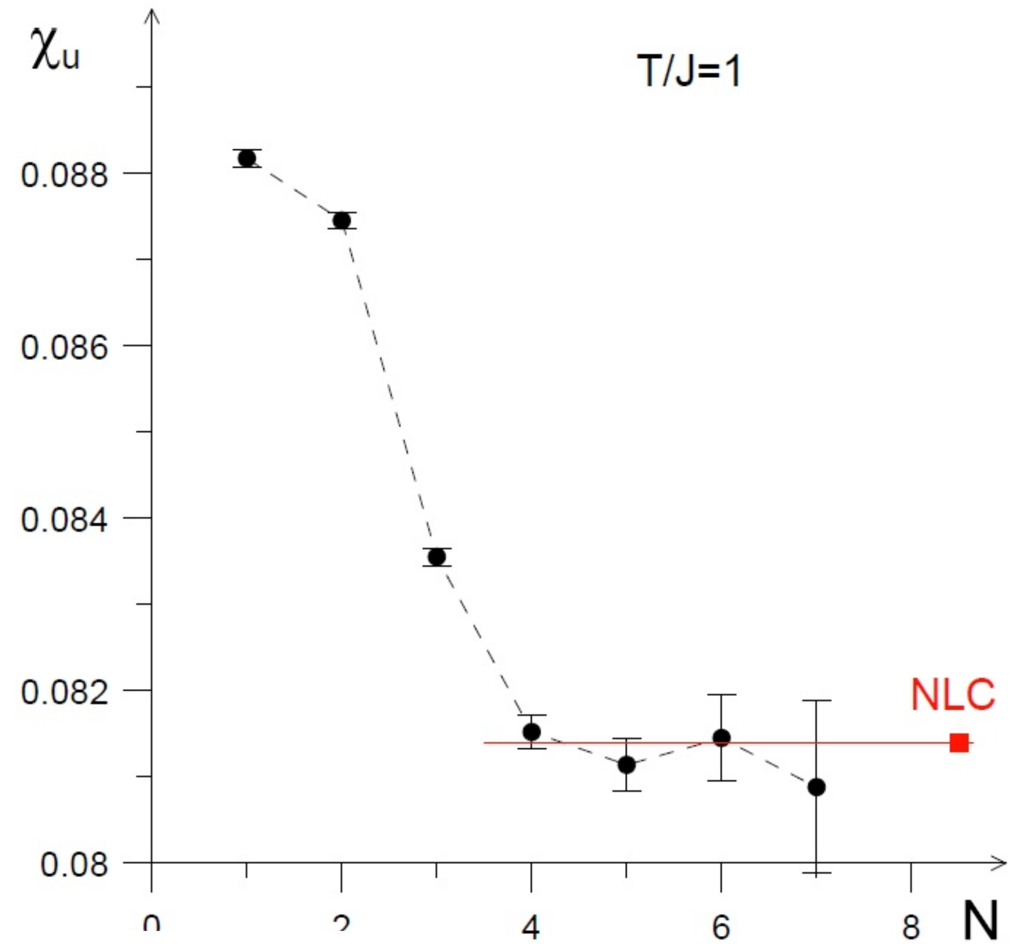
Quantum soup (cooperative paramagnet): not ordered but strongly correlated

$$T / zJ < 1$$

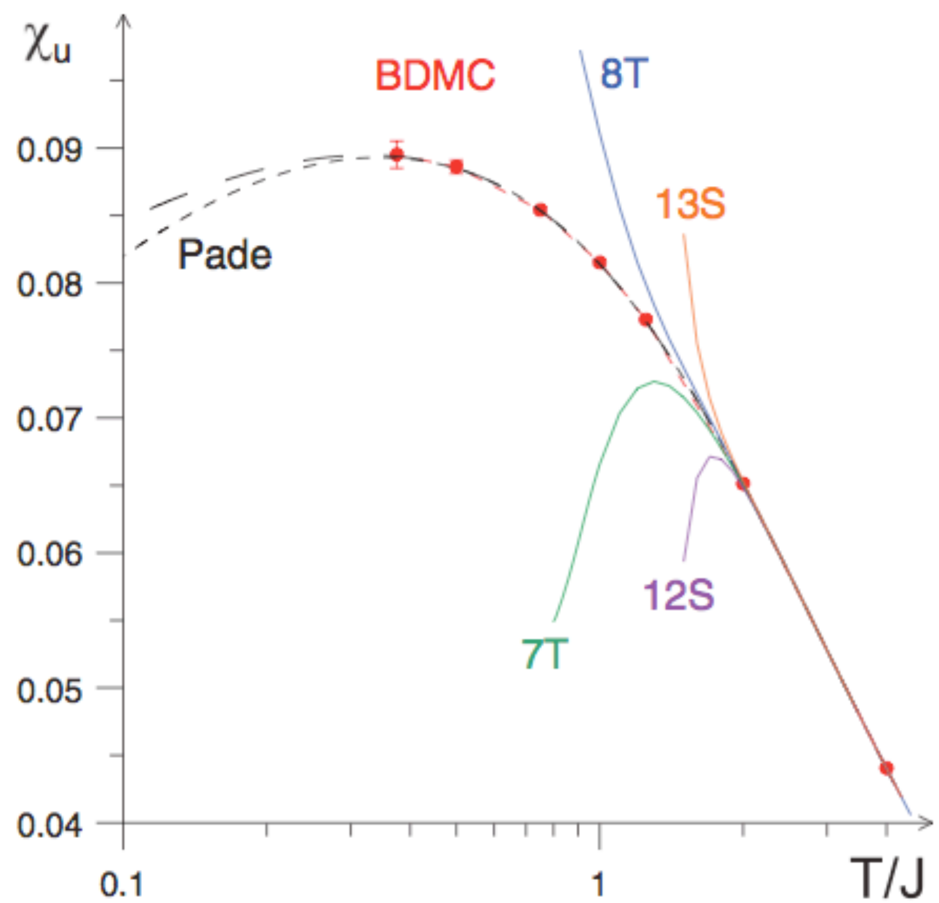
Sign-blessing (cancellation of high-order diagrams)

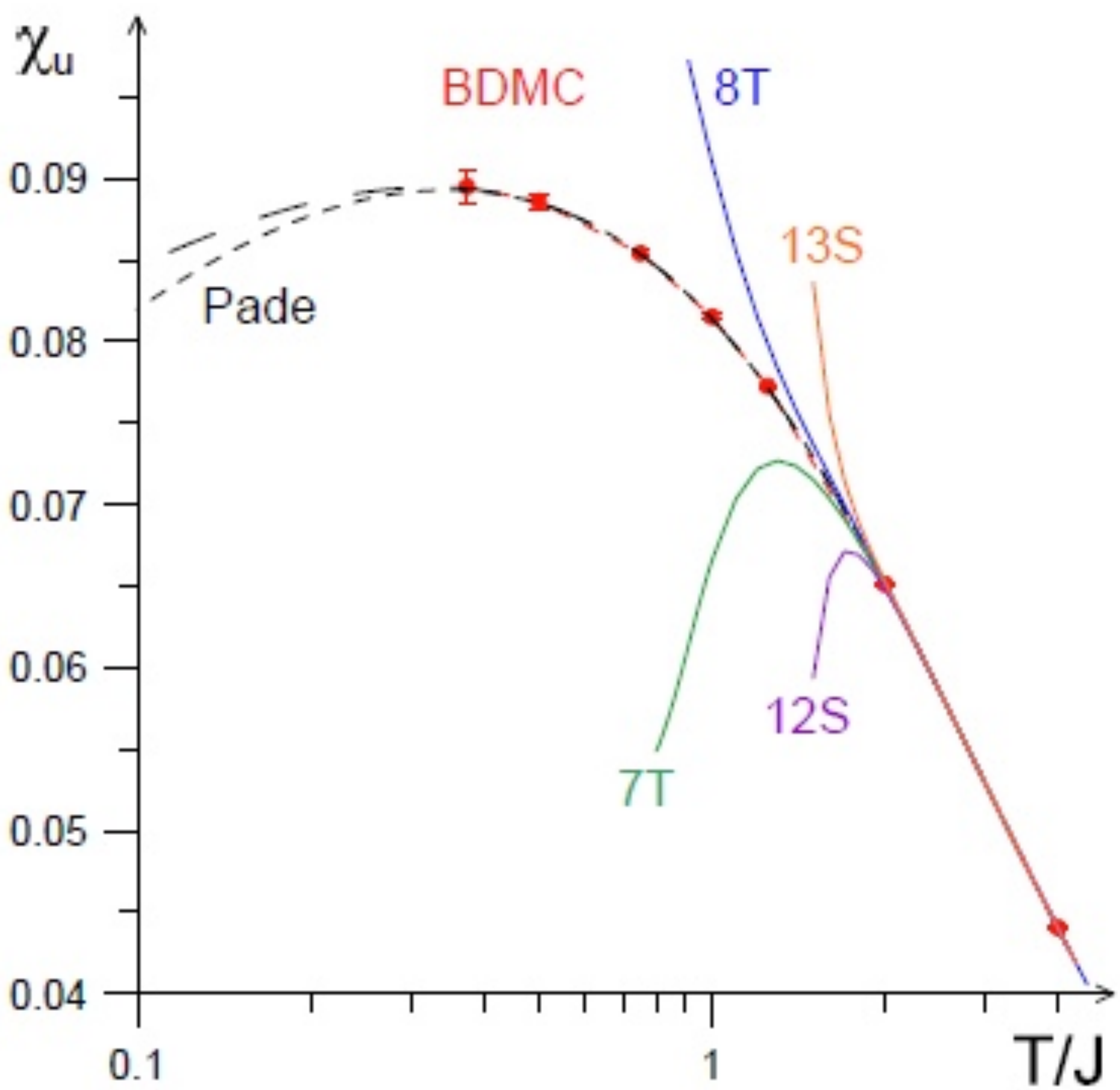


113824
7-th order
diagrams
cancel out!

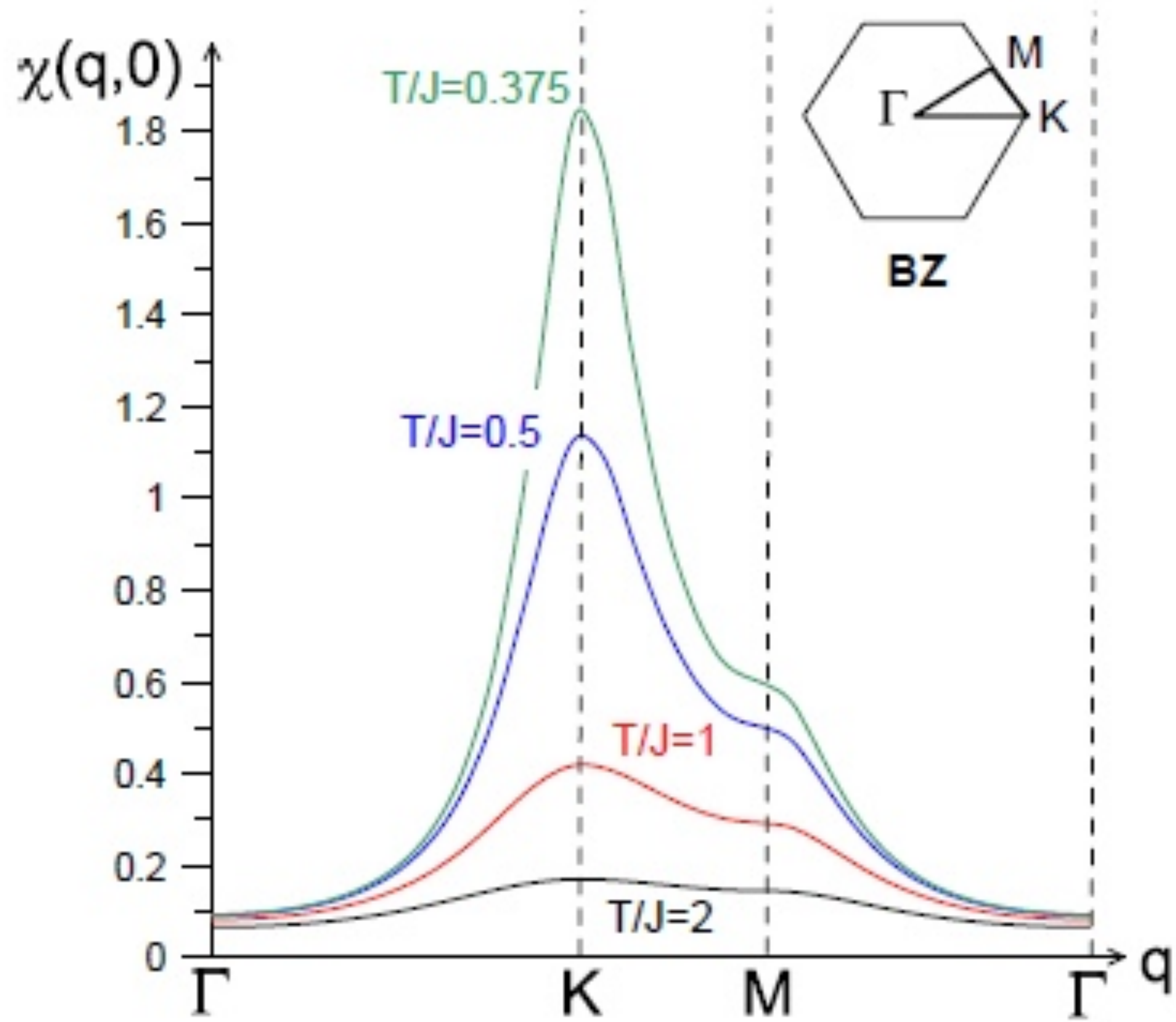


High-temperature
series expansions
(sites or clusters,
Rigol, Bryant, Singh 2007)
vs BDMC





Uniform susceptibility $\chi(q=0) = \dfrac{\partial M(h=0)}{\partial h}$



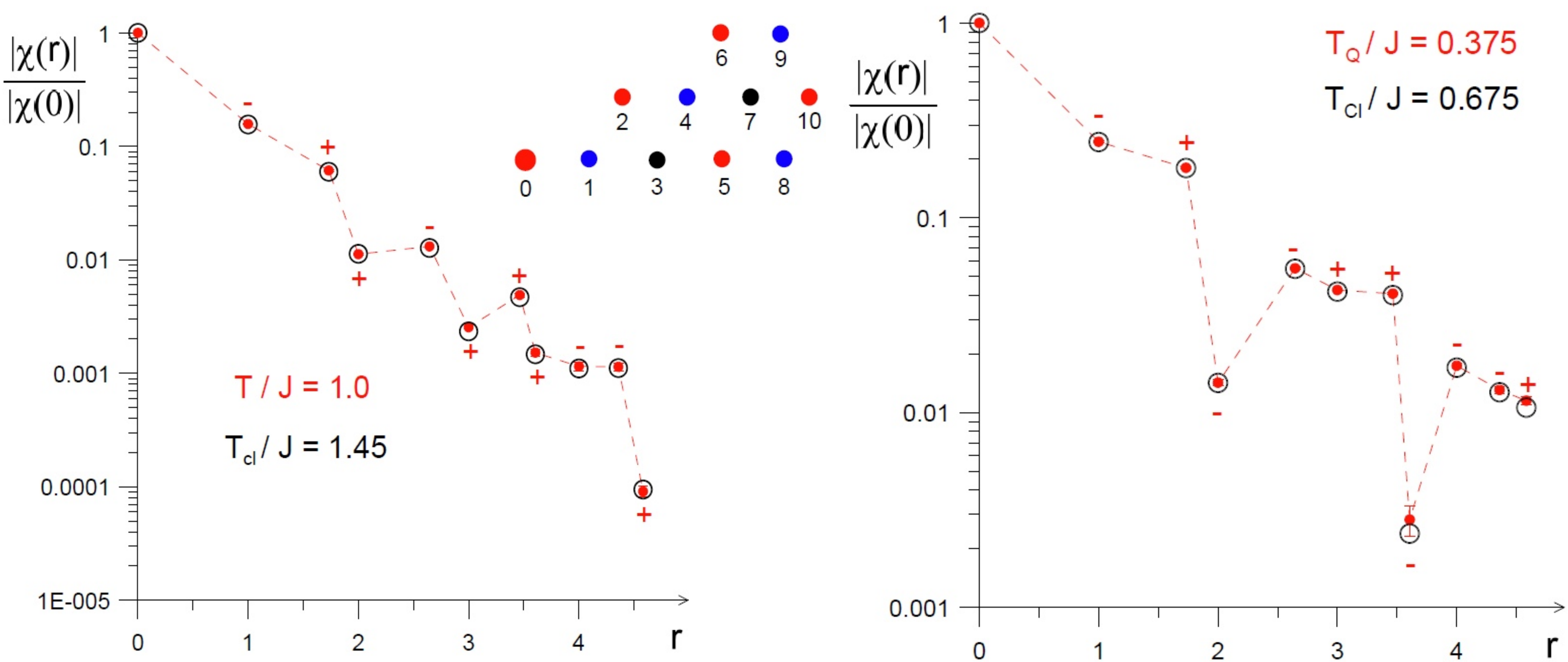
Static susceptibility $\chi(\mathbf{q}, \omega_n = 0)$
measures ordering tendency
at momentum **q**
[series expansion cannot access
finite **q**]

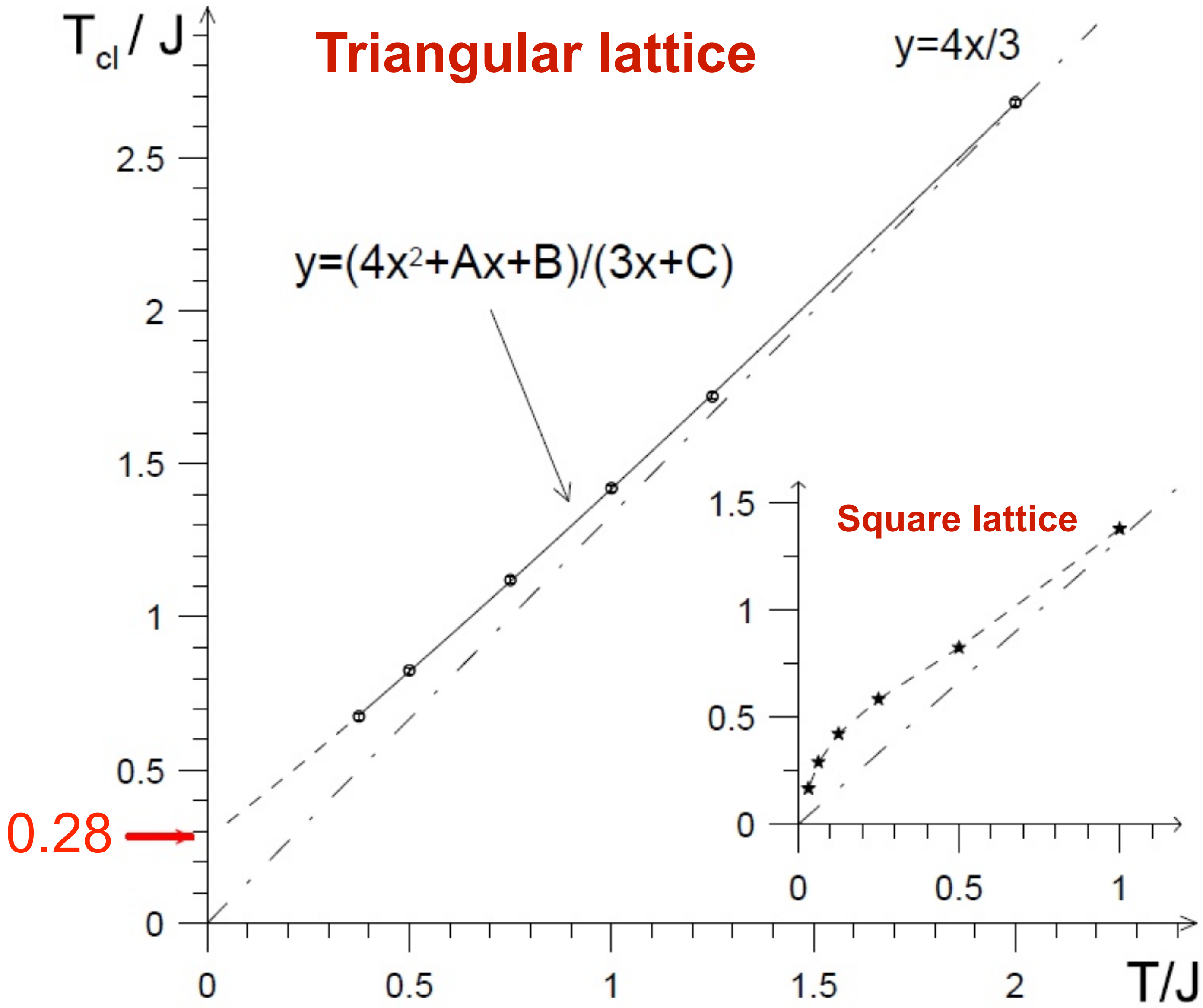
Quantum-to-classical (QCC) correspondence for static response:

Quantum $\chi(q,T)$ is the same as classical $\chi(q,T_{cl})$ for some $T_{cl}(T)$ (relative accuracy of 1%)

(this correspondence also takes place for the square lattice with relative accuracy 0.3% at all T)

$$\chi(\mathbf{r},\omega=0)=\int_0^{1/T} d\tau \langle S_0^z(0) S_{\mathbf{r}}^z(\tau)\rangle$$





QCC, if confirmed, implies (in 2D):

1. If $T_{cl}(T=0) \neq 0$ then the quantum ground state is disordered, i.e. it is a spin liquid

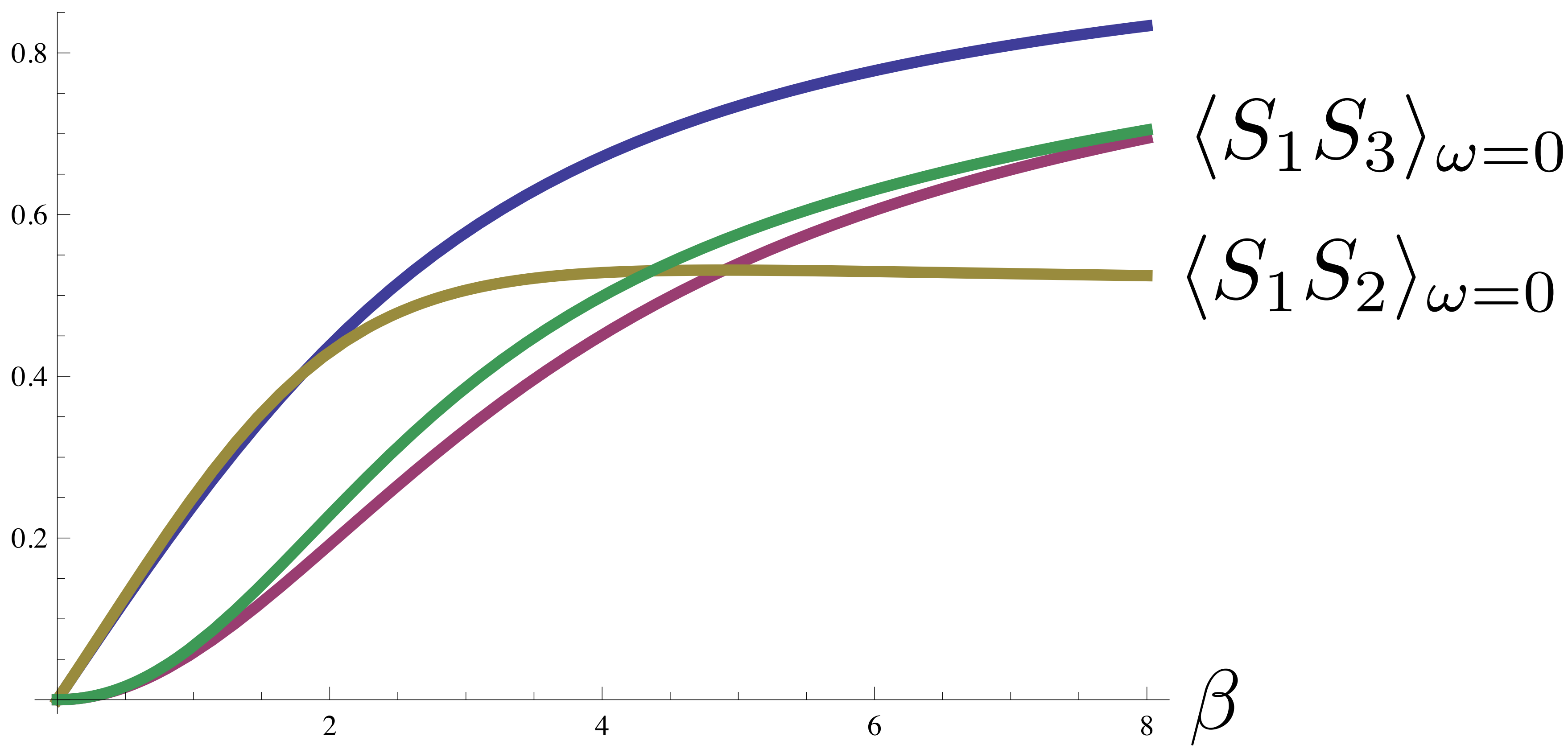
2. If the classical ground state is disordered (macro degeneracy) then the quantum ground state is a spin liquid
   Example: Kagome antiferromagnet

Efficient tool in the search for spin liquids

Triangular lattice: Naive extrapolation suggests: T_{cl} = 0.28 J for T_q=0.
This coincides with a crossover, at T_v = 0.285 J, from high-T Z_2-vortex dominated regime to low-T spin-fluctuation dominated regime ["spin-gel" state, Kawamura (2010)].
Square lattice: $T_{cl}(T)$ turns around at low T so that T_{cl} = 0 for T_q=0. Thus both models, classical and quantum, predict ordered magnetic state (as they should).

Triangular AFM: Low-T regime is not reached yet

3 spin "chain": QCC is not the law of nature



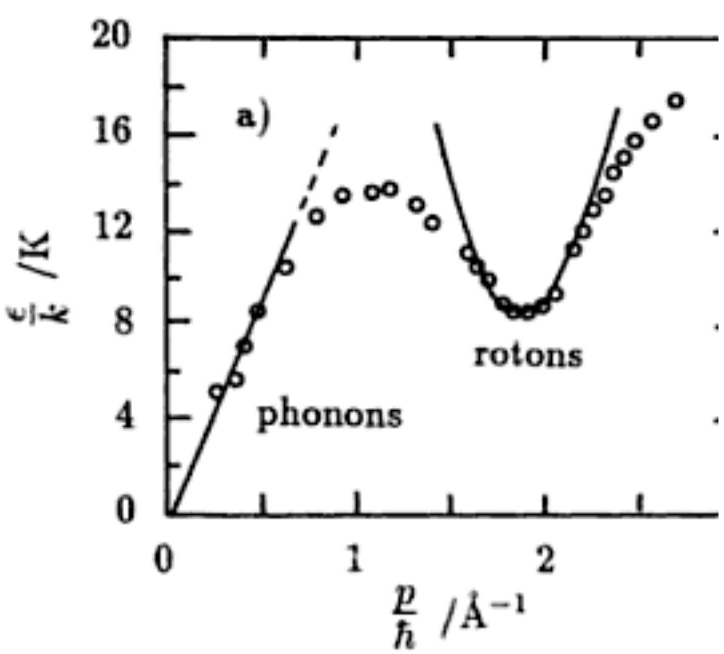
Quantum-Classical correspondence is a result of **approximate** extended high-T scaling

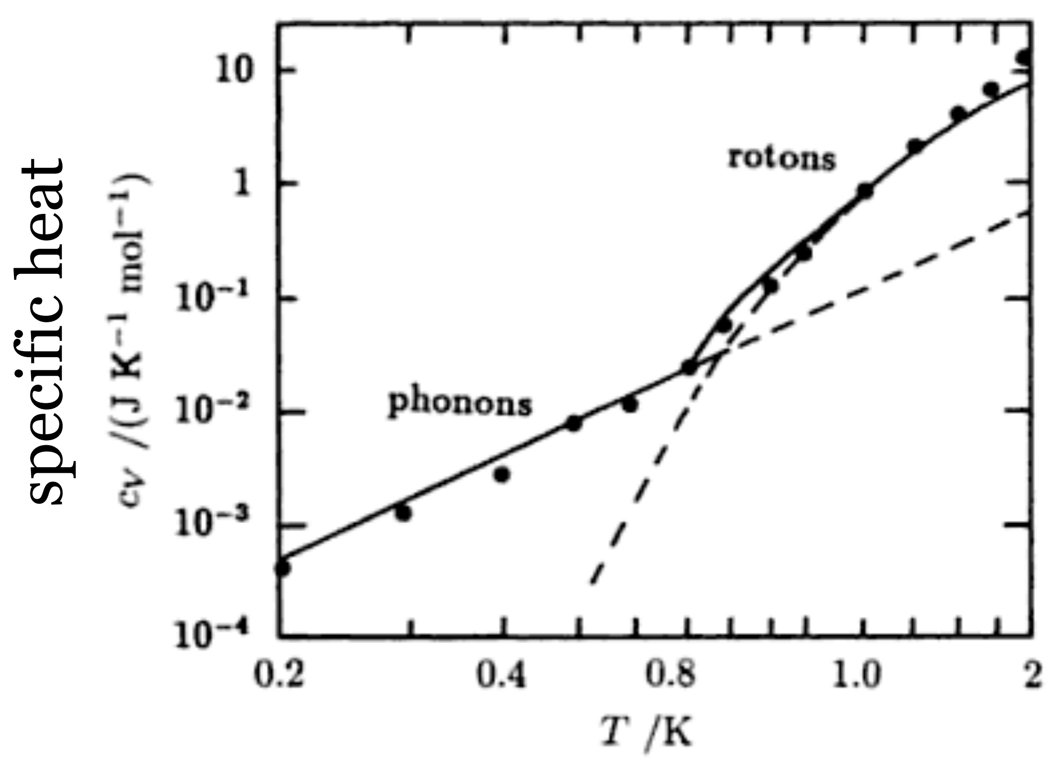
$$\langle S_1 S_n \rangle_{\text{classical}} = \left(\coth[\frac{3\beta}{4}] - \frac{4}{3\beta} \right)^{n-1} \to (\beta/4)^{n-1}$$

[also, 5σ deviations on a square lattice]

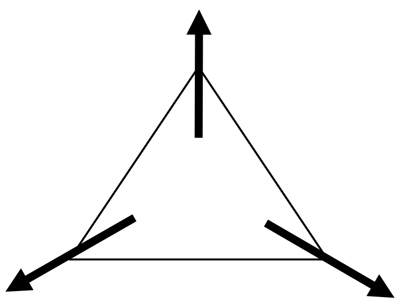
Possible reason for strongly delayed universal (field-theoretical) scaling limit?

- Non-universal "roton" [almost **flat** band] regime due to non-collinear short-range spin order
- Strong quantum renormalization of the dispersion (specific no non-collinear short-range order) leads to strong enhancement of the density of states at ~ J
- Strong similarity with He II: high-energy rotons (with $\varepsilon_{min} = \Delta = 8.6$ K) control thermodynamics down to T = 1 K [this is large density of states effect].





The minimal explanation: non-collinear spin structure is the key!



- Rotated basis: order along S^z (via rotation about S^x)

$$H = \sum_{ij} \underbrace{-\frac{1}{2}(S_i^z S_j^z + S_i^y S_j^y) + S_i^x S_j^x}_{H_{coll}} + \underbrace{\sin[\phi_i - \phi_j](S_i^z S_j^y - S_i^y S_j^z)}_{H_{non\text{-}coll}}$$

H_{coll} collinear piece: 2, 4, 6…magnons
(1, S^{-1}, S^{-2} terms)

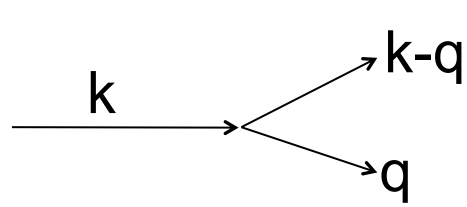
$H_{non\text{-}coll}$ non-collinear piece: 3, 5, … magnons
($S^{-1/2}$, $S^{-3/2}$ terms)

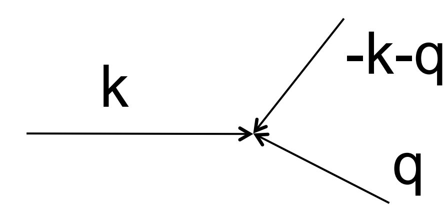
$\phi_i = \{0, 2\pi/3, 4\pi/3\}$ [angle w.r.t. fixed direction]

Spin wave expansion: S >> 1

$$S^z = S - a^\dagger a \ , \ S^x = \sqrt{\frac{S}{2}}(a^\dagger + a) \ , \ S^y = i\sqrt{\frac{S}{2}}(a^\dagger - a)$$

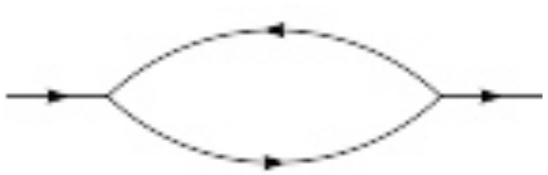
- $H_{non\text{-}coll}$ describes magnon decay (a a^+ a^+) and creation/annihilation (a a a + h.c.)





Absent in collinear AFM (where $\phi_i = 0, \pi$)

✓ *Similar to anharmonic phonons and He⁴*



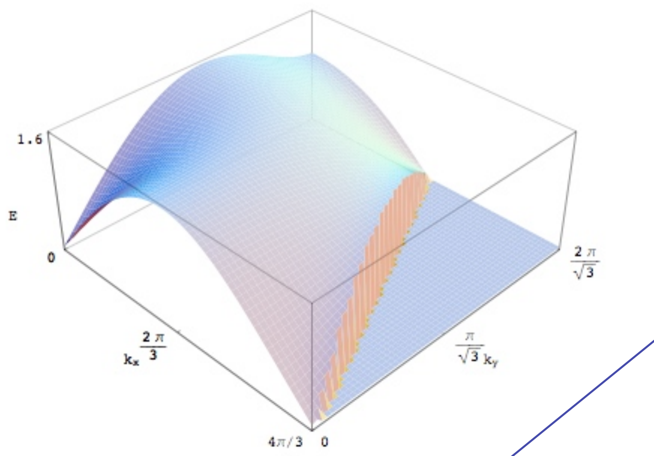
- Produces 1/S (!) correction to magnon spectrum: renormalization + lifetime

[Square lattice: corrections only at $1/S^2$ order, numerically small]

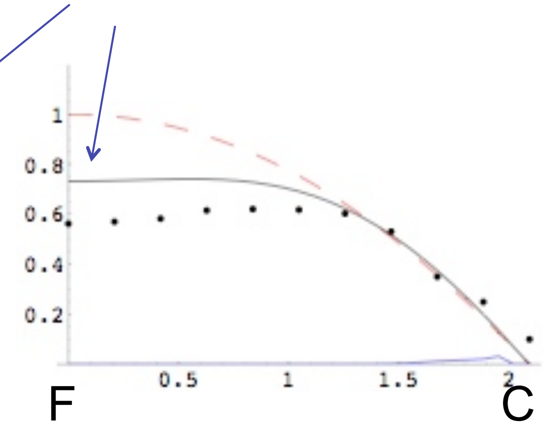
Results: 1/S corrections are HUGE

(shown in 1/4 of the Brillouin zone)

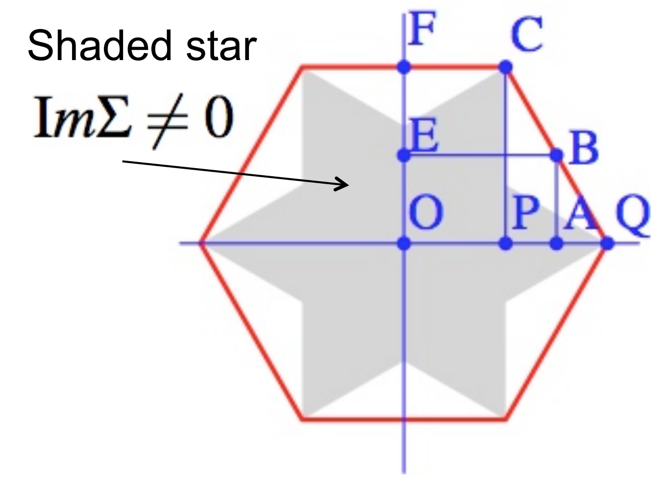
Bare dispersion



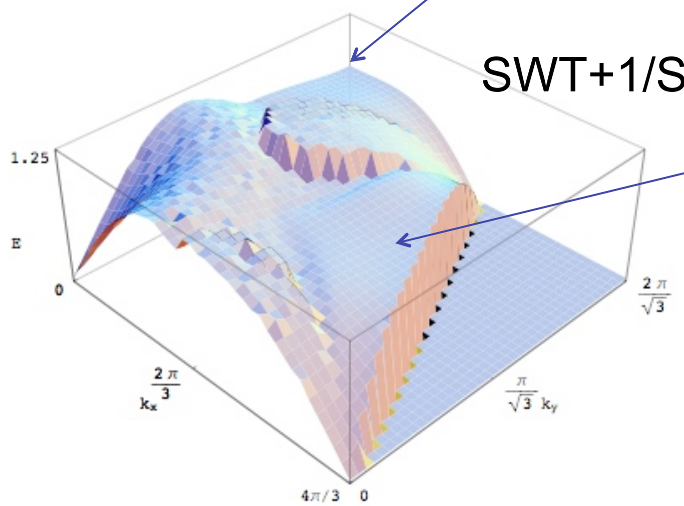
"Roton" minimum



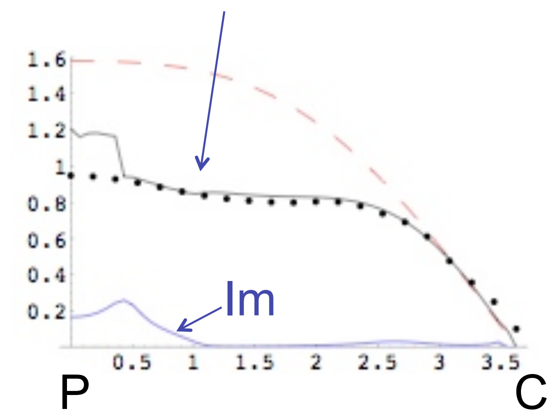
Im part (lifetime)

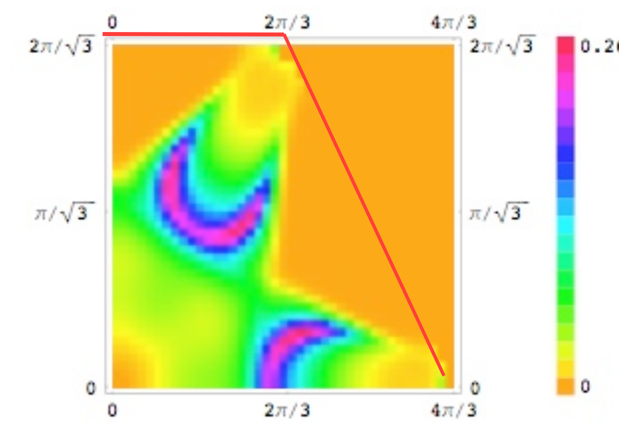


SWT+1/S



Flat dispersion

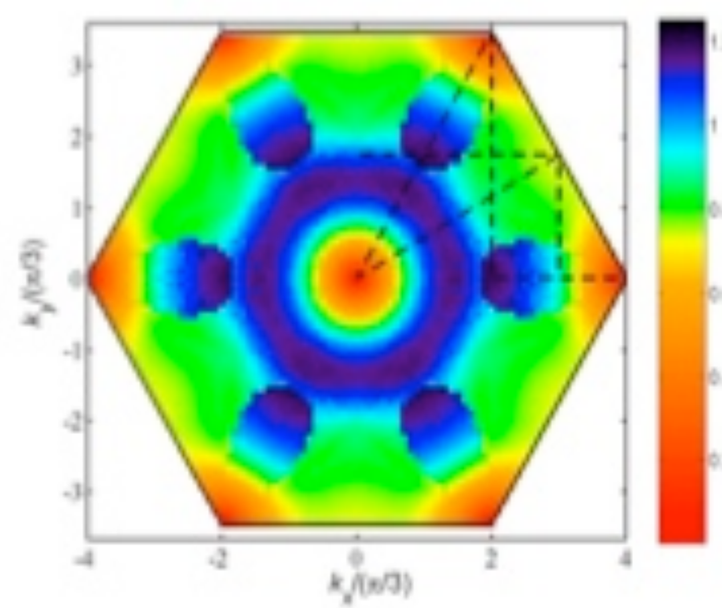




Renormalized dispersion,
with 1/S correction

Semi-quantitative agreement with sophisticated series expansion technique with *no adjustable parameters* (except for S=1/2).

- "rotons" are part of global renormalization (weak local minimum)
- large regions of (almost) flat dispersion;
- finite lifetime [not present in numerics].

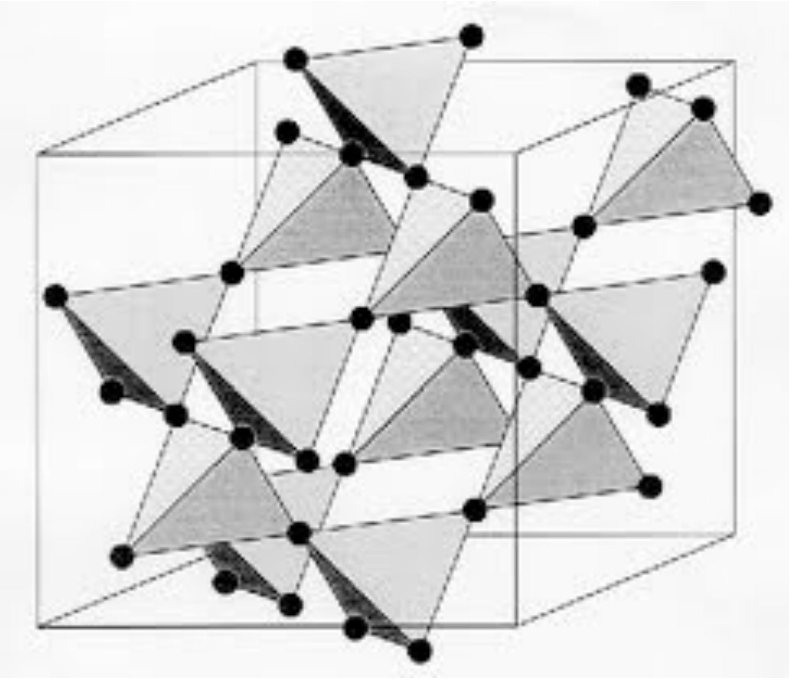


OS, Chubukov, Abanov 2006; Numerics (dots) - Zheng et al, 2006

Conclusions

- We need (**k**, ω) BDMC results at finite T for the ***retarded*** spin susceptibility $\chi(\mathbf{k}, \omega)$

- Apply to strongly frustrated 3D systems: s=½ pyrochlore antiferromagnet



disordered classically.
quantum model - not known.
expect $\xi \sim 1/T$, hence
no slowing down due to incipient ordering

A puzzling coincidence

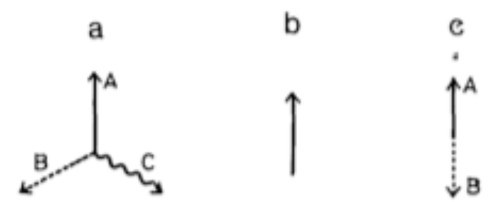


Fig. 1. Order parameter of the Heisenberg antiferromagnet on the triangular lattice (a), the Heisenberg ferromagnet (b) and the antiferromagnet on the bipartite lattice (c). Symbols A-C represent each sublattice of the original lattice.

Journal of the Physical Society of Japan
Vol. 53, No. 12, December, 1984, pp. 4138–4154

Phase Transition of the Two-Dimensional Heisenberg Antiferromagnet on the Triangular Lattice

Hikaru KAWAMURA and Seiji MIYASHITA†

order parameter space = that of rigid body = SO(3)

$$\Pi_1(\mathrm{SO}(3)) = Z_2$$

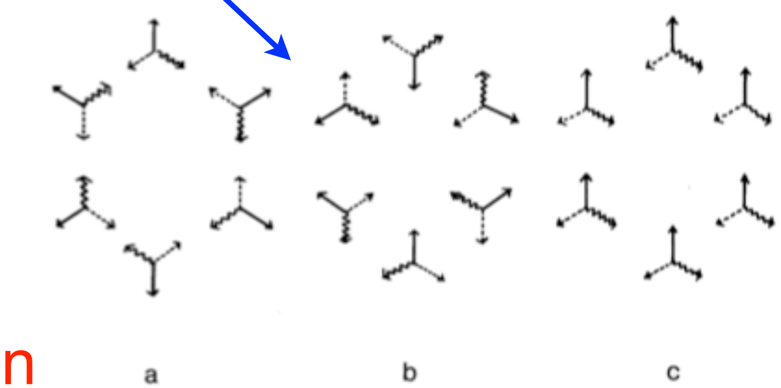
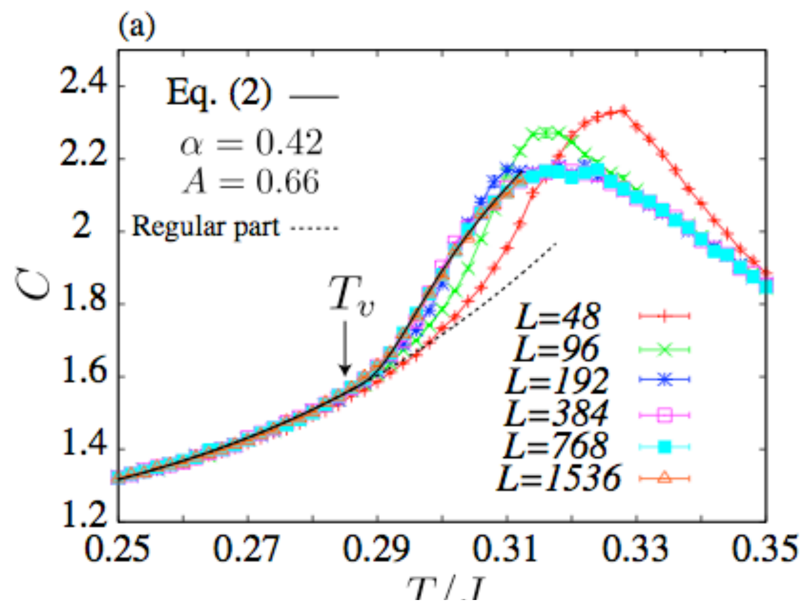


Fig. 2. An example of vortex configuration. Configuration (a) can be continuously transformed into (b) and vice versa, but neither (a) nor (b) can be continuously transformed into (c). The chirality vector defined by (2.2) is perpendicular to the plane of the page for all configurations.

Z_2 vortex binding transition

$T_v = 0.285$ J



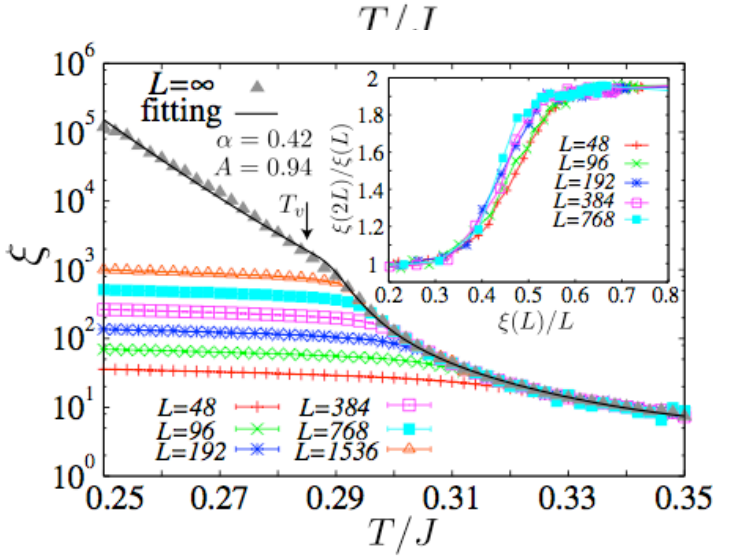
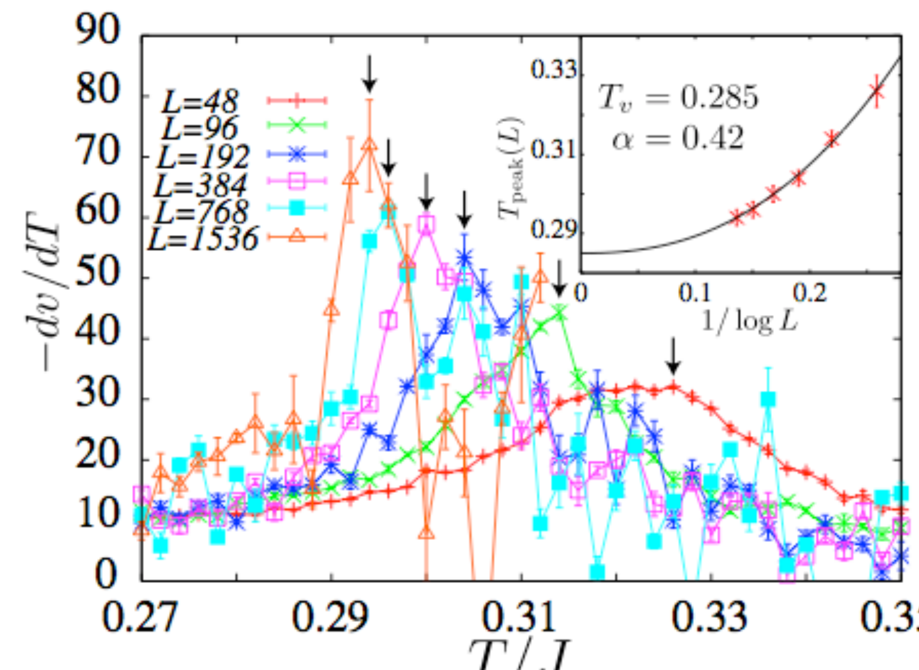


Fig. 2. (Color online) Temperature dependence of the finite-size spin correlation length, together with the bulk one. The inset is a scaling plot, i.e., ξ_{2L}/ξ_L plotted vs ξ_L/L.



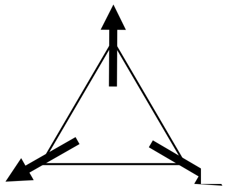
(T-derivative of) vorticity modulus, Kawamura, Yamamoto, Okubo 2010

PRL 96, 057201 (2006) PHYSICAL REVIEW LETTERS week ending 10 FEBRUARY 2006

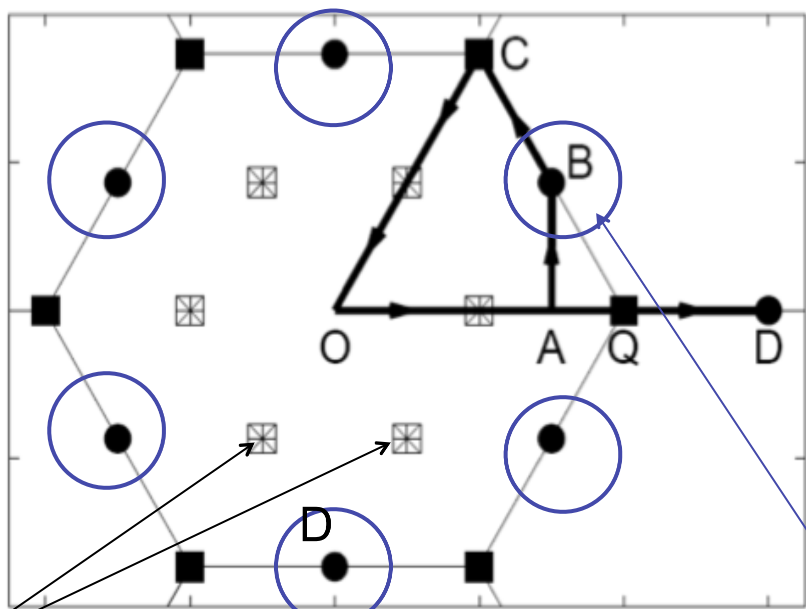
Anomalous Excitation Spectra of Frustrated Quantum Antiferromagnets

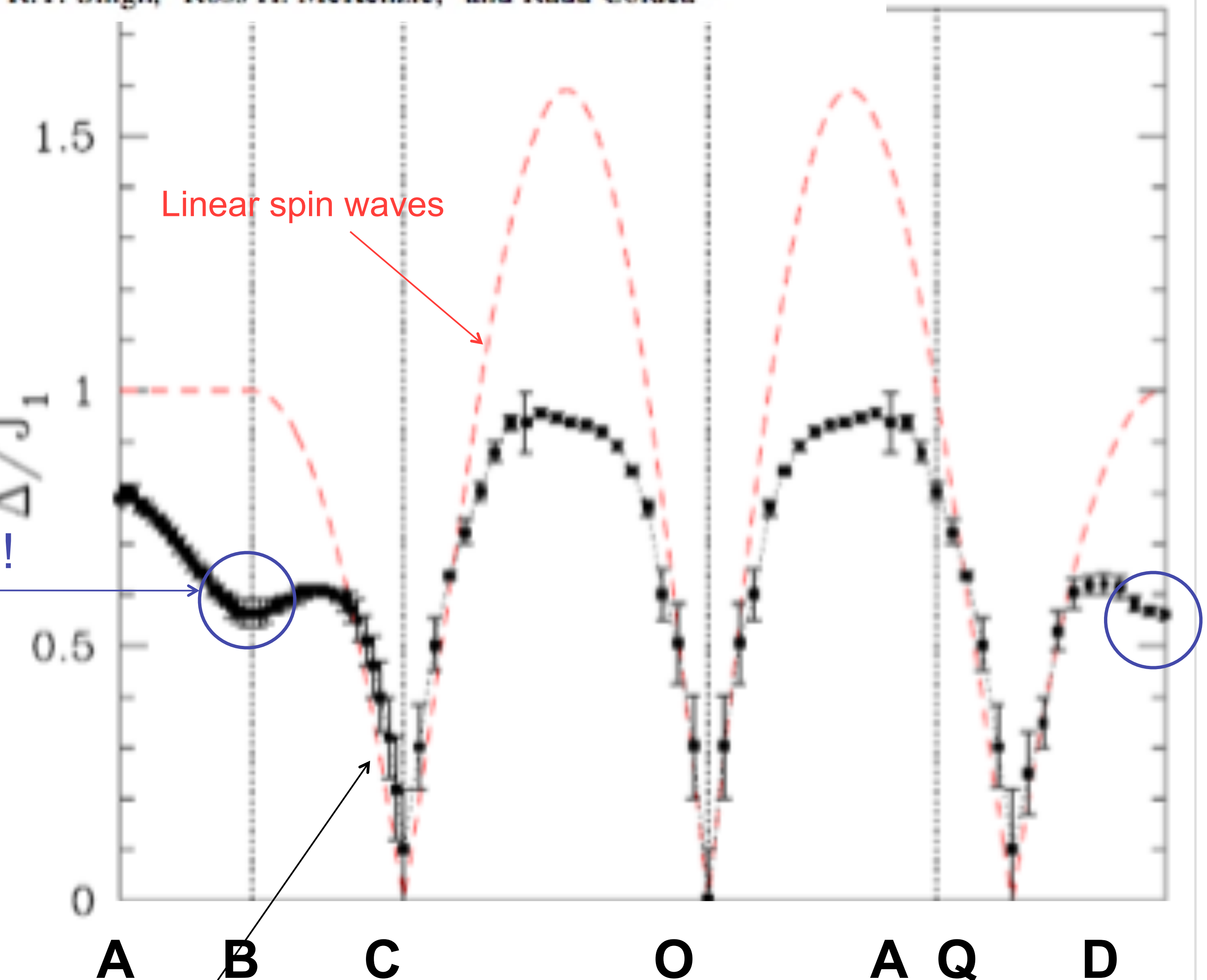
Weihong Zheng,[1] John O. Fjærestad,[2] Rajiv R. P. Singh,[3] Ross H. McKenzie,[2] and Radu Coldea[4]

S=½ data



Brillouin zone:



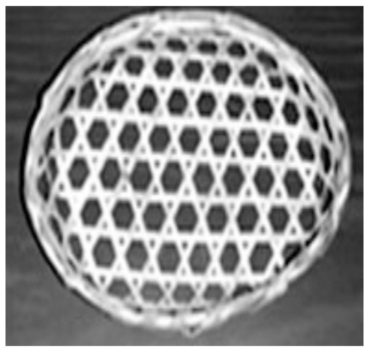


Dots: Series expansion for S=1/2 antiferromagnet

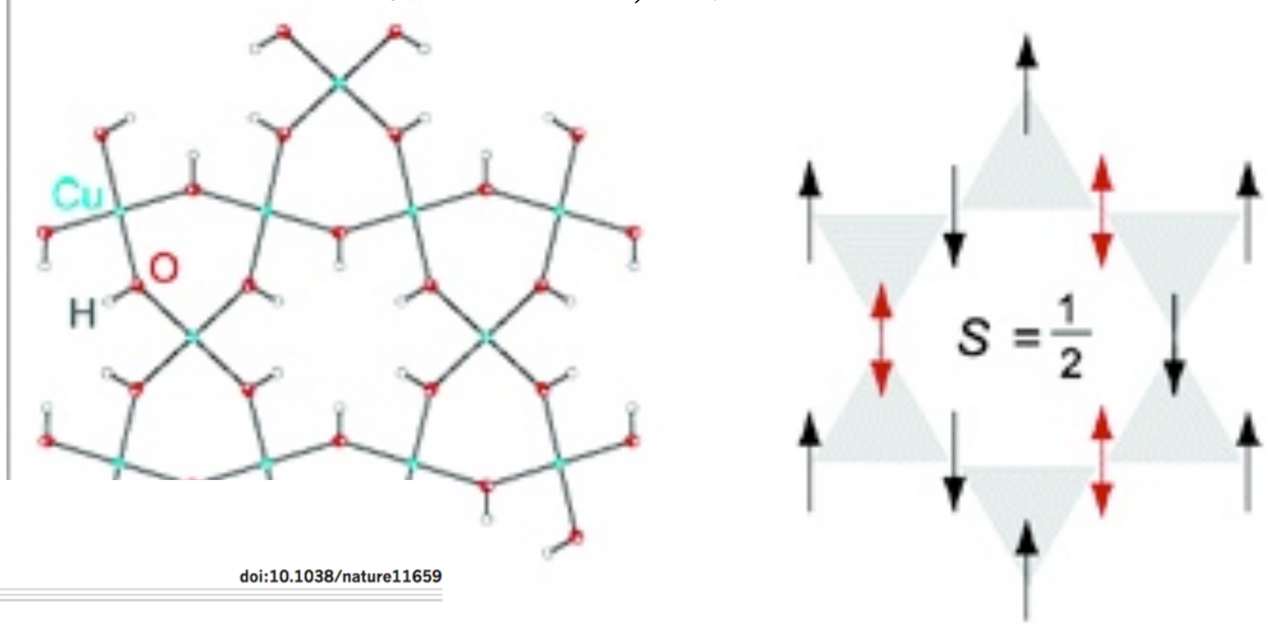
✳ Series expansion: ***Huge*** renormalization of the dispersion for s=½ antiferromagnet. (*Note*: cannot probe finite lifetime.)

★ Agrees in details with the leading 1/S spin wave renormalization of the dispersion.

Structurally perfect S=1/2 Kagome antiferromagnets: Herbersmithite $ZnCu_3(OH)_6Cl_2$ and spatially anisotropic Volborthite $Cu_3V_2O_7(OH)_2\,2H_2O$

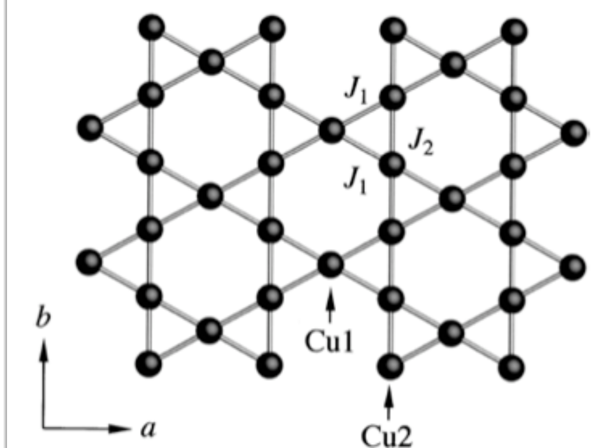


θ_{cw} =-300K, T_N<0.05K



Shores et al 2005

θ_{cw}=-115K, T_N<1.8K



Hiroi et al 2001

LETTER

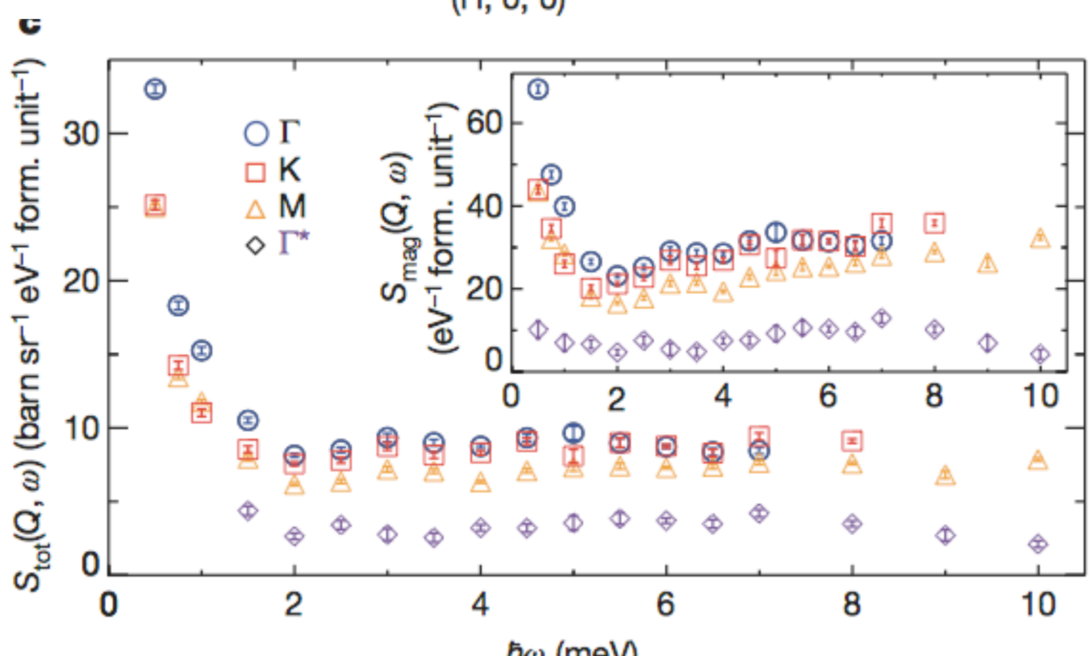
doi:10.1038/nature11659

Fractionalized excitations in the spin-liquid state of a kagome-lattice antiferromagnet

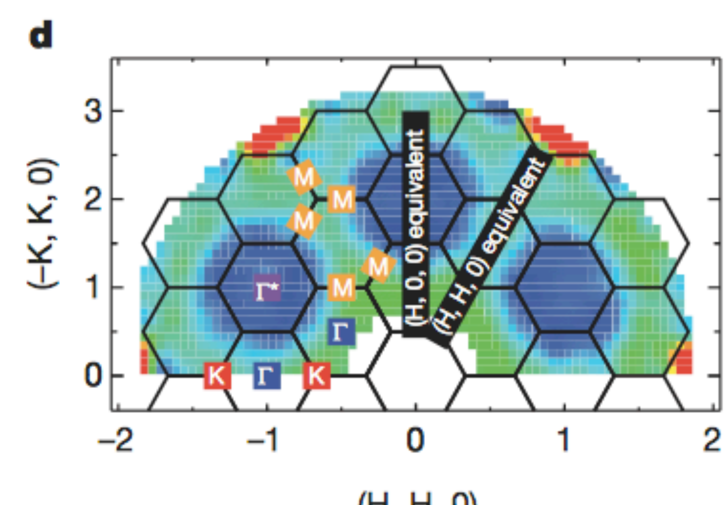
Tian-Heng Han[1], Joel S. Helton[2], Shaoyan Chu[3], Daniel G. Nocera[4], Jose A. Rodriguez-Rivera[2,5], Collin Broholm[2,6] & Young S. Lee[1]

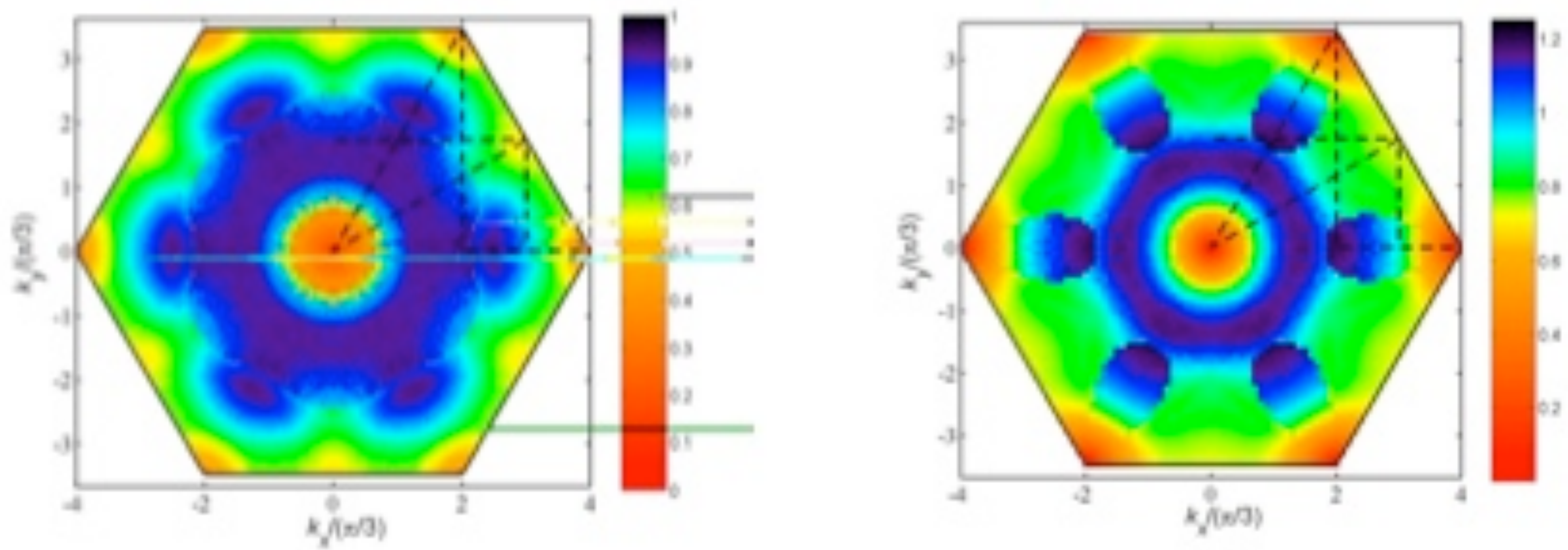
Han et al, Nature 2012

(H, 0, 0)



(H, H, 0)





k_y/(π/3)
k_x/(π/3)