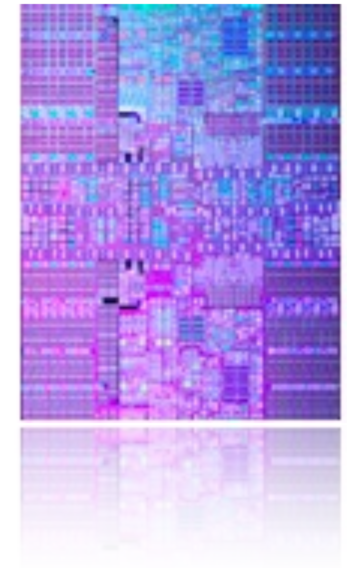
$$\mathcal{H}|\psi\rangle = E|\psi\rangle$$



# Introduction to Exact Diagonalization & Applications


Andreas Läuchli,
“New states of quantum matter”
MPI für Physik komplexer Systeme - Dresden

http://www.pks.mpg.de/~aml
aml@pks.mpg.de

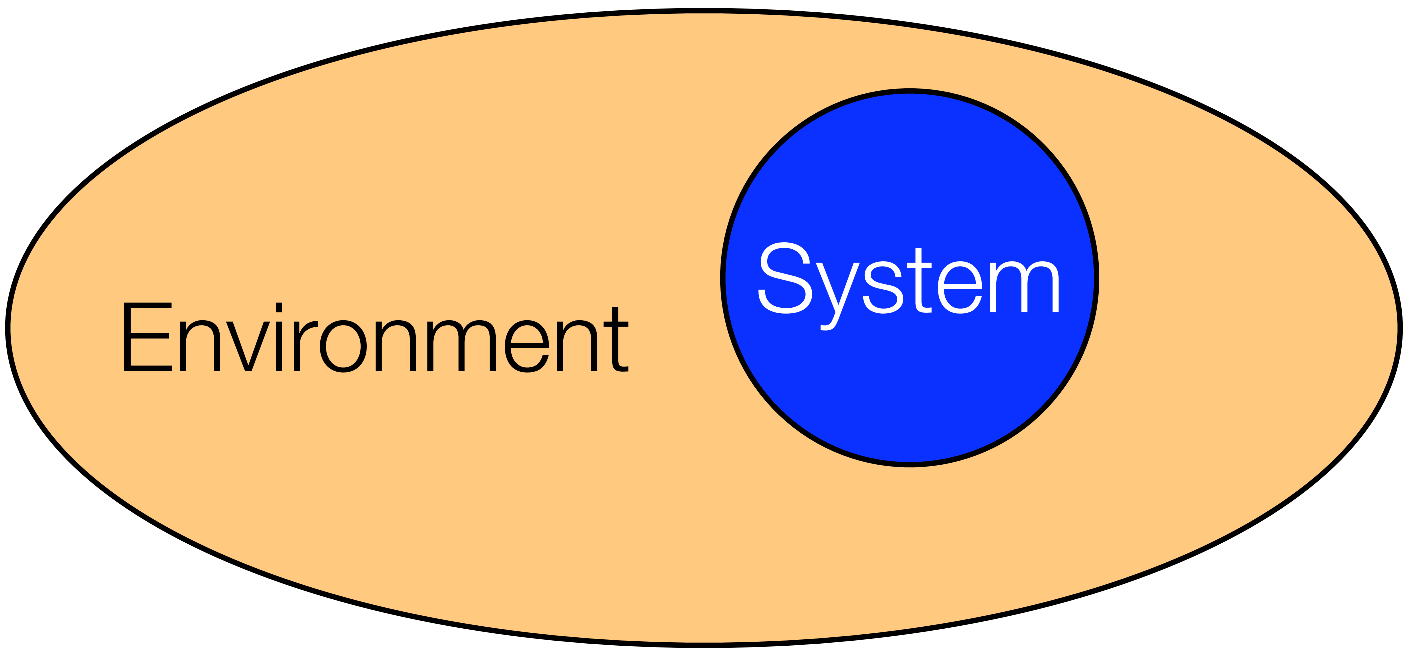

Boulder Summer School 2010 - Boulder - 15/7/2010

# Exact Diagonalization: Applications

- Quantum Magnets: nature of novel phases, critical points in 1D, dynamical correlation functions in 1D & 2D
- Fermionic models (Hubbard/t-J): gaps, pairing properties, correlation exponents, etc
- Fractional Quantum Hall states: energy gaps, overlap with model states, entanglement spectra
- Quantum dimer models or other constrained models (anyon chain..)
- Full Configuration Interaction in Quantum Chemistry

# (Topological) Entanglement Entropy

- Let us look at reduced density matrices, and their entanglement entropies




$$\rho = \mathrm{Tr}_E |\psi\rangle\langle\psi|$$

$$S(\rho) = \mathrm{Tr}[-\rho \log \rho]$$

For topologically ordered phases:

Area Law

$$S(\rho) = \boxed{\alpha L} - \boxed{\gamma} + \cdots$$

Topological entanglement entropy

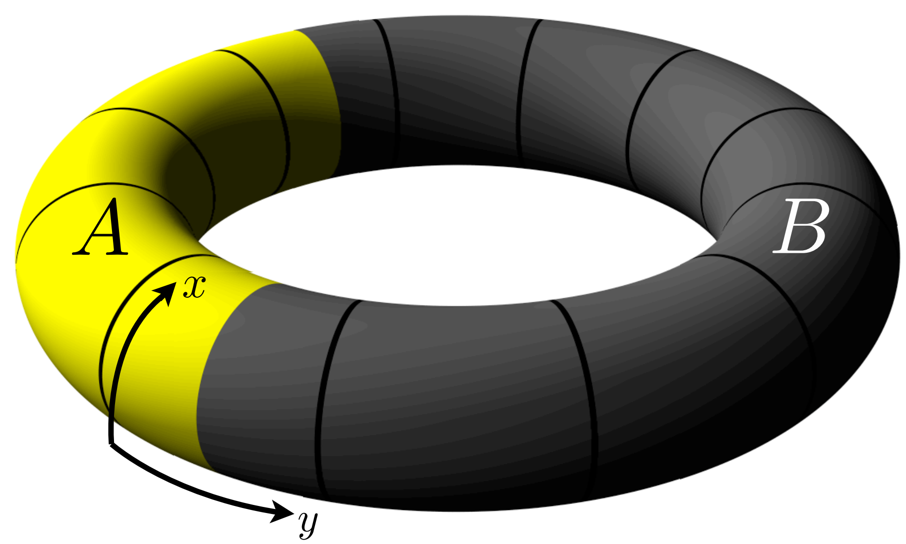
$$\gamma = \log \mathcal{D}$$

$\mathcal{D}$ Total quantum dimension

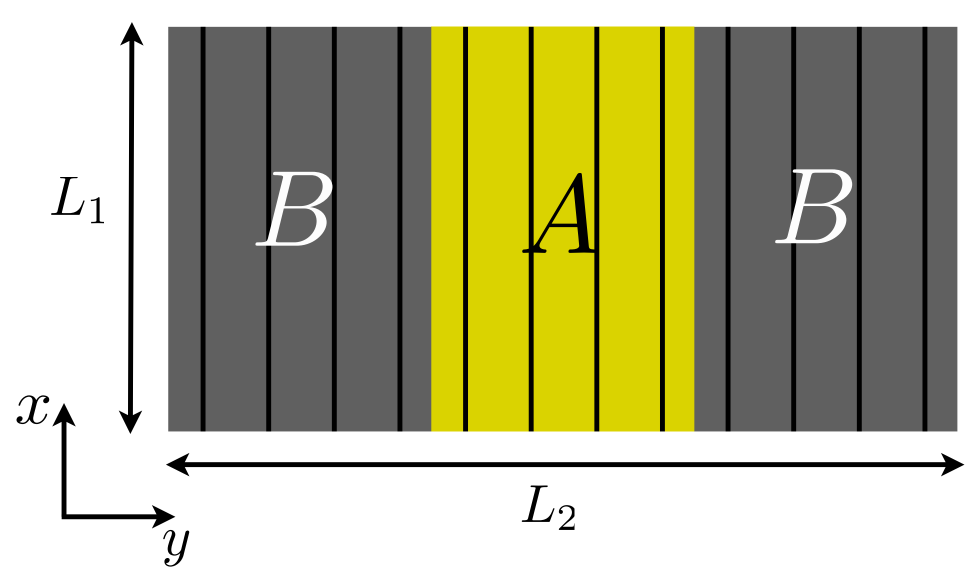
Kitaev & Preskill PRL '06
Levin & Wen PRL '06

# Fractional QH states on the torus

- The torus can be tuned continuously by varying $L_1$ and $L_2$ ($L_1 L_2 = 2\pi N_s$).

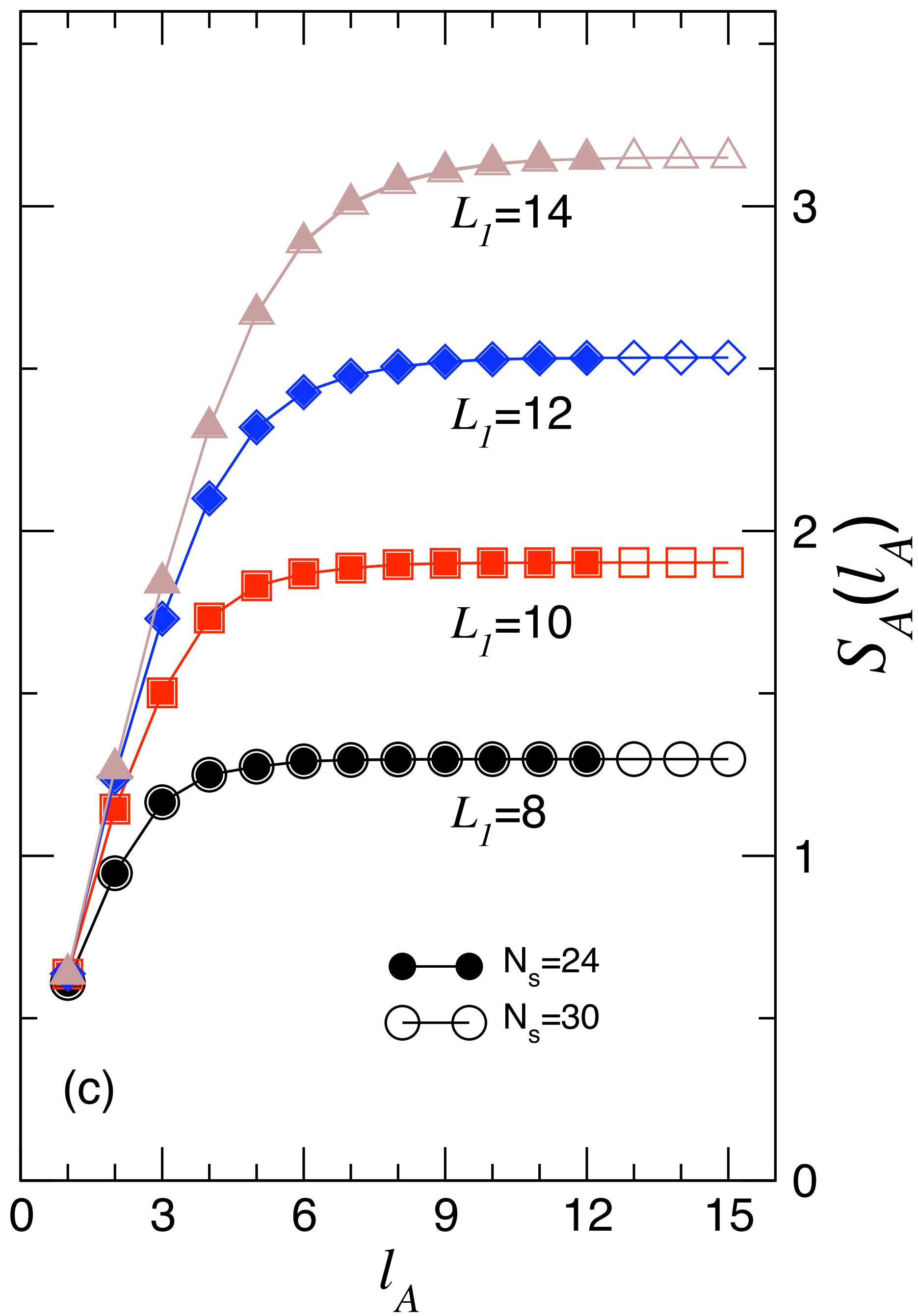


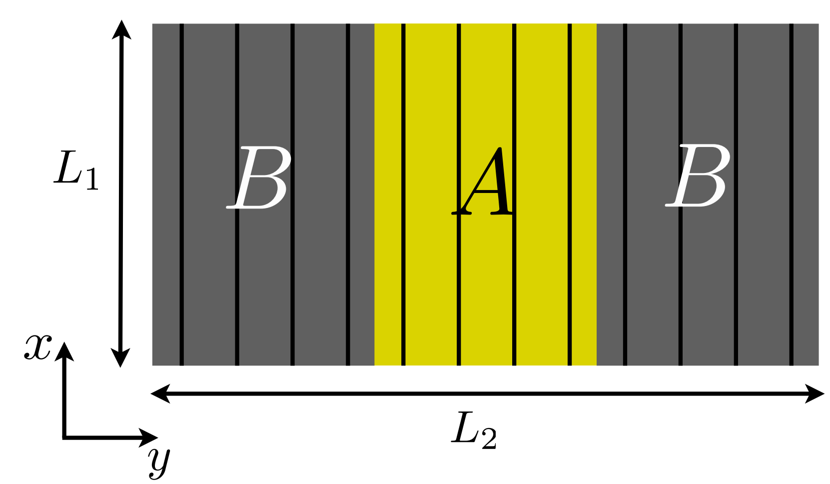

- We study orbital partitioning, which is expected to correspond to real space partitioning



# Area law at constant $L_1$ ($\nu$=1/3 Laughlin)

- Increasing $N_s$ (and thus $L_2$) at constant $L_1$ ⇒ Saturation at large $l_A$

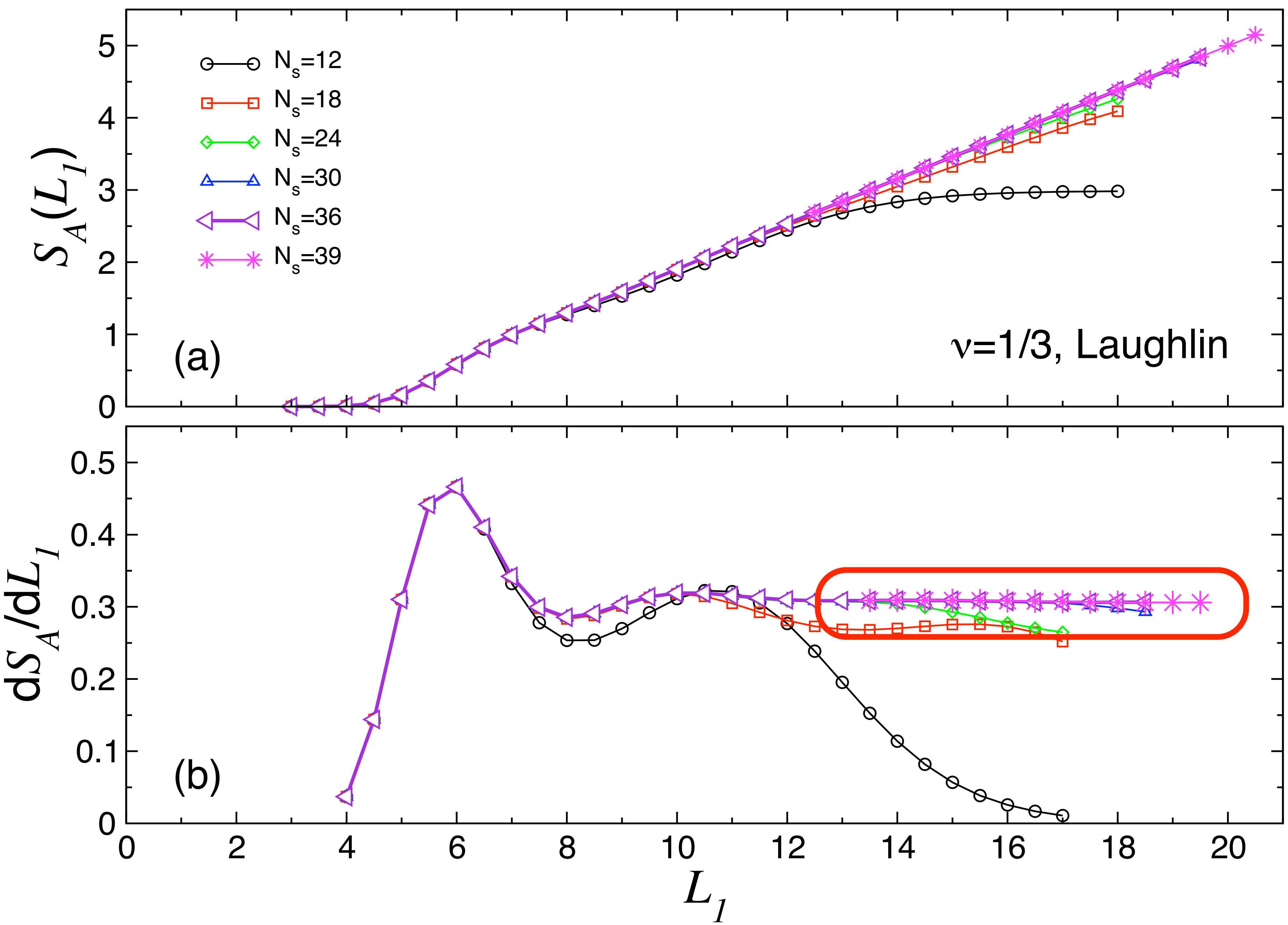



AML, Bergholtz & Haque, NJP (2010)

# Entanglement entropy $S(L_1)$ ($\nu$=1/3 Laughlin)

- For large enough $N_s$, $S(L_1)$ converges for each $L_1$



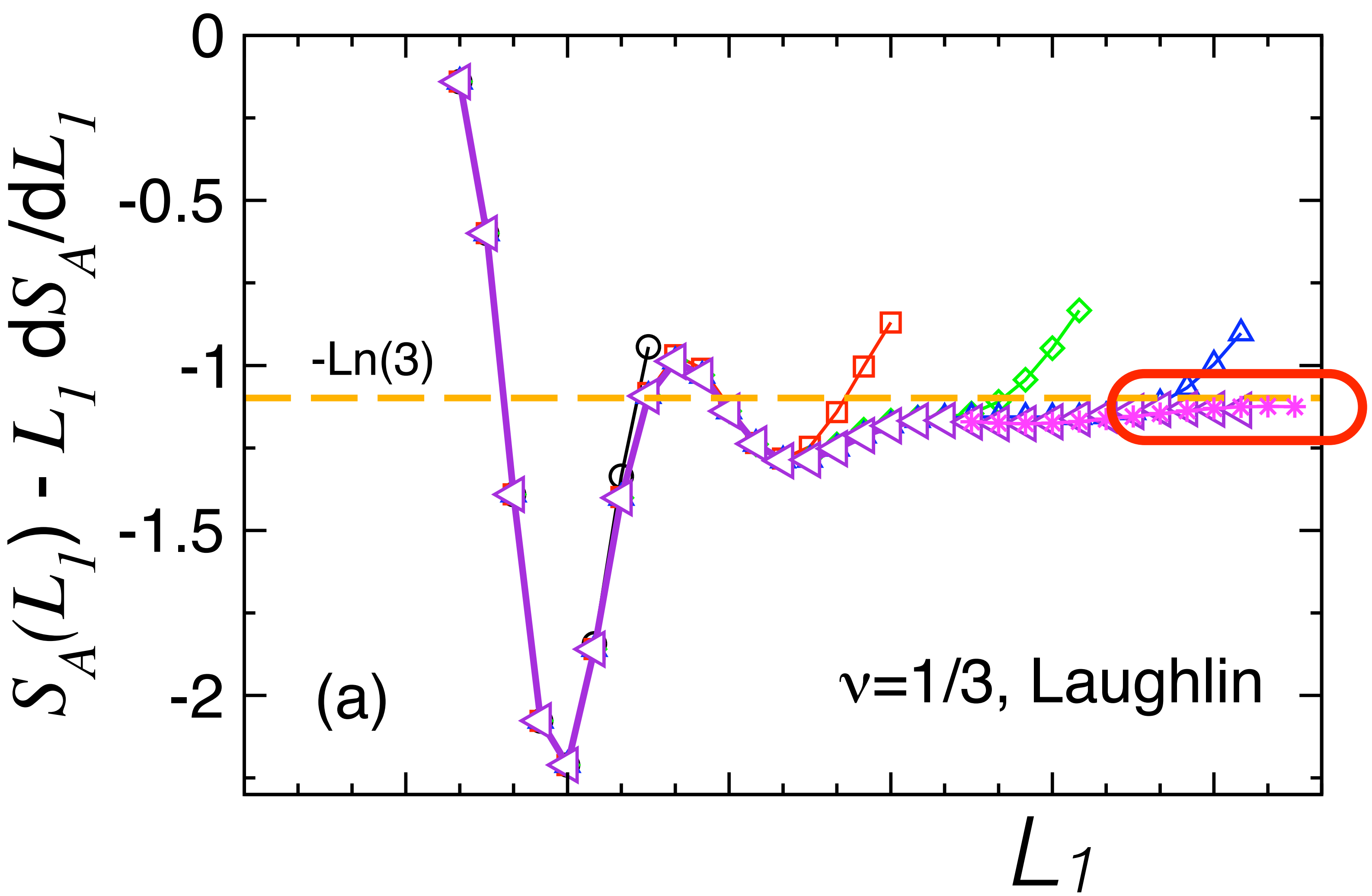

$$S(L_1) = 2\alpha L_1 - 2\gamma + \dots$$

Boundary entropy density (**α**)

AML, Bergholtz & Haque, NJP (2010)

# Extracting the topological entanglement entropy

- Use a running $\gamma$ extraction, and monitor $L_1$ convergence




$$S(L_1) = 2\alpha L_1 - 2\gamma + \ldots$$

- $2\gamma$ converges towards expected Log(3) !
  Most accurate numerical determination for FQH states to date.

AML, Bergholtz & Haque, NJP (2010)

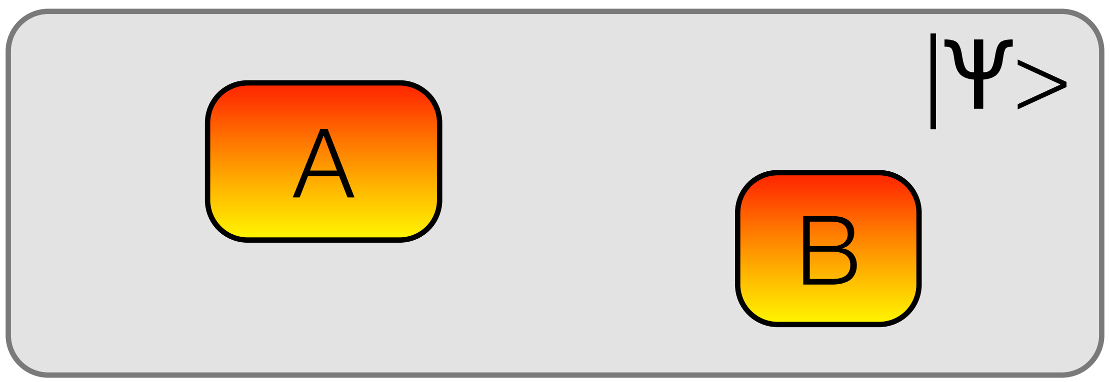
# Exact Diagonalization: Applications

- Quantum Magnets: nature of novel phases, critical points in 1D, dynamical correlation functions in 1D & 2D
- Fermionic models (Hubbard/t-J): gaps, pairing properties, correlation exponents, etc
- Fractional Quantum Hall states: energy gaps, overlap with model states, entanglement spectra
- Quantum dimer models or other constrained models (anyon chain..)
- Full Configuration Interaction in Quantum Chemistry

# Outline

- Correlation Density Matrices
  - Concept
  - Applications to spin chains and the Kagome AFM
- "Tower of States" spectroscopy
  - Continuous symmetry breaking: magnetic vs spin nematic order

# The correlation density matrix (CDM)




- Is there a systematic way to detect important correlations between parts A and B embedded in a larger system ?
- The correlation density matrix:

$$\rho^{c}_{AB} = \rho_{AB} - \rho_A \otimes \rho_B$$

contains all the required information

# The correlation density matrix (CDM)

$$\rho^c_{AB} = \rho_{AB} - \rho_A \otimes \rho_B$$


- Contains all information on any connect correlation function between A and B:

$$\mathrm{Tr}(\rho^c_{AB}\widehat{O}_A\widehat{O}_B) = \langle \widehat{O}_A\widehat{O}_B\rangle - \langle\widehat{O}_A\rangle\langle\widehat{O}_B\rangle$$

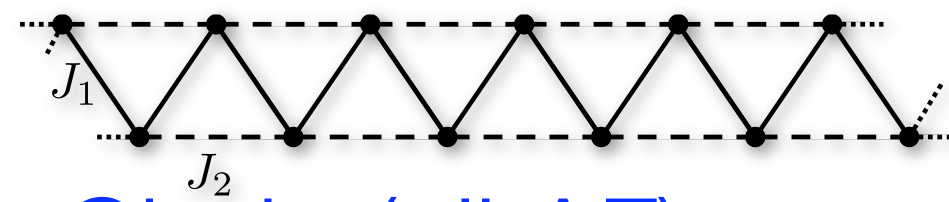
- The key step is to perform a singular value decomposition

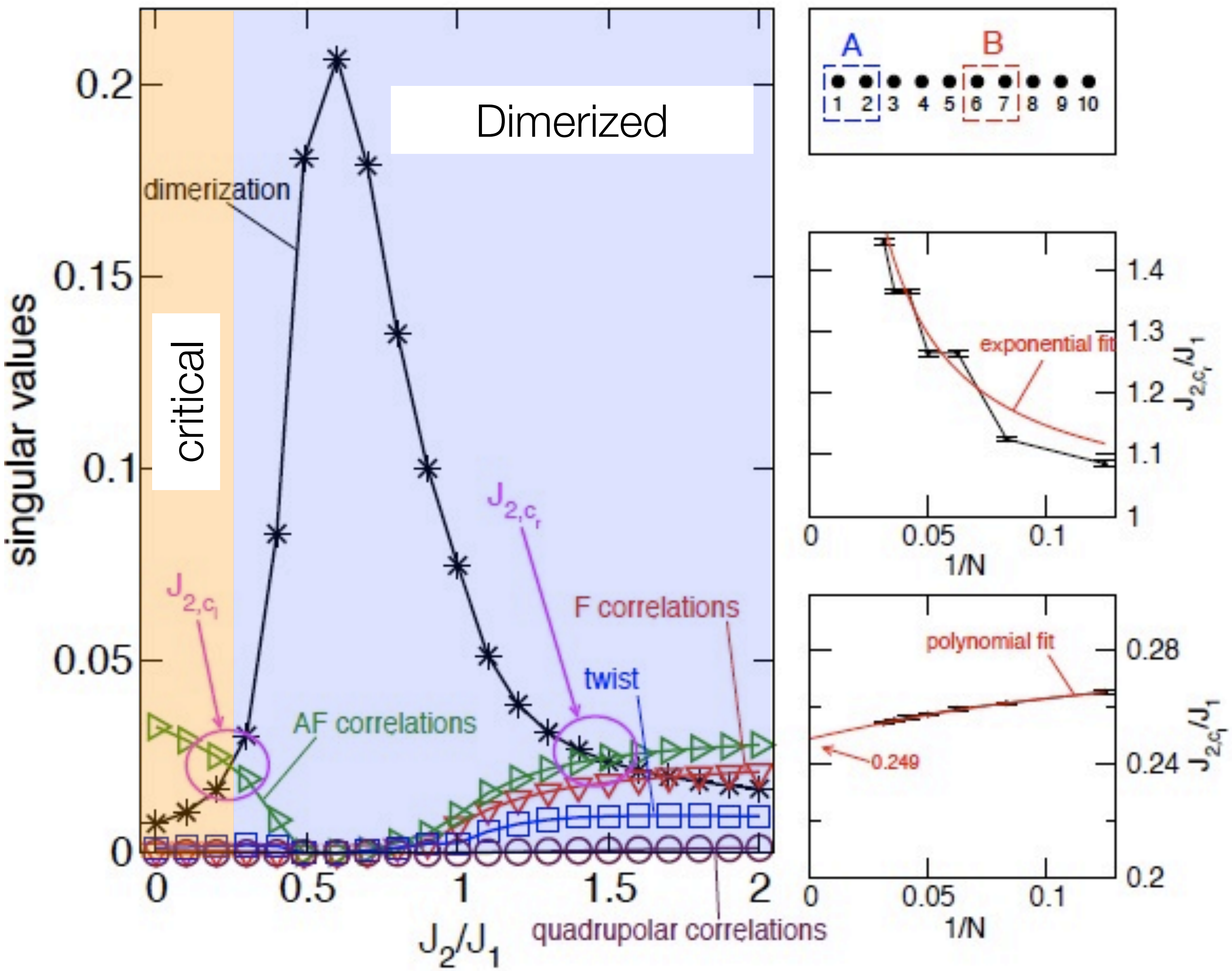
$$\rho^c_{AB} = \sum_{i=1} \sigma_i X'_i Y'^{\dagger}_i$$

where the $\boldsymbol{\sigma}_i$ give the strength of the correlation i and the $X_i$ and $Y_i$ are the operators of the correlator acting in A and B.

S.-A. Cheong & C.L. Henley, PRB 2009

# CDM
# $J_1$-$J_2$ frustrated Heisenberg Chain (all AF)



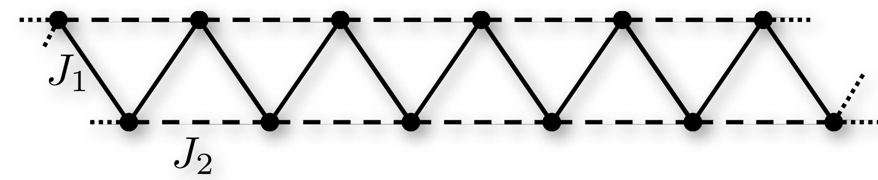



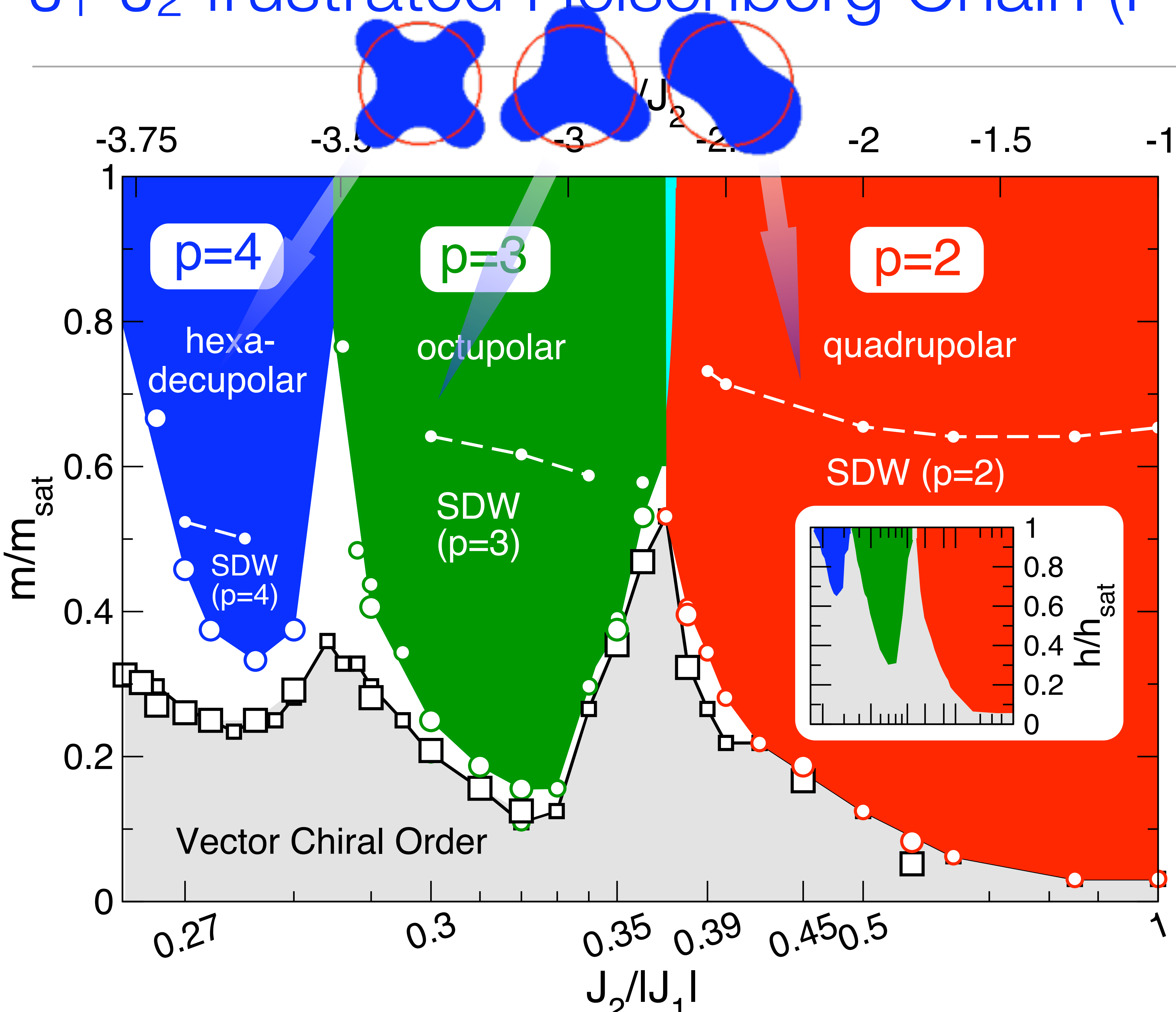

- Benchmark on existing phase diagrams.
- singular values respect SU(2) symmetry in S=0 GS (multiplicities).
- works very well for the well understood Majumdar-Ghosh chain.

J. Sudan & AML

# CDM

# $J_1$-$J_2$ frustrated Heisenberg Chain (F-AF)



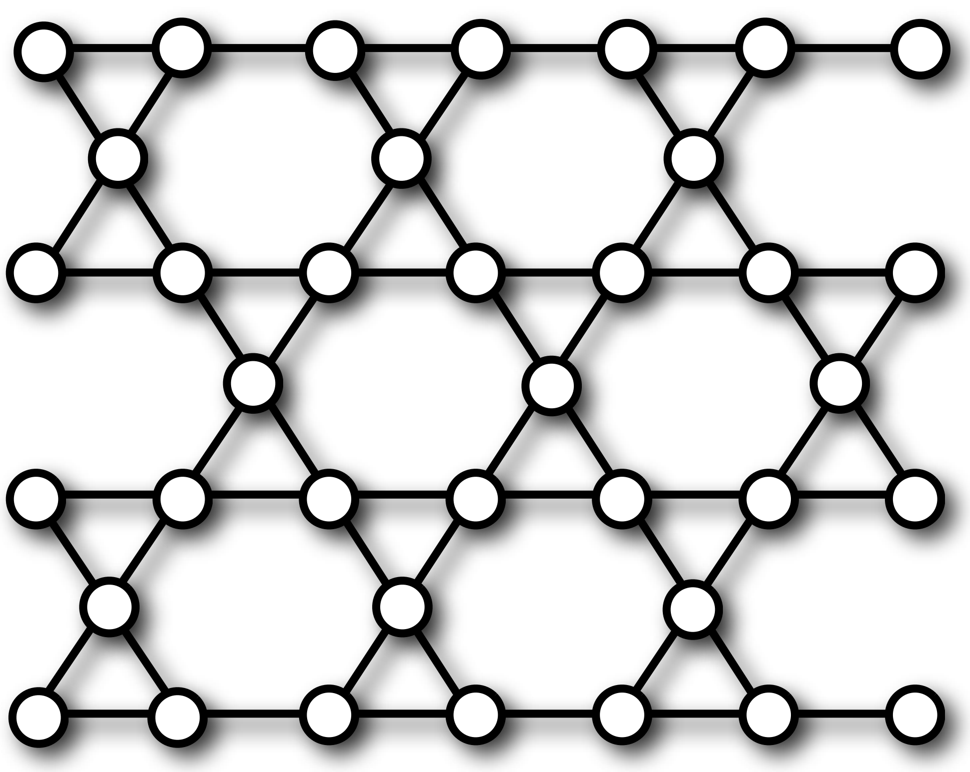




- vector chiral phase at low m
- spin multipolar liquids at high m
- CDM helped us understand that spin multipolar phases are generically imprinted in close-by magnetically ordered states

J. Sudan, A. Lüscher, AML, PRB 2009, ED/DMRG

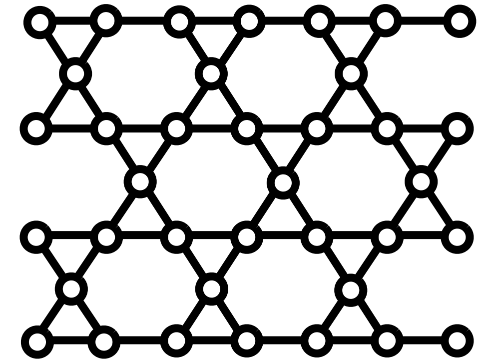
F. Heidrich-Meisner et al. PRB '06
T. Hikihara et al., PRB '08

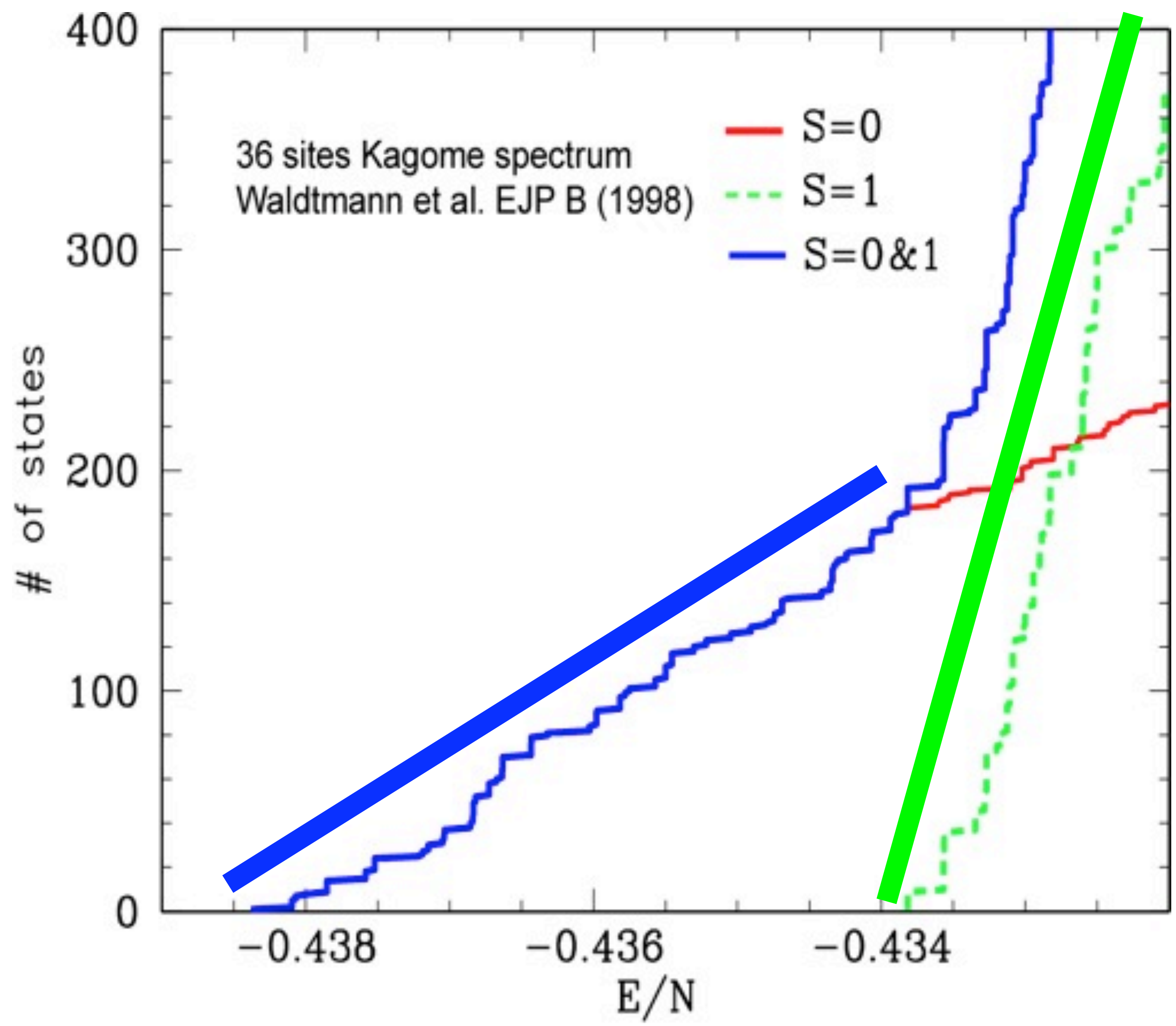
# The Kagome Antiferromagnet



$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

# Some kagome facts so far

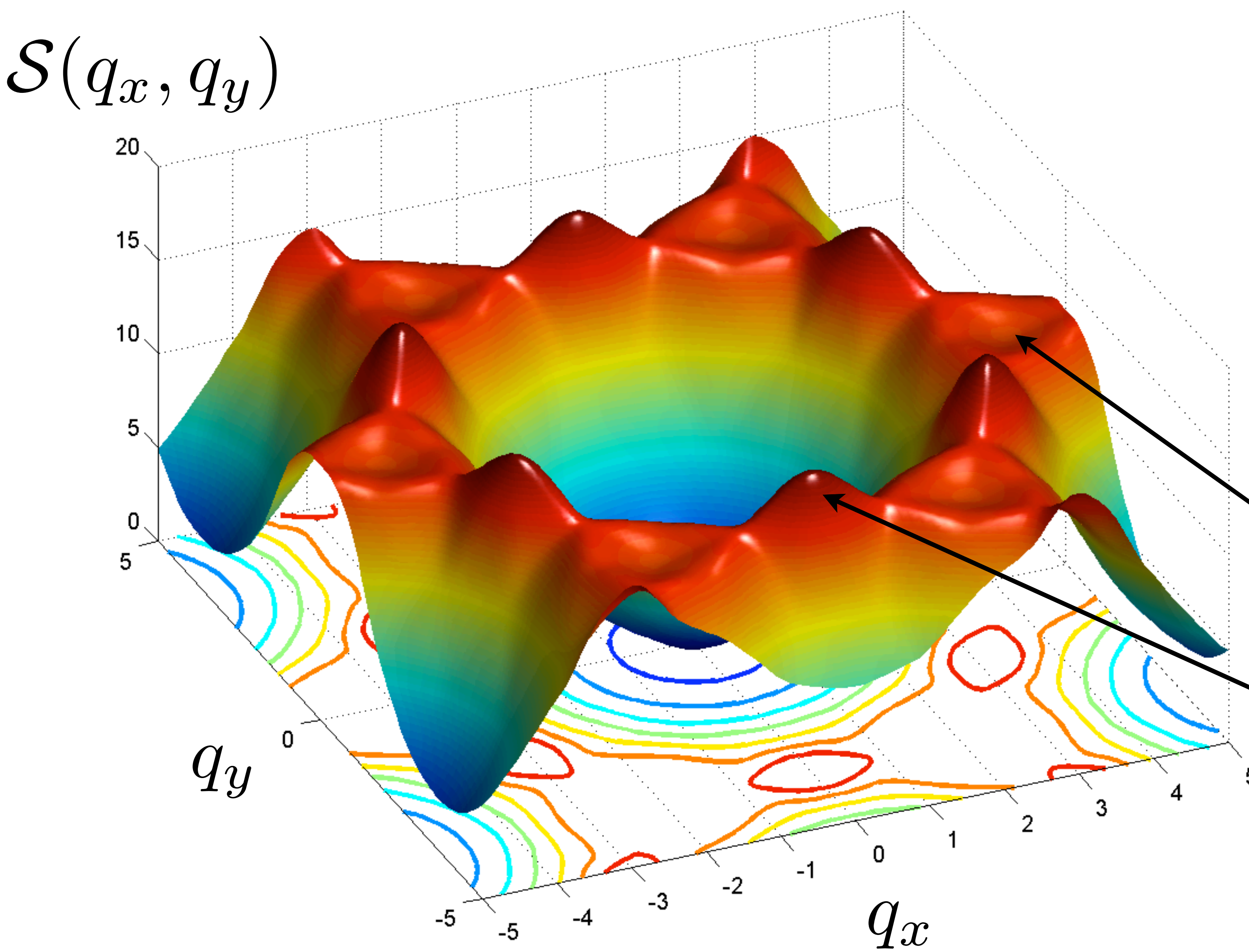




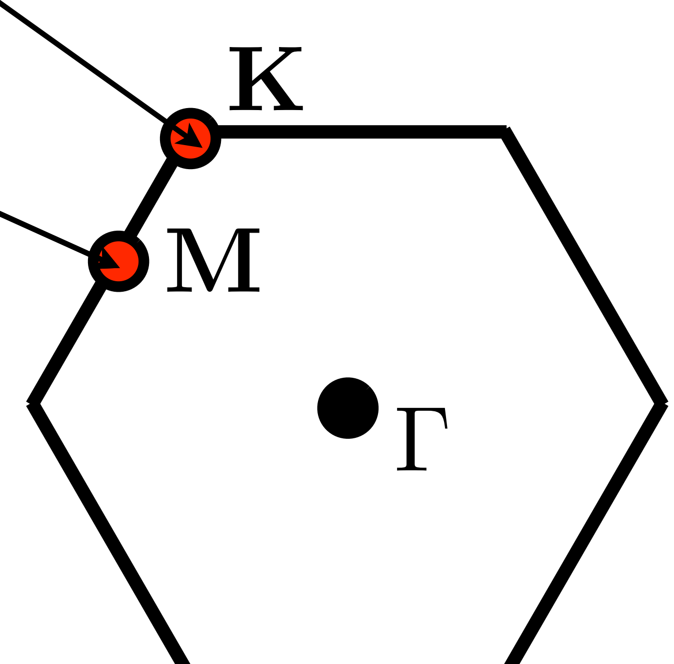

- Absence of magnetic order for S=1/2, Spin gap probably finite ~0.05 - 0.1 J
  Waldtmann et al, EPJB '98, Jiang et al, PRL 08
- Puzzlingly high density of singlets below the finite size spin gap.
  Lecheminant et al PRB '97, Mila PRL '98
- Nature of the ground state unclear, nature and origin of high singlet density not really understood

mpipks

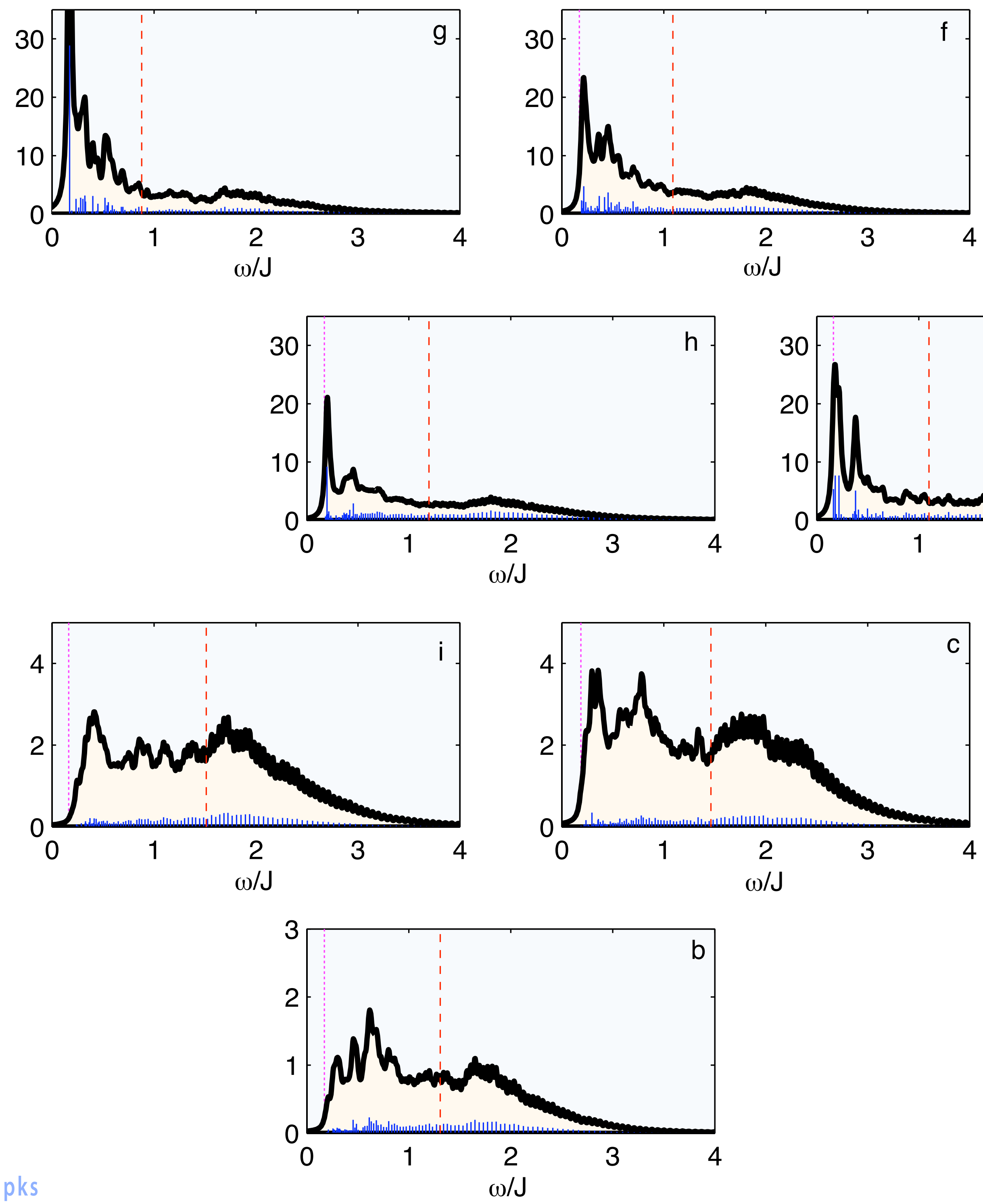
# Kagome AFM
# Static Spin Structure Factor



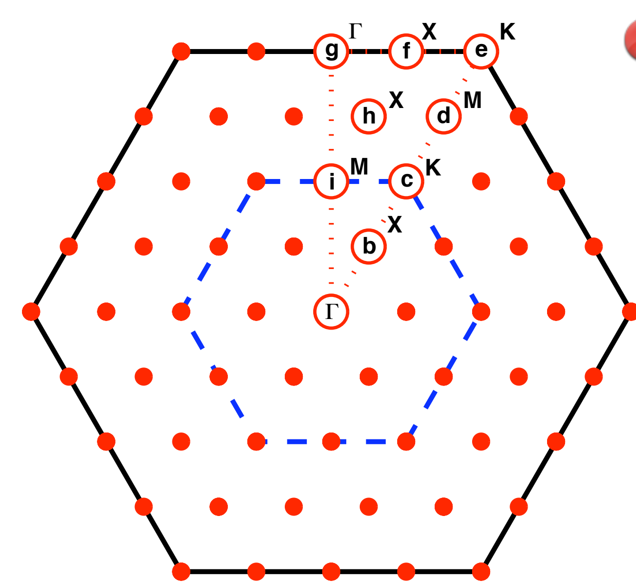

- Ring of enhanced scattering at the extended BZ boundary
- No magnetic order!



# Kagome AFM
# Dynamical Spin Structure Factor (~ INS)




ED, 36 sites

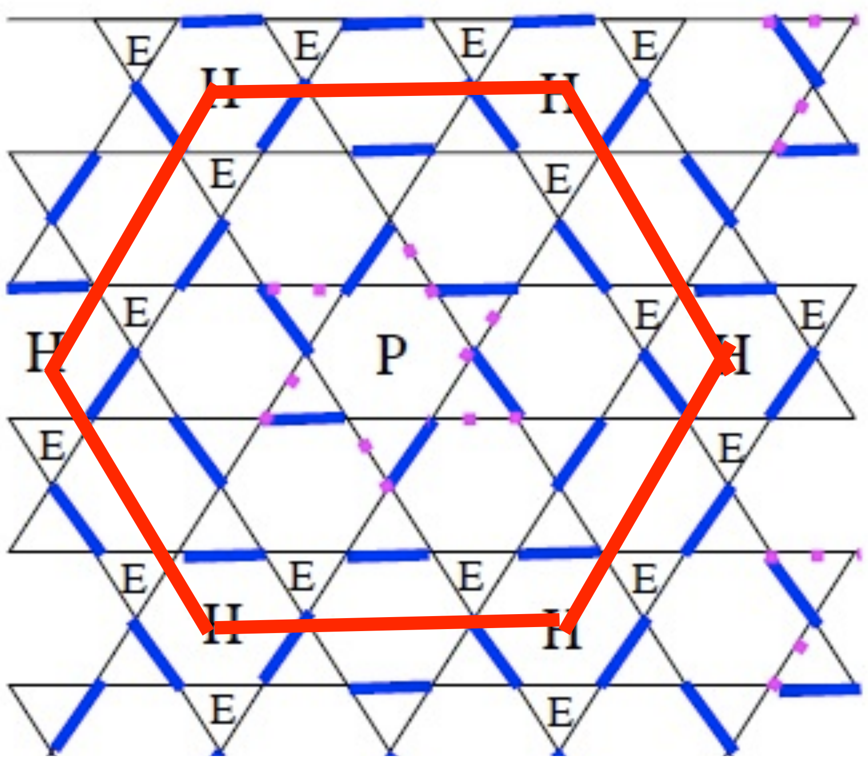



- Broad response in energy
- Spiky features at lowest energies, Remnant of VBC?
- Relation to INS experiments on Herbertsmithite ?
  Lee et al ‘07,
  Helton et al. ‘07,
  deVries et al, ‘09

AML, C. Lhuillier, arXiv:0901.1065

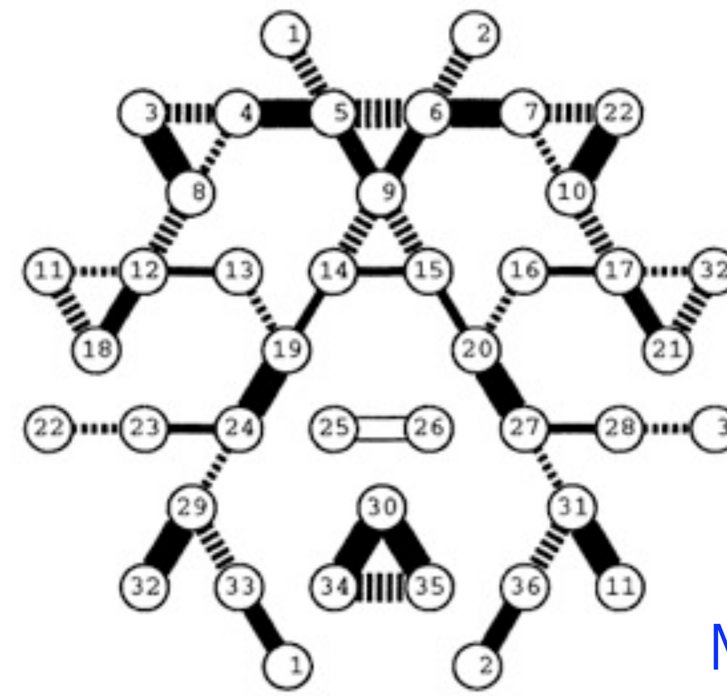
# Groundstate of the Kagome AFM

- Valence Bond Solid ?

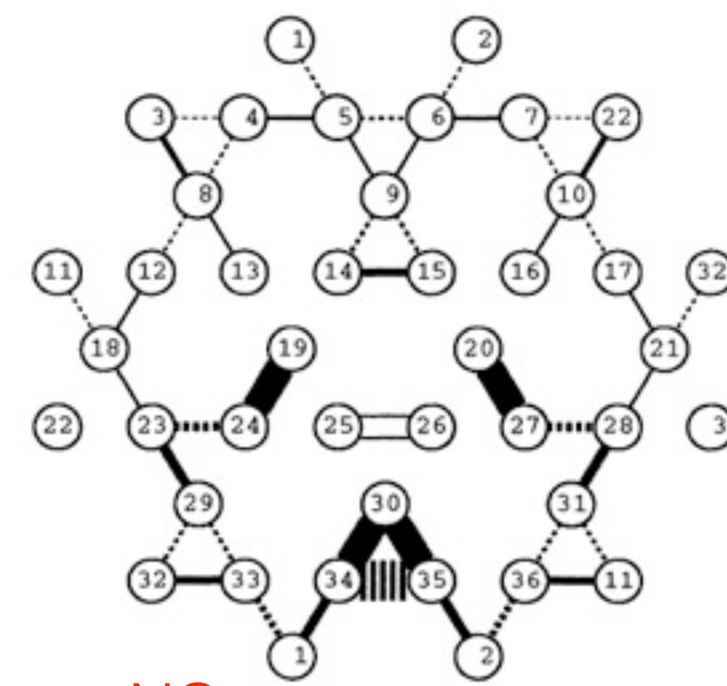


Marston & Zheng, JAP '91
...
Singh & Huse, PRB 07
Evenbly & Vidal, arXiv:0903

} YES



Model state



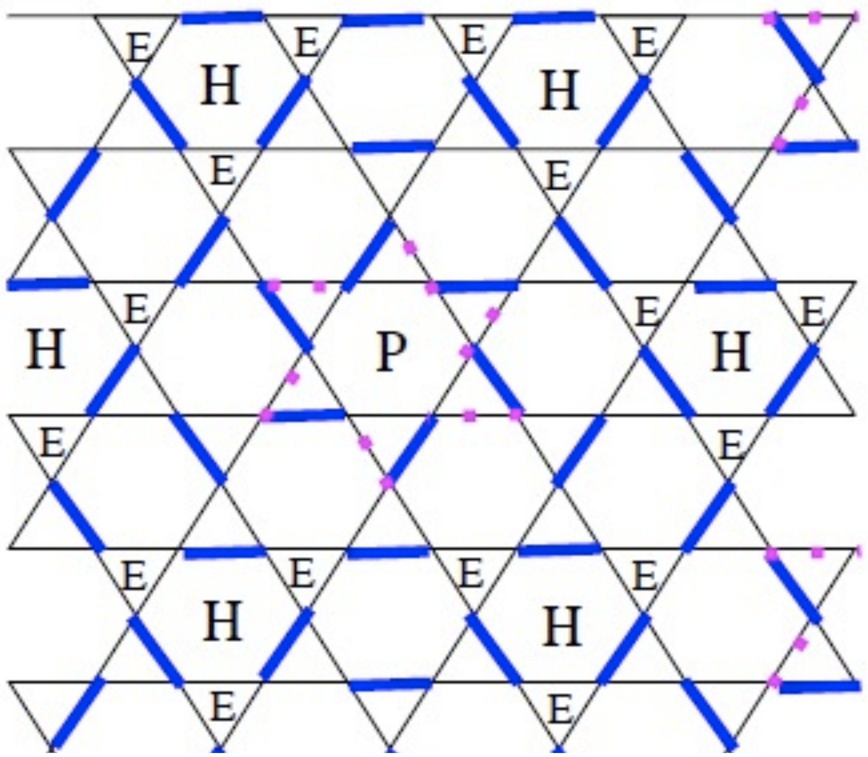
ED Results
36 sites

NO,
or very weak

Leung & Elser, PRB 93

# Groundstate of the Kagome AFM

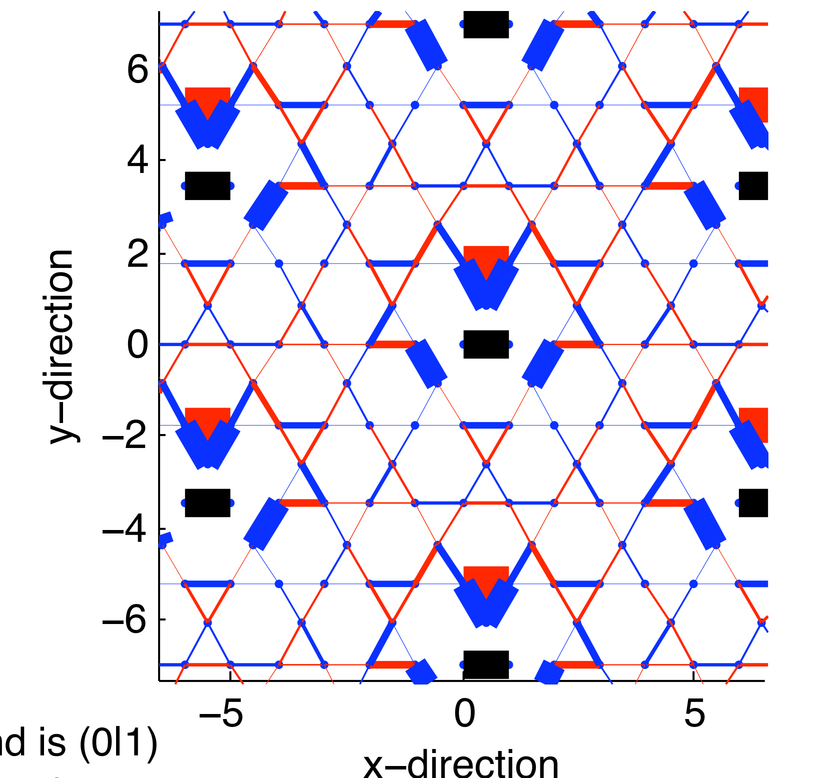
- Valence Bond Solid ?

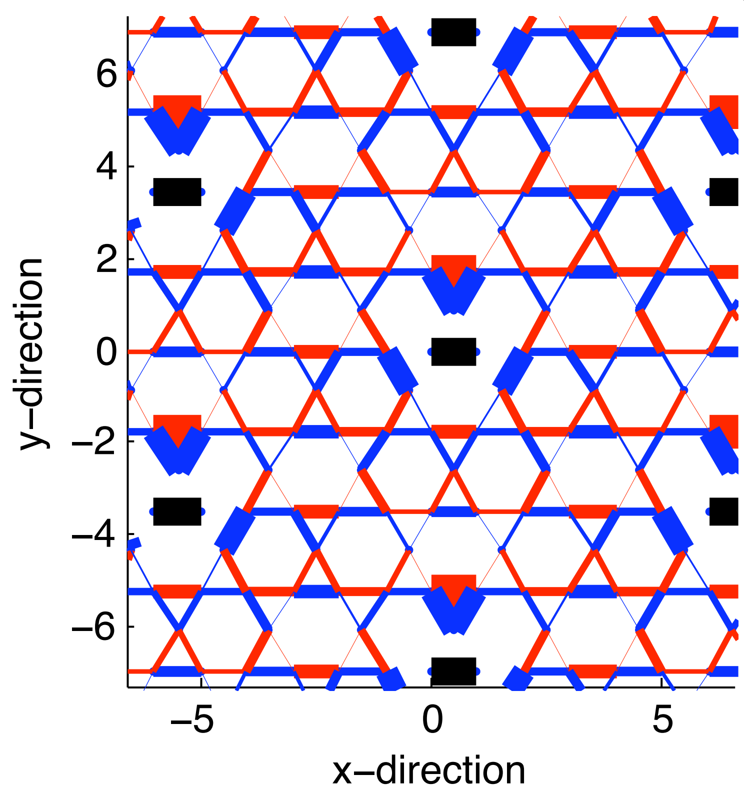


Marston & Zheng, JAP '91
...
Singh & Huse, PRB 07
Evenbly & Vidal, arXiv:0903

} YES

GS 36 sites



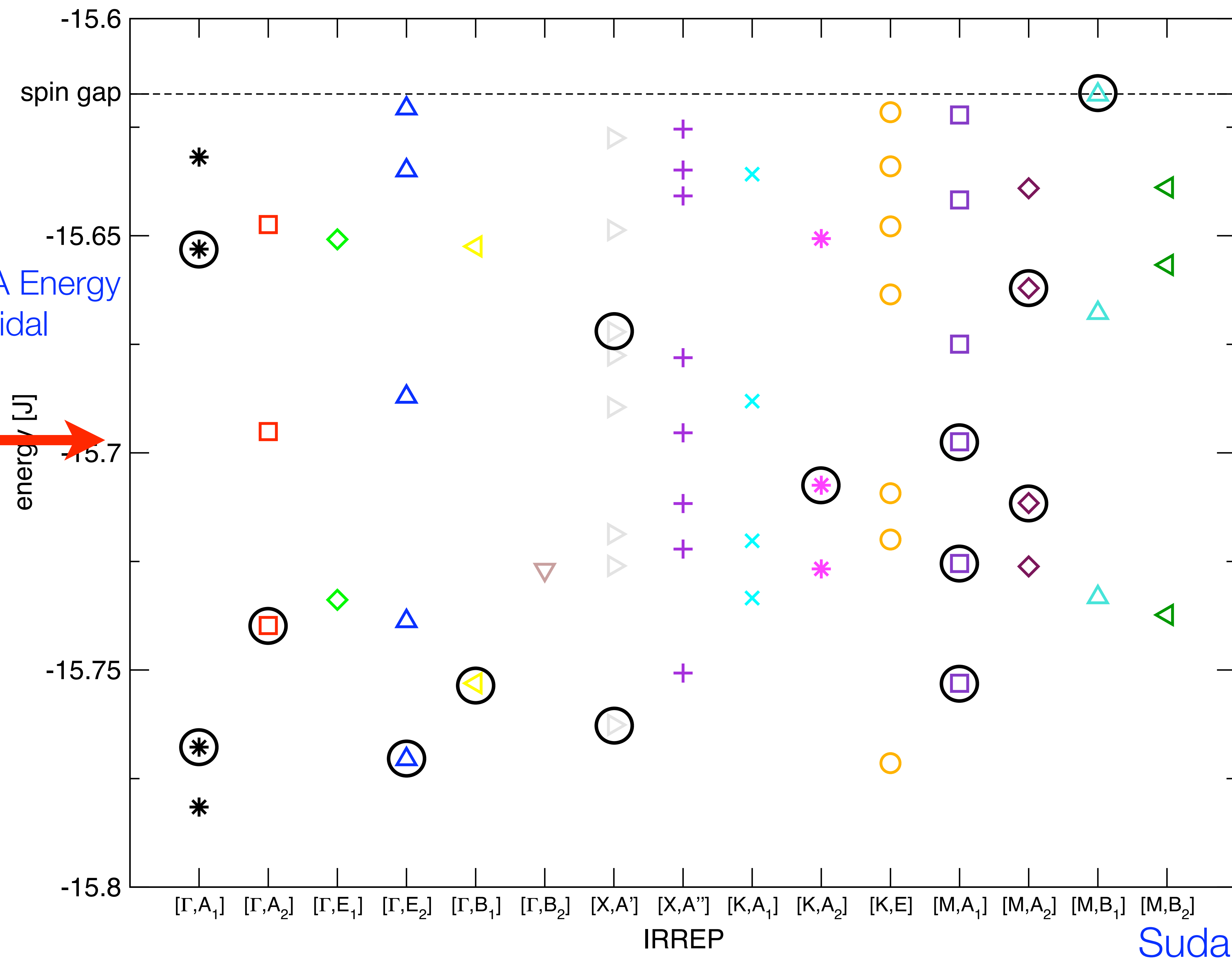

Excited state at
ΔE=0.03 J

likely VBC,
but not MZ crystal
on 36 sites

Sudan & AML, '09

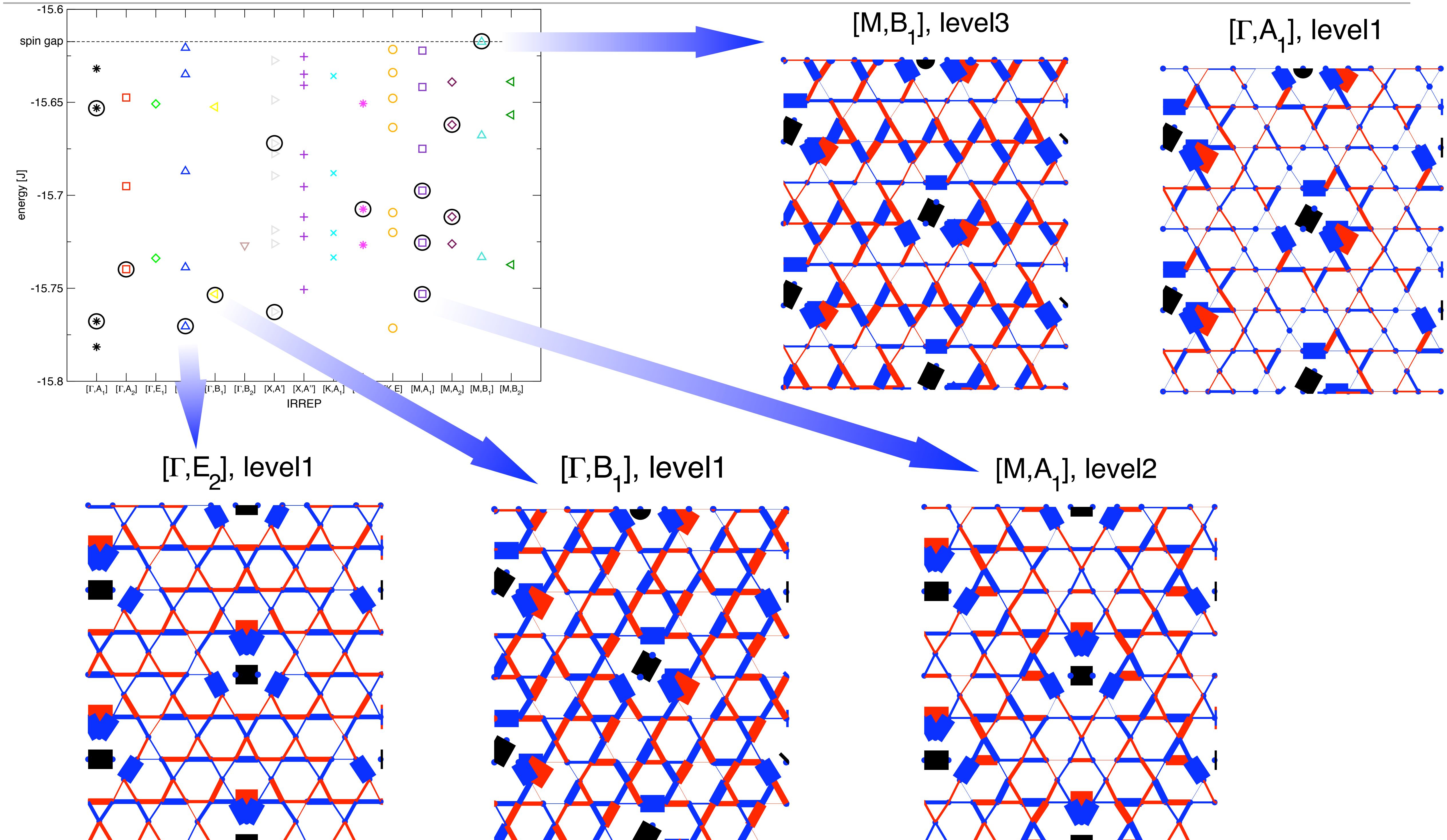
# Low Energy Singlet Spectrum (N=36 sites)

N=36 MERA Energy
Evenbly & Vidal
PRL 2010




Sudan & AML, '09

# Dimer correlations of low lying singlets (N=36)

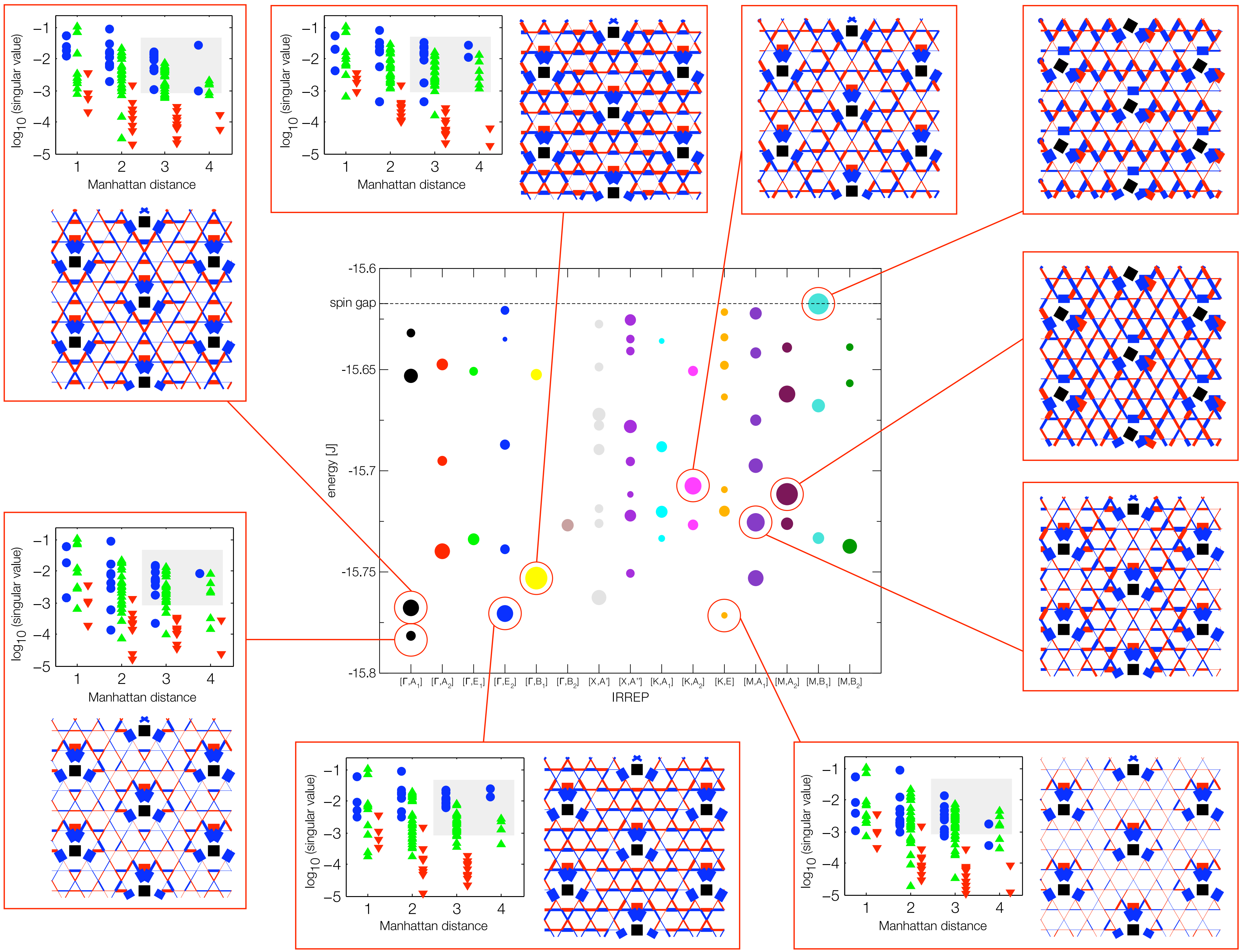



Sudan & AML, '09

mpipks

New States of Quantum Matter

# Dimer correlations of low lying singlets (N=36)

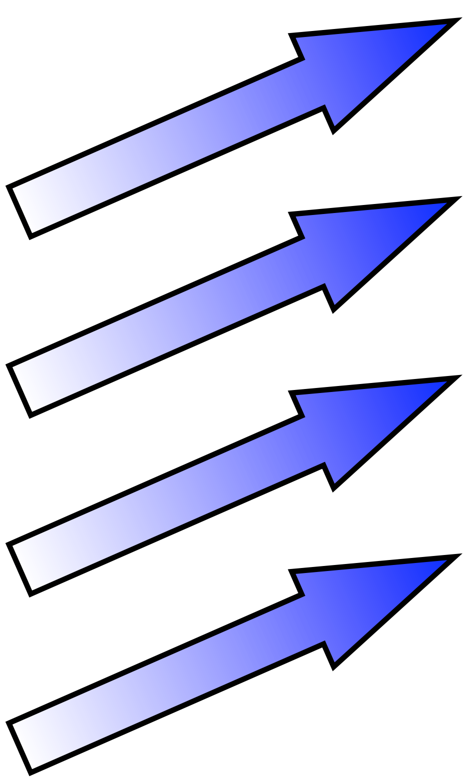


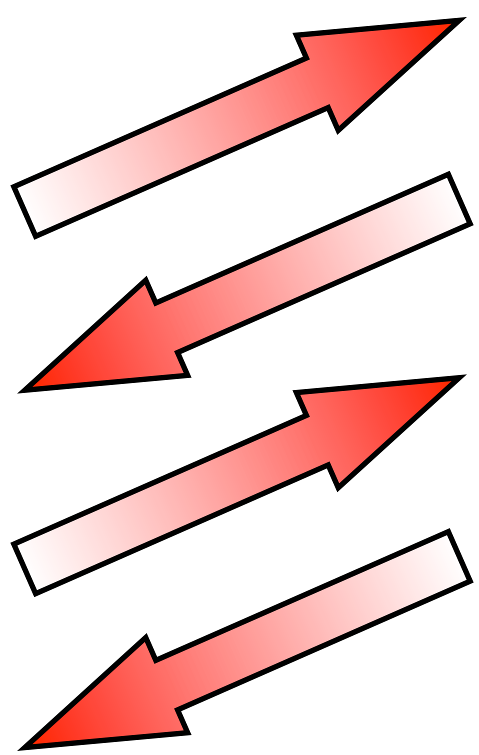
# Outline

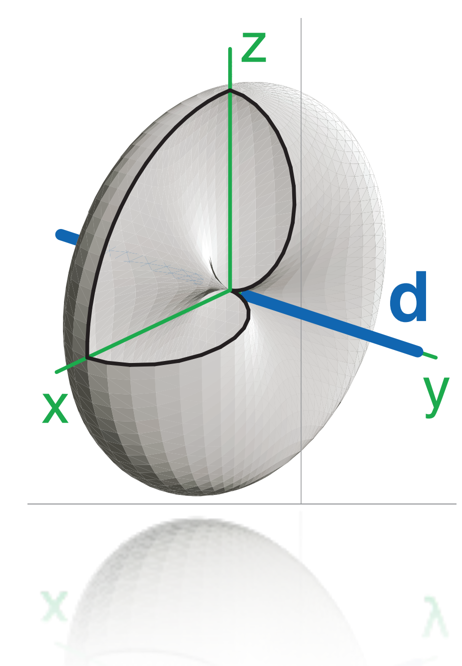
- Correlation Density Matrices
  - Concept
  - Applications to spin chains and the Kagome AFM
- “Tower of States” spectroscopy
  - Continuous symmetry breaking: magnetic vs spin nematic order

# “Tower of States” spectroscopy

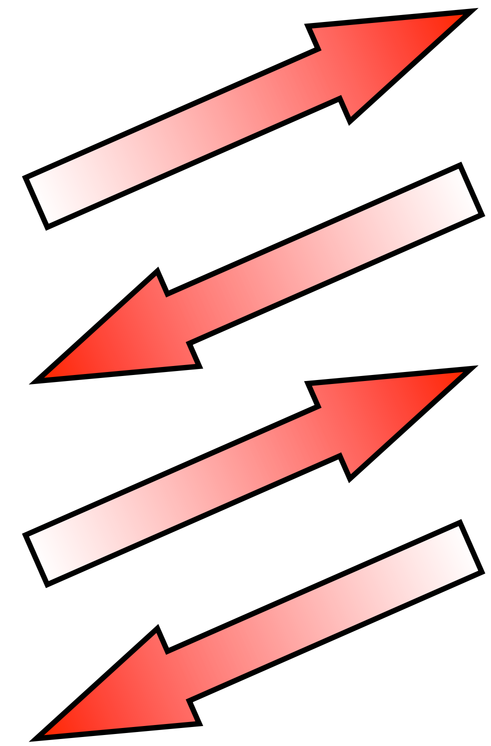
- What are the finite size manifestations of a continuous symmetry breaking ? (eg in superfluids/superconductors, magnetic order, spin nematic order)
- Order parameter is zero on a finite system ! (symmetric partition function)
- So usually one looks into order parameter correlations [(order parameter)$^2$]







# “Tower of States” spectroscopy

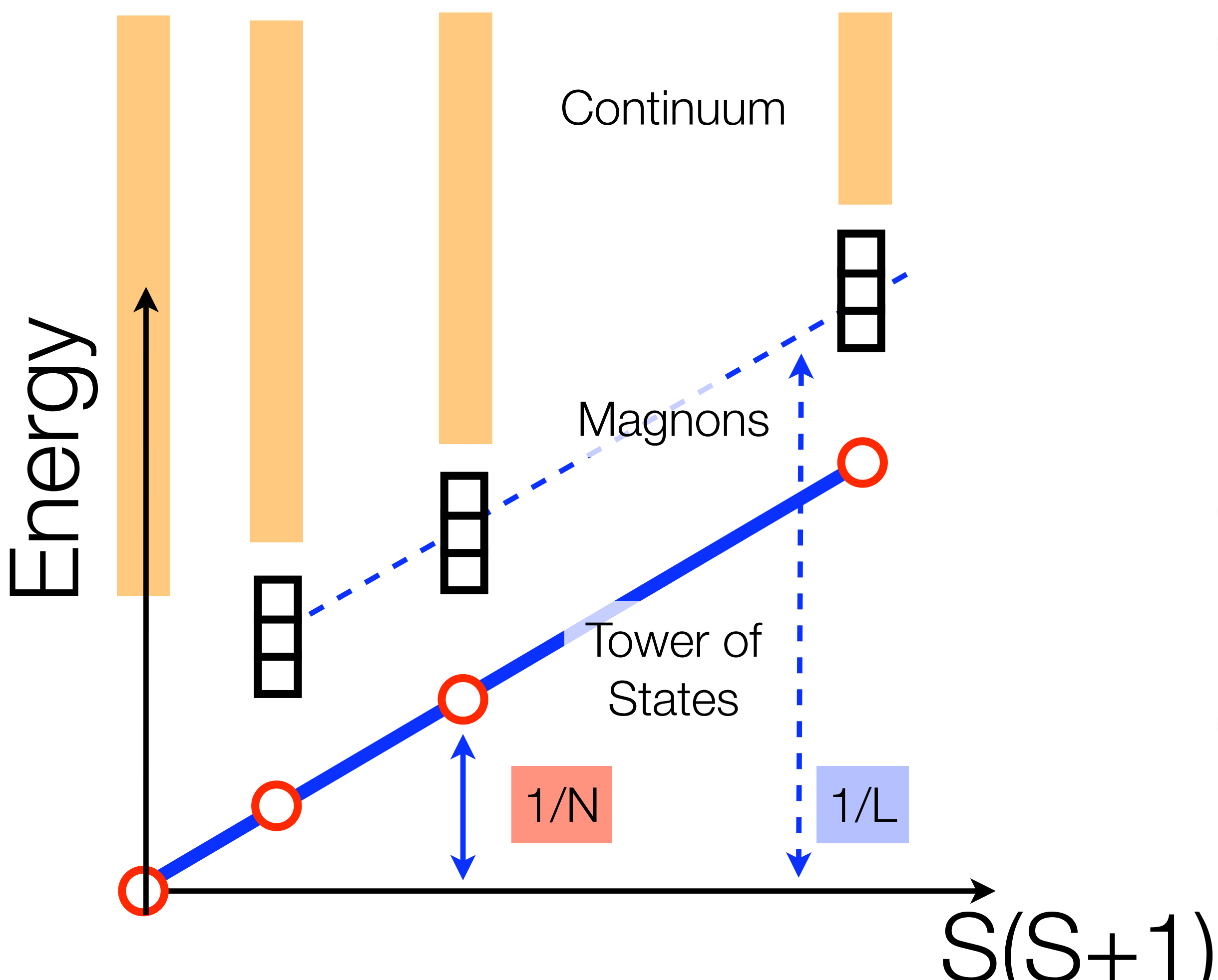


- Order parameter is not a conserved quantity
- Order parameter is zero on a finite size sample (Wigner-Eckart)
- How does one get spontaneous symmetry breaking anyway ?
- Ground state degeneracy is building up as we approach the thermodynamic limit, which will allow to form a symmetry breaking wave packet at zero energy cost

# "Tower of States" spectroscopy

- What are the finite size manifestations of a continuous symmetry breaking ?
(eg in superfluids/superconductors, magnetic order, spin nematic order)

- Low-energy dynamics of the order parameter
Theory: P.W. Anderson 1952, Numerical tool: Bernu, Lhuillier and others, 1992 -




- Dynamics of the free order parameter is visible in the finite size spectrum. Depends on the continuous symmetry group.

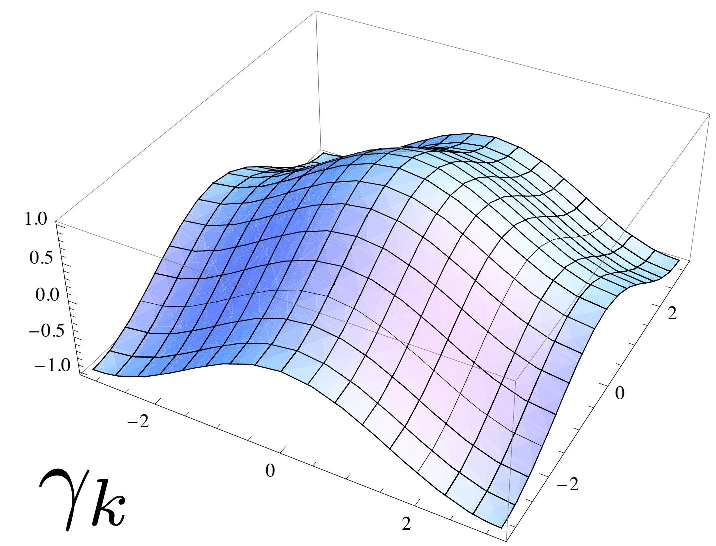
- U(1): $(S^z)^2$ SU(2): $S(S+1)$

- Symmetry properties of levels in the Tower states are crucial and constrain the nature of the broken symmetries.

# Square lattice Heisenberg antiferromagnet

- Hamiltonian $$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

- Fourier transform $$H = 2J \sum_k \gamma_k \, \mathbf{S}_k \cdot \mathbf{S}_{-k}$$

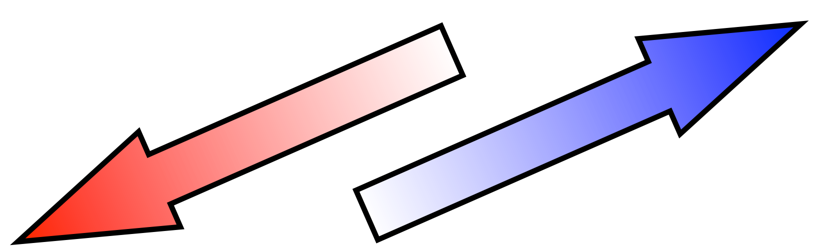


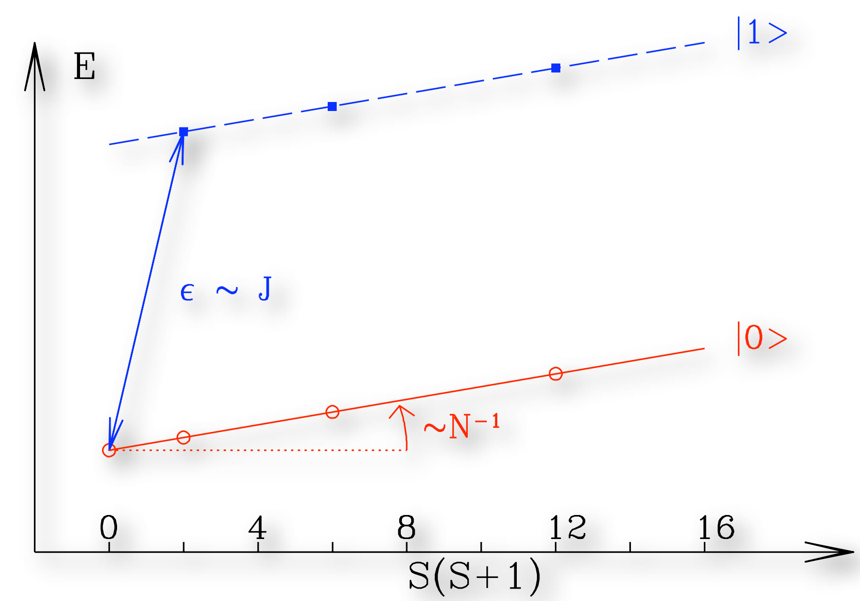

$\gamma_k$

- Keep only the (0,0) and (π,π) mode

- Lieb Mattis model recovered

$$H_0 = \frac{4J}{N}(S_{\text{tot}}^2 - S_A^2 - S_B^2)$$

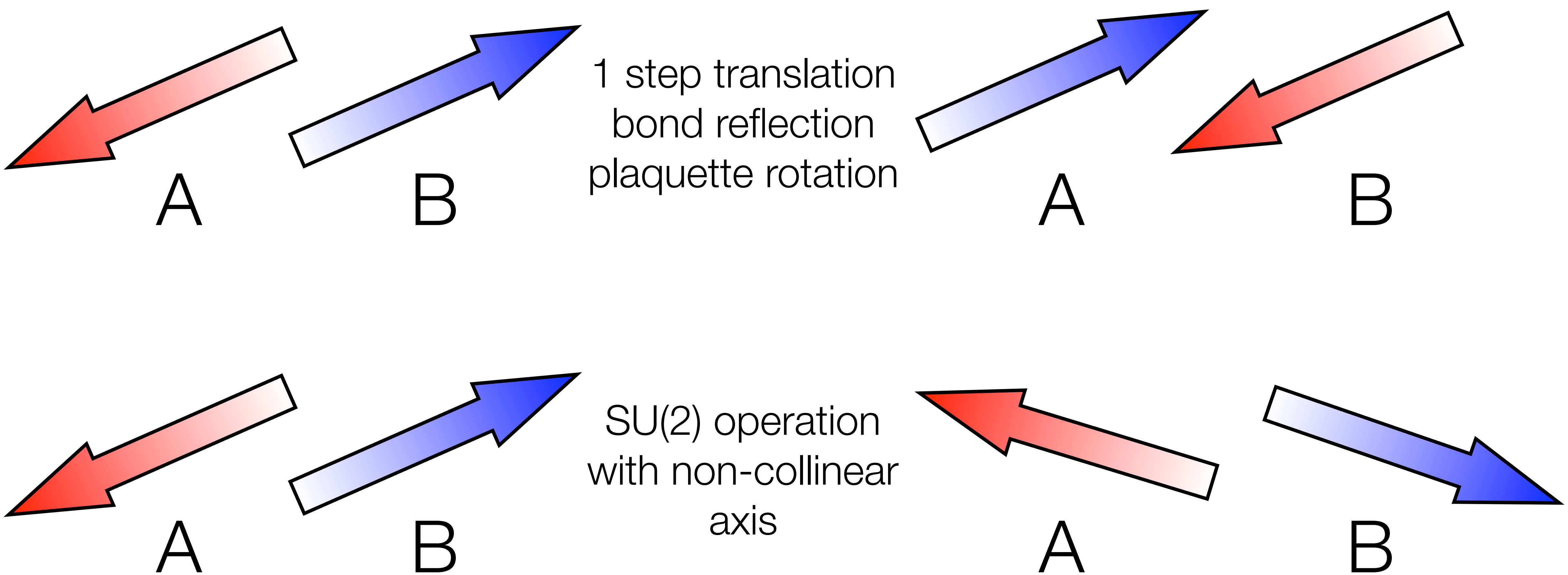





C. Lhuillier, cond-mat/0502464

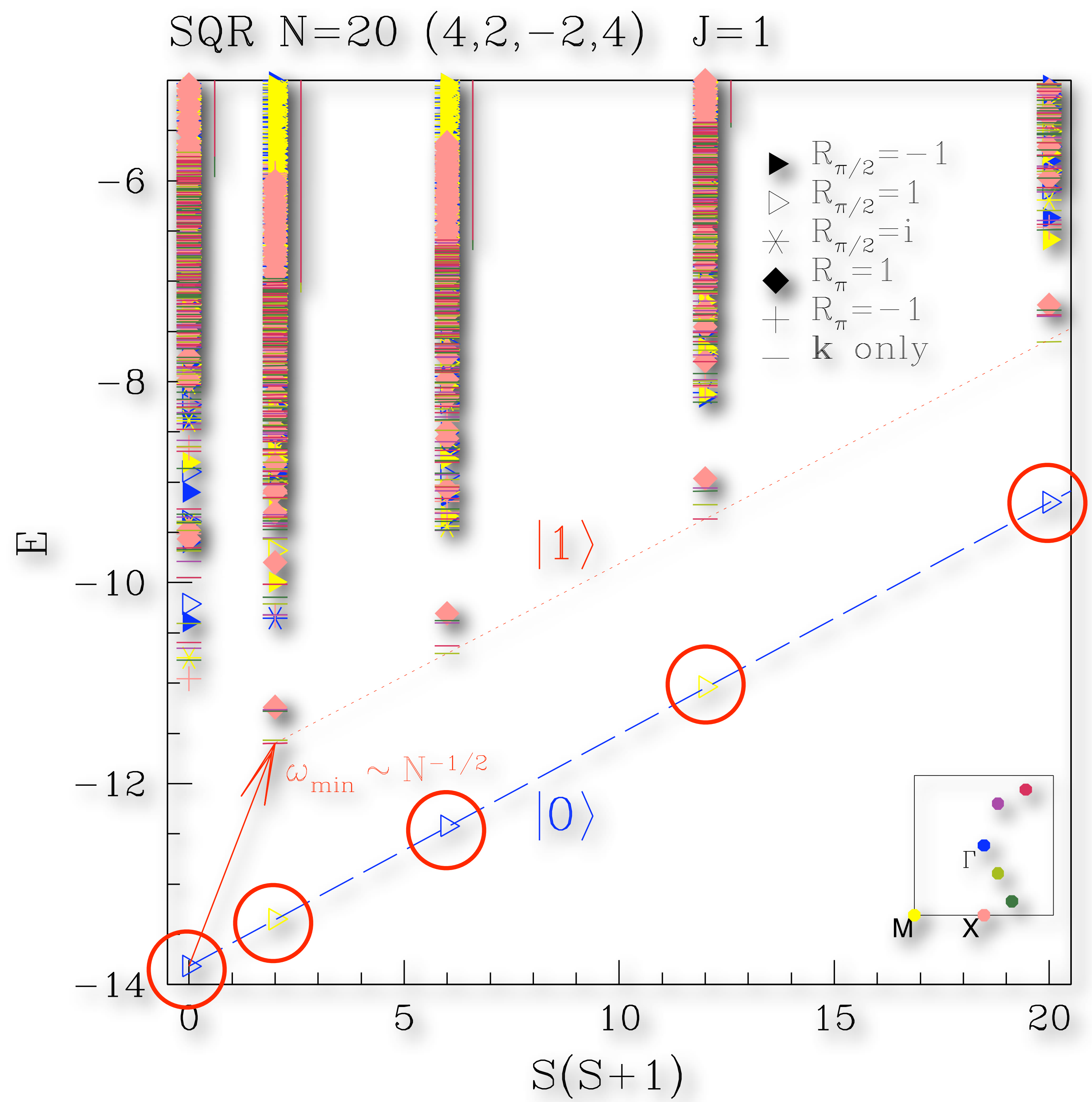
# Symmetry decomposition of order parameter

- Order parameter manifold forms a representation space for the symmetry group of the Hamiltonian
- Decompose this (reducible) representation into irreducible representations



# Symmetry decomposition of order parameter

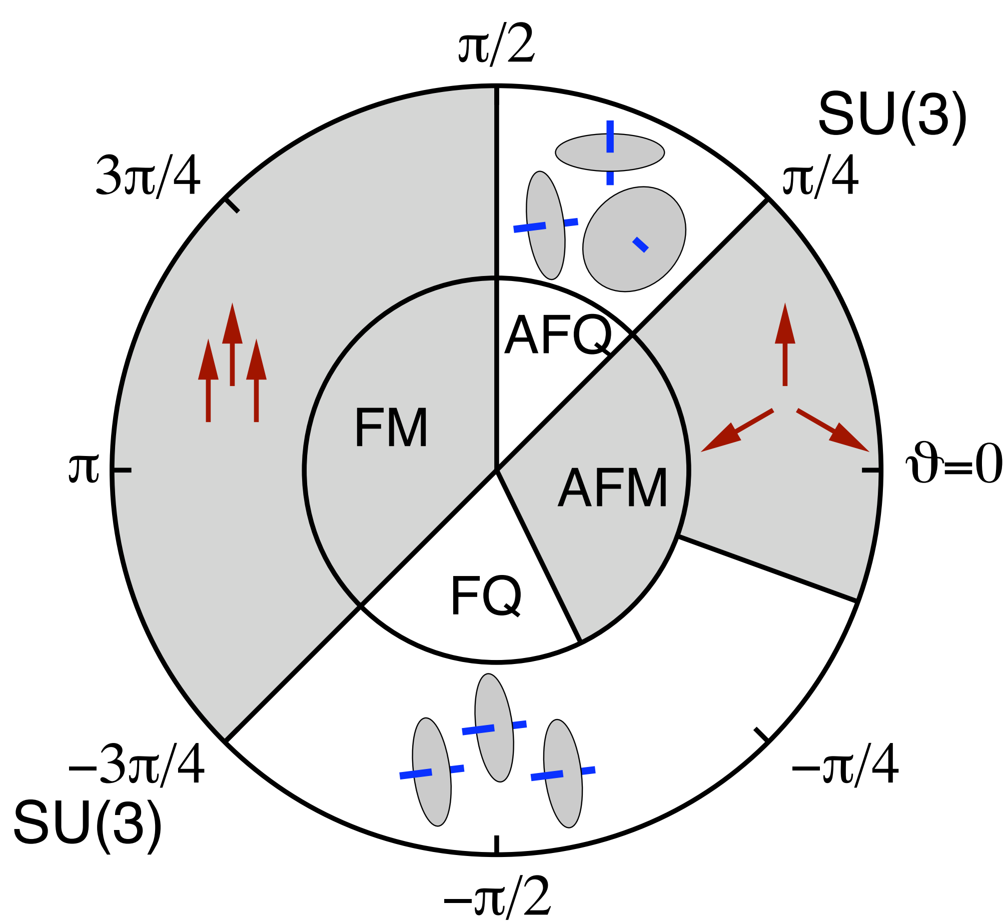
- As a result of the group theoretical analysis one obtains
  - 1 irrep with S=0, (0,0) A1
  - 1 irrep with S=1, (π,π) A1
  - 1 irrep with S=2, (0,0) A1
  - 1 irrep with S=3, (π,π) A1
  - ...



# Beyond the collinear Neel state

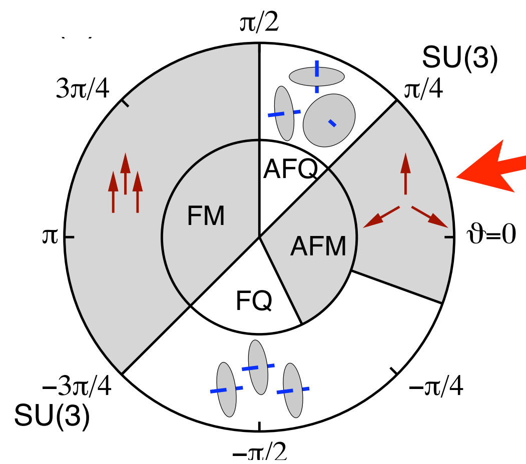
- Bilinear-biquadratic S=1 model on the triangular lattice (model for $NiGaS_4$).

$$H = \sum_{\langle i,j \rangle} \cos(\theta)\ \mathbf{S}_i \cdot \mathbf{S}_j + \sin(\theta)\ \ (\mathbf{S}_i \cdot \mathbf{S}_j)^2$$

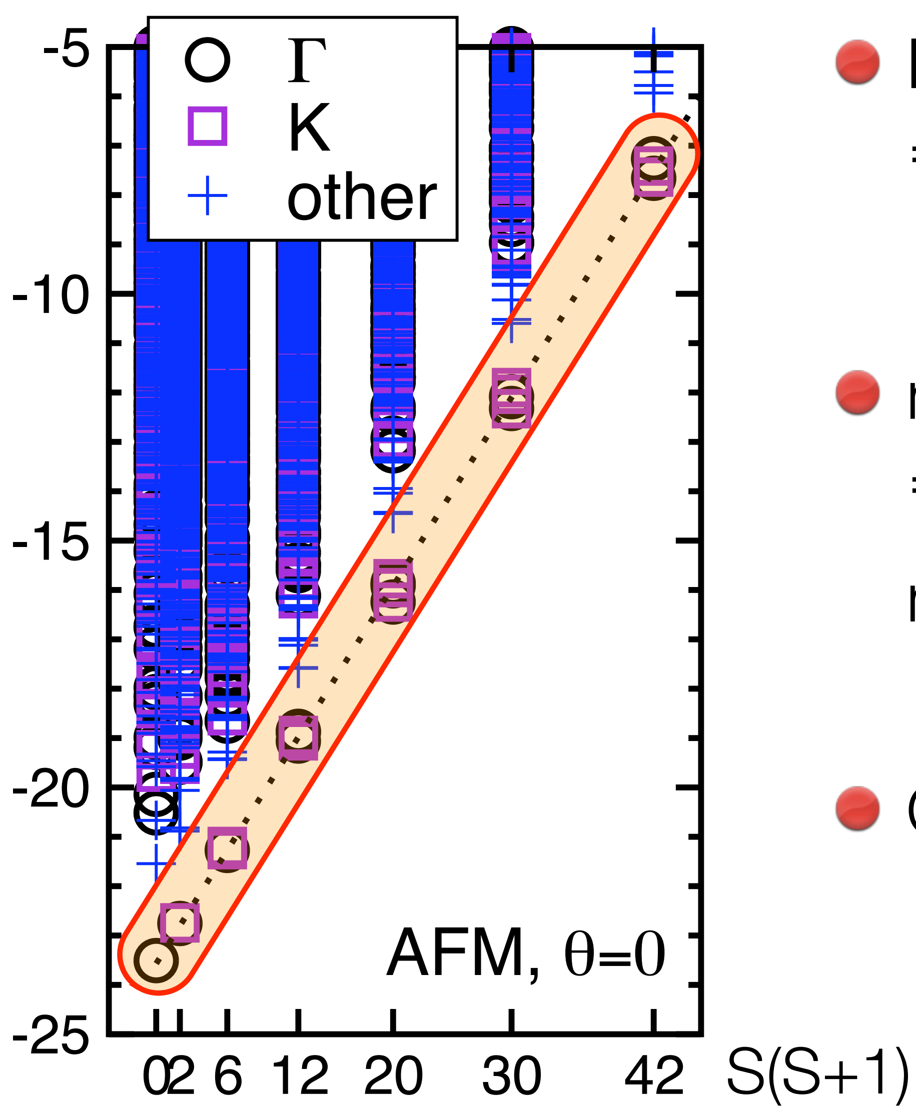



AML, F. Mila, K. Penc, PRL ‘06

# Tower of States
# S=1 on triangular lattice: Antiferromagnetic phase




- ϑ=0 : coplanar magnetic order,
  120 degree structure



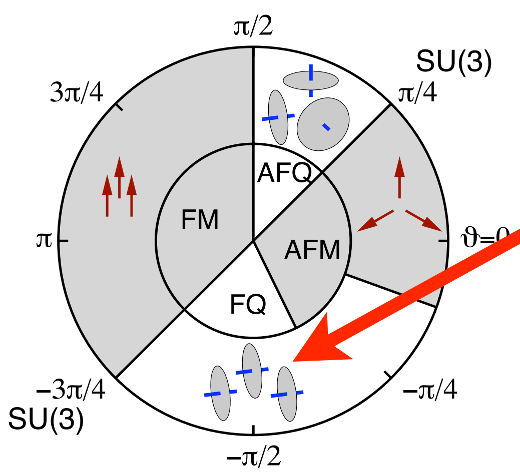

- Breaks translation symmetry. Tree site unit cell
  ⇒ nontrivial momenta must appear in TOS

- non-collinear magnetic structure
  ⇒ SU(2) is completely broken,

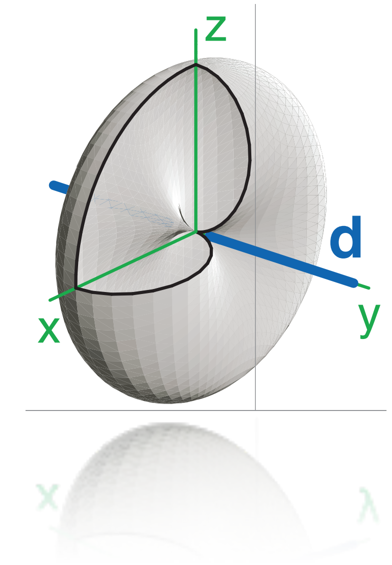
  number of levels in TOS increases with S

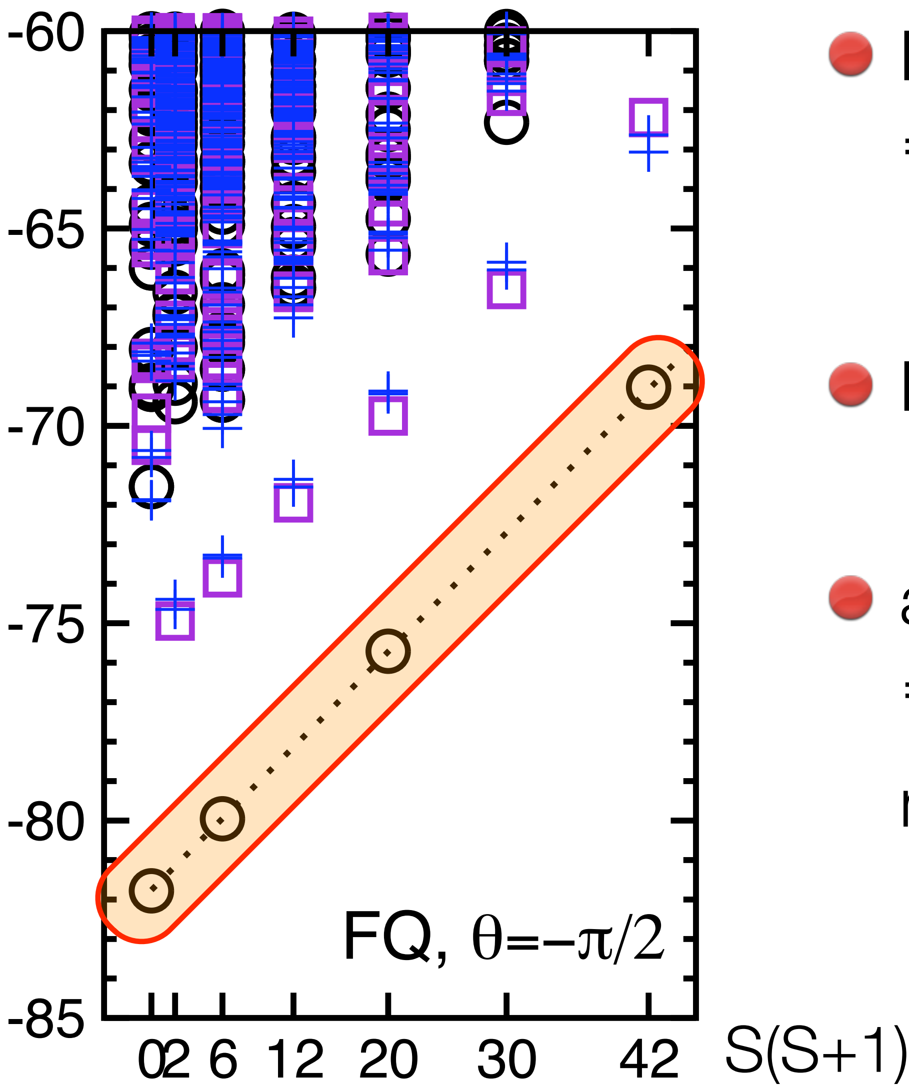
- Quantum number are identical to the S=1/2 case

# Tower of States
# S=1 on triangular lattice: Ferroquadrupolar phase




- ϑ=-π/2 : ferroquadrupolar phase, finite quadrupolar moment,  no spin order

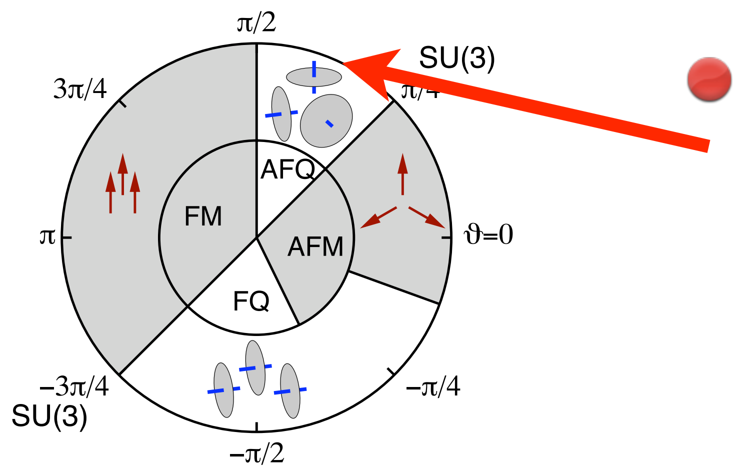


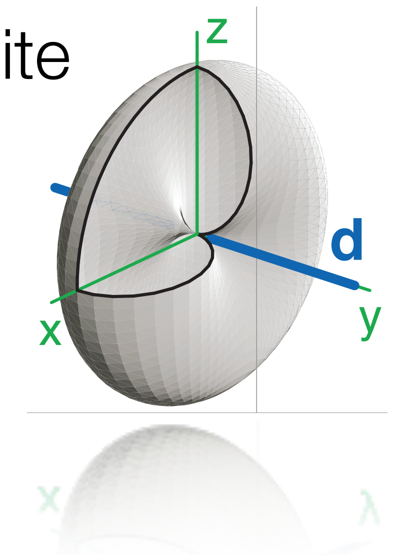

- No translation symmetry breaking.
  ⇒ only trivial momentum appears in TOS
- Ferroquadrupolar order parameter, only even S
- all directors are collinear
  ⇒ SU(2) is broken down to U(1),

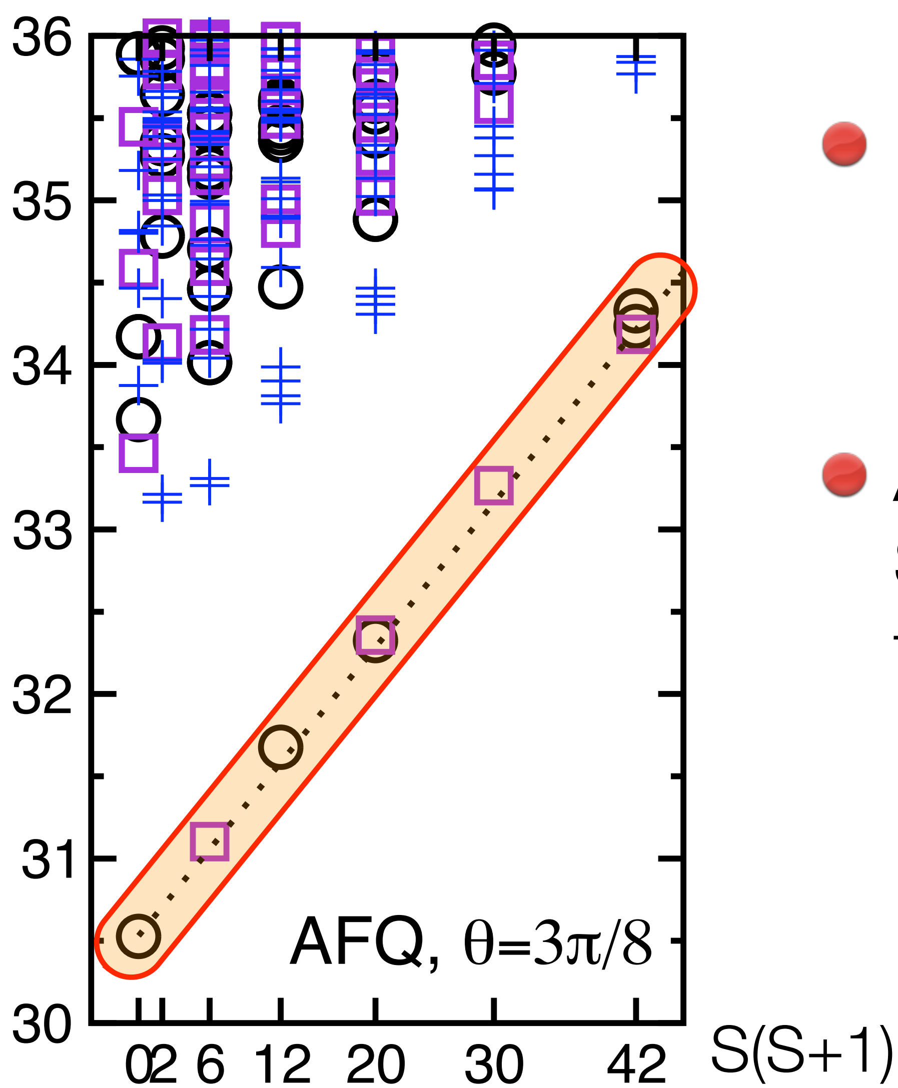
  number of states in TOS is *independent* of S.

# Tower of States
## S=1 on triangular lattice: Antiferroquadrupolar phase




- $\vartheta=3\pi/8$ : antiferroquadrupolar phase, finite quadrupolar moment, no spin order, three sublattice structure.




- Breaks translation symmetry. Tree site unit cell ⇒ nontrivial momenta must appear in TOS

- Antiferroquadrupolar order parameter, complicated S dependence. Can be calculated using group theoretical methods.

# Exact Diagonalization: Applications

- Quantum Magnets: nature of novel phases, critical points in 1D, dynamical correlation functions in 1D & 2D
- Fermionic models (Hubbard/t-J): gaps, pairing properties, correlation exponents, etc
- Fractional Quantum Hall states: energy gaps, overlap with model states, entanglement spectra
- Quantum dimer models or other constrained models (anyon chain..)
- Full Configuration Interaction in Quantum Chemistry

# Tower of states in a quantum dimer model

- We study the quantum dimer model on the square lattice

$$H = -\, t \sum_{\mathrm{plaq}} \left( |\,\mathbf{||}\,\rangle\langle\,\mathbf{=}\,| + \mathrm{H.c.} \right) + V \sum_{\mathrm{plaq}} \left( |\,\mathbf{||}\,\rangle\langle\,\mathbf{||}\,| + |\,\mathbf{=}\,\rangle\langle\,\mathbf{=}\,| \right)$$

- RK point (V/t=1) is gapless, all other points are believed to be confining, i.e. VBS phases.

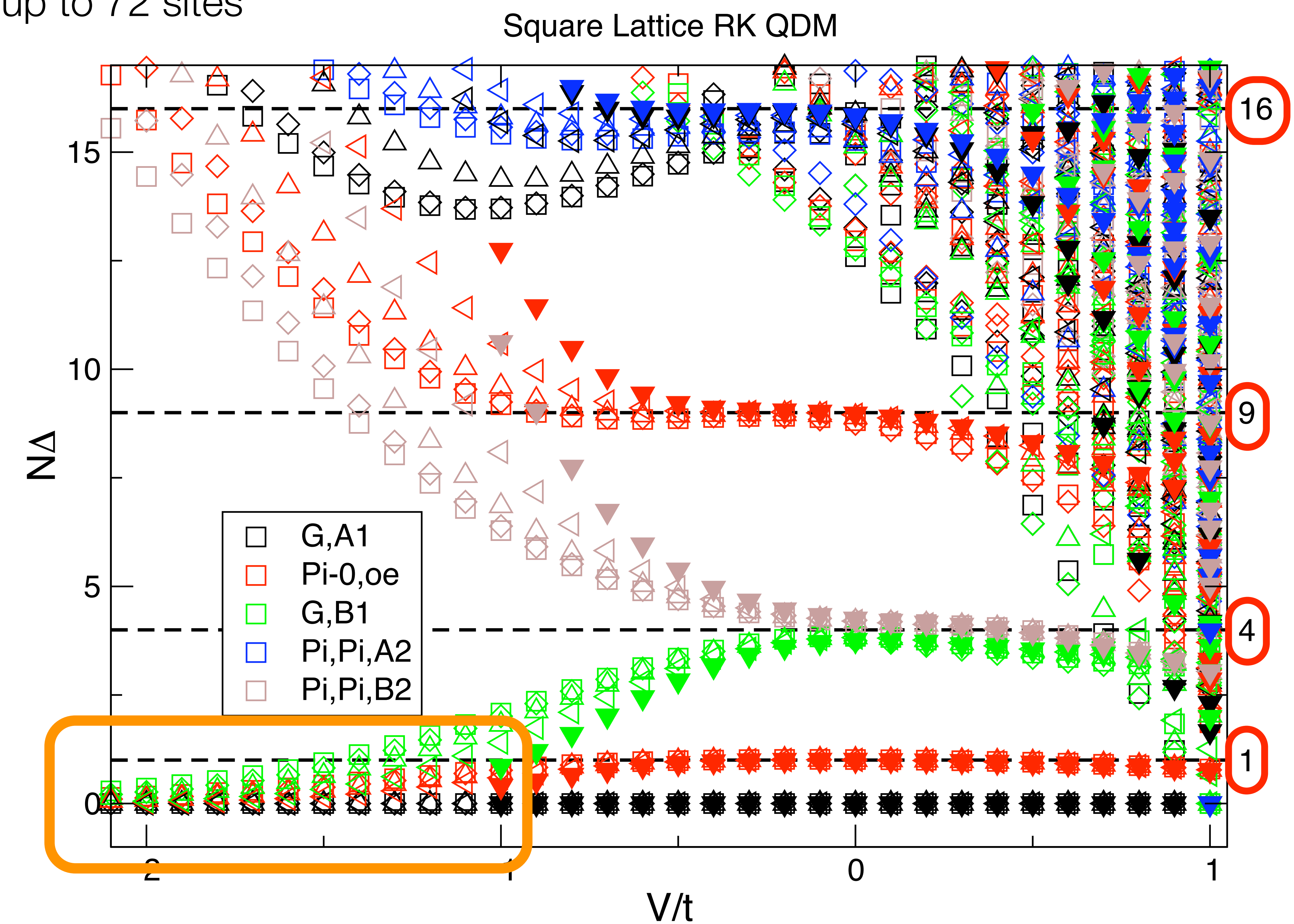
- For V/t very large and negative a columnar phase is expected.

- Still ongoing debate on the nature of phase(s) for -1 <V/t <1
  columnar, plaquette, mixed columnar-plaquette, ...
  Leung, Syljuasen, Poilblanc, ...

# Energy spectrum of the square lattice RK QDM

D. Schwandt, S. Capponi, AML

ED up to 72 sites

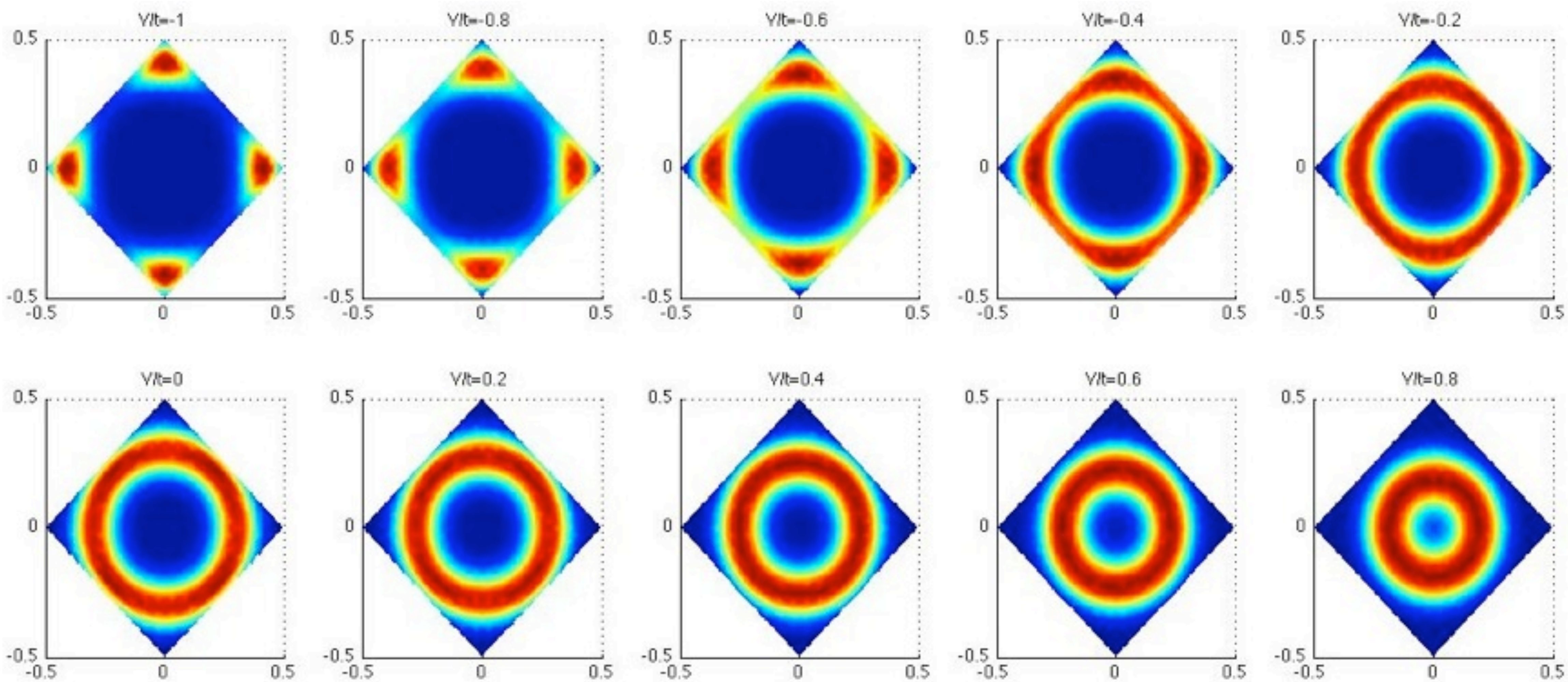



Collapse of levels associated to columnar VBS

Quadratic prefactor of 1/N

# U(1) Tower in a Dimer model

- Appearance of a divergent U(1) to VBS crossover length scale in dimer histograms upon approaching the RK point




- “Sz”$^2$ tower despite non-obvious “Sz” in dimer model

D. Schwandt, S. Capponi, AML

Thank you !