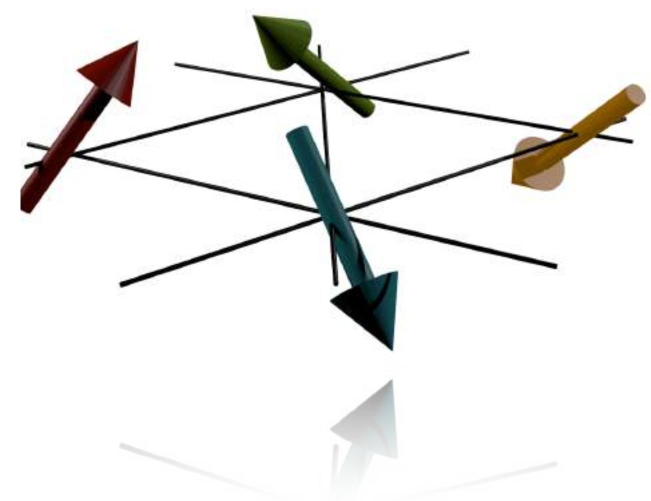
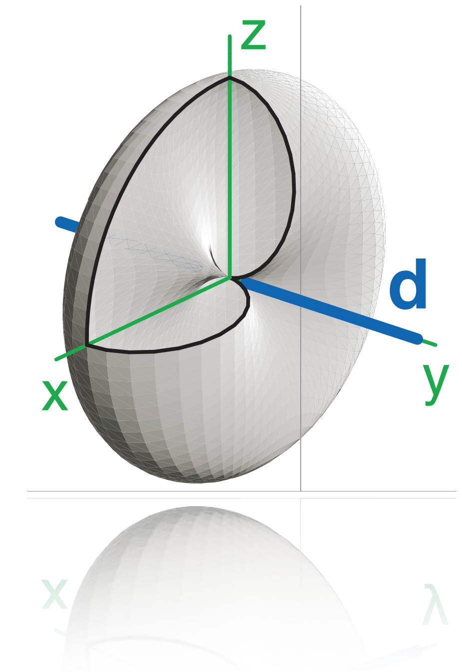
$$\mathcal{H}|\psi\rangle = E|\psi\rangle$$



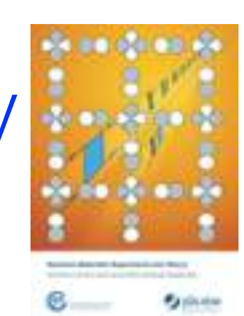



# Studying Continuous Symmetry Breaking with Exact Diagonalization

Andreas Läuchli
Institute for Theoretical Physics
University of Innsbruck, Austria

andreas.laeuchli@uibk.ac.at
http://laeuchli-lab.uibk.ac.at/group-page

Quantum Materials, Experiment & Theory
Correl 16, Jülich, 15.9.2016



# Outline of the lecture

- Short Overview on Exact Diagonalization
- Introduction to Continuous Symmetry Breaking, Lieb-Mattis Model
- General Formalism
- Many Examples …
- Outlook: other symmetry groups than SO(3), quantum critical points, …

# Outline of the lecture

- Short Overview on Exact Diagonalization
- Introduction to Continuous Symmetry Breaking, Lieb-Mattis Model
- General Formalism
- Many Examples …
- Outlook: other symmetry groups than SO(3), quantum critical points, …

# Exact Diagonalization: Main Idea

- Solve the Schrödinger equation of a quantum many body system numerically

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

- Sparse matrix, but for quantum many body systems the vector space dimension grows exponentially!

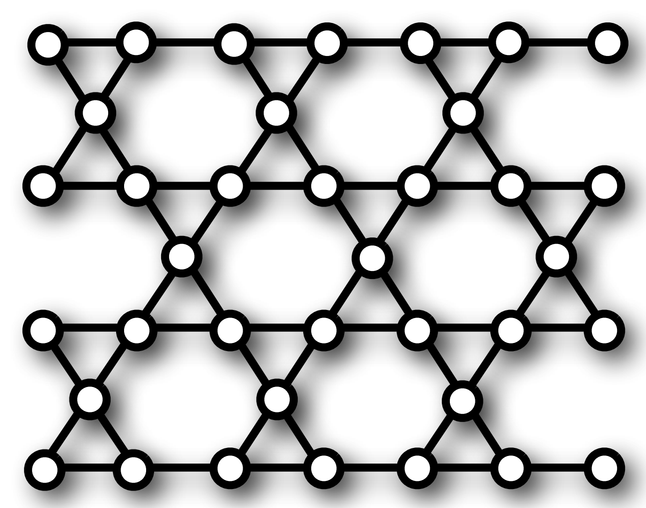
- Some people will tell you that's all there is.

- But if you want to get a maximum of physical information out of a finite system there is a lot more to do and the reward is a powerful:

**Quantum Mechanics Toolbox**

# Hilbert space sizes

- The Hilbert space of a quantum many body system grows exponentially in general
- For N spin 1/2 particles, the complete Hilbert space has dim=$2^N$ states
- 10 spins dim=1‘024
- 20 spins dim=1‘048‘576
- 30 spins dim=1‘073‘741‘824
- 40 spins dim=1’099’511’627’776
- 50 spins dim=1‘125‘899‘906‘842’624 ...
- The quantum mechanical wave function is a vector in this Hilbert (vector) space and we would like to know the ground state and a few other low lying eigenstates



○ $|\uparrow\rangle$ or $|\downarrow\rangle$

# Symmetries

- Consider a XXZ spin model on a lattice. What are the symmetries of the problem ?

$$H = \sum_{i,j} J^{xy}_{i,j} (S^x_i S^x_j + S^y_i S^y_j) + J^z_{i,j} S^z_i S^z_j$$

- The Hamiltonian conserves total $S^z$, we can therefore work within a given $S^z$ sector This easily implemented while constructing the basis, as we discussed before.

- The Hamiltonian is invariant under the space group, typically a few hundred elements. (in many cases = Translations x Pointgroup). Needs some technology to implement...

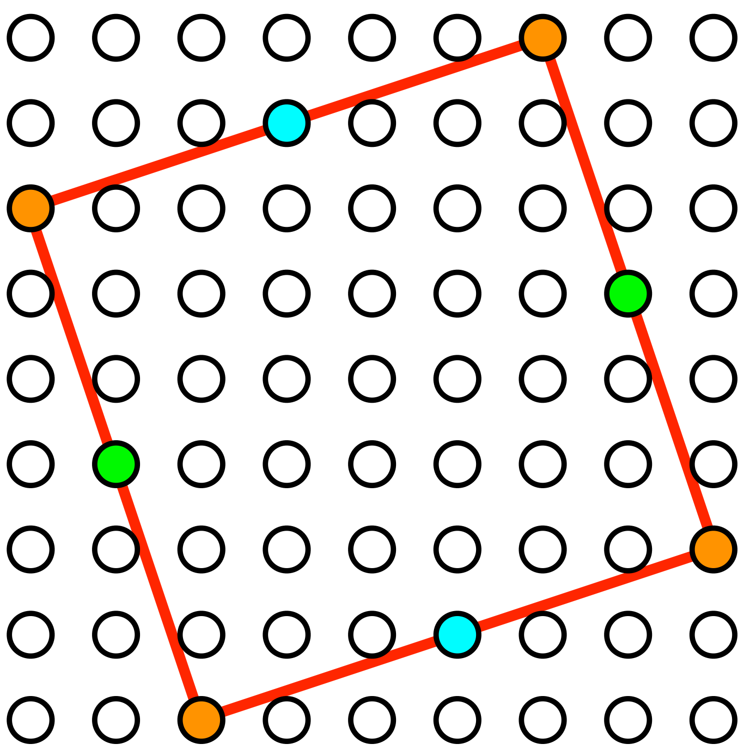
- At the Heisenberg point, the total spin is also conserved. It is however very difficult to combine the SU(2) symmetry with the lattice symmetries in a computationally useful way (non-sparse and computationally expensive matrices).

- At $S^z$=0 one can use the spin-flip (particle-hole) symmetry which distinguishes even and odd spin sectors at the Heisenberg point. Simple to implement.

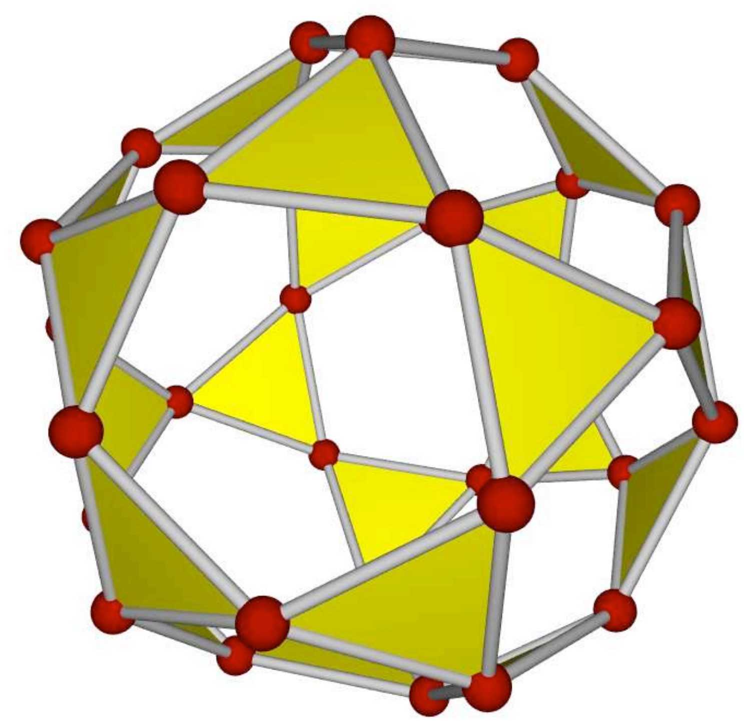
# Spatial Symmetries

- Spatial symmetries are important for reduction of Hilbert space
- Symmetry resolved eigenstates teach us a lot about the physics at work, dispersion of excitations, symmetry breaking tendencies, topological degeneracy, ... ⇒ more about this in the second lecture

40 sites square lattice
$T \otimes PG$ =40 x 4 elements



Icosidodecahedron (30 vertices)
$I_h$:120 elements



# 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, cluster spectra, etc
- Fractional Quantum Hall states: energy gaps, overlap with model states, entanglement spectra
- Quantum dimer models / constrained models (anyon chains, ...)
- Full Configuration Interaction in Quantum Chemistry, Nuclear structure
- Quantum Field Theory

# Exact Diagonalization: Present Day Limits

- Spin S=1/2 models:
  40 spins square lattice, 39 sites triangular, 42 sites Honeycomb lattice
  48 sites kagome lattice, soon 50-52 spins square lattice
  64 spins or more in elevated magnetization sectors
  up to ~500 billion basis states

- Fractional quantum hall effect
  different filling fractions ν, up to 16-20 electrons
  up to 3.5 billion basis states

- Hubbard models (~ Full CI in Quantum Chemistry)
  20 sites square lattice at half filling, 21 sites triangular lattice
  24 sites honeycomb lattice
  up to 160 billion basis states

low-lying eigenvalues, not full diagonalization

# Exact Diagonalization Literature

- N. Laflorencie & D. Poilblanc,
  *"Simulations of pure and doped low-dimensional spin-1/2 gapped systems"*
  Lecture Notes in Physics **645**, 227 (2004).

- R.M. Noack & S. Manmana,
  *"Diagonalization- and Numerical Renormalization-Group-Based Methods for Interacting Quantum Systems"*,
  AIP Conf. Proc. **789**, 93 (2005).

- A. Weisse, H. Fehske
  *"Exact Diagonalization Techniques"*
  Lecture Notes in Physics 739, 529 (2008).

- A. Läuchli
  *"Numerical Simulations of Frustrated Systems"*
  in "Highly Frustratred Magnetism", Springer, Eds. Lacroix, Mendels, Mila, (2011).
  available upon e-mail request.

# Outline of the lecture

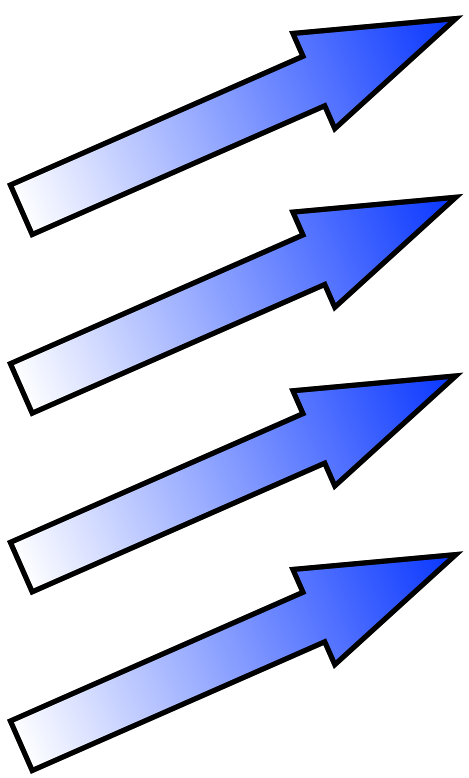
- Short Overview on Exact Diagonalization
- Introduction to Continuous Symmetry Breaking, Lieb-Mattis Model
- General Formalism
- Many Examples …
- Outlook: other symmetry groups than SO(3), quantum critical points, …

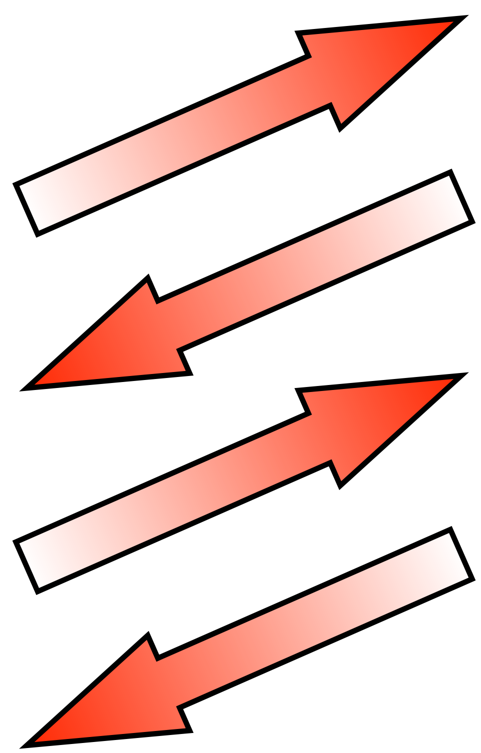
# “Tower of States” spectroscopy

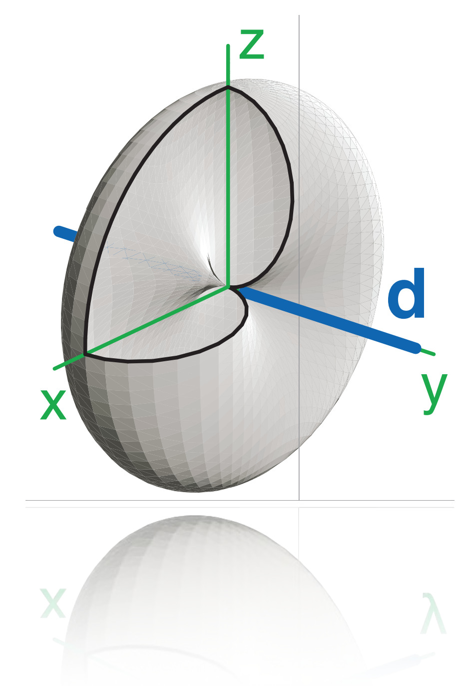
- What are the finite size manifestations of a continuous symmetry breaking ?
  (eg in superfluids/superconductors, magnetic order, spin nematic order)

- Order parameter is zero on a finite system ! (symmetric partition function)

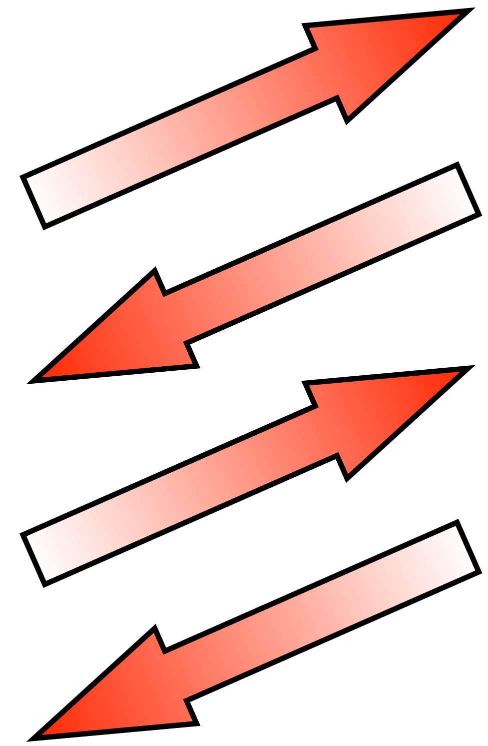
- So usually one looks into order parameter correlations [(order parameter)$^2$]







# “Tower of States” spectroscopy

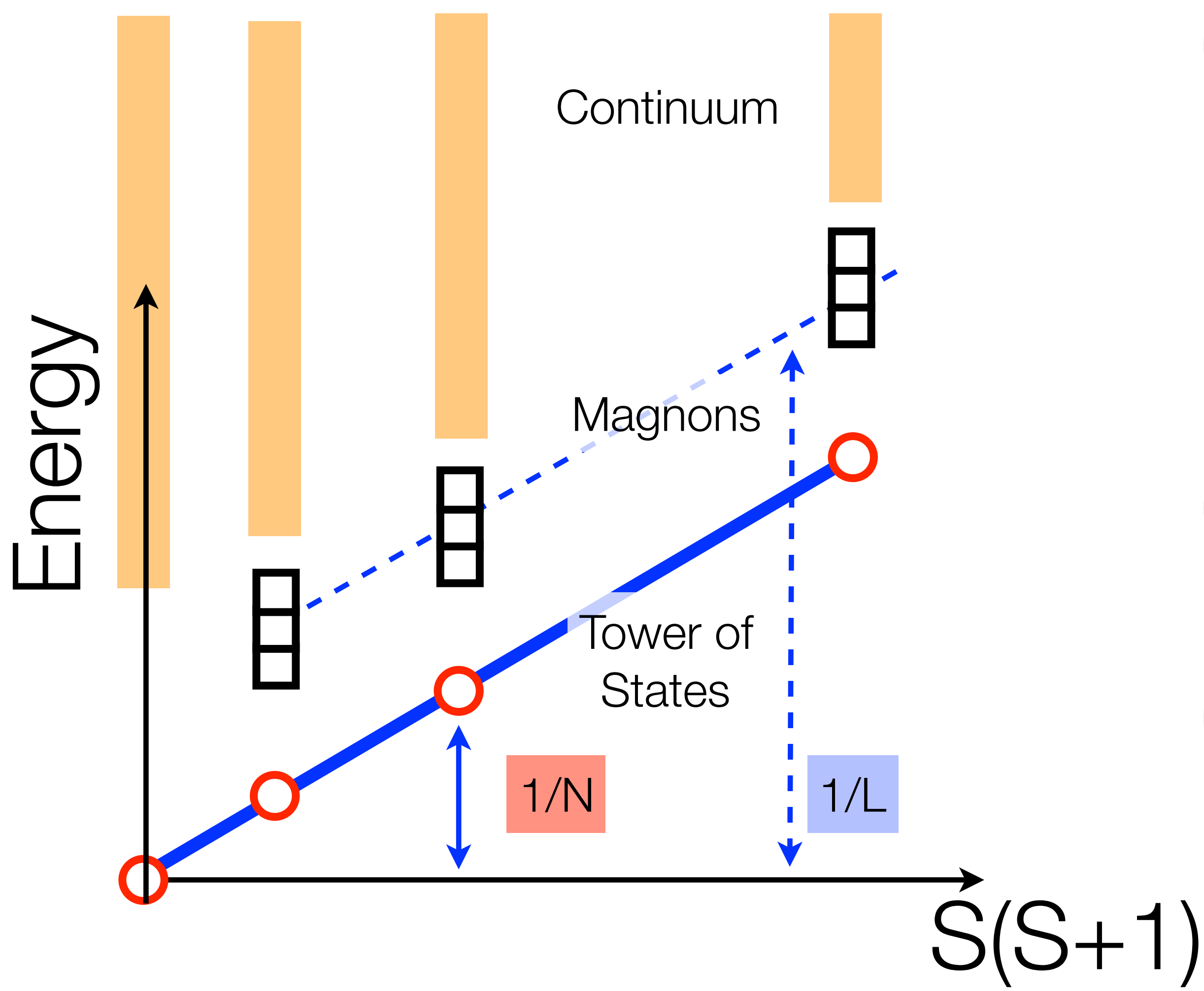


- Order parameter is not a conserved quantity
- Order parameter is zero on a finite size sample (Wigner-Eckart)
- How does one get spontaneous symmetry breaking anyway ?
- Ground state degeneracy is building up as we approach the thermodynamic limit, which will allow to form a symmetry breaking wave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



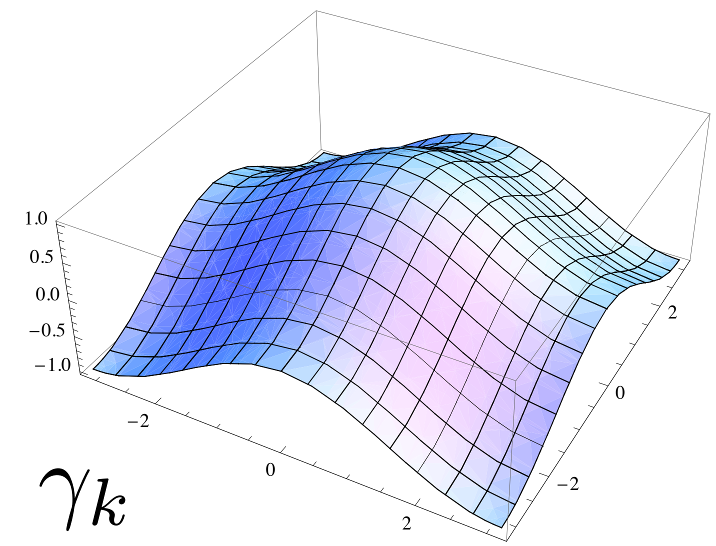

- Dynamics of the free order parameter is visible in the finite size spectrum. Depends on the continuous symmetry group. ED is good at spectra.

- 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.

# Toy model: from square lattice Heisenberg antiferromagnet to the Lieb-Mattis model

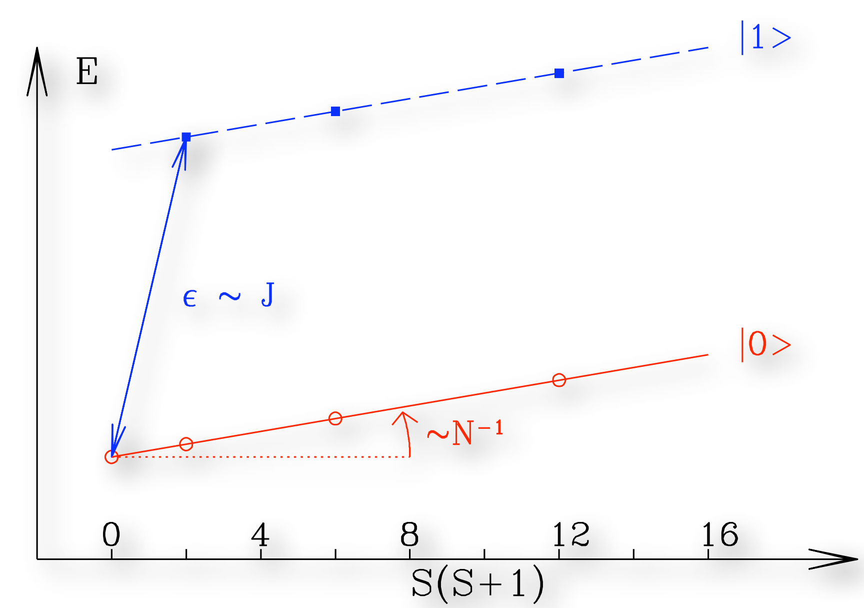
- Hamiltonian $$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$
- Fourier transform $$H = 2J \sum_{k} \gamma_k \, \mathbf{S}_k \cdot \mathbf{S}_{-k}$$




$\gamma_k$

- Keep only the (0,0) and (π,π) mode
- Lieb Mattis model recovered

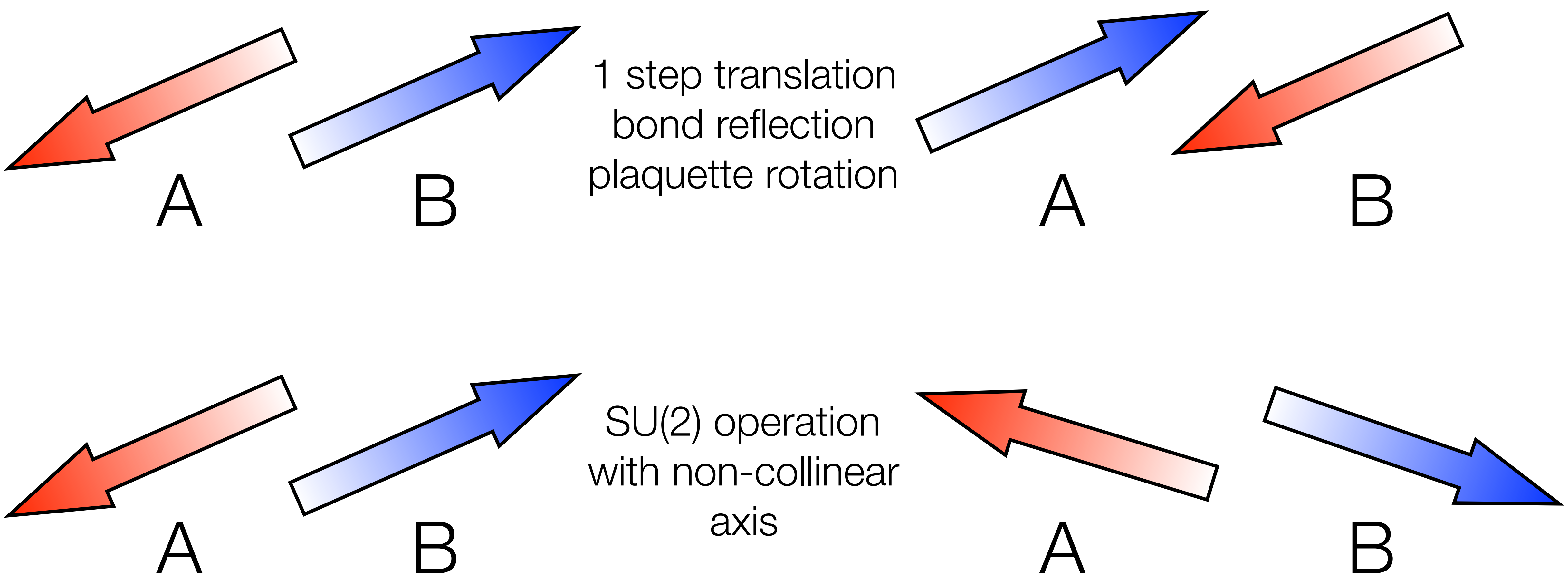
$$H_0 = \frac{4J}{N}(S_{\rm tot}^2 - S_A^2 - S_B^2)$$




C. Lhuillier, cond-mat/0502464

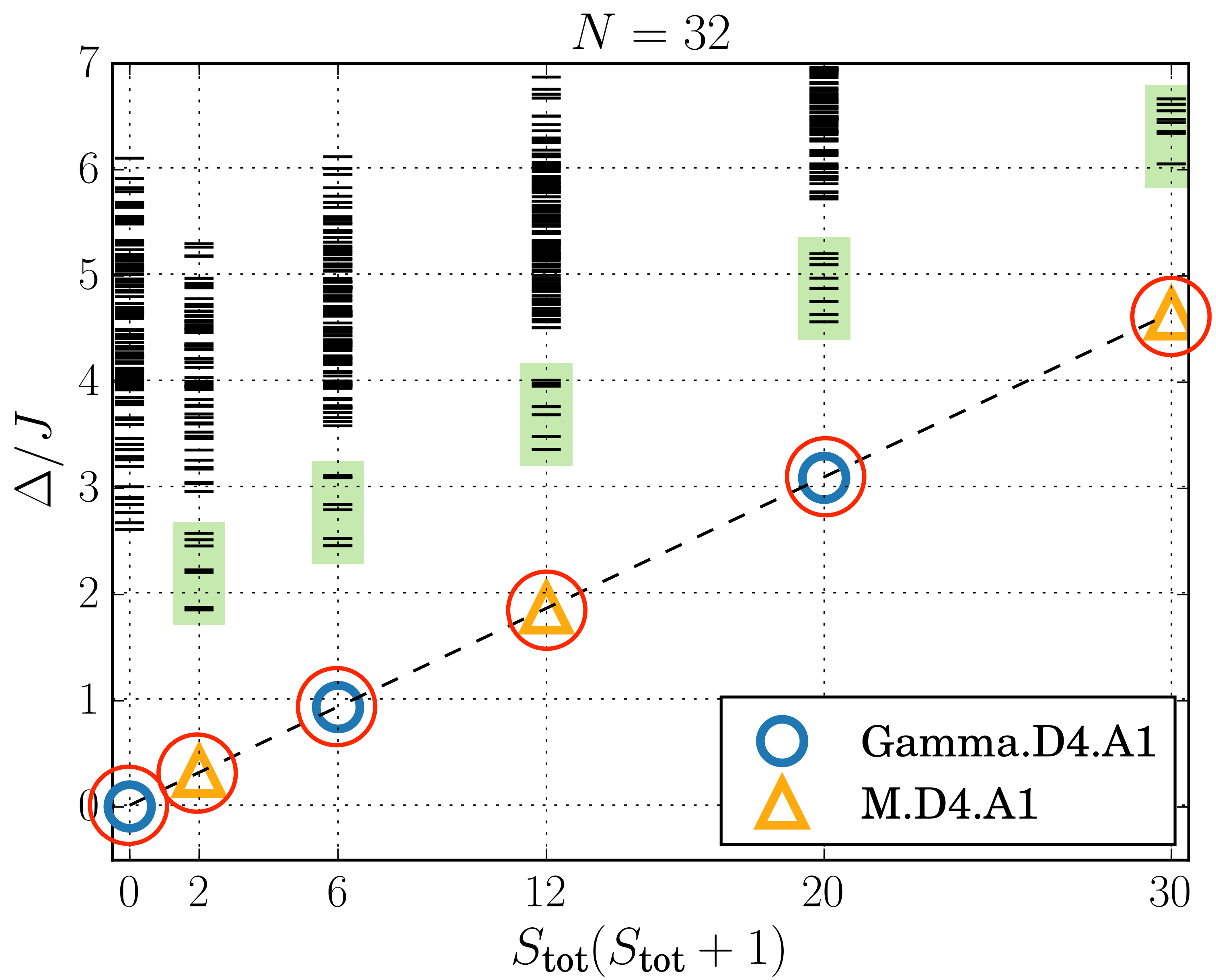
# Symmetry decomposition of order parameter

- Order parameter manifold forms a representation space for the symmetry group of the Hamiltonian (more details later)
- 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
    - ...




actual ED results for square lattice Heisenberg model

# Outline of the lecture

- Short Overview on Exact Diagonalization
- Introduction to Continuous Symmetry Breaking, Lieb-Mattis Model
- General Formalism
- Many Examples …
- Outlook: other symmetry groups than SO(3), quantum critical points, …

# General Formalism for Symmetry Decomposition

- Ground state manifold: span of all $|\psi_{\mathrm{GS}}\rangle$ a *prototypical state* (e.g. product state)

$$V_{\mathrm{GS}} = \mathrm{span}\left\{|\psi^i_{\mathrm{GS}}\rangle\right\}$$

where $|\psi^i_{\mathrm{GS}}\rangle$ are the degenerate ground states in the thermodynamic limit. This space is finite dimensional for discrete symmetry breaking and infinite dim. for continuous symmetry breaking.

- The symmetry group acts nontrivially within this subspace (prototypical states “break” symmetries), it forms a (reducible) representation $\Gamma$

$$\begin{aligned} \mathit{\Gamma} :& \mathcal{G} \to \mathrm{Aut}(V_{\mathrm{GS}}) \\ & g \mapsto \left(\langle\psi^i_{\mathrm{GS}}|O_g|\psi^j_{\mathrm{GS}}\rangle\right)_{i,j} \end{aligned}$$

$$\mathit{\Gamma} = \bigoplus_\rho n_\rho \rho$$

- The representation can be decomposed into irreducible representations of the symmetry group according to standard group theory formula:

$$n_\rho = \frac{1}{|\mathcal{G}|}\sum_{g\in\mathcal{G}} \overline{\chi_\rho(g)}\,\mathrm{Tr}(\mathit{\Gamma}(g))$$

# General Formalism: Simplification using “stabiliser”

- General action

$$\Gamma : \mathcal{G} \to \mathrm{Aut}(V_{\mathrm{GS}})$$
$$g \mapsto \left(\langle \psi^i_{\mathrm{GS}} | O_g | \psi^j_{\mathrm{GS}} \rangle\right)_{i,j}$$

- Often we have

$$\langle \psi_{\mathrm{GS}} | O_g | \psi'_{\mathrm{GS}} \rangle = \begin{cases} 1 \text{ if } O_g \left|\psi'_{\mathrm{GS}}\right\rangle = \left|\psi_{\mathrm{GS}}\right\rangle \\ 0 \text{ otherwise} \end{cases}$$

i.e. ~ Permutation matrix

- Then we can simplify the representation reduction formula

$$n_\rho = \frac{1}{|\mathrm{Stab}(|\psi_{\mathrm{GS}}\rangle)|} \sum_{g \in \mathrm{Stab}(|\psi_{\mathrm{GS}}\rangle)} \chi_\rho(g)$$

using the “stabiliser” subgroup concept

$$\mathrm{Stab}(|\psi_{\mathrm{GS}}\rangle) \equiv \{ g \in \mathcal{G} : \; O_g \left|\psi_{\mathrm{GS}}\right\rangle = \left|\psi_{\mathrm{GS}}\right\rangle \}$$

- we only need:
  - the stabilizer $\mathrm{Stab}(|\psi_{\mathrm{GS}}\rangle)$ of a prototypical state $|\psi_{\mathrm{GS}}\rangle$ in the groundstate manifold
  - the characters of the irreducible representations of the symmetry group $\mathcal{G}$

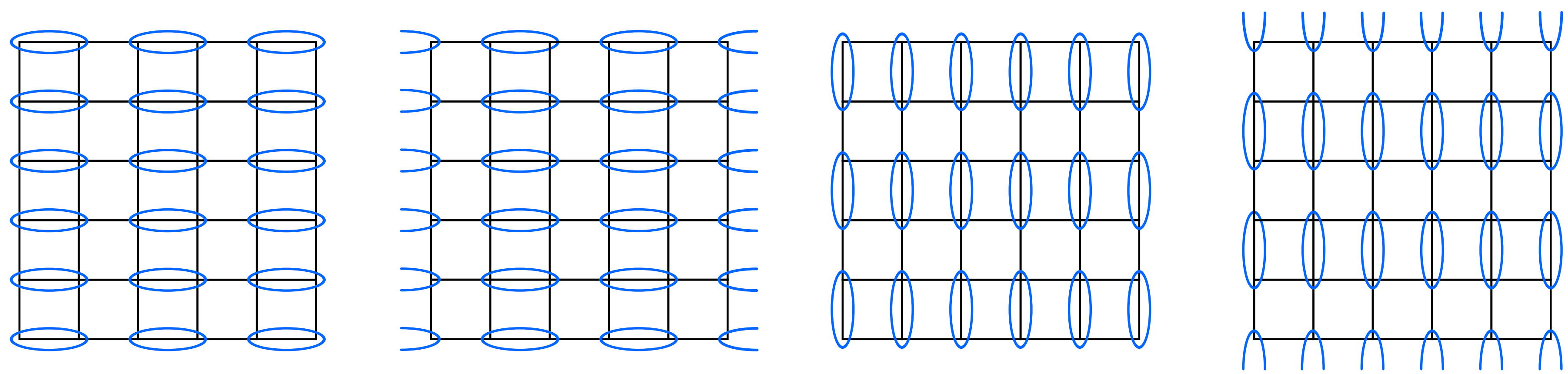
# Outline of the lecture

- Short Overview on Exact Diagonalization
- Introduction to Continuous Symmetry Breaking, Lieb-Mattis Model
- General Formalism
- Many Examples …
- Outlook: other symmetry groups than SO(3), quantum critical points, …

# First a simple example:
# Discrete Symmetry Breaking

| Irreps | cVBS | sVBS |
|---|---|---|
| $(0,0)$ A | 1 | 1 |
| $(0,0)$ B | 1 | 1 |
| $(\pi,0)$ A | 1 | 0 |
| $(0,\pi)$ A | 1 | 0 |
| $(\pi,\pi)\mathrm{E}_a$ | 0 | 1 |
| $(\pi,\pi)\mathrm{E}_b$ | 0 | 1 |

- Columnar Dimer Valence Bond Crystal (4 different singlet states) occurs in Quantum Dimer models and some frustrated quantum magnets



$$\mathcal{G} = \mathcal{D} = \mathcal{T} \times \mathrm{PG} \qquad \mathbf{t}_1 = (0,0), \quad \mathbf{t}_x = (1,0), \quad \mathbf{t}_y = (0,1), \quad \mathbf{t}_{xy} = (1,1) \qquad \mathrm{PG} = \mathrm{C}_4$$

$$\chi_{\mathbf{k}}(t) = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{t}}$$

| $\mathrm{C}_4$ | 1 | $C_4$ | $C_2$ | $(C_4)^3$ |
|---|---|---|---|---|
| A | +1 | +1 | +1 | +1 |
| B | +1 | -1 | +1 | -1 |
| $\mathrm{E}_a$ | +1 | +i | -1 | -i |
| $\mathrm{E}_b$ | +1 | -i | -1 | +i |

Table 1: Character table for pointgroup $\mathbf{C}_4$.

$\mathrm{Stab}(|\Psi_{cVBS}\rangle) = \{1 \times 1\} \cup \{1 \times C_2\} \cup \{t_y \times 1\} \cup \{t_y \times C_2\}$
where $C_2$ denotes the rotation about an angle $\pi$ around the center of a plaquette.

$$n_{(\pi,0)A} = \frac{1}{|\mathrm{Stab}(|\Psi_{cVBS}\rangle)|} \sum_{d \in \mathrm{Stab}(|\Psi_{cVBS}\rangle)} \chi_A(d)\chi_{\mathbf{k}=(\pi,0)}(d)$$

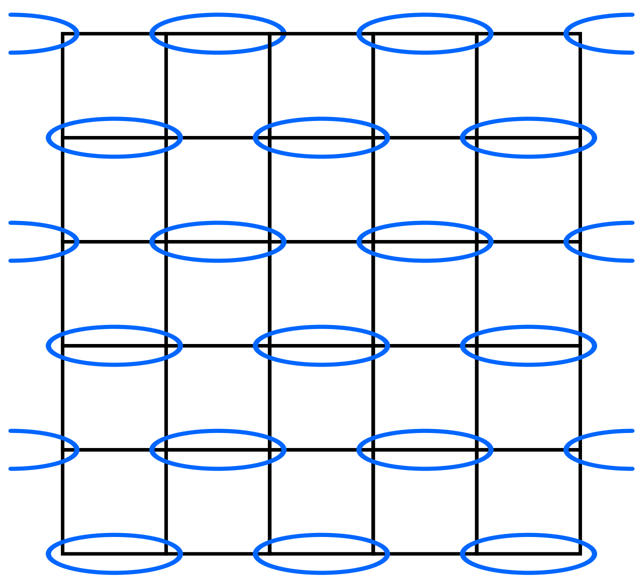
$$= \frac{1}{4}\left[1\ e^{i\mathbf{k}\cdot(0,0)} + 1\ e^{i\mathbf{k}\cdot(0,0)} + 1\ e^{i\mathbf{k}\cdot(0,1)} + 1\ e^{i\mathbf{k}\cdot(0,1)}\right] = 1$$

$$n_{(\pi,0)B} = \frac{1}{|\mathrm{Stab}(|\Psi_{cVBS}\rangle)|} \sum_{d \in \mathrm{Stab}(|\Psi_{cVBS}\rangle)} \chi_B(d)\chi_{\mathbf{k}=(\pi,0)}(d)$$

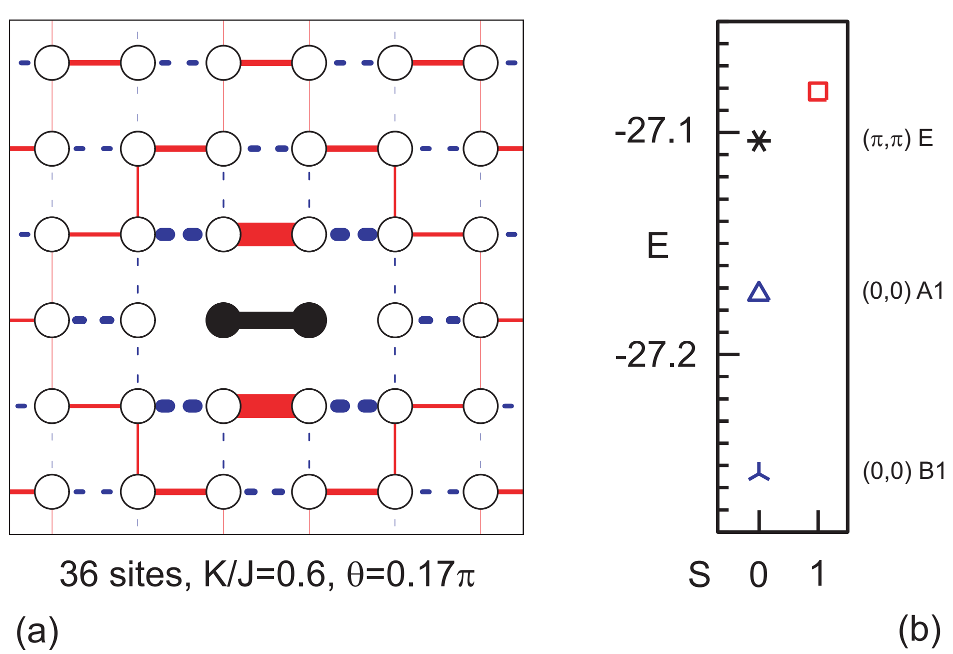
$$= \frac{1}{4}\left[1\ e^{i\mathbf{k}\cdot(0,0)} + (-1)\ e^{i\mathbf{k}\cdot(0,0)} + 1\ e^{i\mathbf{k}\cdot(0,1)} + (-1)\ e^{i\mathbf{k}\cdot(0,1)}\right] = 0$$

# First a simple example:
# Discrete Symmetry Breaking

- Staggered Valence Bond Crystal, also fourfold degenerate



| Irreps | cVBS | sVBS |
| --- | --- | --- |
| $(0,0)$ A | 1 | 1 |
| $(0,0)$ B | 1 | 1 |
| $(\pi,0)$ A | 1 | 0 |
| $(0,\pi)$ A | 1 | 0 |
| $(\pi,\pi)\mathrm{E}_a$ | 0 | 1 |
| $(\pi,\pi)\mathrm{E}_b$ | 0 | 1 |




Found in a ring-exchange model:
AML *et al*, PRL 2005

# Continuous Symmetry Breaking
# Collinear magnetic order

- collinear magnetic order: spins are all (anti)parallel to a common axis in spin space

$$|\psi\rangle = |\uparrow\downarrow\uparrow\downarrow\cdots\rangle$$

- (simplified) square lattice space group, SO(3) spin symmetry group

$$\mathcal{G} = \mathcal{D} \times \mathcal{C} \qquad \mathcal{D} = \mathbb{Z}_2 \times \mathbb{Z}_2 = \{1, t_x, t_y, t_{xy}\} \qquad \mathcal{C} = \mathrm{SO}(3)$$

- Ground state manifold $\qquad V_{\mathrm{GS}} = \{O_g\,|\psi\rangle\,;\, g \in \mathcal{G}\}$

- Stabilizer of a single Néel state:

  - No translation in real space or a diagonal $t_{xy}$ translation together with a spin rotation $R_z(\alpha)$ around the $z$-axis with an arbitrary angle $\alpha$.
  - Translation by one site, $t_x$ or $t_y$, followed by a rotation $R_a(\pi)$ of $180°$ around an axis $a \perp z$ perpendicular to the $z$-axis.

$$\mathrm{Stab}(|\psi\rangle) = \{1 \times R_z(\alpha)\} \cup \{t_{xy} \times R_z(\alpha)\} \cup \{t_x \times R_a(\pi)\} \cup \{t_y \times R_a(\pi)\}$$

# Continuous Symmetry Breaking
# Collinear magnetic order

- Irreducible representations of the symmetry group

$$\chi_{\mathbf{k}}(t) = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{t}} \qquad \mathbf{k} \in \{(0,0),\ (0,\pi),\ (\pi,0),\ (\pi,\pi)\} \qquad \chi_S(R) = \frac{\sin\left[(S+\frac{1}{2})\phi\right]}{\sin\frac{\phi}{2}}$$

- Multiplicity of irreducible representations (general formula)

$$\begin{aligned} n_{(\mathbf{k},S)} =& e^{i\mathbf{k}\cdot 0}\frac{1}{4\,|R_z(\alpha)|}\int_0^{2\pi} d\alpha\chi_S(R_z(\alpha)) + e^{i\mathbf{k}\cdot(\mathbf{e}_x+\mathbf{e}_y)}\frac{1}{4\,|R_z(\alpha)|}\int_0^{2\pi} d\alpha\chi_S(R_z(\alpha)) \\ &+ e^{i\mathbf{k}\cdot\mathbf{e}_x}\frac{1}{4\,|R_a(\pi)|}\int_0^{2\pi} d\alpha\chi_S(R_a(\pi)) + e^{i\mathbf{k}\cdot\mathbf{e}_y}\frac{1}{4\,|R_a(\pi)|}\int_0^{2\pi} d\alpha\chi_S(R_a(\pi)) \end{aligned}$$

- evaluated for the present case (details in lecture notes)

$$n_{((0,0),S)} = \frac{1}{4}\left(1\cdot 1 + 1\cdot 1 + 1\cdot(-1)^S + 1\cdot(-1)^S\right) = \begin{cases} 1 \text{ if } S \text{ even} \\ 0 \text{ if } S \text{ odd} \end{cases}$$

$$n_{((\pi,\pi),S)} = \frac{1}{4}\left(1\cdot 1 + 1\cdot 1 - 1\cdot(-1)^S - 1\cdot(-1)^S\right) = \begin{cases} 0 \text{ if } S \text{ even} \\ 1 \text{ if } S \text{ odd} \end{cases}$$

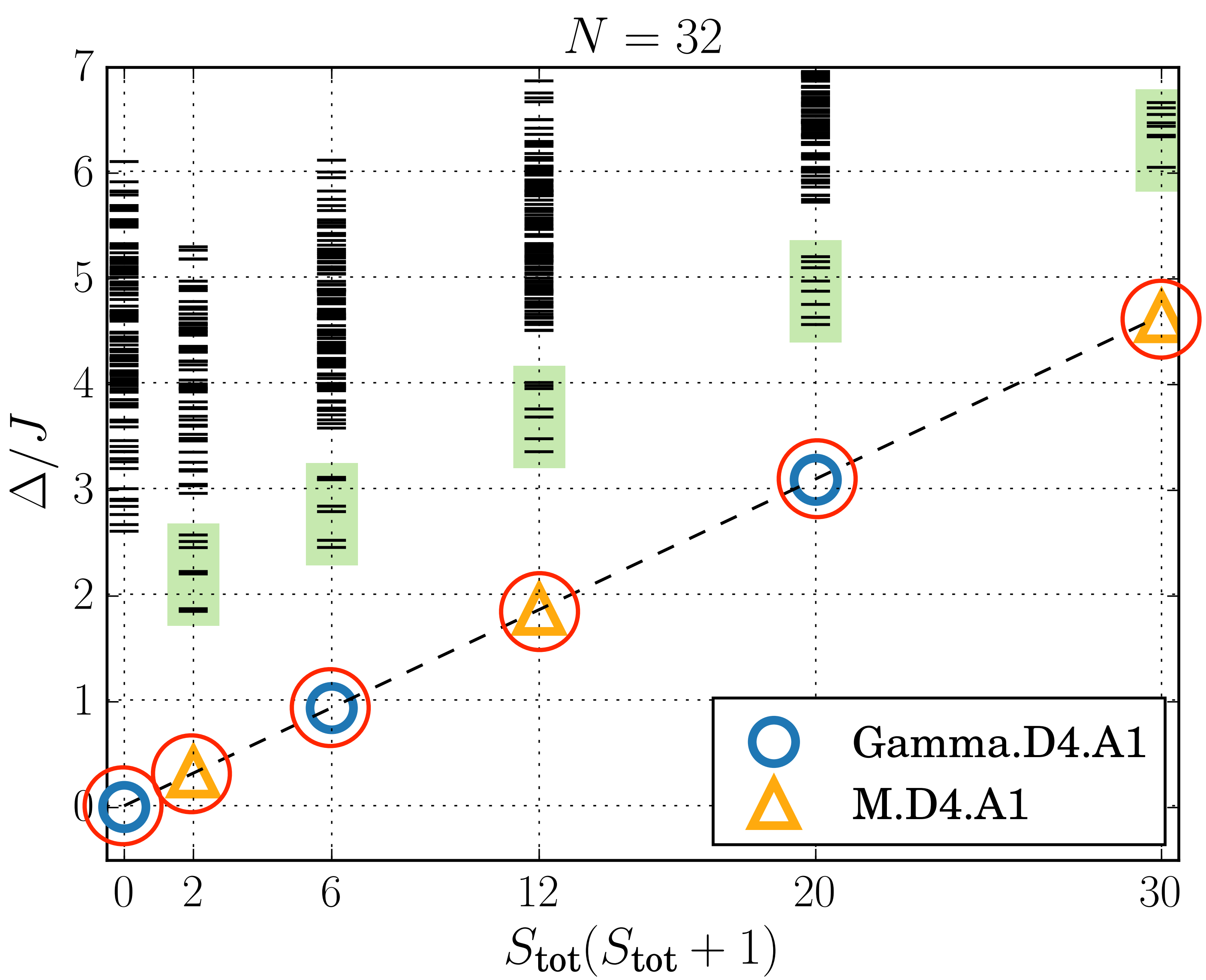
$$n_{((0,\pi),S)} = \frac{1}{4}\left(1\cdot 1 - 1\cdot 1 + 1\cdot(-1)^S - 1\cdot(-1)^S\right) = 0$$

$$n_{((\pi,0),S)} = \frac{1}{4}\left(1\cdot 1 - 1\cdot 1 - 1\cdot(-1)^S + 1\cdot(-1)^S\right) = 0$$

| $S$ | $\Gamma$.A1 | $M$.A1 |
|---|---|---|
| 0 | 1 | 0 |
| 1 | 0 | 1 |
| 2 | 1 | 0 |
| 3 | 0 | 1 |

# Continuous Symmetry Breaking
# Collinear magnetic order

- Exact Diagonalization for a N=32 site square lattice Heisenberg model

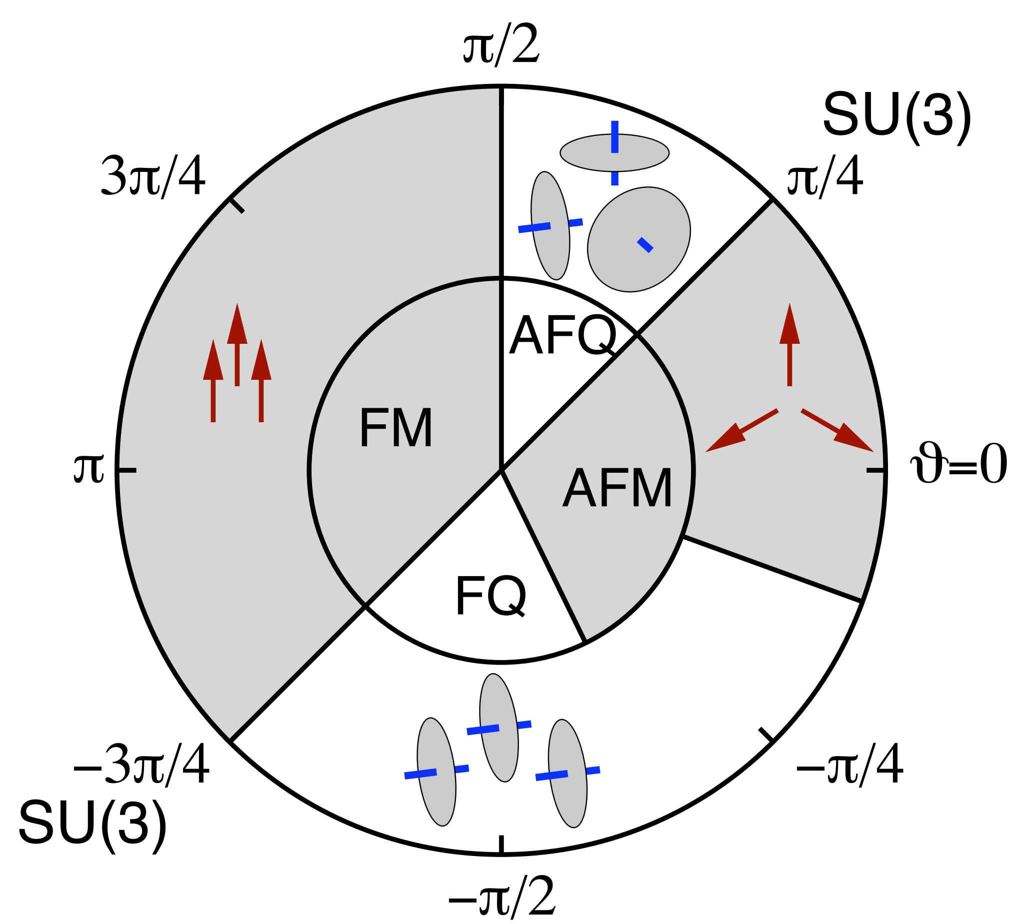



| $S$ | $\Gamma$.A1 | $M$.A1 |
|---|---|---|
| 0 | 1 | 0 |
| 1 | 0 | 1 |
| 2 | 1 | 0 |
| 3 | 0 | 1 |

# Beyond the collinear Neel state

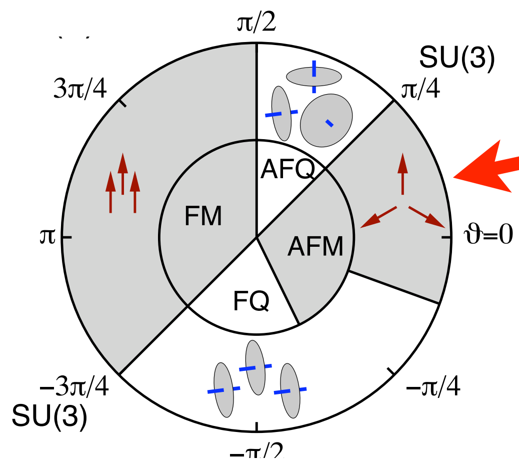
- Bilinear-biquadratic S=1 model on the triangular lattice (model for $NiGaS_4$).

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

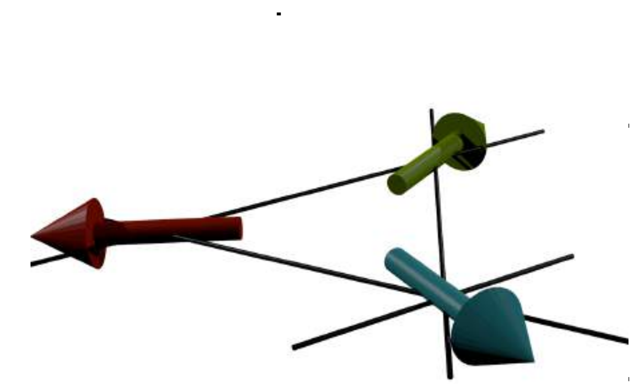


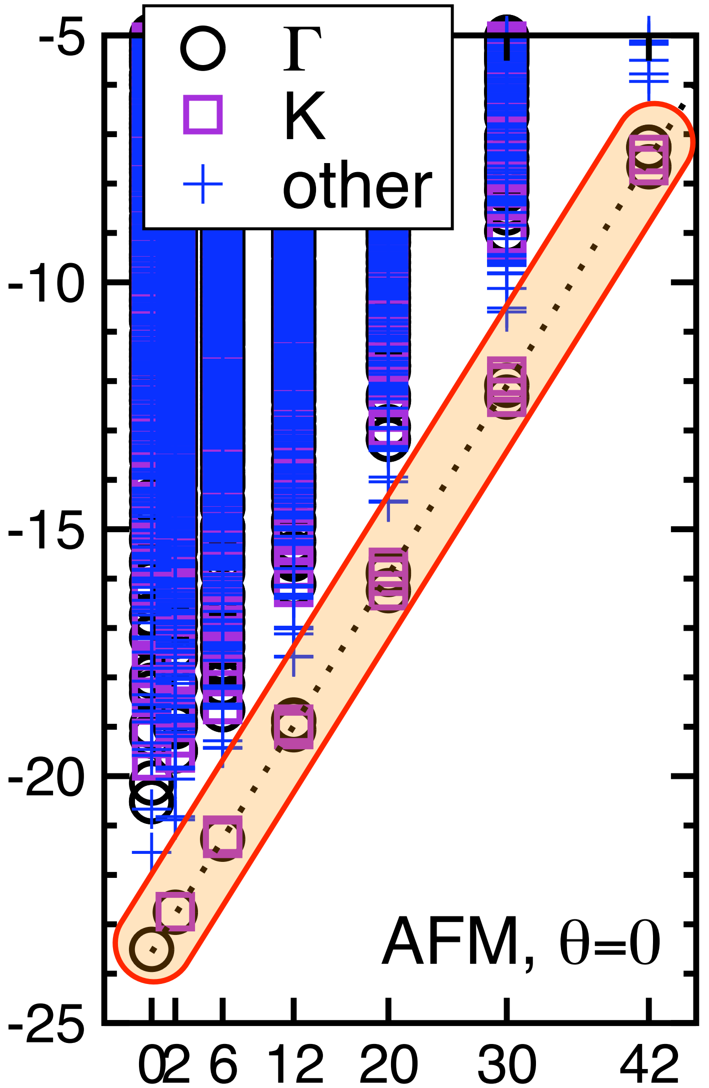

AML, F. Mila, K. Penc, PRL ‘06

# 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

120° Néel

| S | $\Gamma$.A1 | $\Gamma$.B1 | $K$.A1 |
|---|---|---|---|
| 0 | 1 | 0 | 0 |
| 1 | 0 | 1 | 1 |
| 2 | 1 | 0 | 2 |
| 3 | 1 | 2 | 2 |

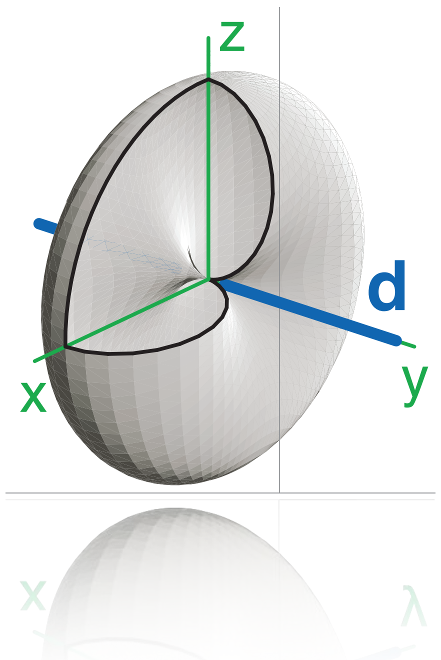
- non-collinear magnetic structure
  ⇒ SU(2) is completely broken,

  number of levels in TOS increases with S

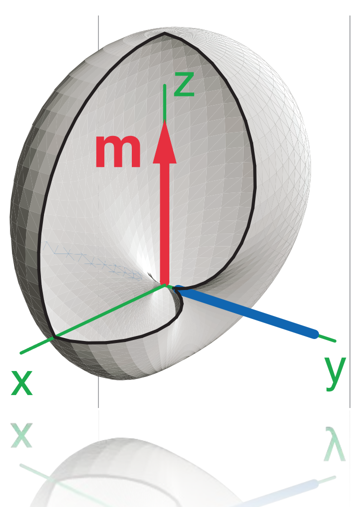
- Quantum numbers are identical to the S=1/2 case

# Spin Quadrupolar Order

Andreev & Grishchuk, Chubukov, Papanicolaou




pure quadrupole




polarized quadrupole

- Order parameter is not a vector as usual, but instead a tensor of rank two.
- Belongs to the class of spin nematic states, i.e. $\langle \mathbf{S}_i \rangle = 0$ , but SU(2) is broken nevertheless.
- Single site example: $|S^y = 0\rangle$, S=1

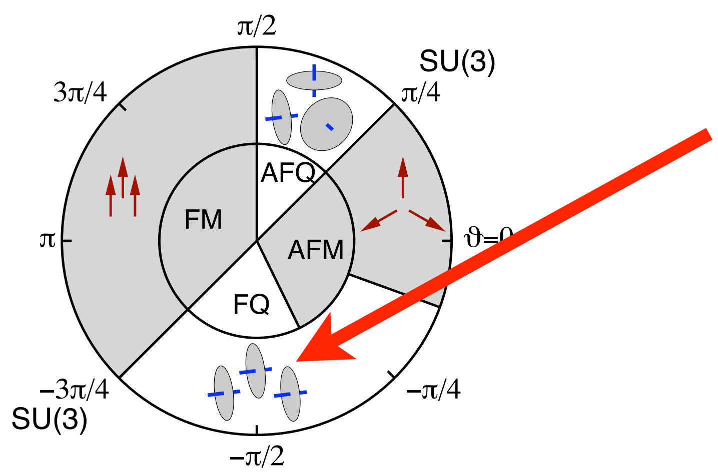
$$\langle S^\alpha \rangle = 0$$

- anisotropic fluctuations break SU(2) symmetry

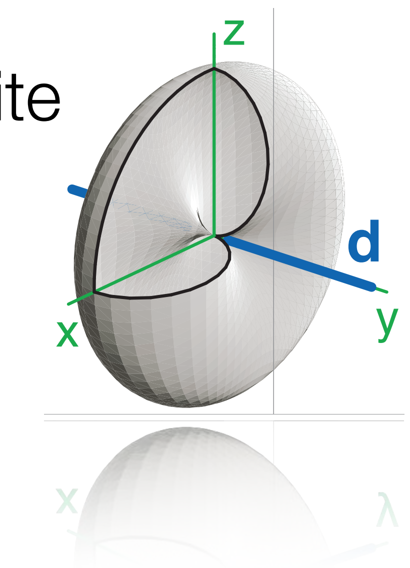
$$\langle (S^y)^2 \rangle = 0 \qquad \langle (S^{x,z})^2 \rangle \neq 0$$

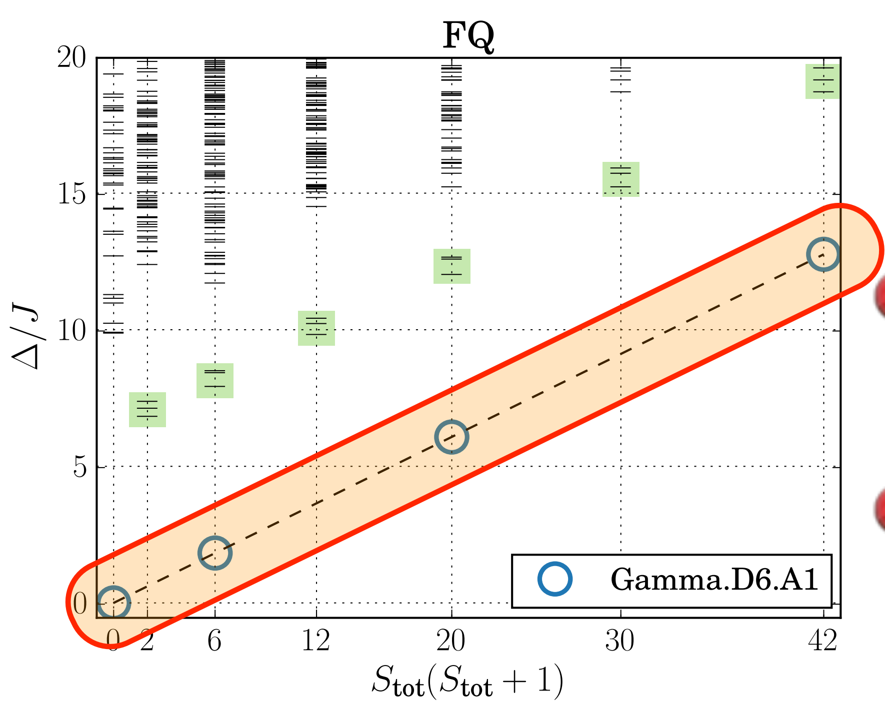
# Tower of States

## S=1 on triangular lattice: Ferroquadrupolar phase




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




- No spatial symmetry breaking.
  ⇒ only trivial spatial irrep appears in TOS

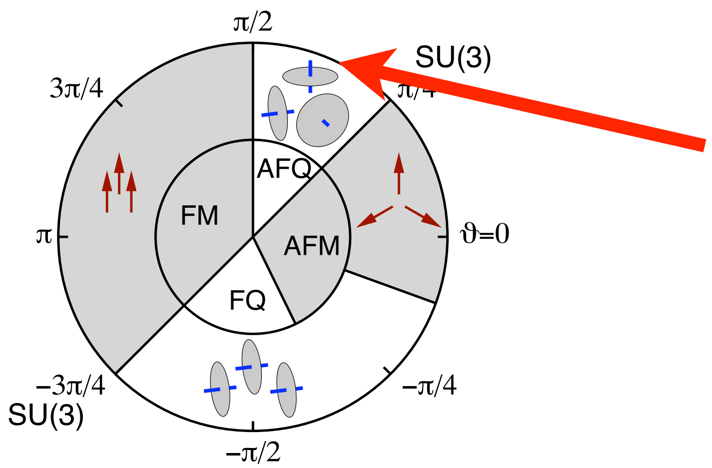
- Ferroquadrupolar order parameter, only even S

- all directors are collinear
  ⇒ SU(2) is broken down to U(1),

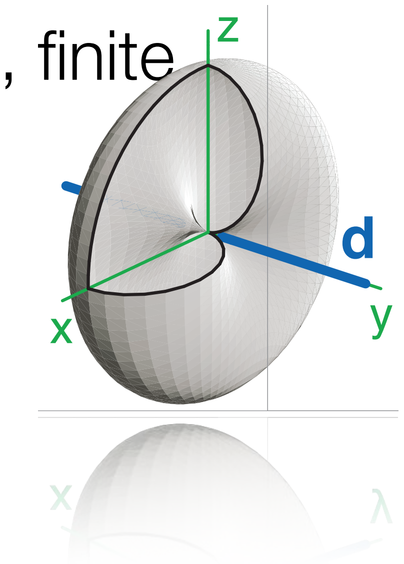
number of states in TOS is *independent* of S.

S(S+1)

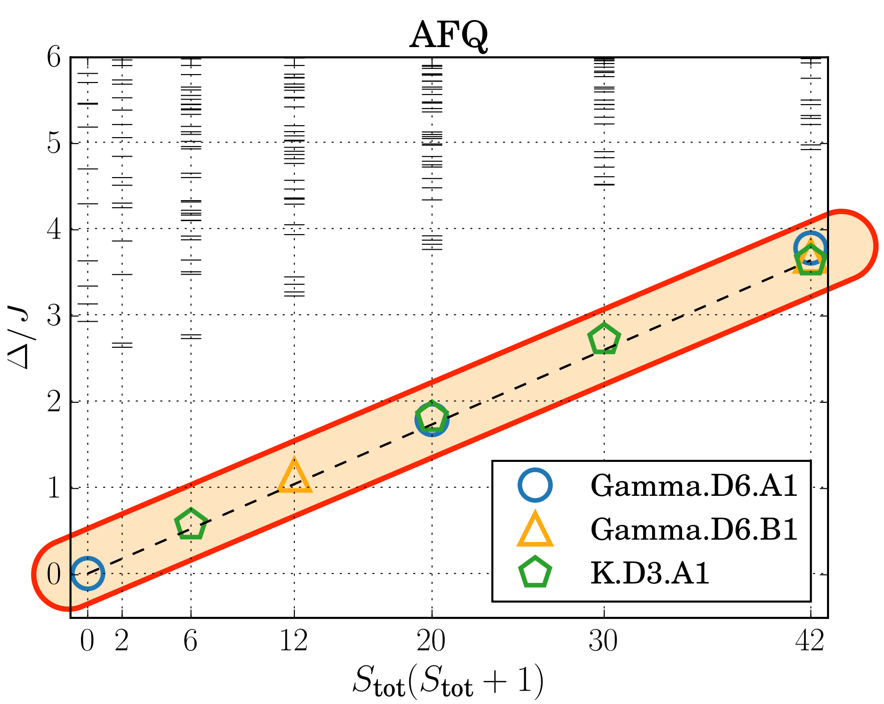
# Tower of States
# S=1 on triangular lattice: Antiferroquadrupolar phase




- ϑ=3π/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.

AFQ

| S | $\Gamma$.A1 | $\Gamma$.B1 | $K$.A1 |
|---|---|---|---|
| 0 | 1 | 0 | 0 |
| 1 | 0 | 0 | 0 |
| 2 | 0 | 0 | 1 |
| 3 | 0 | 1 | 0 |

S(S+1)

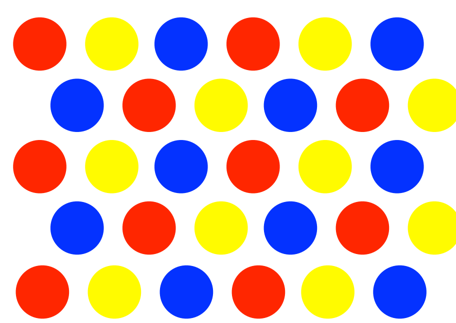
# Outline of the lecture

- Short Overview on Exact Diagonalization
- Introduction to Continuous Symmetry Breaking, Lieb-Mattis Model
- General Formalism
- Many Examples …
- Outlook: other symmetry groups than SO(3), quantum critical points, …

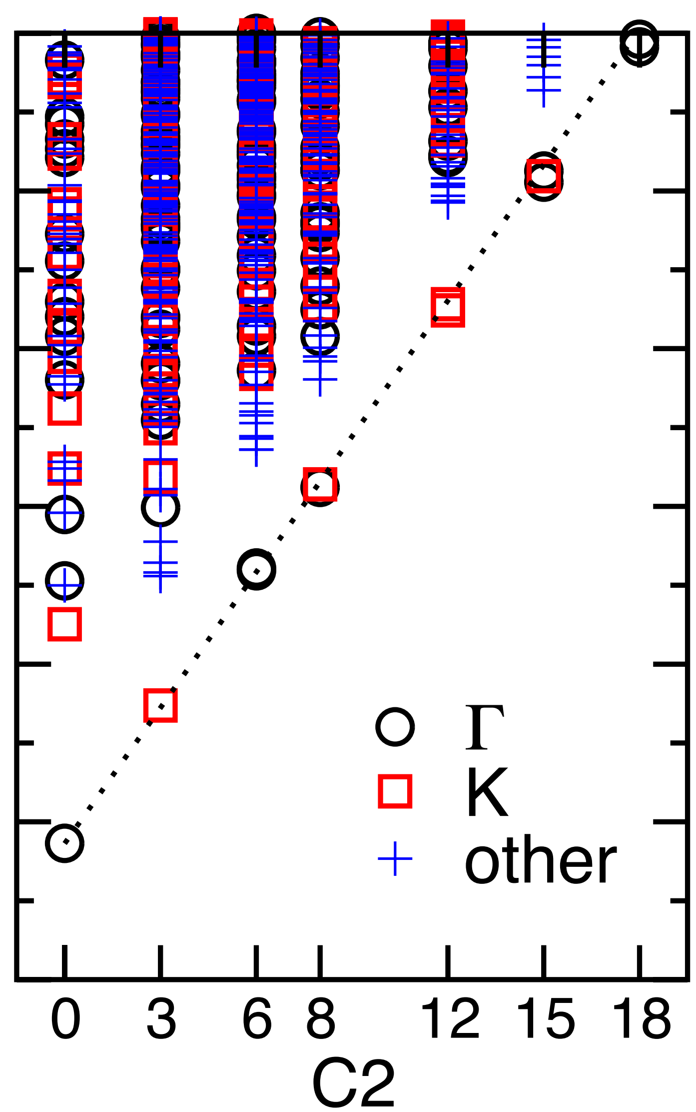
# Continous symmetry breaking with other groups

- SU(N) quantum magnetism in ultracold atomic gases
- Here an SU(3) example on the triangular lattice:

AML, F. Mila, K. Penc
PRL (2006)



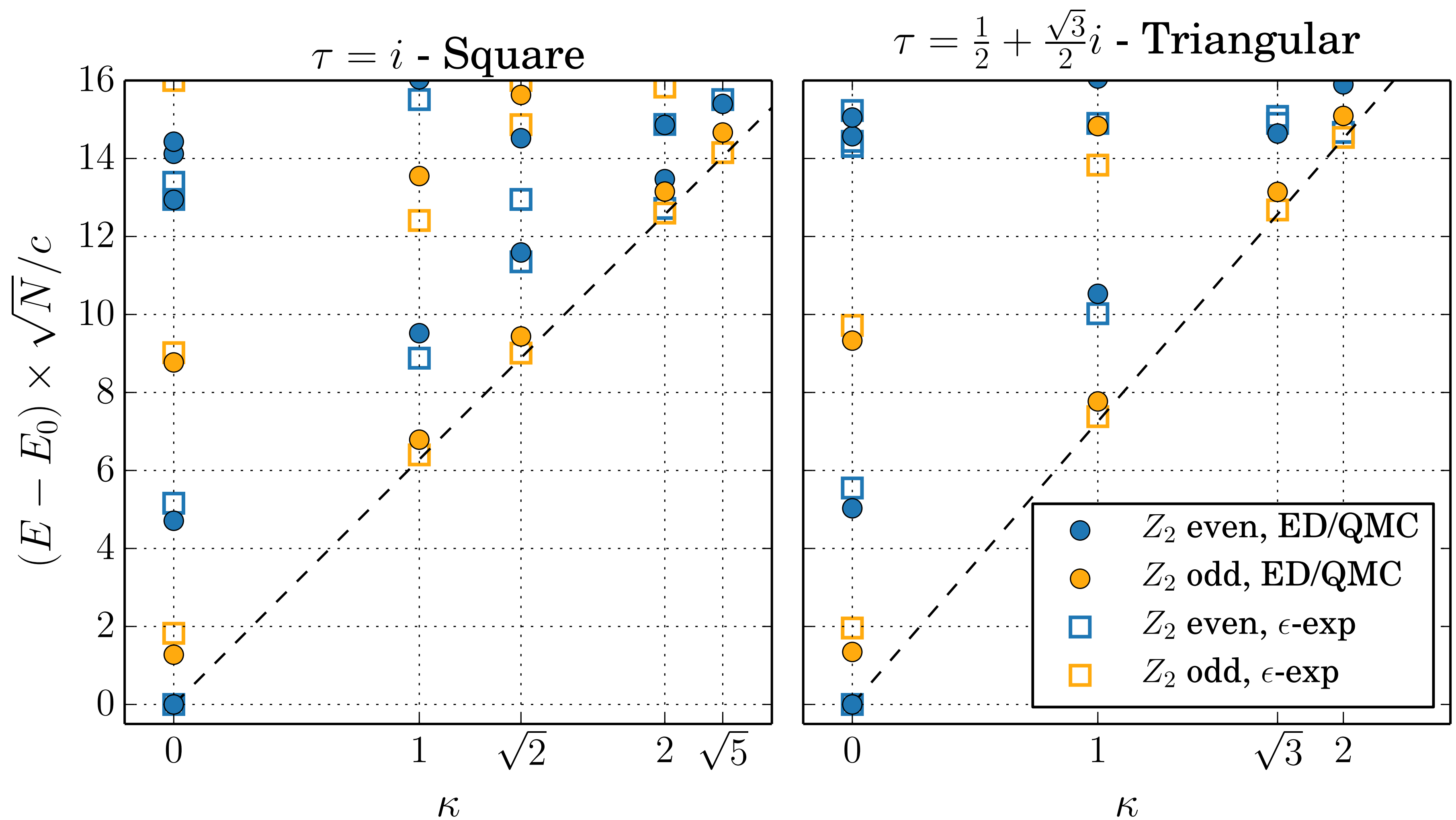
triangular lattice




- S(S+1) scaling gets replaced by quadratic Casimir of irreducible representations of symmetry group.

# Quantum Critical Points

- Universal spectrum of the critical field theory at the quantum critical point
- Spectrum scales as 1/L. Here an example for the Ising CFT in 2+1D:



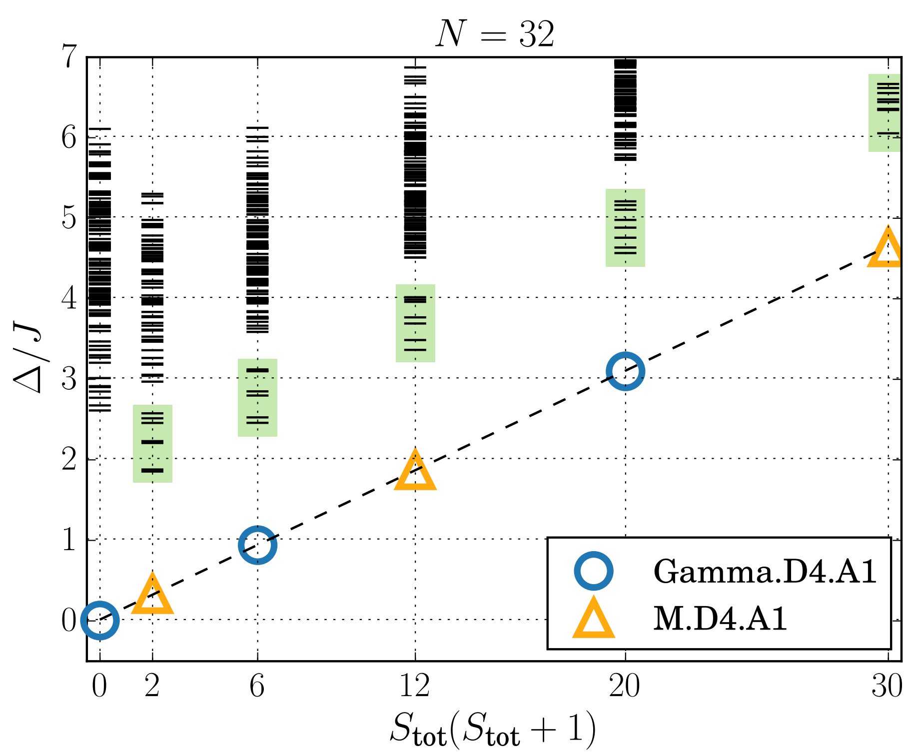

M. Schuler, S. Whitsitt, L.P. Henry, S.Sachdev & AML, arXiv:1603.03042

# Conclusions

- Exact Diagonalization based spectroscopy of quantum many body Hamiltonians is a very powerful technique.

- Well developed framework to diagnose and characterise (continuous) symmetry breaking on finite size systems. Recent extensions to quantum critical points

- More details in lecture notes written together with M. Schuler and A. Wietek




Thank you for your attention !