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

Introduction to Exact Diagonalization

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Outline of the four lectures (tentative)

- Lecture 1 (now):
  Introduction to Exact Diagonalization
- Lecture 2 (today 10:30-12:00):
  Exact Diagonalization: Symmetries & Dynamics
- Lecture 3 (tomorrow 10:30-12:00)
  Exact Diagonalization: Spectroscopy
- Lecture 4 (tomorrow 14:00-15:30)
  Exact Diagonalization: Tutorial

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!

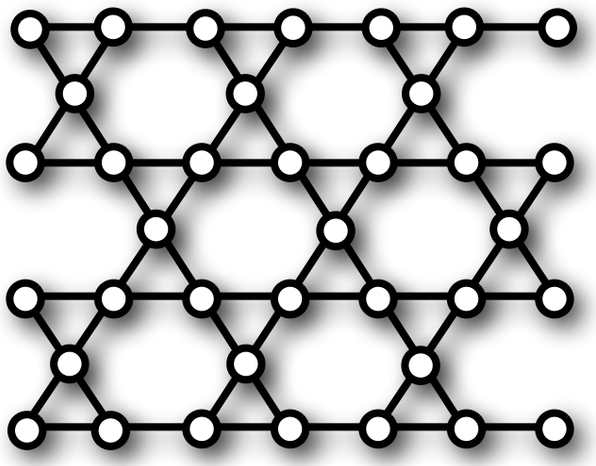
- Some people will tell you that's all there is.

- 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 $|\downarrow\rangle$

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 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
  64 spins or more in elevated magnetization sectors
  up to ~500 billion basis states

- Fractional quantum hall effect
  different filling fractions v, 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

Structure of an Exact Diagonalization code

Ingredients

- Hilbert space
  - Basis represention, Lookup techniques
  - Symmetries
- Hamiltonian Matrix
  - Sparse Matrix representation (memory/disk)
  - Matrix recalculation on the fly (matrix-free)
- Linear Algebra : Eigensolver / Time propagation
  - LAPACK full diagonalization
  - Lanczos type diagonalization (needs only $|v\rangle = H|u\rangle$ operations)
  - More exotic eigensolver techniques, real oder imaginary-time propagation,
- Observables
  - Static quantities (multipoint correlation functions, correlation density matrices,...)
  - Dynamic observables (spectral functions, density of states,...)
  - Real-time evolution

Hilbert Space

Basis representation

- States of the Hilbert space need to be represented in the computer.

- Choose a representation which makes it simple to act with the Hamiltonian or other operators on the states, and to localize a given state in the basis

- Simple example: ensemble of S=1/2 sites in binary coding

$$|\uparrow\uparrow\downarrow\uparrow\rangle \rightarrow [1\ 1\ 0\ 1]_2 = 13$$

detection of up or down spin can be done with bit-test.
transverse exchange $S^+S^- + S^-S^+$ can be performed by an XOR operation:

$$[1\ 1\ 0\ 1]_2\ \mathrm{XOR}\ [0\ 1\ 1\ 0]_2 = [1\ 0\ 1\ 1]_2$$

initial config — bit 1 at the two sites coupled — final config

- For S=1, one bit is obviously not sufficient. Use ternary representation or simply occupy two bits to label the 3 states.

Basis representation

- For t-J models at low doping it is useful to factorize hole positions and spin configurations on the occupied sites.

- For Hubbard models one can factorize the Hilbert space in up and down electron configurations.

- For constrained models - such as dimer models - the efficient generation of all basis states requires some thought.

- One of the key challenges for a fast ED code is to find the index of the new configuration in the list of all configurations (index f in $H_{i,f}$).

- Let us look at the example of S=1/2 spins at fixed S^z

Basis lookup procedures (Lin tables)

- One of the key problems for a fast ED code is to find the index of the new configuration in the list of all configurations (index f in $H_{i,f}$).

$$[1\ 0\ 1\ 1]_2 = 11_{10}$$

- But is 11 the index of this configuration in a list of all S^z=1 states ? no !

- Use Lin tables to map from binary number to index in list of allowed states:
  (generalization of this idea works for arbitrary number of additive quantum numbers)

- Two tables with $2^{(N/2)}$ [=sqrt(2^N)] entries, one for MSBs and one for LSBs

$$\begin{array}{lcl} [0\ 0] & = & X \\ [0\ 1] & = & 0 \\ [1\ 0] & = & 1 \\ [1\ 1] & = & 2 \end{array}$$

MSB

$$\begin{array}{lcl} [0\ 0] & = & X \\ [0\ 1] & = & 0 \\ [1\ 0] & = & 1 \\ [1\ 1] & = & 0 \end{array}$$

LSB

$$\begin{array}{lcl} \mathrm{Ind}([0\ 1\ 1\ 1]) = 0+0 & = & 0 \\ \mathrm{Ind}([1\ 0\ 1\ 1]) = 1+0 & = & 1 \\ \mathrm{Ind}([1\ 1\ 0\ 1]) = 2+0 & = & 2 \\ \mathrm{Ind}([1\ 1\ 1\ 0]) = 2+1 & = & 3 \end{array}$$

Basis lookup procedures (Lin tables)

- Lookup can therefore be done with two direct memory reads. This is a time and memory efficient approach (at least in many interesting cases).
- An alternative procedure is to build a hash list [const access time] or to perform a binary search [log access time].
- This becomes somewhat more involved when using spatial symmetries...

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...

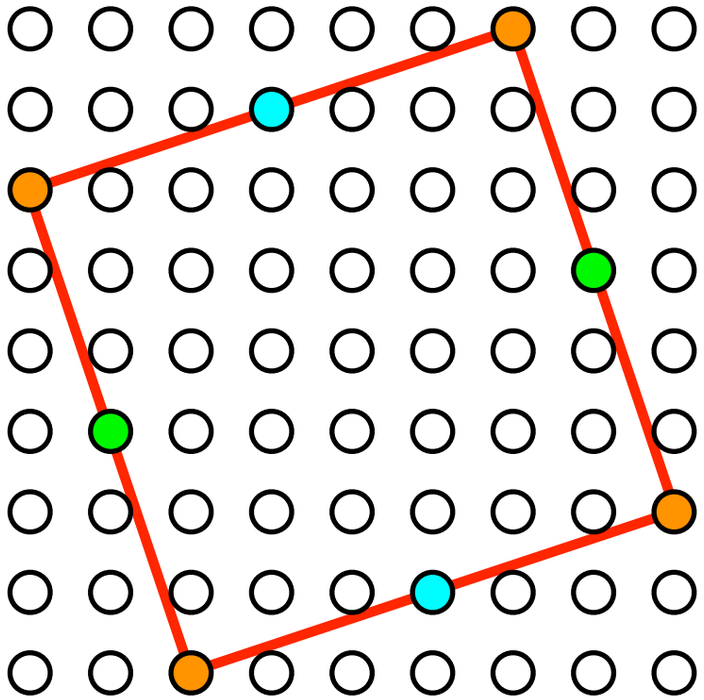
- At the Heisenberg point, the total spin is also conserved. It is however very difficult to combine the SU(2) symmetry with the lattice symmetries in a computationally useful way (non-sparse and computationally expensive matrices).

- 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.

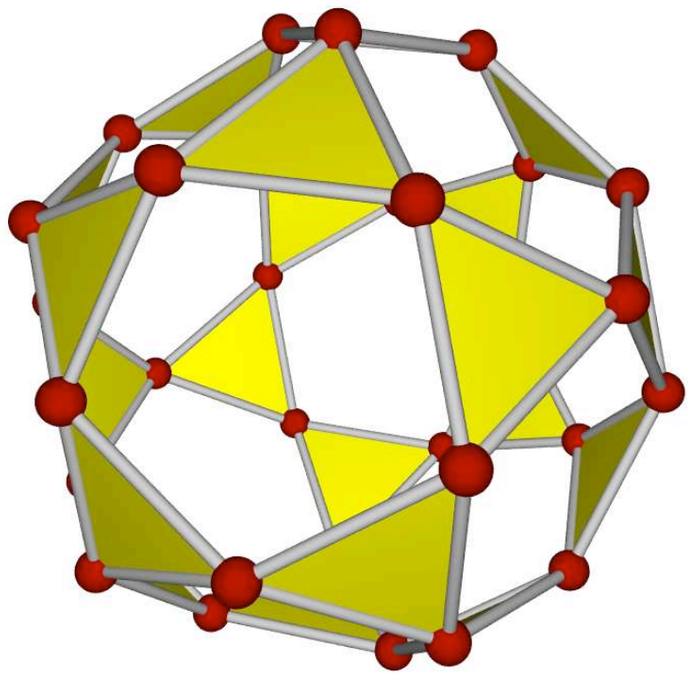
Spatial Symmetries

- 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 ⊗ PG =40 x 4 elements



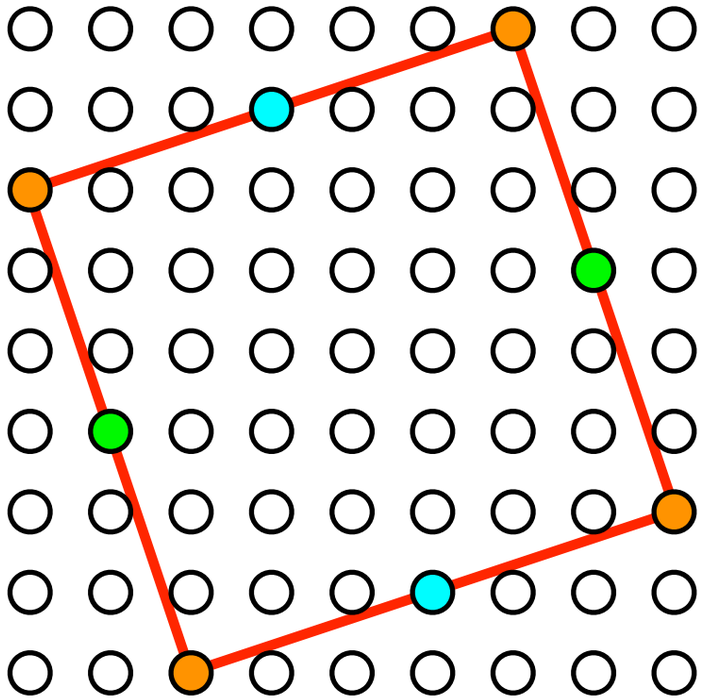
Icosidodecahedron (30 vertices)
I_h:120 elements



Spatial Symmetries

- Symmetries are sometimes not easily visible, use graph theoretical tools to determine symmetry group [nauty, grape].
- In an ED code a spatial symmetry operation is a site permutation operation.
  (could become more complicated with spin-orbit interactions and multiorbital sites)

40 sites square lattice
T ⊗ PG =40 x 4 elements



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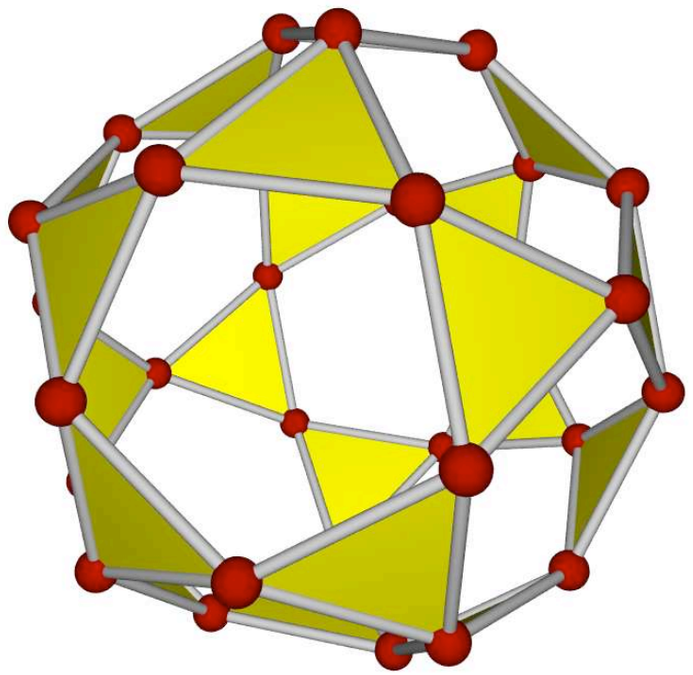
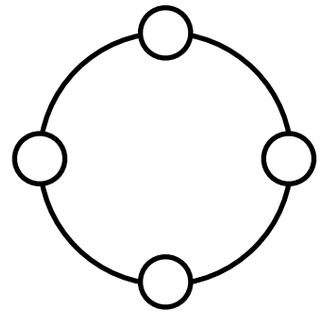


Spatial Symmetries: Building the basis

- Build a list of all allowed states satisfying the “diagonal” constraints, like particle number, total S^z, ...

- for each state we apply all symmetry operations and keep the state as a representative if it has the smallest integer representation among all generated states in the orbit.
Example: 4 site ring with cyclic translation *T*, S^z=1 sector



$$T^0([0\ 1\ 1\ 1]) \rightarrow [0\ 1\ 1\ 1]$$
$$T^1([0\ 1\ 1\ 1]) \rightarrow [1\ 0\ 1\ 1]$$
$$T^2([0\ 1\ 1\ 1]) \rightarrow [1\ 1\ 0\ 1]$$
$$T^3([0\ 1\ 1\ 1]) \rightarrow [1\ 1\ 1\ 0]$$

keep state

$$T^0([1\ 0\ 1\ 1]) \rightarrow [1\ 0\ 1\ 1]$$
$$T^1([1\ 0\ 1\ 1]) \rightarrow [1\ 1\ 0\ 1]$$
$$T^2([1\ 0\ 1\ 1]) \rightarrow [1\ 1\ 1\ 0]$$
$$T^3([1\ 0\ 1\ 1]) \rightarrow [0\ 1\ 1\ 1]$$

discard state

...

Spatial Symmetries: Building the basis

- For one-dimensional representations χ of the spatial symmetry group:
  - "Bloch" state $$|\tilde{r}\rangle = \frac{1}{\mathcal{N}\sqrt{|G|}} \sum_{g\in G} \chi(g)|g(r)\rangle$$
  - Norm of the state is given as: $$\mathcal{N} = \sqrt{\sum_{g\in G, g(r)=r} \chi(g)}$$
  - The norm (and therefore the state itself) can vanish if it has a nontrivial stabilizer combined with a nontrivial representation χ.

- Example: 4 site S=1/2 ring with cyclic translations:

	$K=0$	$K=\pm\pi/2$	$K=\pi$	**2^4=16**
S^z=2	$\|1\ 1\ 1\ 1\rangle, \mathcal{N}=2$			1+1
S^z=1	$\|0\ 1\ 1\ 1\rangle, \mathcal{N}=1$	$\|0\ 1\ 1\ 1\rangle, \mathcal{N}=1$	$\|0\ 1\ 1\ 1\rangle, \mathcal{N}=1$	4+4
S^z=0	$\|0\ 1\ 0\ 1\rangle, \mathcal{N}=\sqrt{2}$		$\|0\ 1\ 0\ 1\rangle, \mathcal{N}=\sqrt{2}$	2
	$\|0\ 0\ 1\ 1\rangle, \mathcal{N}=1$	$\|0\ 0\ 1\ 1\rangle, \mathcal{N}=1$	$\|0\ 0\ 1\ 1\rangle, \mathcal{N}=1$	4

The Hamiltonian Matrix

The Hamiltonian Matrix

- Now that we have a list of representatives and their norms, can we calculate the matrix elements of the Hamiltonian ? $\langle \tilde{s}|H|\tilde{r}\rangle = ?$

- Let us look at an elementary, non-branching term in the Hamiltonian:

$$h^{\alpha}|r\rangle = h^{\alpha}(r)|s\rangle$$

- We can now calculate the matrix element $\langle \tilde{s}|h^{\alpha}|\tilde{r}\rangle$ without double expanding the Bloch states:

$$\langle \tilde{s}|h^{\alpha}|\tilde{r}\rangle = \frac{\mathcal{N}_s}{\mathcal{N}_r}\chi(g^*)h^{\alpha}(r)$$

- key algorithmic problem: given a possibly non-representative $|s\rangle$, how do we find the associated representative $|\tilde{s}\rangle$, as well as a symmetry element g^* relating $|s\rangle$ to $|\tilde{s}\rangle$?

The Hamiltonian Matrix

- key algorithmic problem: given a possibly non-representative $|s\rangle$, how do we find the associated representative $|\tilde{s}\rangle$, as well as a symmetry element g^* relating $|s\rangle$ to $|\tilde{s}\rangle$?

  - Brute force: loop over all symmetry operations applied on $|s\rangle$ and retain $|\tilde{s}\rangle$ and g^*. This is however often not efficient (many hundred symmetries).

  - Prepare a lookup list, relating each allowed configuration with the index of its representative, and also the associated group element linking the two. Gives fast implementation, but needs a list of the size of the non spatially-symmetrized Hilbert space.

  - For specific lattices and models (Hubbard models) clever tricks exist which factorize the symmetry group into a sublattice conserving subgroup times a sublattice exchange. They give $|\tilde{s}\rangle$ fast, then a hash or binary search is needed to locate $|\tilde{s}\rangle$ in the list of representatives in order to get its index.

Hamiltonian Matrix Storage

- Different possibilities exist:

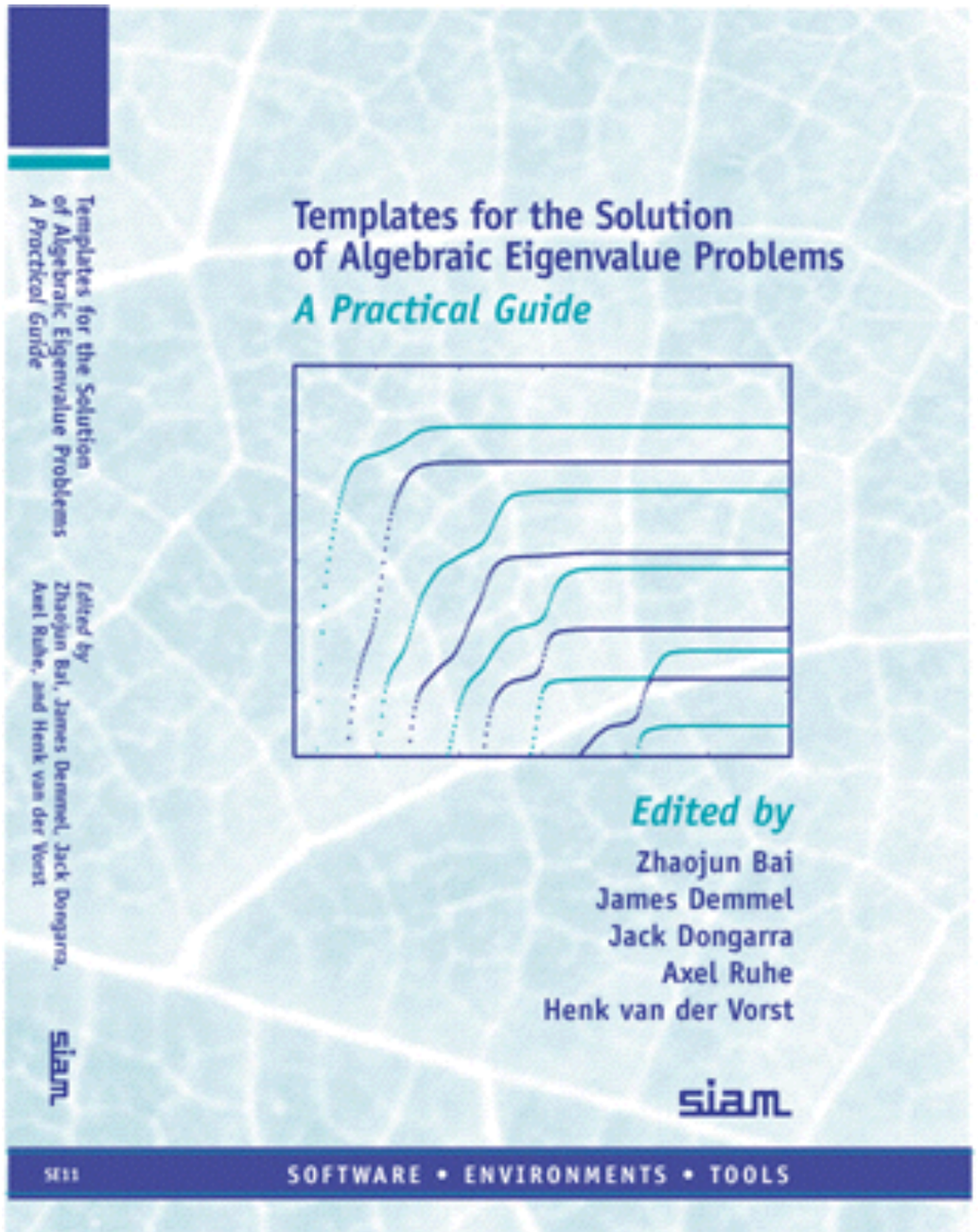
  - Store hamiltonian matrix elements in memory in a sparse matrix format
    Fast matrix vector multiplies, but obviously limited by available memory.

  - Store hamiltonian matrix elements on disk in a sparse matrix format.
    In principle possible due to the vast disk space available, but I/O speed is much slower than main memory access times. Difficult to parallelize.

  - Recalculate the hamiltonian matrix elements in each iterations “on the fly”.
    Needed for the cutting edge simulations, where the whole memory is used by the Lanczos vectors. Can be parallelized on most architectures.

The Linear Algebra Backend

The Reference:



- Online book at: http://www.cs.utk.edu/~dongarra/etemplates/index.html

Linear Algebra:
The most popular: Lanczos Algorithm

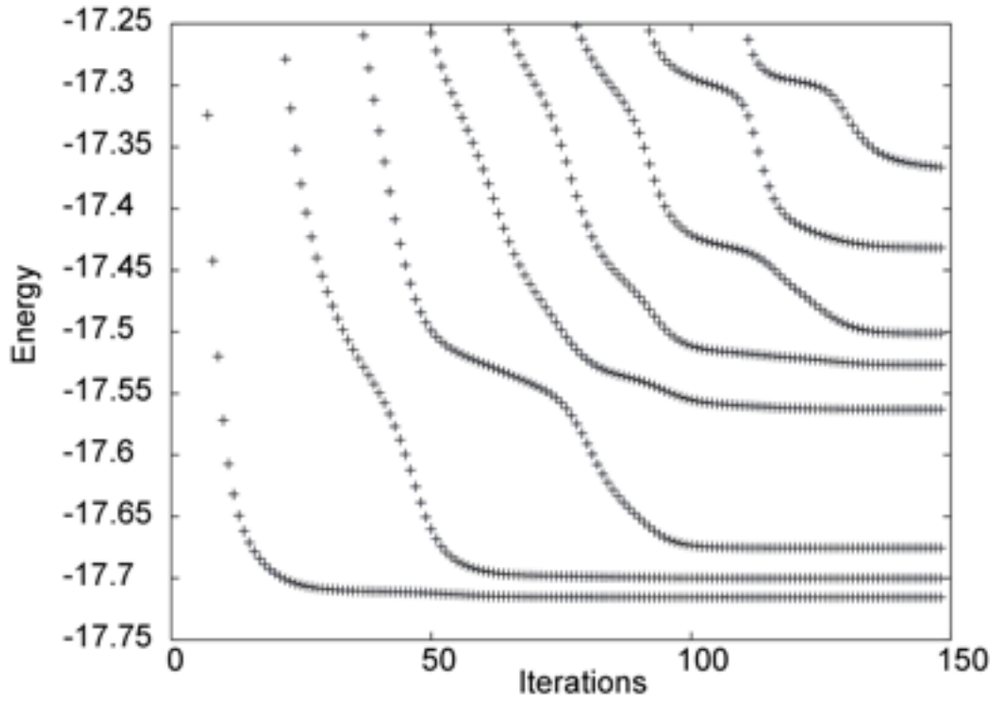
- Lanczos Algorithm (C. Lanczos, 1950)

Three vector recursion

$$
\begin{aligned}
|\phi'\rangle &= H|\phi_n\rangle - \beta_n|\phi_{n-1}\rangle\,, \\
\alpha_n &= \langle\phi_n|\phi'\rangle\,, \\
|\phi''\rangle &= |\phi'\rangle - \alpha_n|\phi_n\rangle\,, \\
\beta_{n+1} &= ||\phi''|| = \sqrt{\langle\phi''|\phi''\rangle}\,, \\
|\phi_{n+1}\rangle &= |\phi''\rangle/\beta_{n+1}\,,
\end{aligned}
\qquad
\tilde{H}_N = \begin{bmatrix}
\alpha_0 & \beta_1 & 0 & \cdots & \cdots & 0 \\
\beta_1 & \alpha_1 & \beta_2 & 0 & \cdots & 0 \\
0 & \beta_2 & \alpha_2 & \beta_3 & 0 & 0 \\
 & & \ddots & \ddots & \ddots & \\
0 & \cdots & 0 & \beta_{N-2} & \alpha_{N-2} & \beta_{N-1} \\
0 & \cdots & \cdots & 0 & \beta_{N-1} & \alpha_{N-1}
\end{bmatrix}
$$

- Eigenvalues of H_N converge rapidly towards eigenvalues of H.

- Once desired eigenvalue is converged, restart recursion and assemble the eigenvector.



very quick convergence for extremal eigenvalues !

Linear Algebra: Lanczos Algorithm

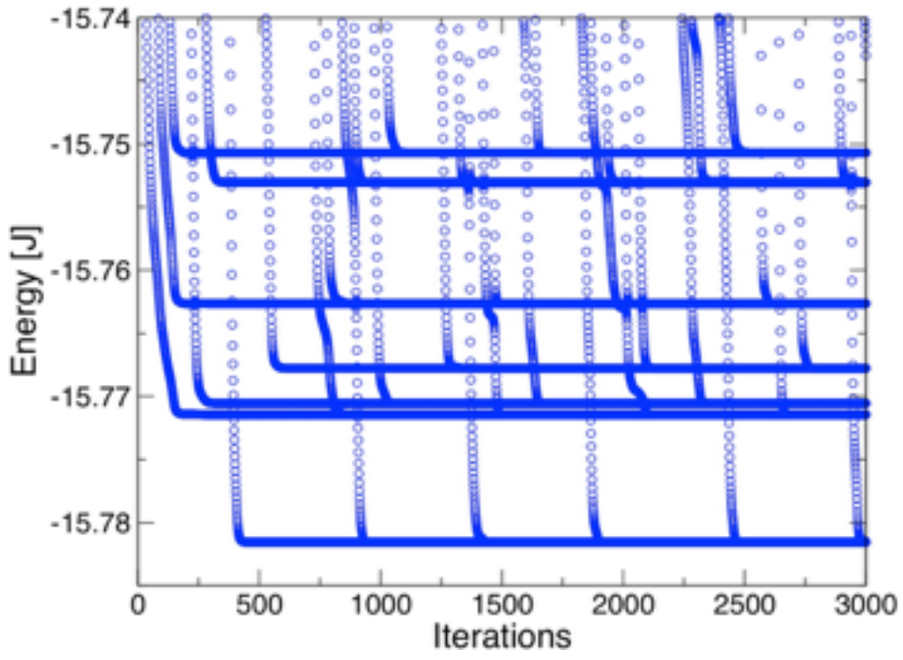
- The same algorithm according to the book:

ALGORITHM 4.6: **Lanczos Method for HEP**

(1) *start with* $r = v$, *starting vector*
(2) $\beta_0 = \|r\|_2$
(3) **for** $j = 1, 2, \ldots,$ **until** *convergence*,
(4) $v_j = r/\beta_{j-1}$
(5) *operate* $r = Av_j$
(6) $r = r - v_{j-1}\beta_{j-1}$
(7) $\alpha_j = v_j^* r$
(8) $r = r - v_j\alpha_j$
(9) *reorthogonalize if necessary*
(10) $\beta_j = \|r\|_2$
(11) *compute approximate eigenvalues* $T_j = S\Theta^{(j)}S^*$
(12) *test bounds for convergence*
(13) **end for**
(14) *compute approximate eigenvectors* $X = V_j S$

Linear Algebra:
Lanczos Algorithm

- Once the ground state has converged, the vectors in the recursion tend to lose their orthogonality. As a consequence fake new eigenvalues show up in the approximate spectrum. These can be removed by heuristic techniques



- Degeneracies of eigenvalues can not be resolved by construction. For this task one would need a band lanczos or the (Jacobi-)Davidson technique. However multiply degenerate eigenvalues are converged.

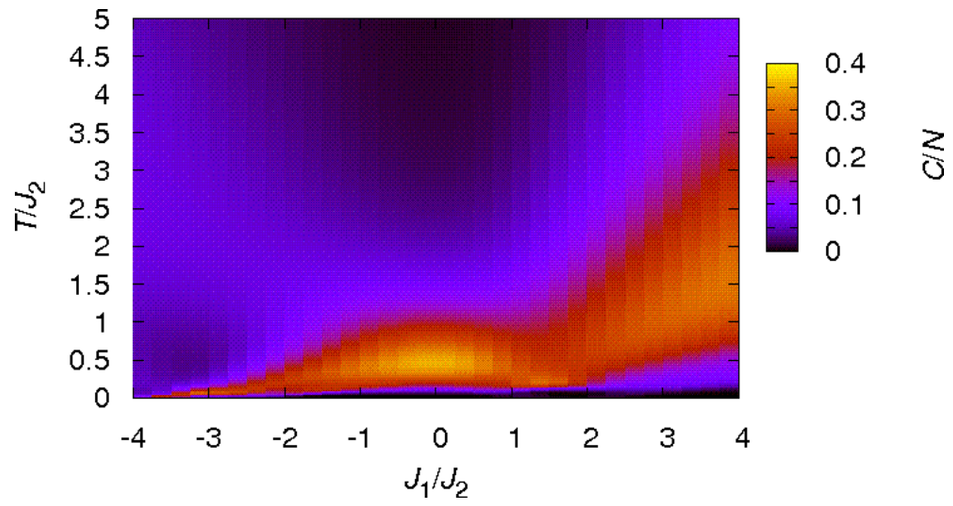
- Checkpointing is useful when performing large-scale simulations.

Full Diagonalization: Thermodynamics

- Lapack / Householder complete diagonalization of the spectrum.

- Calculate partition function and all the thermodynamic quantities you want, often the only pedestrian method available for frustrated systems.

- Symmetries are also very important, because the computational requirements scale as $O(D^3)$, where D is the dimension of the block Hilbert space. Typical D's for a workstation are a few 1'000, up to a few 100'000 on supercomputers.



F. Heidrich-Meisner, A. Honecker, T. Vekua, Phys. Rev. B **74**, 020403(R) (2006).

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

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Observables

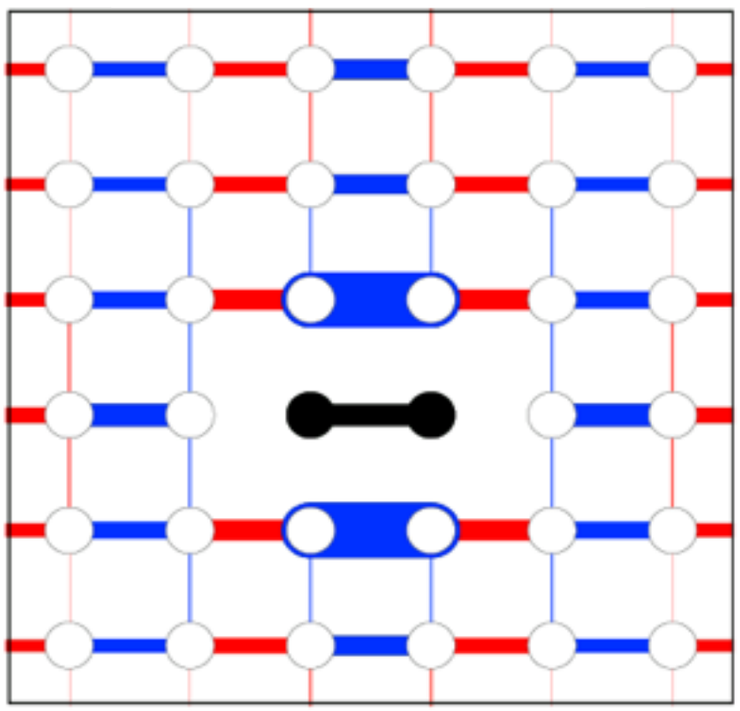
Observables

- In principle once can calculate any correlation function, since one has access to the full many body wave functions. When using spatial symmetries, the correlation functions need to be properly symmetrized too.

- Complicated correlation functions occur in frustrated systems:

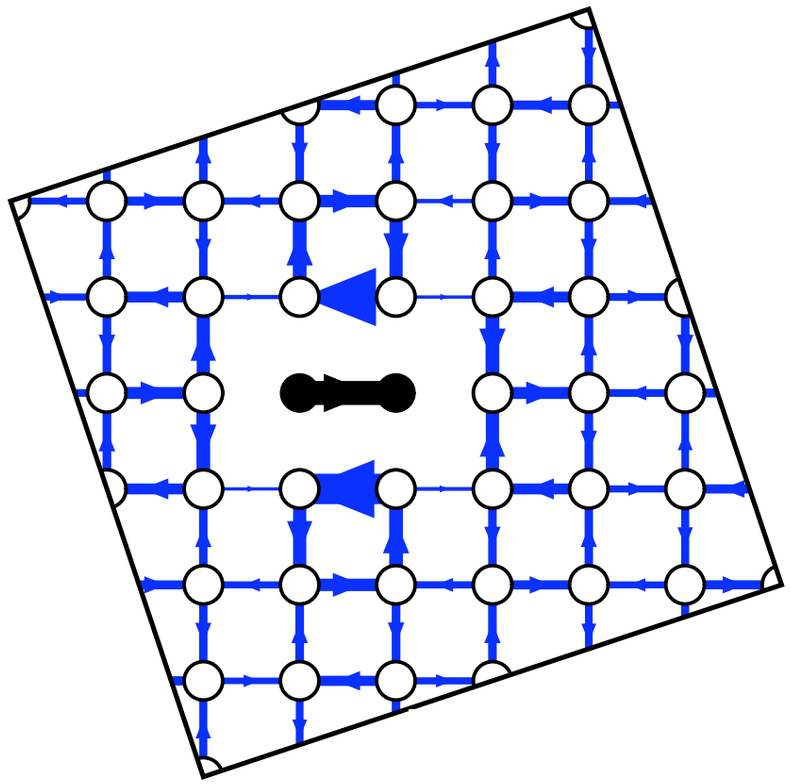
$\langle (\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l) \rangle - \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle \langle \mathbf{S}_k \cdot \mathbf{S}_l \rangle$

Dimer-dimer correlations



$\langle (\mathbf{S}_i \wedge \mathbf{S}_j)^z (\mathbf{S}_k \wedge \mathbf{S}_l)^z \rangle - \langle (\mathbf{S}_i \wedge \mathbf{S}_j)^z \rangle \langle (\mathbf{S}_k \wedge \mathbf{S}_l)^z \rangle$

Spin current correlations

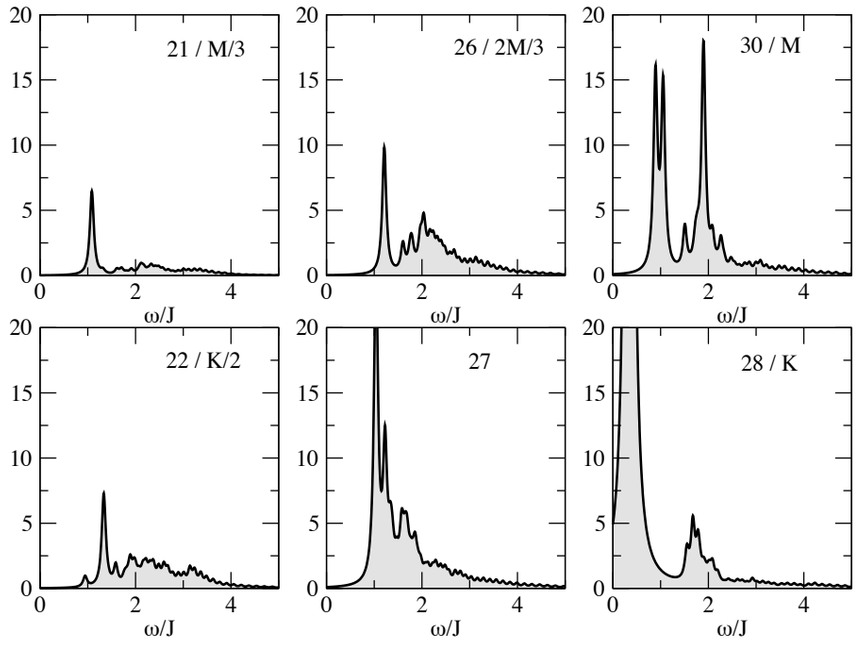


Frequency Dynamics

- $G_A(\omega + i\eta) = \langle\psi|A^\dagger \dfrac{1}{E_0 + \omega + i\eta - H} A|\psi\rangle \quad A = S^\alpha(\mathbf{q}), c_\mathbf{k}, \ldots$

- Generate Krylov space of $A|\psi\rangle$
  Use continued fraction to invert $(E_0 + \omega + i\eta - H)$

- Triangular Lattice Spin Dynamics in zero field



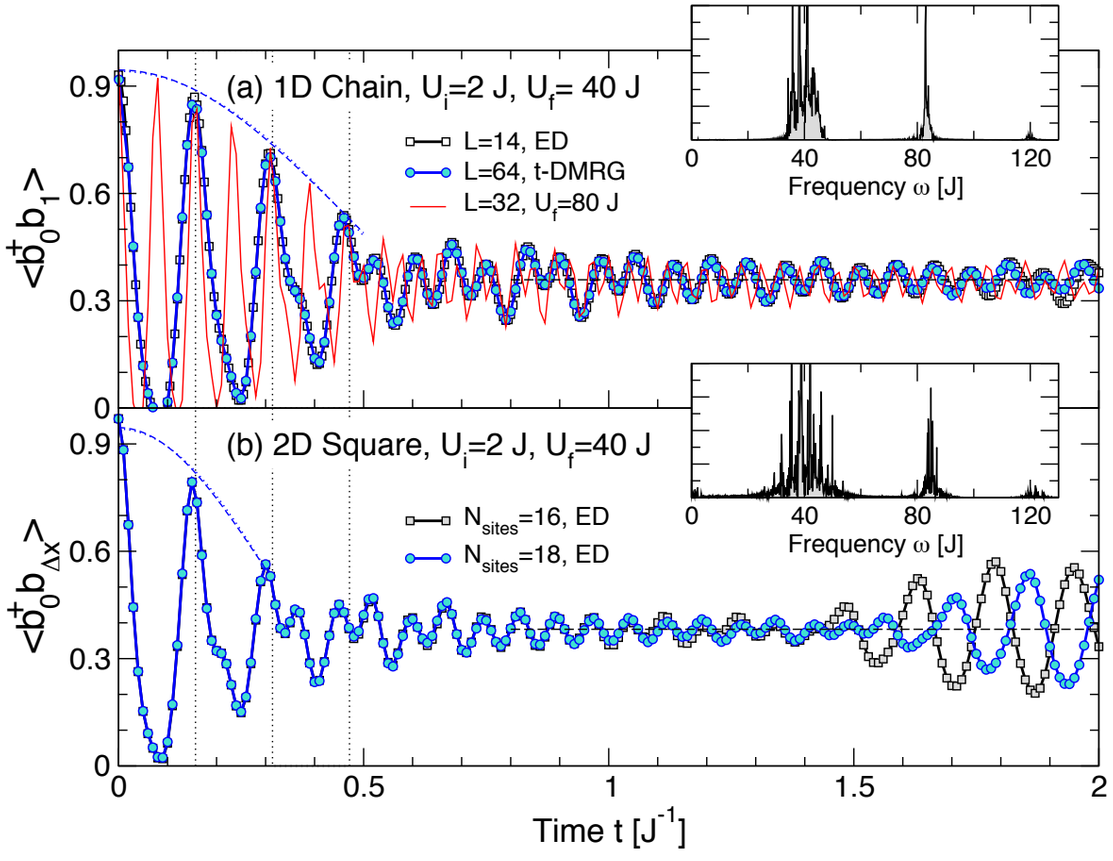
AML unpublished

Exact Diagonalization
Real-Time Dynamics

- It is expensive to obtain the full propagator $\exp[-itH]$

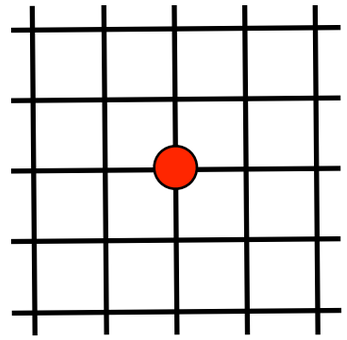
- Krylov methods exist to approximate the propagator for a given state $|\psi(0)\rangle$
  One can get the time propagated state $|\psi(t)\rangle$ with only $|v\rangle = H|u\rangle$ operations.

- Example: time evolution of a strongly correlated quantum systems after an abrupt change in the parameters in the Hamiltonian. Revivals and Relaxation.

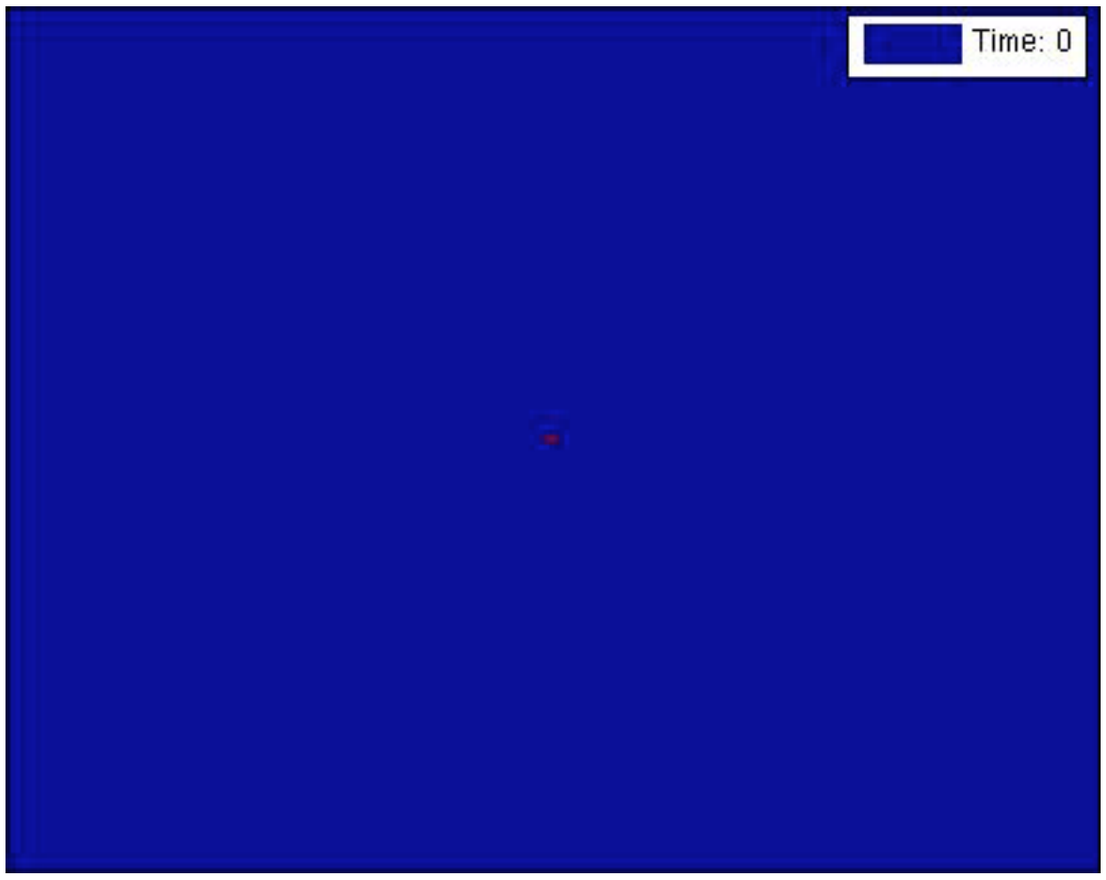


C. Kollath, AML, E. Altman, PRL 2007

Two-dimensional uniform square lattice

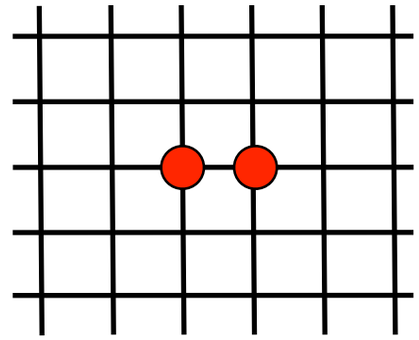


- Single particle spreading (on a ~190x190 lattice)

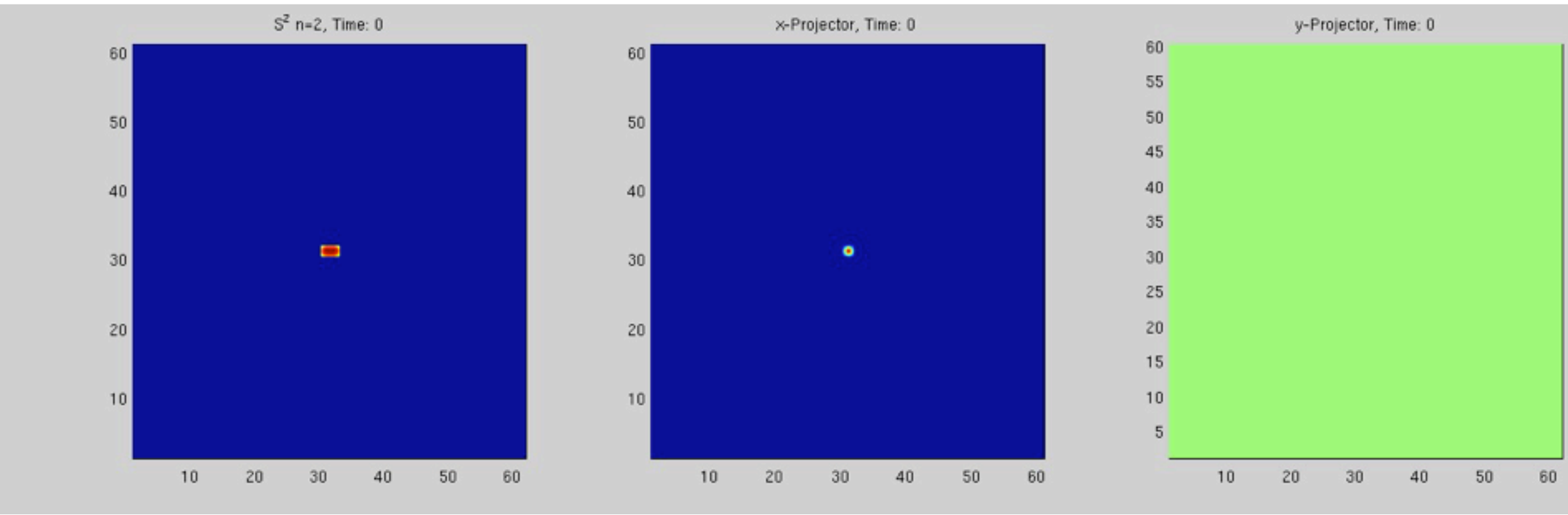


C. Krimphoff, M. Haque, and AML, in progress

Two-dimensional square lattice



- two neighboring particles (aligned in x direction) on a 60x60 lattice

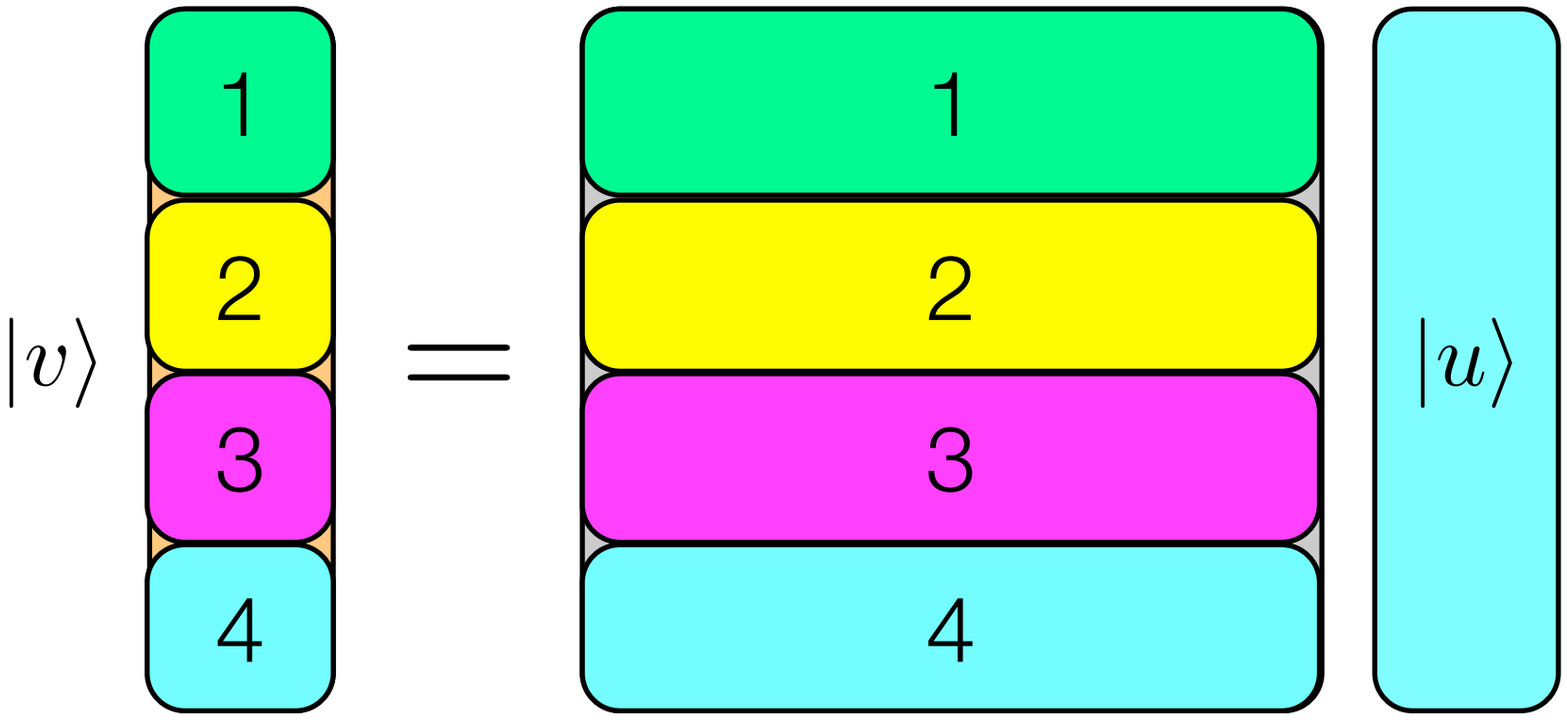


C. Krimphoff, M. Haque, and AML, in progress

Parallelization Strategies

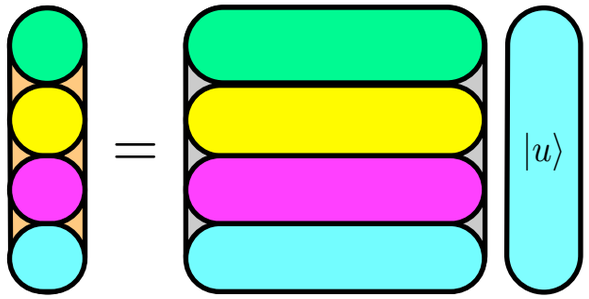
Parallelization:
Shared memory nodes

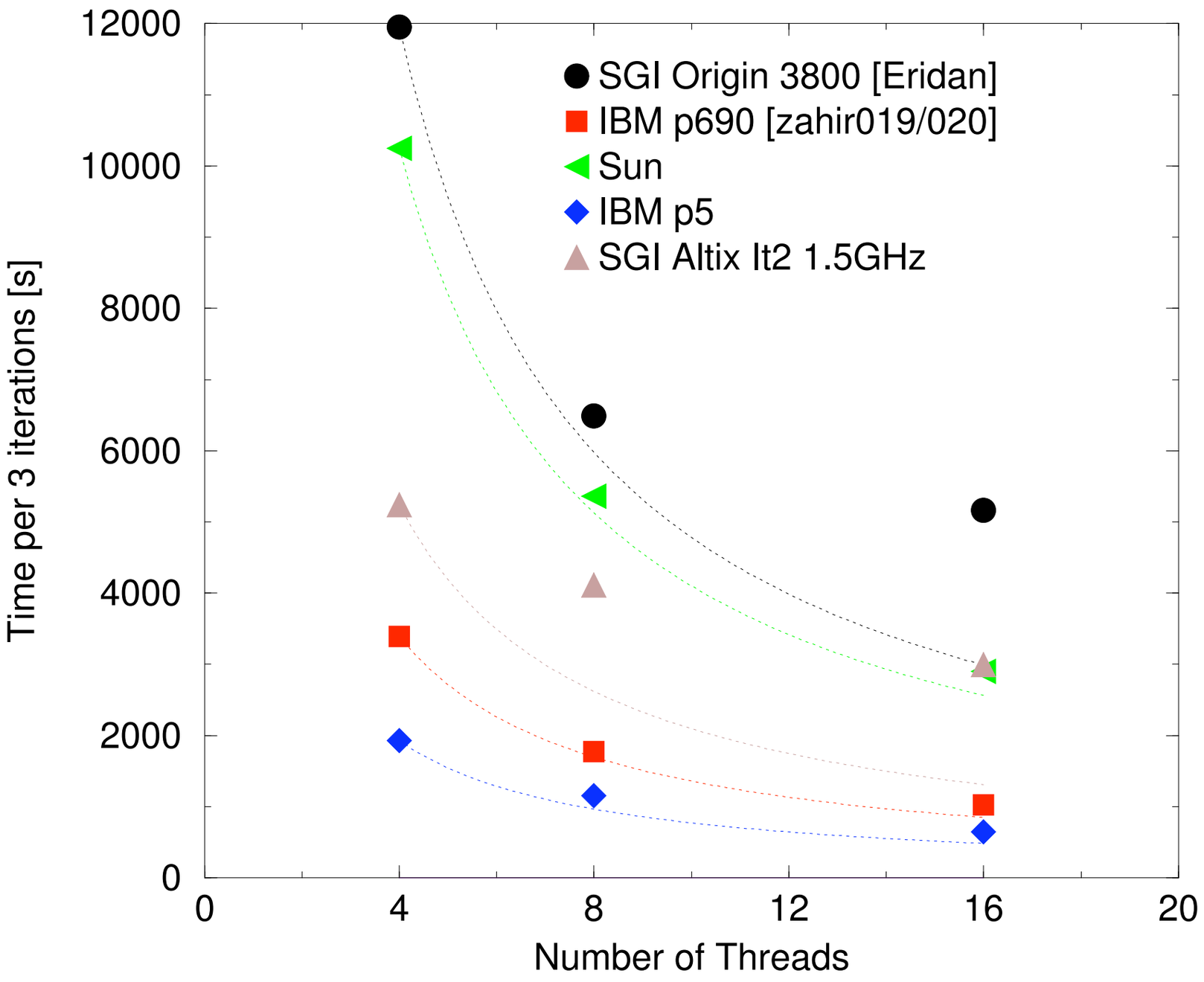
- In the Lanczos algorithm the heaviest part is the elementary matrix-vector multiplication.
- In a matrix-free formulation this part can easily be parallelized using OpenMP pragmas in the code, even on your multi-core workstation.
  Choose the right strategy between pull and push !



In this parallelization we have uncritical concurrent reads, but no concurrent updates of vector v.

Parallelization: Shared memory nodes



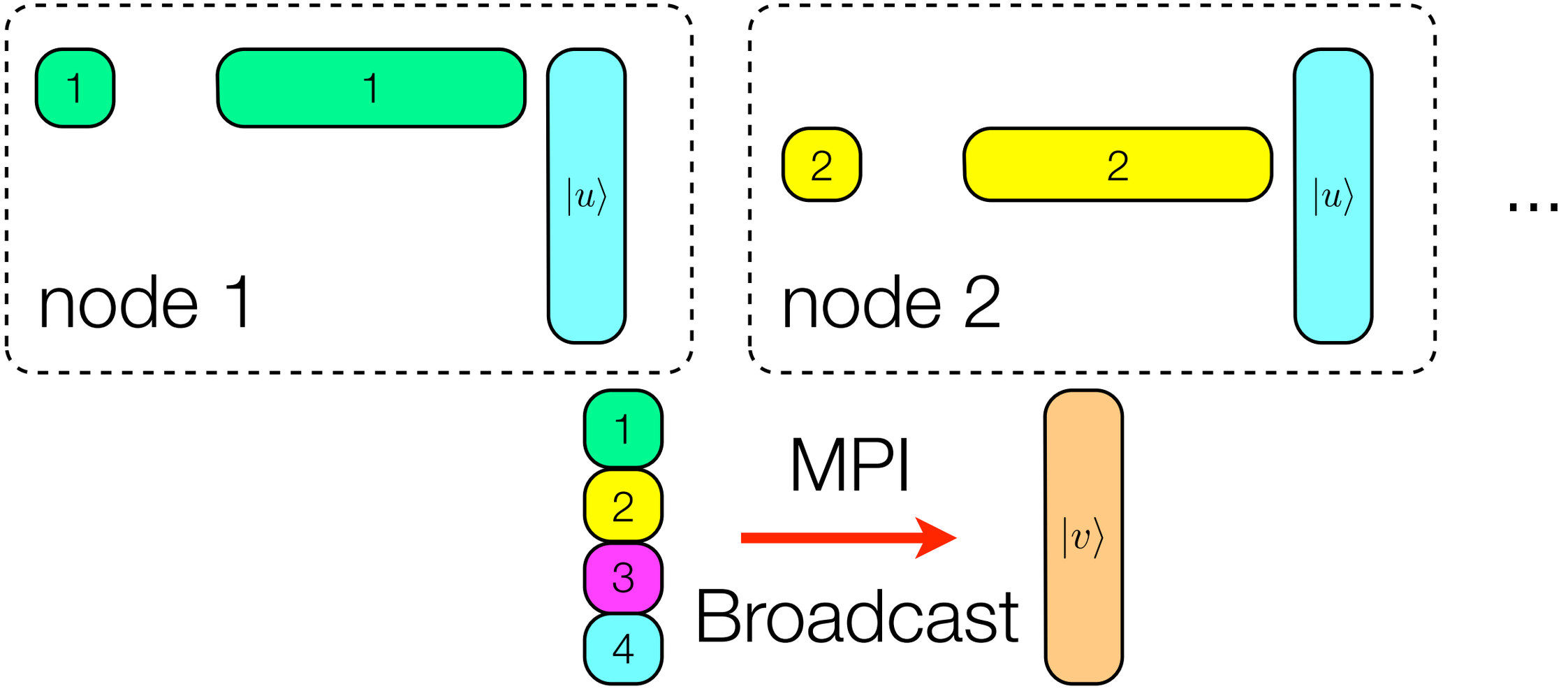


- scales well up to a few ten threads on “memory uniform” SMP machines.

Parallelization:
Distributed memory nodes

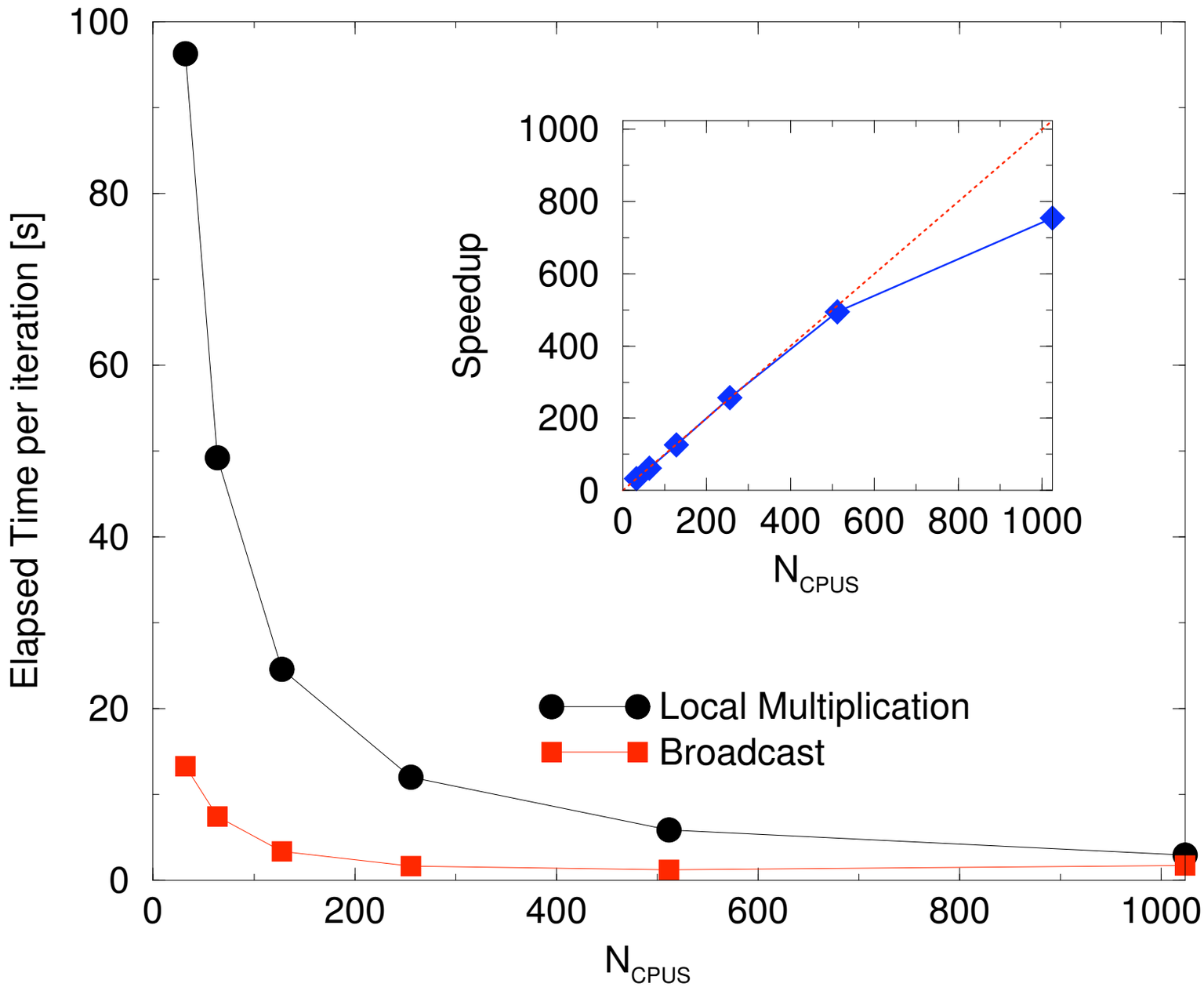
- For some classes of problems the Hilbert space size is not too big, but the vast number of matrix elements is a challenge.
  [ED in momentum space formulation & Quantum Hall problems]

- These problems can be OpenMP parallelized, but are also suitable for large scale Message passing parallelization.



Parallelization:
Distributed memory nodes

- Strong scaling example RG-ED: matrix dimension 10 million performed on a 1024 node Cray XT-3 machine: speedup of ≈ 800 on 1024 procs

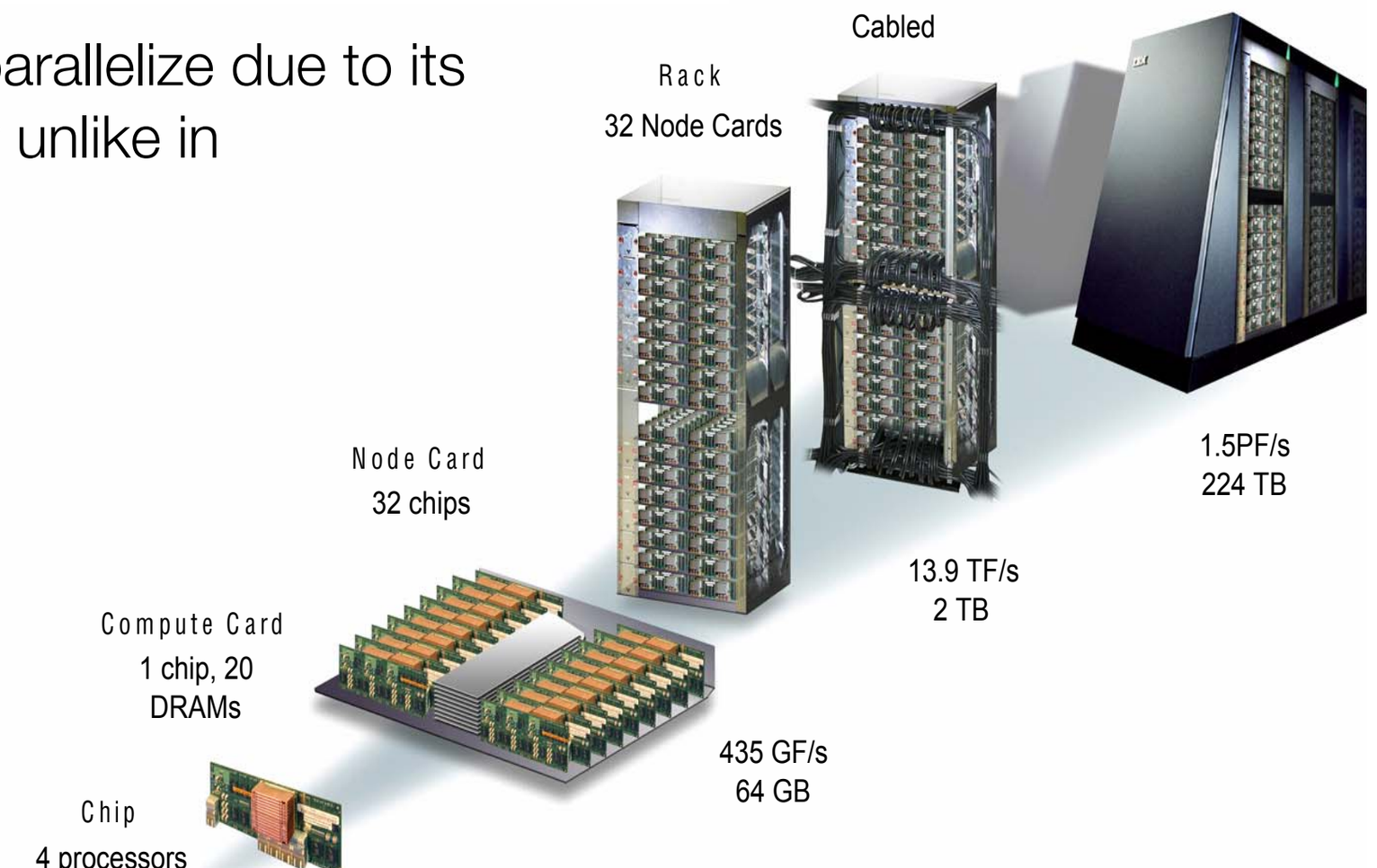


Parallelization:
How to harness the petaflop computers ?

- Cutting edge petaflop systems have a huge number of core, but only a moderate amount of node-local memory.

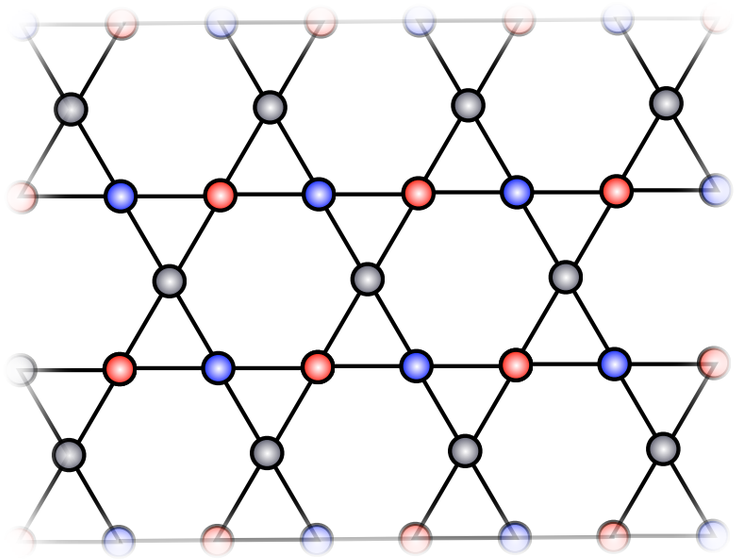
- Next generation ED codes need to be developed in order to attack e.g. the huge Hilbert space of a 48 site kagome antiferromagnet.

- Problem remains difficult to parallelize due to its all-to-all structure. No locality unlike in PDE solvers.



MPI Parallel Kagome ED Code: Technical Aspects

- Three-sublattice stable symmetry implementation for fast lookups



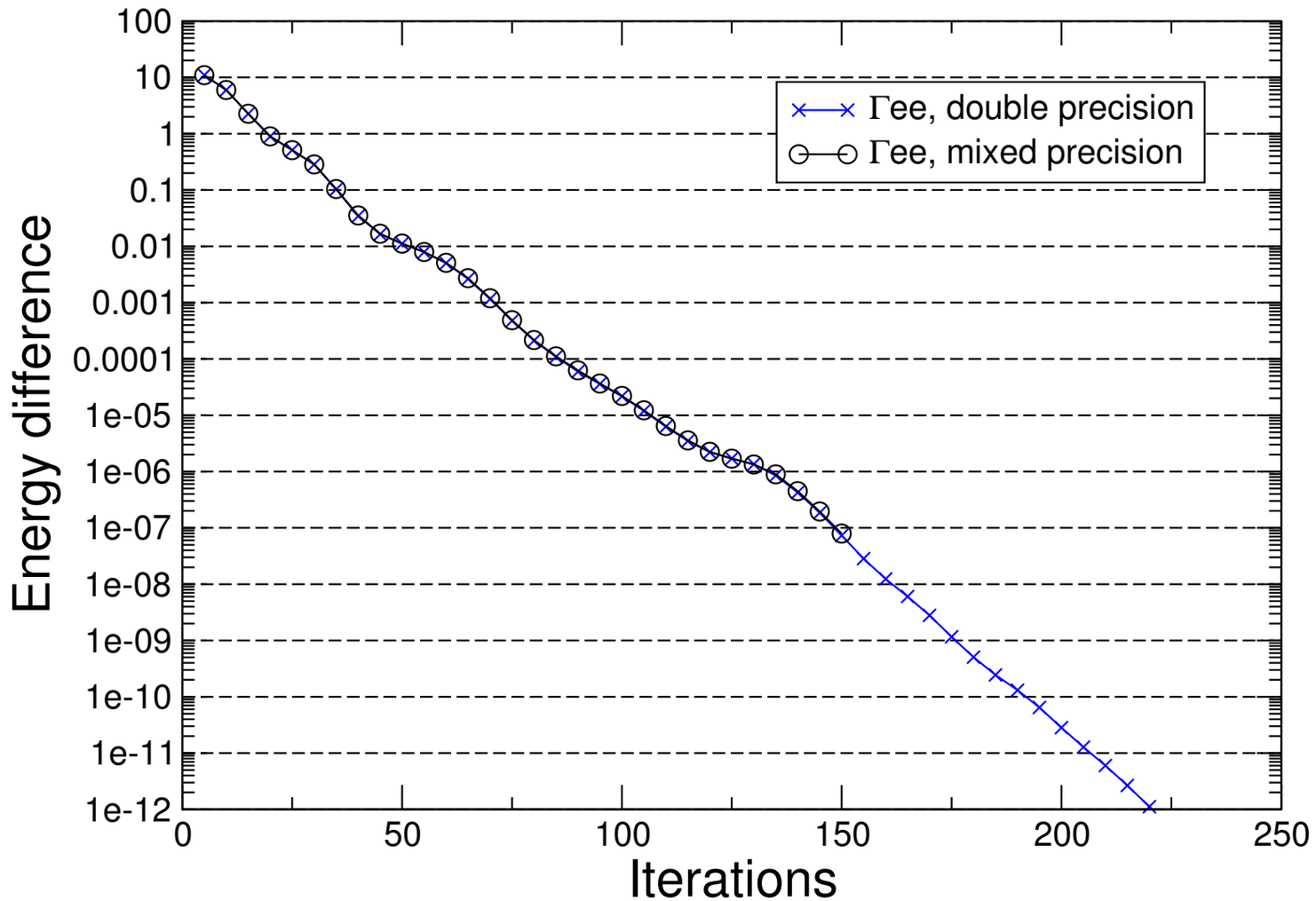
- MPI protocol based implementation for distributed memory architectures

- Performance (memory requirements up to 12 Terabytes)

Lattice	size of Hilbert space	number of tasks (architecture)	time per iteration
kagome $N_s = 42$	19,223,570,420	1,024 (Intel Xeon Infiniband)	74 seconds
kagome $N_s = 48$	251,936,333,376	1,600 (Intel Xeon NUMAlink5)	1,450 seconds
kagome $N_s = 48$	251,936,333,376	3,072 (Intel Xeon Infiniband)	650 seconds
kagome $N_s = 48$	251,936,333,376	16,384 (BlueGene/P)	520 seconds

Convergence

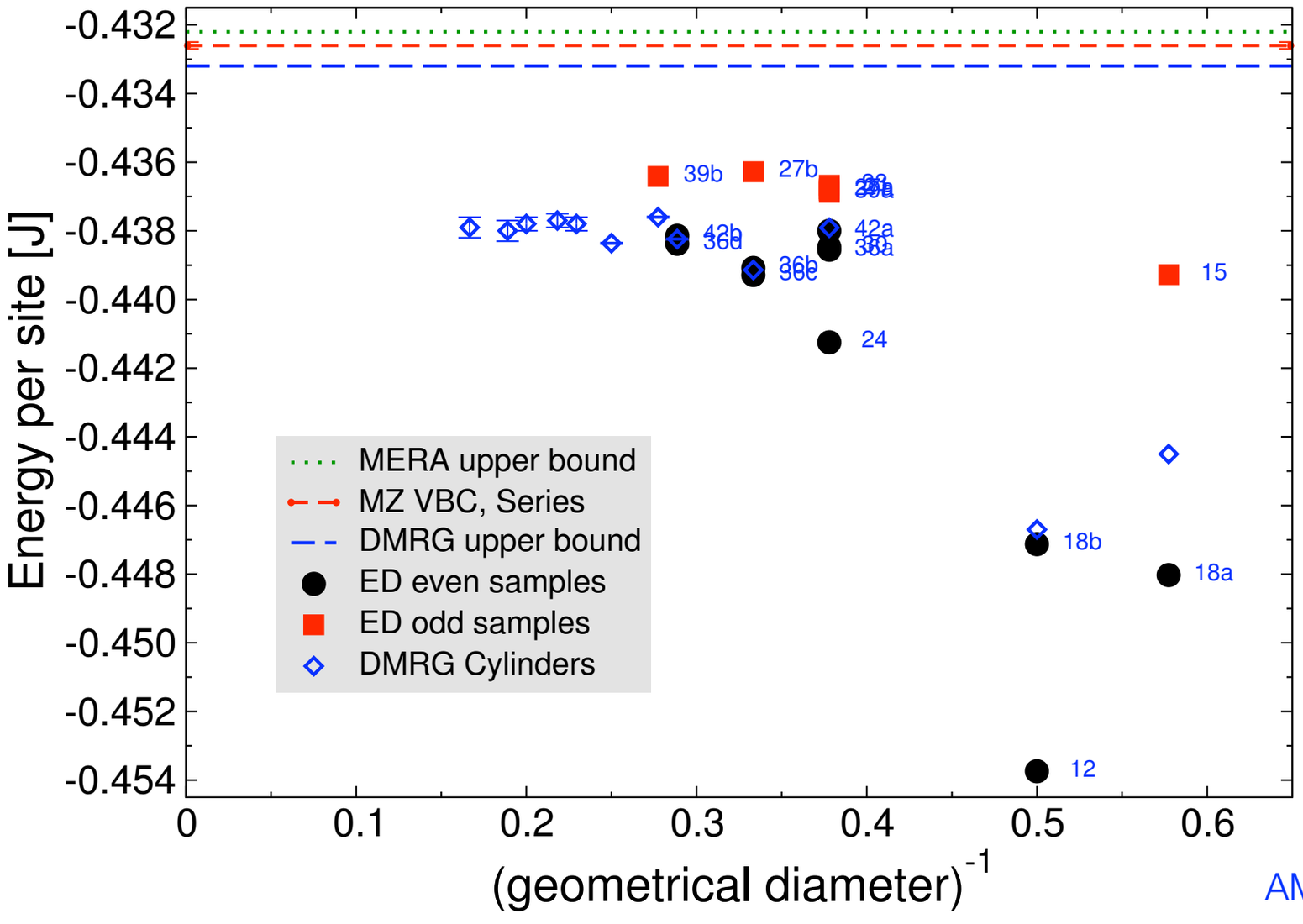
- Convergence for such large Hilbert spaces ? Finite precision arithmetic ?
  Seems ok

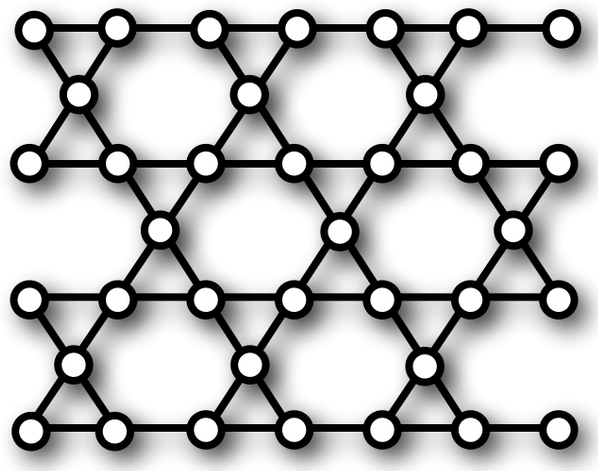


- Upper end of spectrum converges to known energy of the ferromagnetic state !
  ok !

MPI parallel ED for the kagome lattice without spatial symmetries

- ED Energy per site as a function of diameter (N up to 42 sites, dim up 270×10^9).



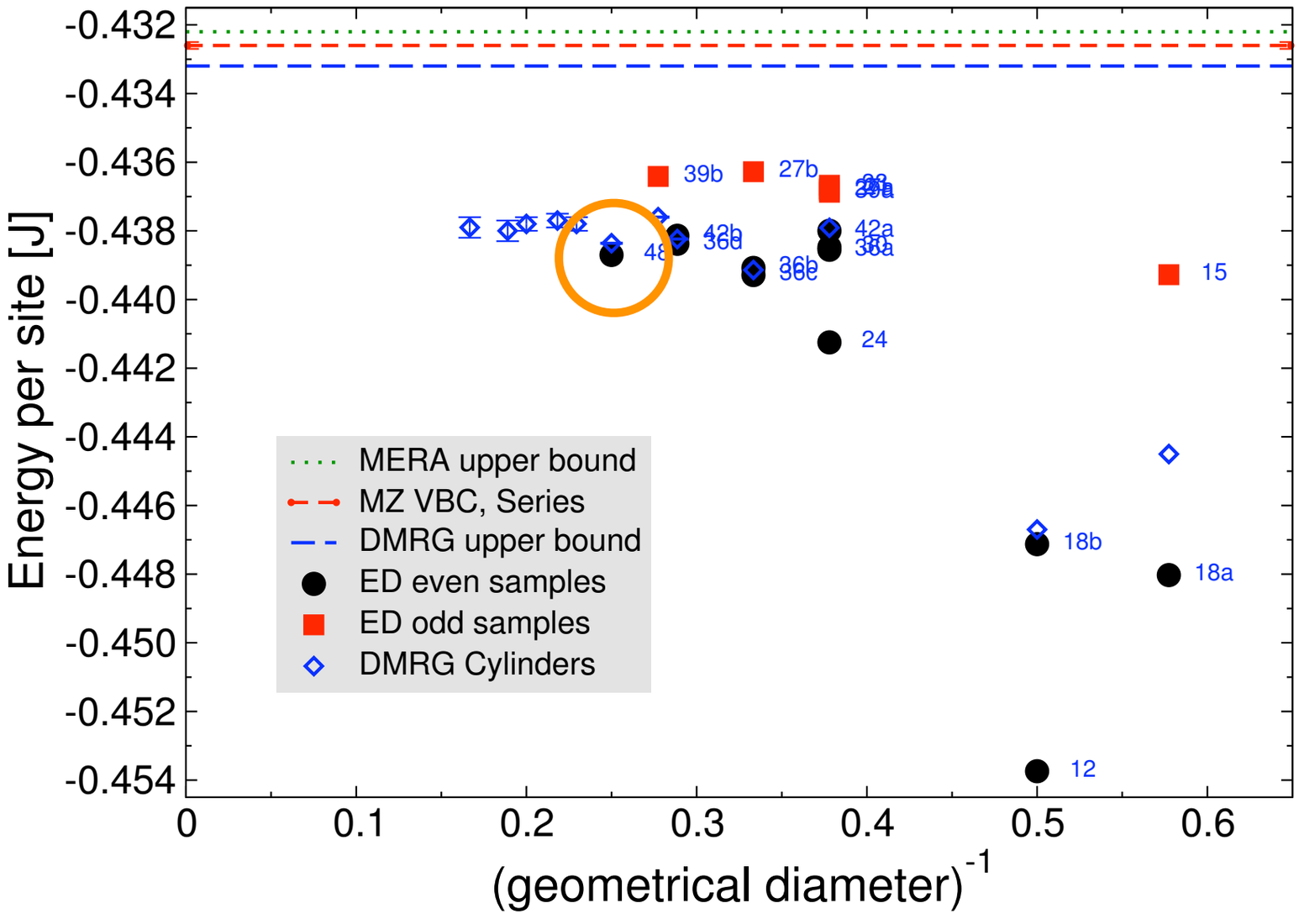


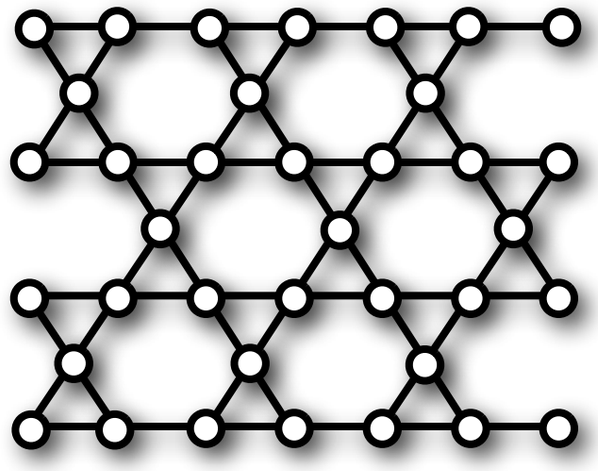
AML, J. Sudan and E. Sorensen, PRB **83**, 212401 (2011)

- MPI implementation (with R. Johanni, MPG RZG):
  180 seconds per iteration on 2048 cores on an 4x QDR IB Xeon cluster

MPI parallel ED for the kagome lattice now including spatial symmetries

- A new data point for N=48 sites (251‘936‘333‘376 states in GS sector)





- MPI implementation (with R. Johanni, MPG RZG):
  520 seconds per iteration on 16‘384 cores on the BlueGene/P @ MPG RZG

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", Eds. Lacroix, Mendels, Mila, (2011).
  available upon e-mail request.

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..)

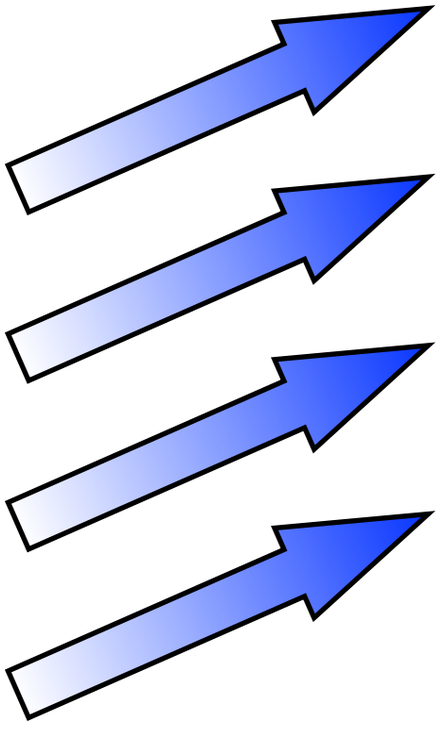
- Full Configuration Interaction in Quantum Chemistry

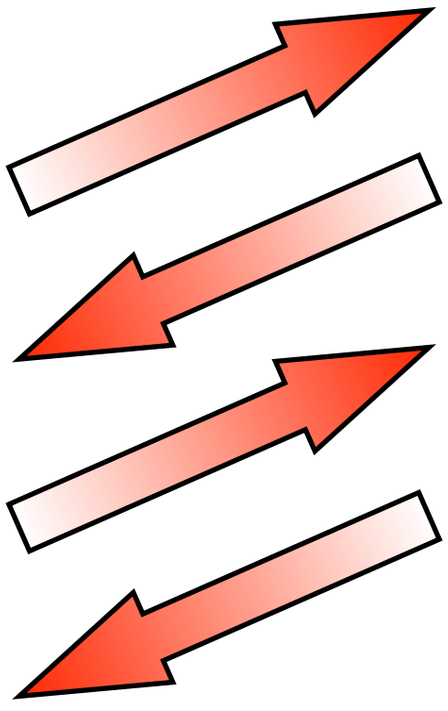
“Tower of States” spectroscopy

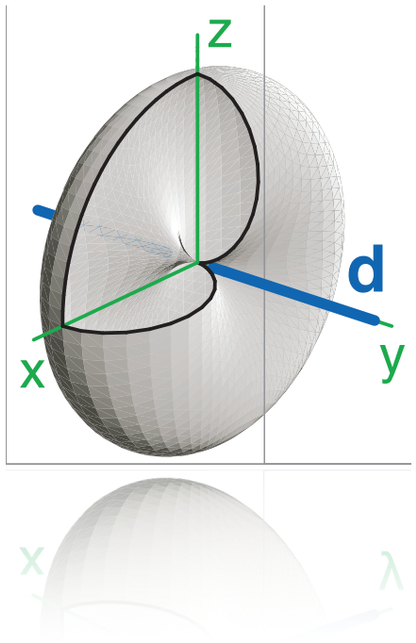
- What are the finite size manifestations of a continuous symmetry breaking ?
  (eg in superfluids/superconductors, magnetic order, spin nematic order)

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

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

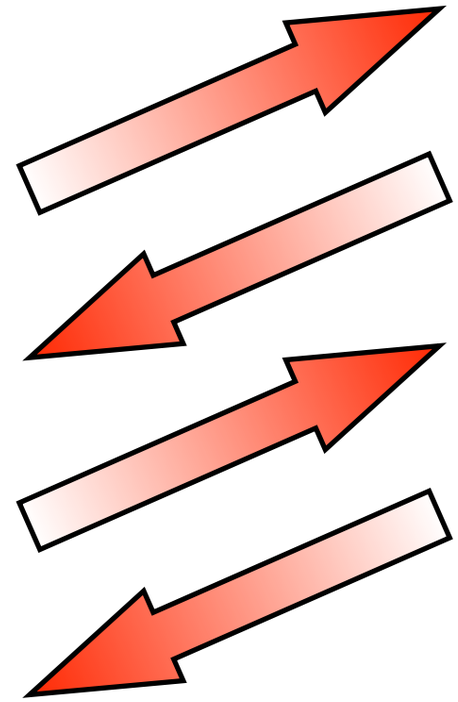






“Tower of States” spectroscopy

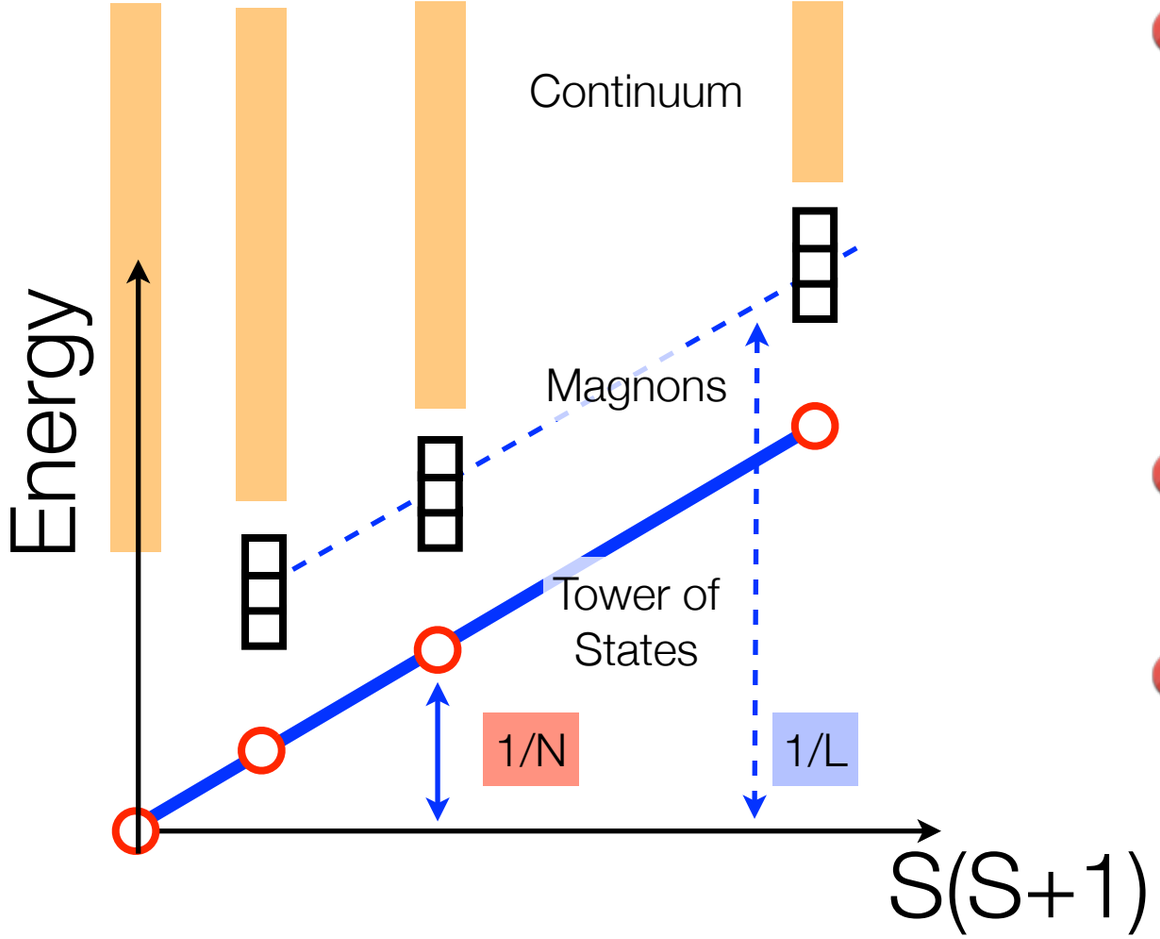
- Order parameter is not a conserved quantity
- Order parameter is zero on a finite size sample (Wigner-Eckart)
- How does one get spontaneous symmetry breaking anyway ?
- Ground state degeneracy is building up as we approach the thermodynamic limit, which will allow to form a symmetry breaking wave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

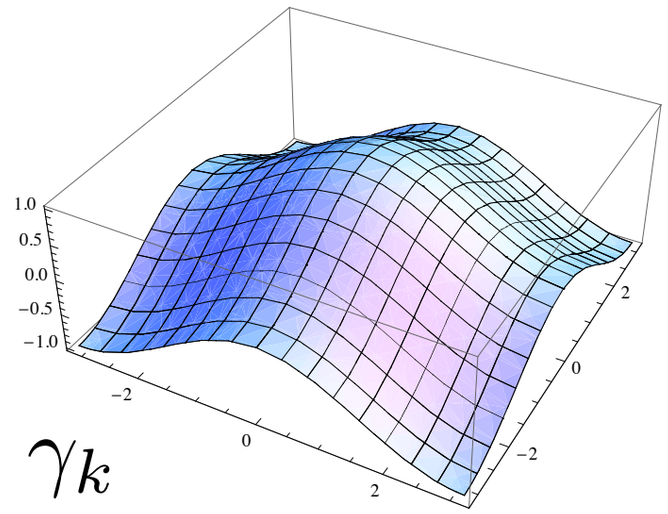
- U(1): $(S^z)^2$ SU(2): S(S+1)

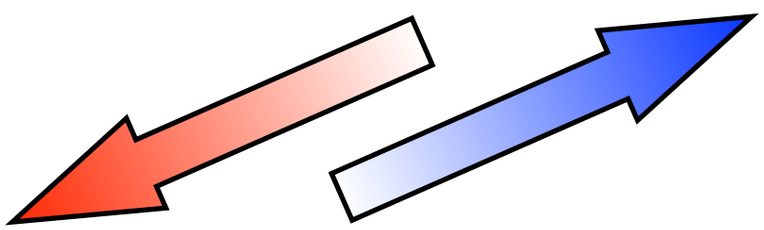
- Symmetry properties of levels in the Tower states are crucial and constrain the nature of the broken symmetries.

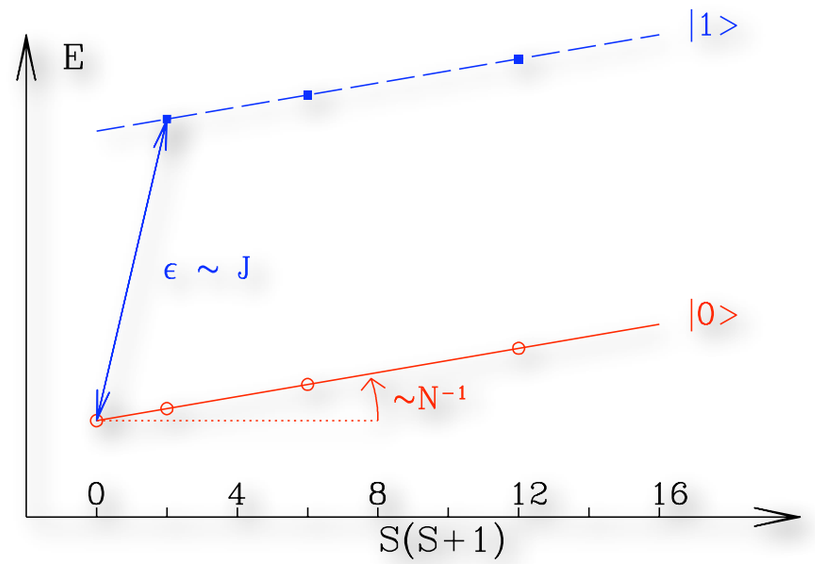
Square lattice Heisenberg antiferromagnet

- Hamiltonian $$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$
- Fourier transform $$H = 2J \sum_k \gamma_k \ \mathbf{S}_k \cdot \mathbf{S}_{-k}$$
- Keep only the (0,0) and (π,π) mode
- Lieb Mattis model recovered

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





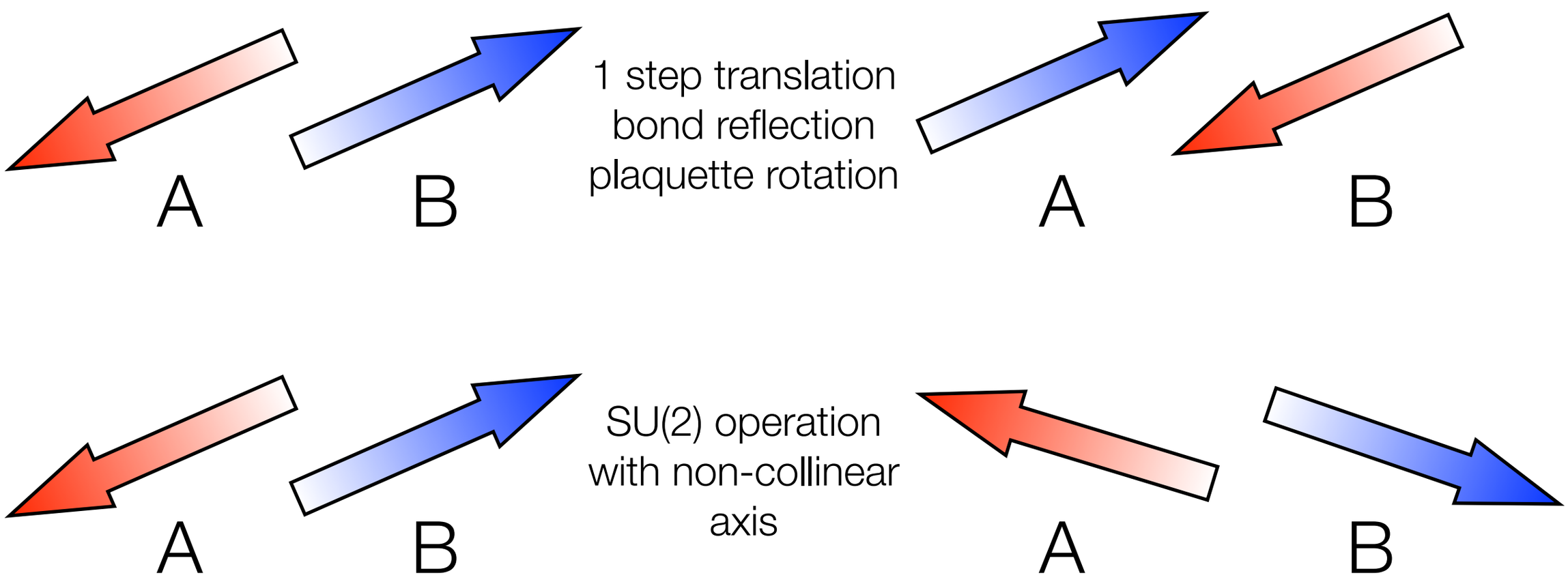


C. Lhuillier, cond-mat/0502464

Symmetry decomposition of order parameter

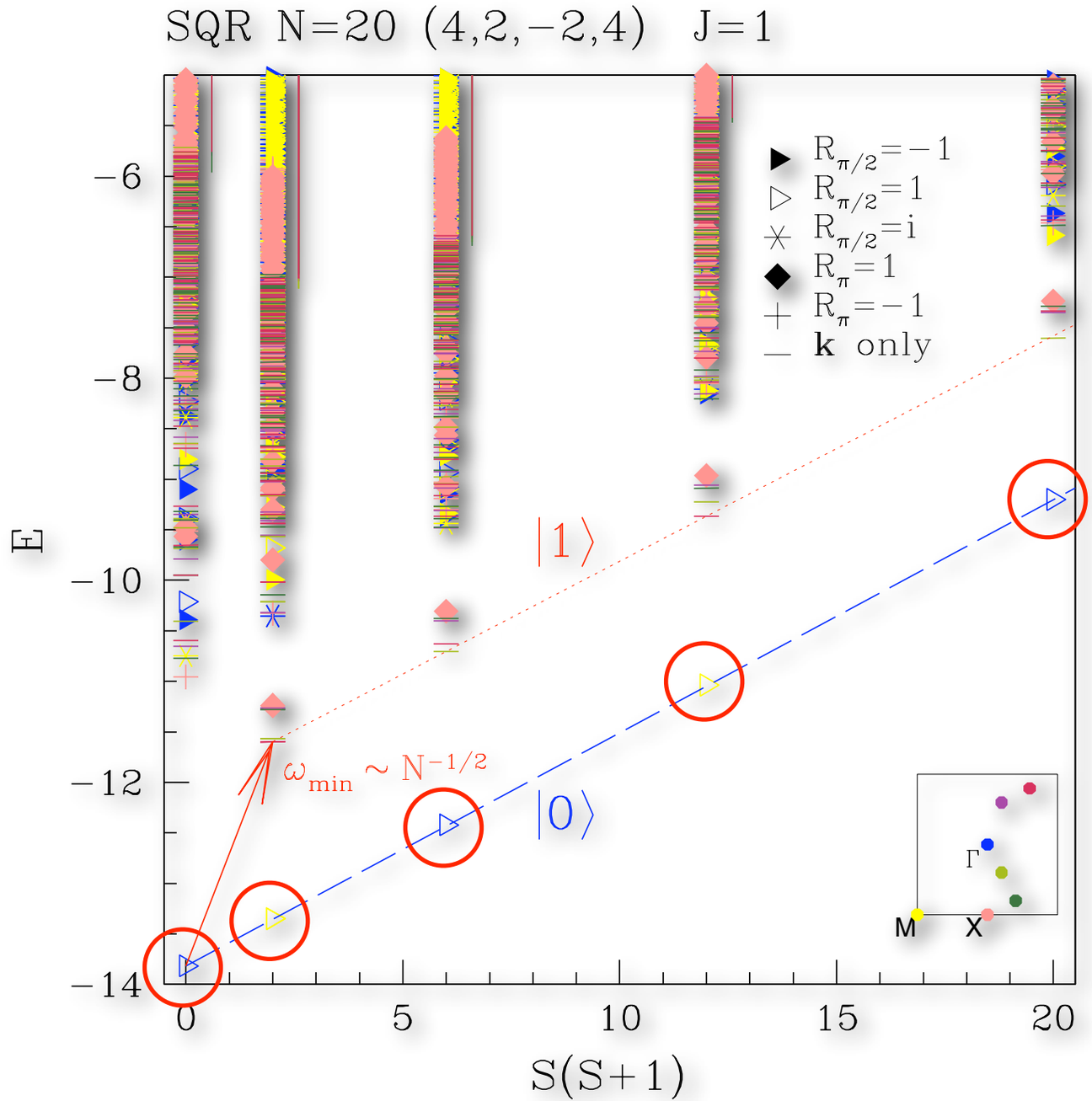
- Order parameter manifold forms a representation space for the symmetry group of the Hamiltonian

- Decompose this (reducible) representation into irreducible representations



Symmetry decomposition of order parameter

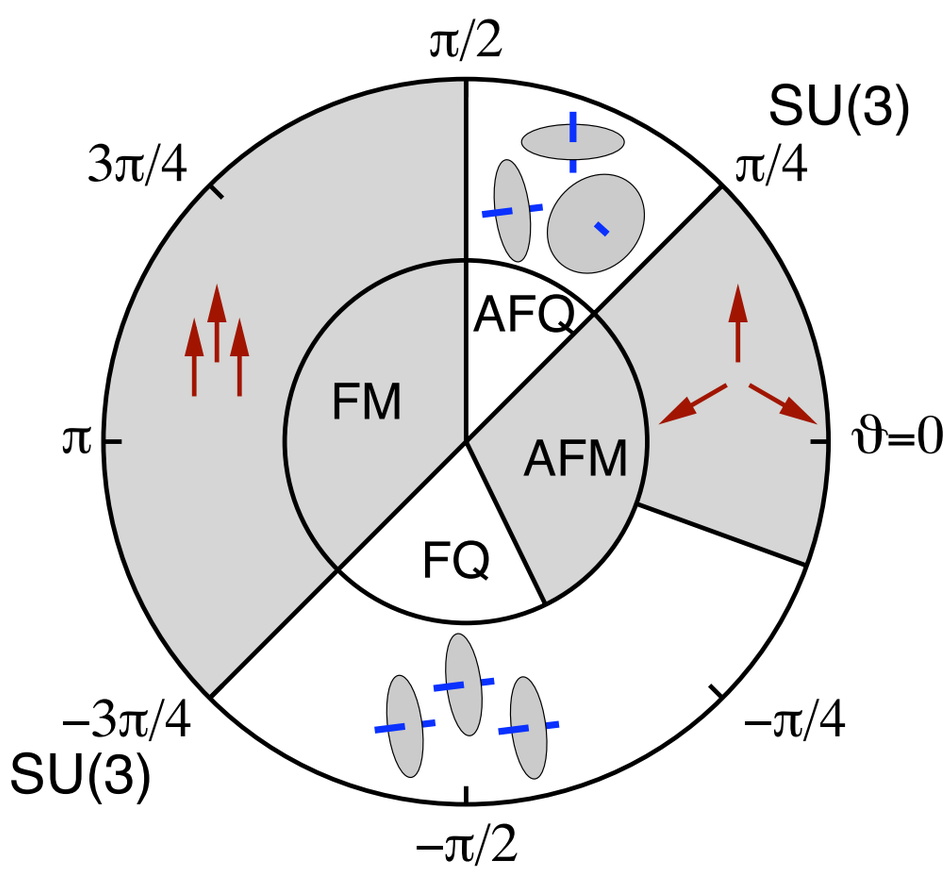
- As a result of the group theoretical analysis one obtains
  - 1 irrep with S=0, (0,0) A1
  - 1 irrep with S=1, (π,π) A1
  - 1 irrep with S=2, (0,0) A1
  - 1 irrep with S=3, (π,π) A1
  - ...



Beyond the collinear Neel state

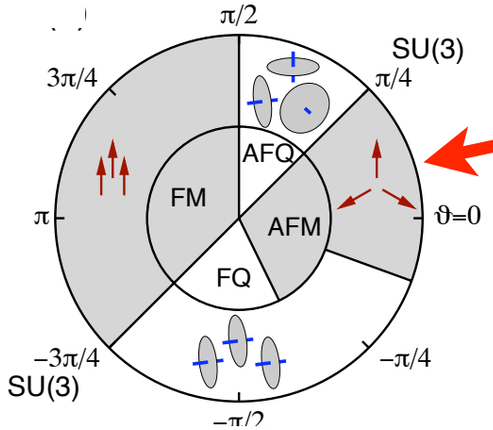
- Bilinear-biquadratic S=1 model on the triangular lattice (model for $NiGaS_4$).

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

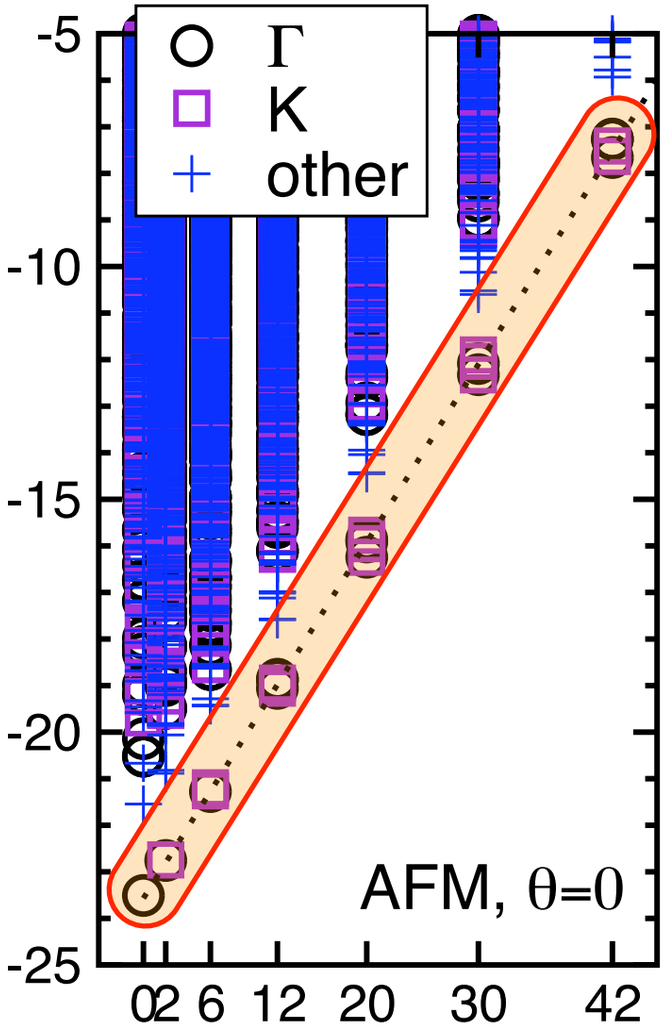


AML, F. Mila, K. Penc, PRL ‘06

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



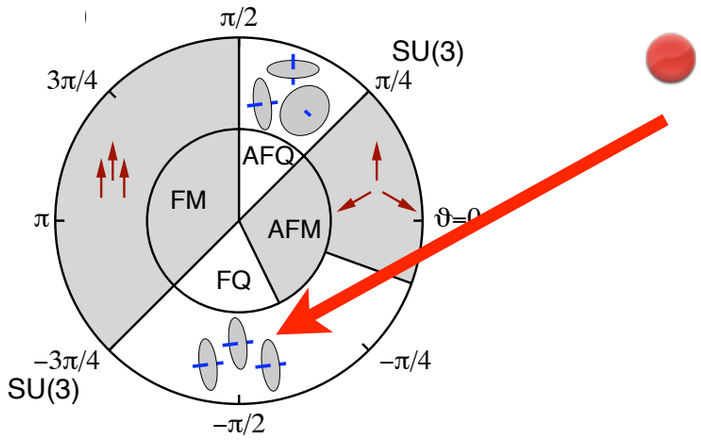
- ϑ=0 : coplanar magnetic order,
  120 degree structure



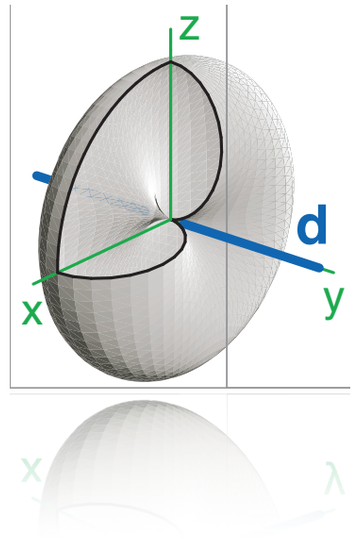
- Breaks translation symmetry. Tree site unit cell
  ⇒ nontrivial momenta must appear in TOS
- non-collinear magnetic structure
  ⇒ SU(2) is completely broken,

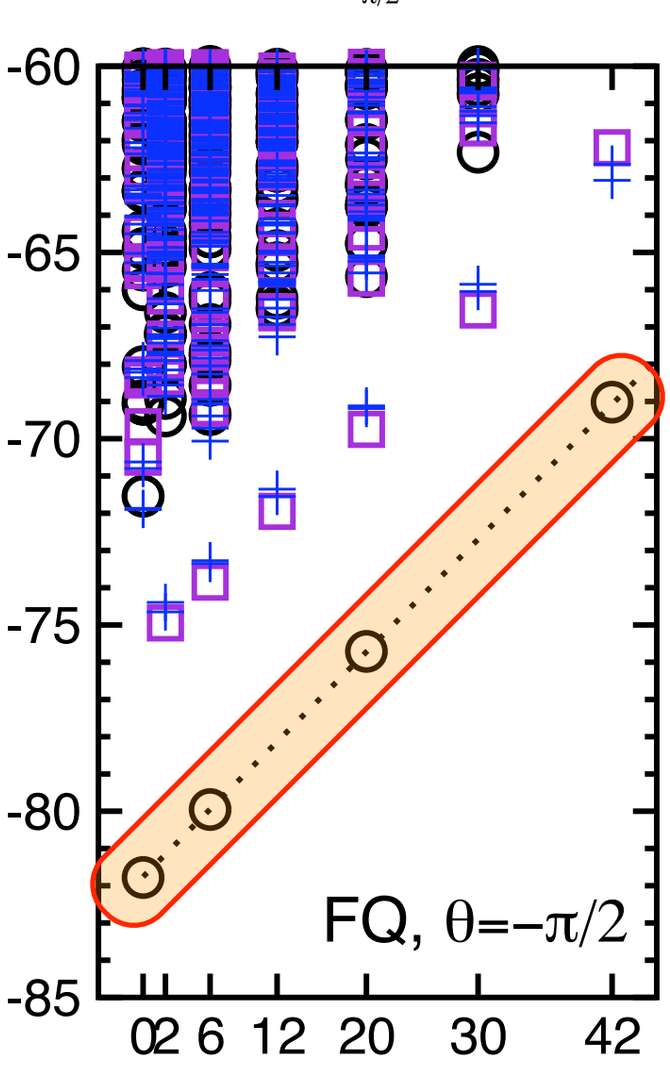
  number of levels in TOS increases with S
- Quantum numbers are identical to the S=1/2 case

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



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

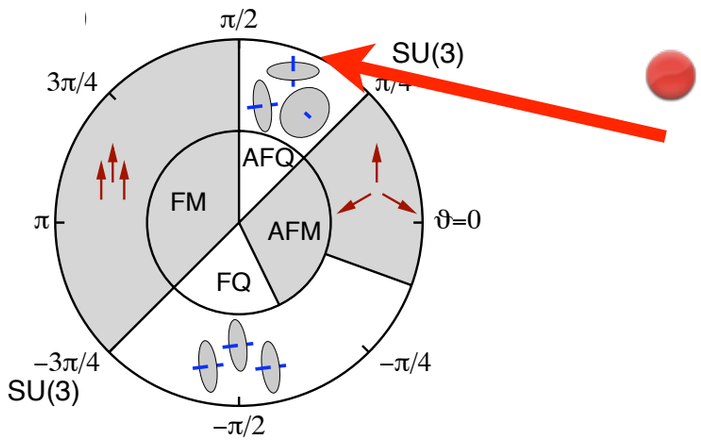




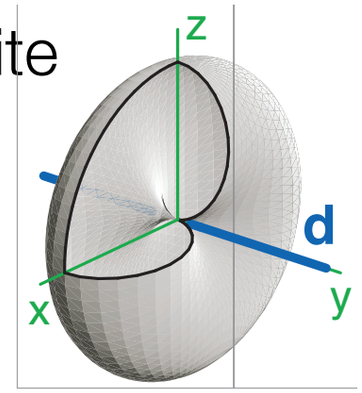
- No translation symmetry breaking.
  ⇒ only trivial momentum appears in TOS
- Ferroquadrupolar order parameter, only even S
- all directors are collinear
  ⇒ SU(2) is broken down to U(1),

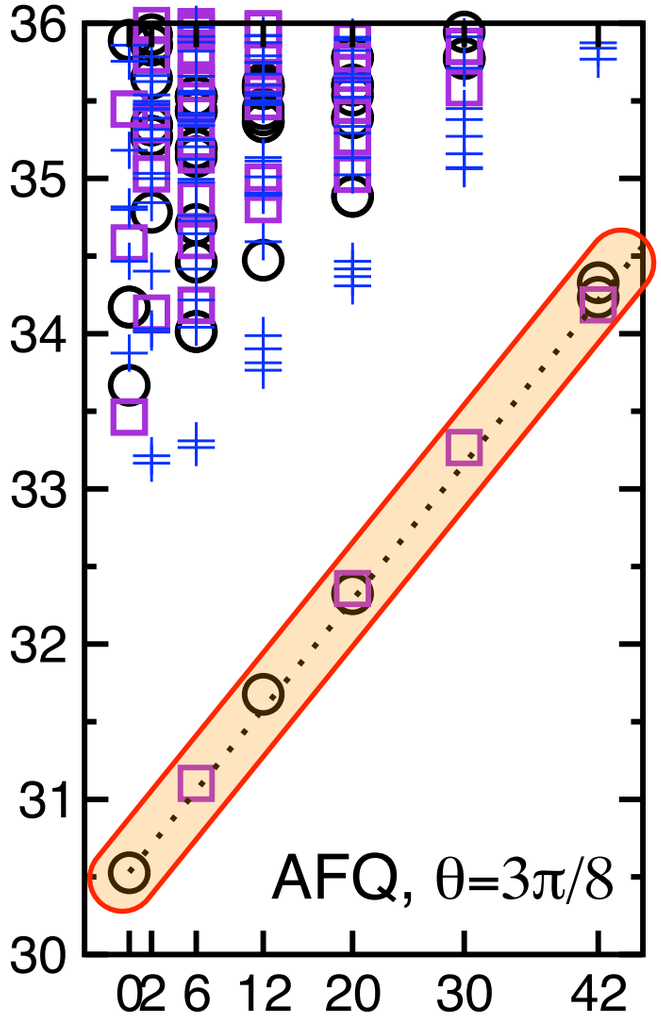
  number of states in TOS is *independent* of S.

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



- ϑ=3π/8 : antiferroquadrupolar phase, finite quadrupolar moment, no spin order, three sublattice structure.

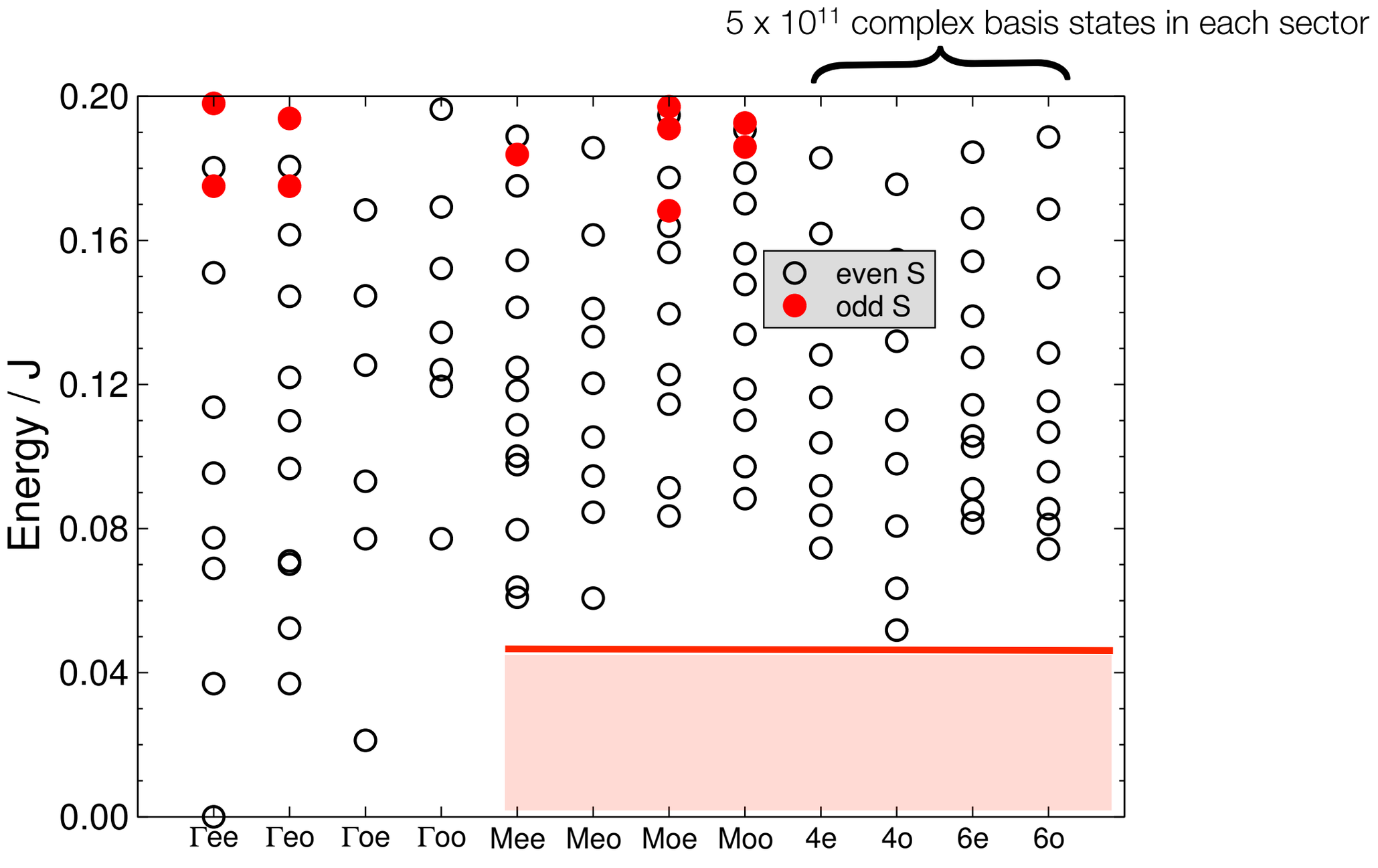




- Breaks translation symmetry. Tree site unit cell ⇒ nontrivial momenta must appear in TOS

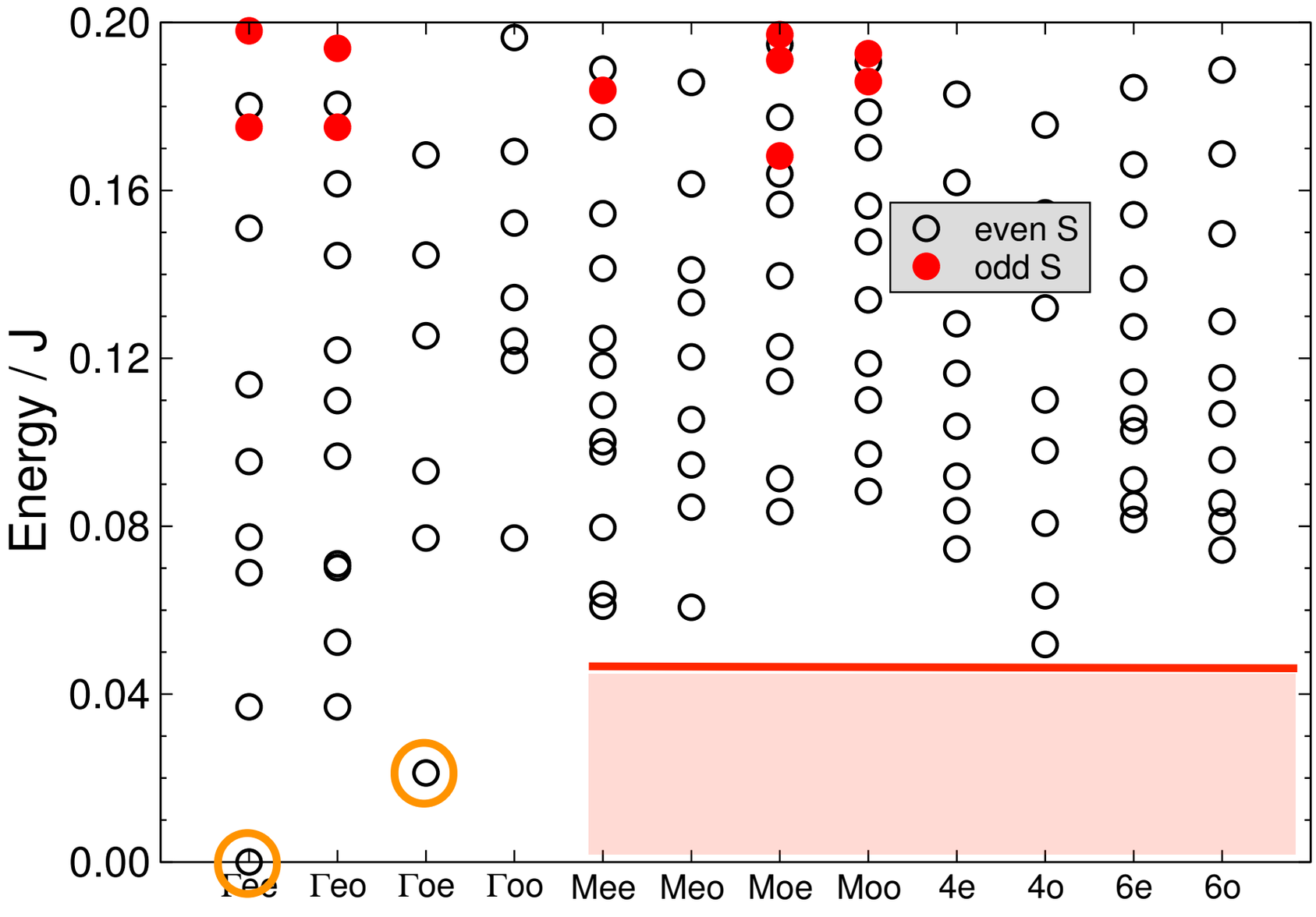
- Antiferroquadrupolar order parameter, complicated S dependence. Can be calculated using group theoretical methods.

Energy Spectroscopy in a putative spin liquid ?
Kagome Low Energy Spectrum (N=48)



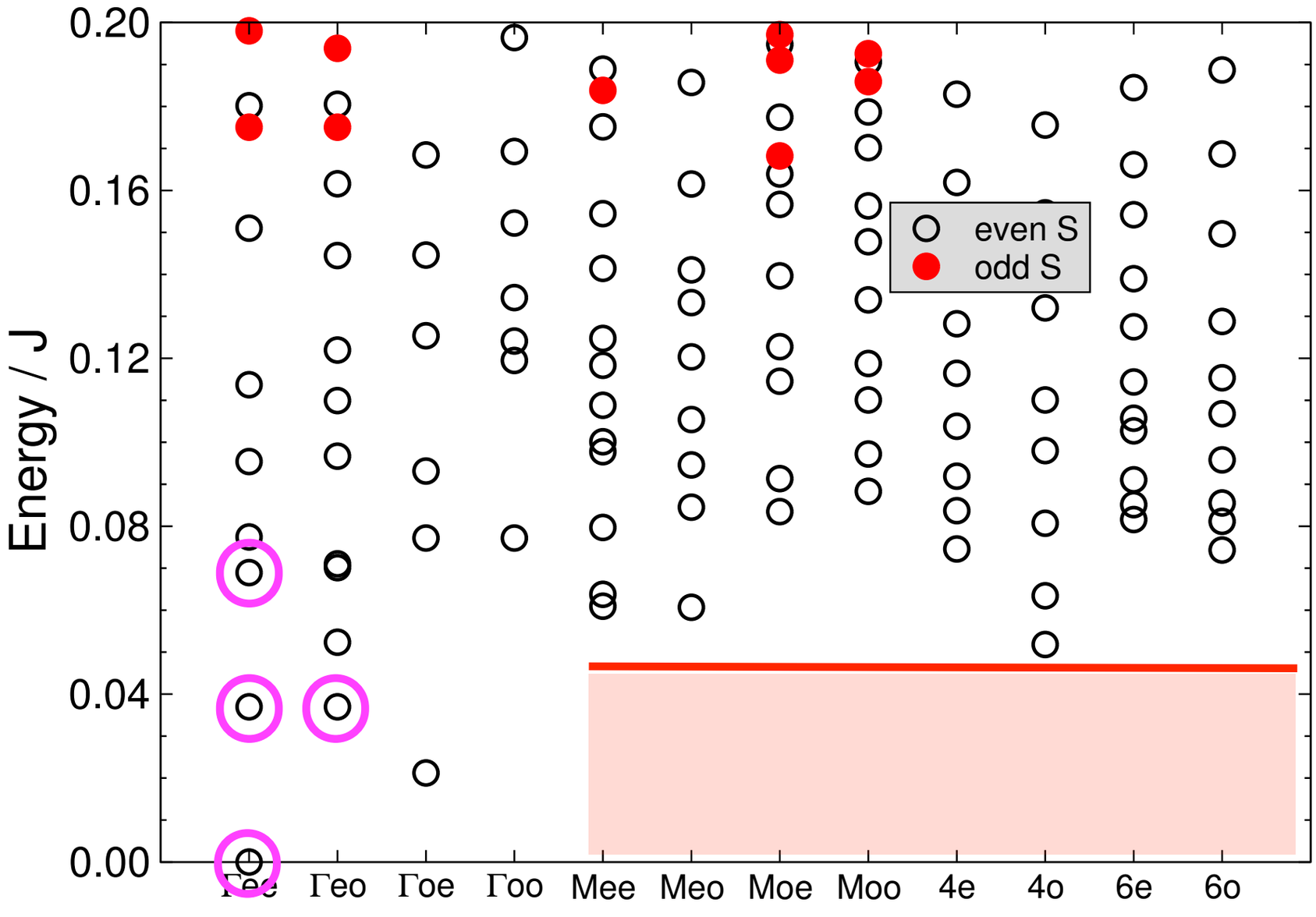
translation symmetry breaking unlikely

Low Energy Spectrum (N=48)



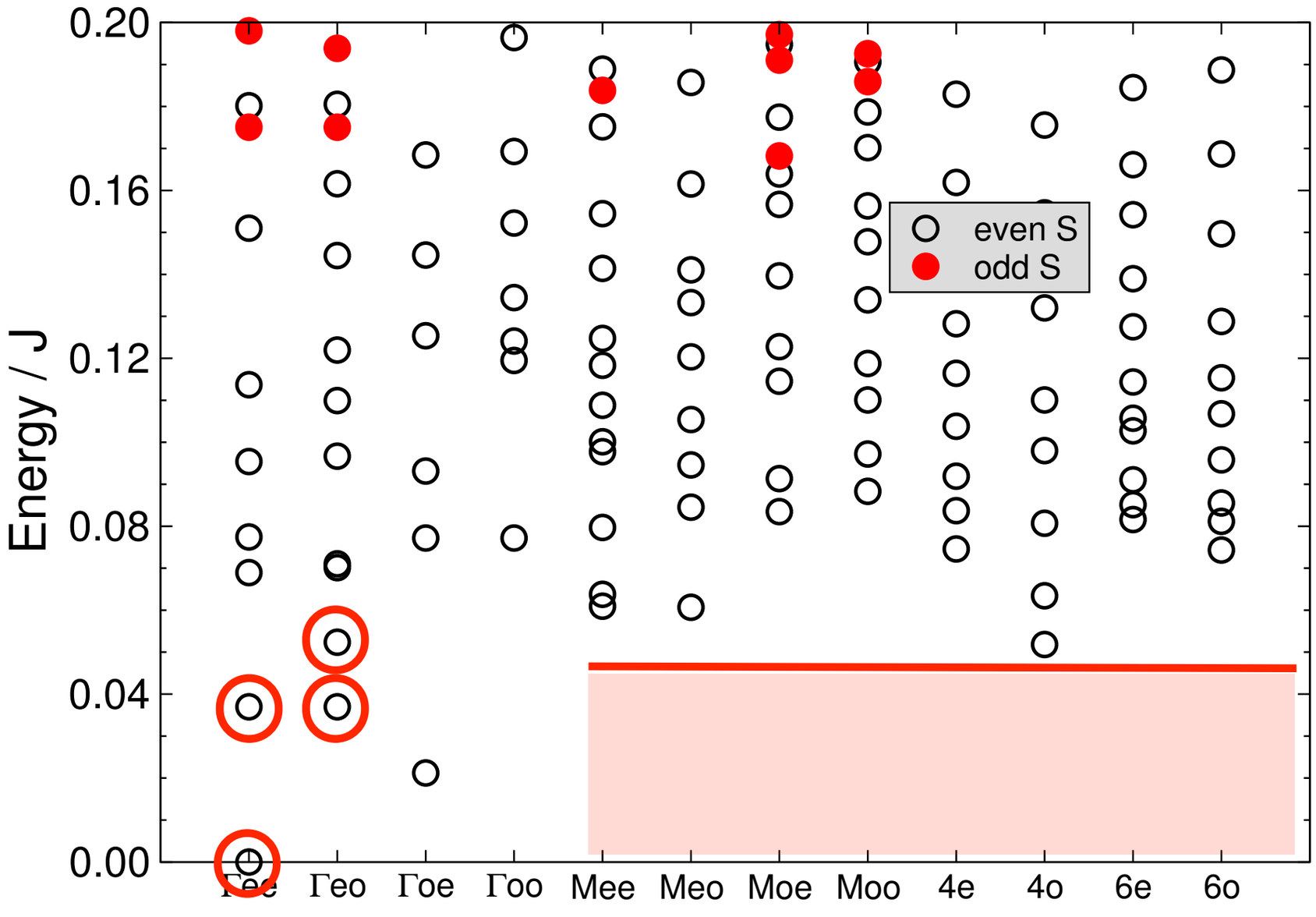
Inversion symmetry breaking ?

Low Energy Spectrum (N=48)



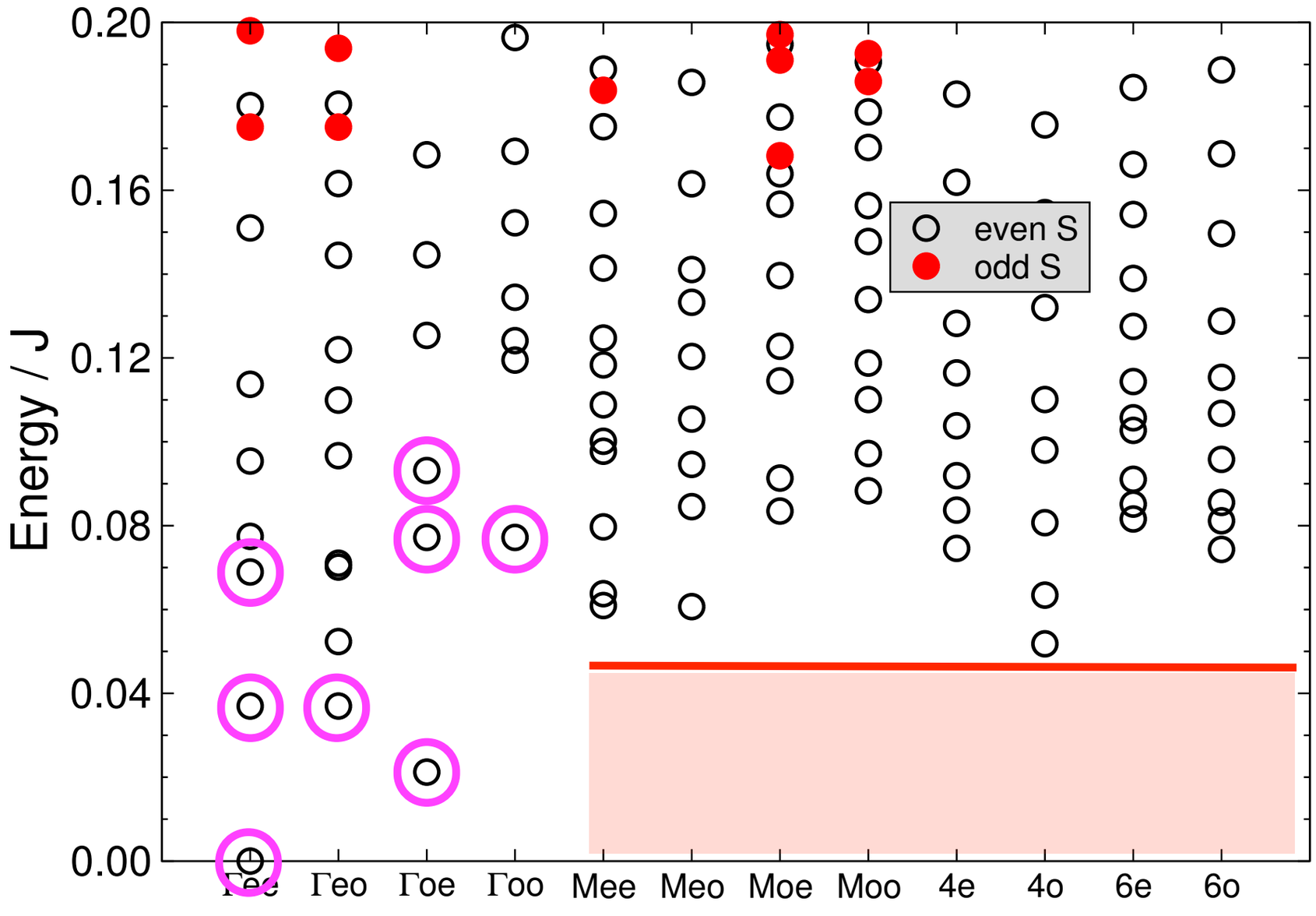
Z_2 topological degeneracy ?

Low Energy Spectrum (N=48)



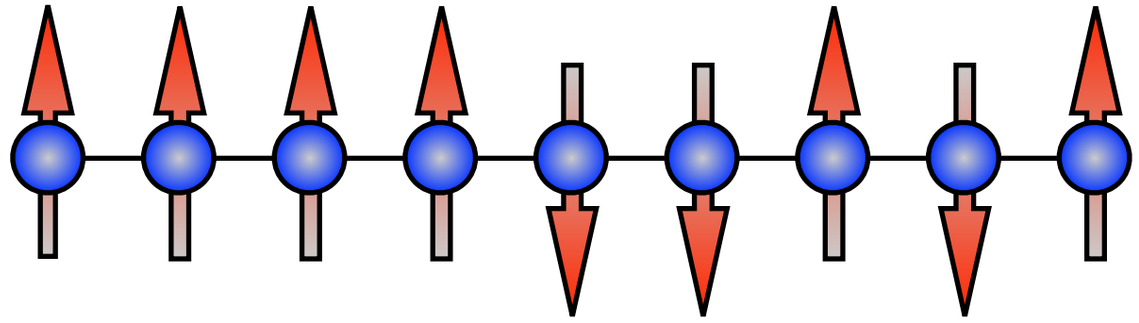
chiral spin liquid ?

Low Energy Spectrum (N=48)



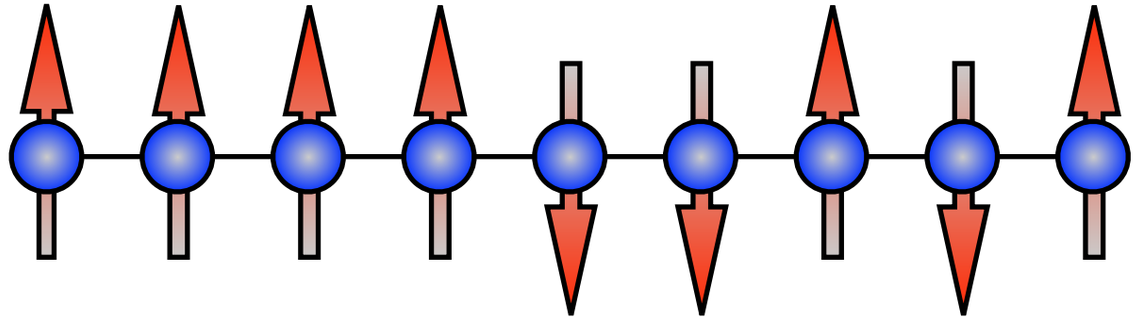
Z_2 topological times Z_2 spatial symmetry breaking ?

Tutorials



- Different options:
  - Play with /and extend/ the code fragment on the following slides
  - Perform the ALPS Tutorial on ED Spectroscopy for a CFT phase transition.
    - http://alps.comp-phys.org/mediawiki/index.php/ALPS_2_Tutorials:ED-04_Criticality
    - http://alps.comp-phys.org/mediawiki/index.php/ALPS_2_Tutorials:ED-05_ED_Phase_Transition
  - Krylov Time Evolution:
    - Understand the Mathematica based Krylov time evolution code available on AFS alauchli
    - Translate into Python or language of your choice and investigate time evolution of two neighbouring flipped spins in a square lattice Heisenberg model as presented in the lecture.

A simple example (1/4):



```
#include <vector>
#include <alps/bitops.h>
class SpinOneHalfBasis {
public:
   typedef unsigned int state_type;
   typedef unsigned int index_type;
   SpinOneHalfBasis (int L, int TwoSz);
   state_type state(index_type i) const {return states_[i];}
   // lookup based on Lin tables
   index_type lookup(state_type s) const {
    return shighlook[alps::gbits(s,sh,sl)]+slowlook[alps::gbits(s,sl,0)];
   }
   unsigned int dimension() const { return states_.size();}
private:
   // list of configurations in Hilbert space
   std::vector<state_type> states_;
   // Lin tables
   int sl,sh;
   std::vector<index_type> slowlook,shighlook;
};
```

A simple example (2/4):

```
SpinOneHalfBasis::SpinOneHalfBasis(int L, int TwoSz)
{
   if (L%2) {
    sl=(L+1)/2;
    sh=(L-1)/2;
     } else
    sl=sh=L/2;

   slowlook.resize(1<<sl);
   shighlook.resize(1<<sh);

   int Nup=(L+TwoSz)/2;

   unsigned int all_states=1U<<L;
   unsigned int index=0;
   unsigned int last_n=0;
    int  lasthigh_nibble=-1;

   // generating all configurations with correct TwoSz
   // and filling of Lin tables
   for (state_type s=0;s<all_states;++s)
    if(alps::bitcount(s)==Nup) {
       // correct number of up spins
       states_.push_back(s);
       //get sl lowest bits of s
       const int low_nibble  =gbits(s,sl,0);
       //get sh highest bits of s
       const int high_nibble =gbits(s,sh,sl);

       if (lasthigh_nibble!=high_nibble) {
          shighlook[high_nibble]=index;
          lasthigh_nibble=high_nibble;
          last_n=index;
       }

       slowlook[low_nibble]=index-last_n;
       index++;
    }
}
```

A simple example (3/4):

```
class HamiltonianMultiplier : public SpinOneHalfBasis {
public:
   HamiltonianMultiplier(int L, int TwoSz, double Jxy, double Jz)
   : SpinOneHalfBasis(L,TwoSz), Jxy_(Jxy), Jz_(Jz), L_(L) {}
   void multiply(std::valarray<double>& v, const std::valarray<double>& w);
private:
   double Jxy_, Jz_;
   int L_;
}
```

A simple example (4/4):

```
void HamiltonianMultiplier::multiply(std::valarray<double>& v,
                                     const std::valarray<double>& w) {
   // check dimensions
   assert(v.size()==dimension()); assert(w.size()==dimension());
   // do the Jz-term
   for (int i=0;i<dimension();++i) {
    state_type s = state(i);
    // count number of parallel spins
    state_type s = state(i);
     for (int r=0;r<L_-1;++r)
        v[i]+=( 0.25*Jz_-0.5*Jz_*(alps::gbit(s,r)^alps::gbit(s,r+1)) )*w[i];
    }
    // do the Jxy-term
    for (int i=0;i<dimension();++i)
    {
     state_type s = state(i);
     for (int r=0;r<L_-1;++r) {
        if(alps:popcnt(s&(3<<r))==1) { // is state flippable ?
           state_type snew = s^(3<<r); // exchange up and down spins
           index_type idx = lookup(snew);
           v[idx]+=w[i]*Jxy_*0.5;
        }
     }
    }
}
```

Homework:

- Take the code fragment from the example and
  - Implement the Hamiltonian with periodic boundary conditions
  - Use the fragment to dump the Hamilton matrix for a toy problem system and diagonalize it in Matlab/Mathematica,....


Write a very basic implemention of a Lanczos eigensolver around it


Implement Sz->-Sz symmetry for the Sz=0 sector


Implement translation symmetry !

- Report any progress or questions to andreas.laeuchli@uibk.ac.at

Thank you !