Quantum Lattice Models
&
Introduction to Exact Diagonalization

$$H\left|\Psi\right\rangle = E\left|\Psi\right\rangle$$

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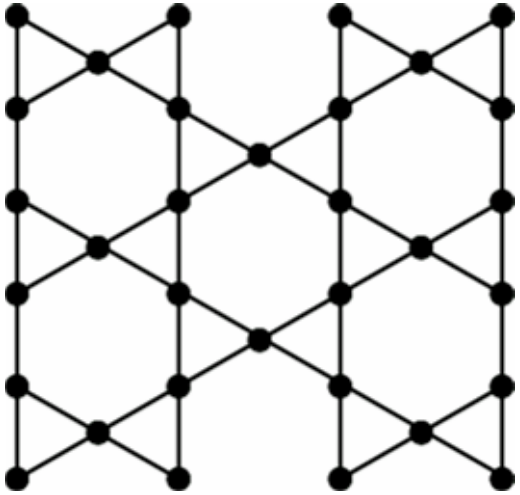
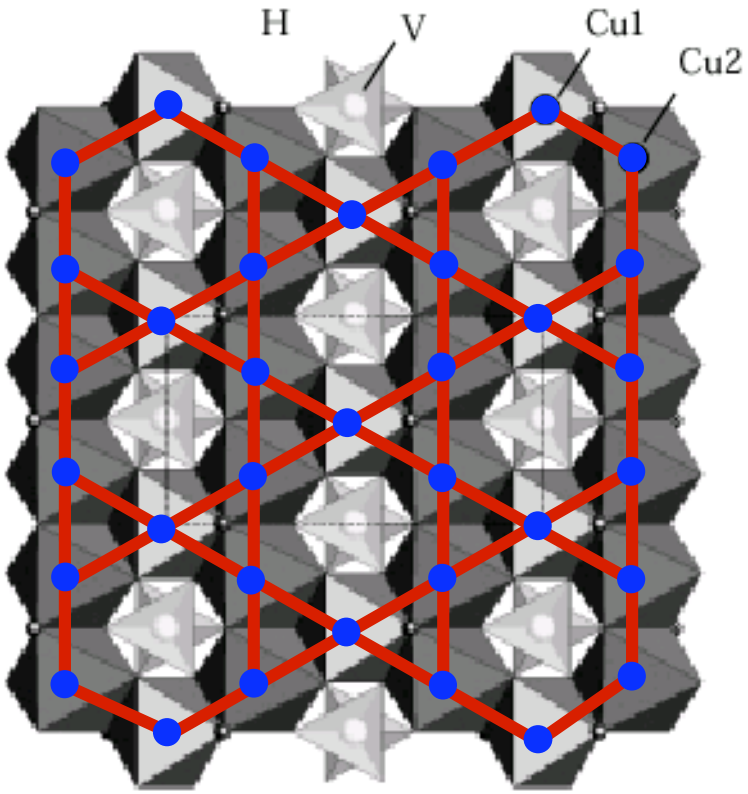
Outline of this lecture:

- Quantum Lattice Models
  - Lattices and Models in general and in ALPS
- Exact Diagonalization (ED)
  - The Method and its applications
  - Ingredients
- ED Extensions
  - Finite Temperature Lanczos Methods
  - Contractor Renormalization (CORE)

Quantum Lattice Models



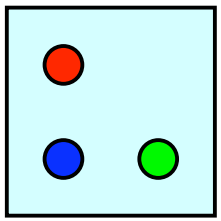
kagome lattice



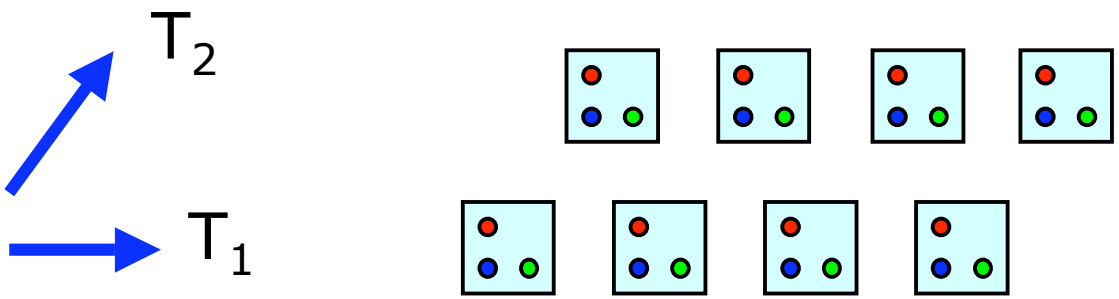
Volborthite

Lattices

- Infinite Lattices are made out of:
  - A Unit Cell, containing n “atoms”

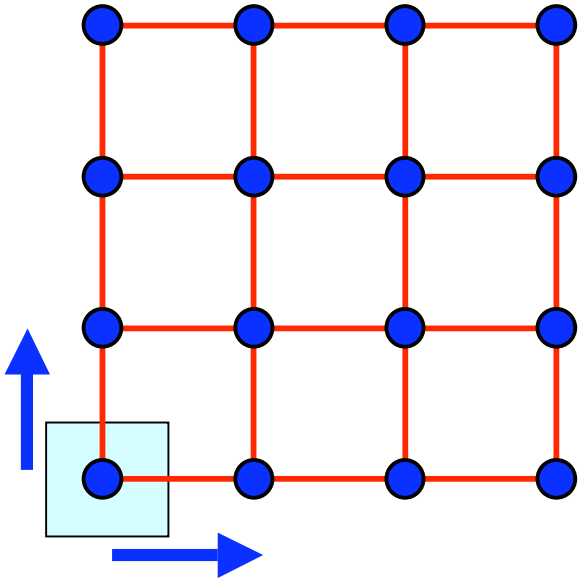


  - Spanning vectors defining the Bravais lattice:

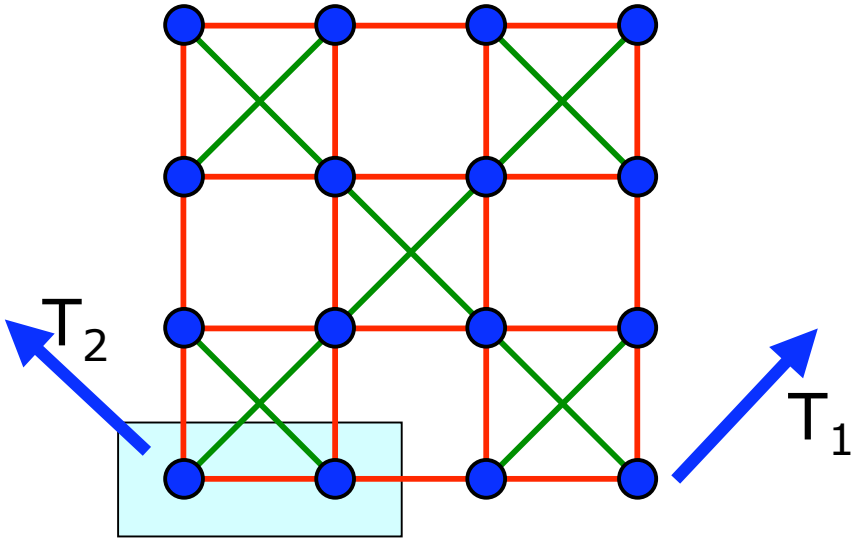


Lattices II

Some Examples:



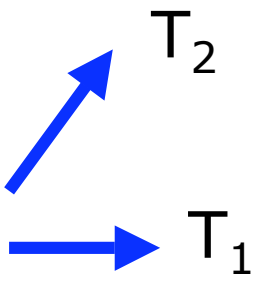
Square Lattice
single site unit cell



Checkerboard Lattice
two sites in unit cell

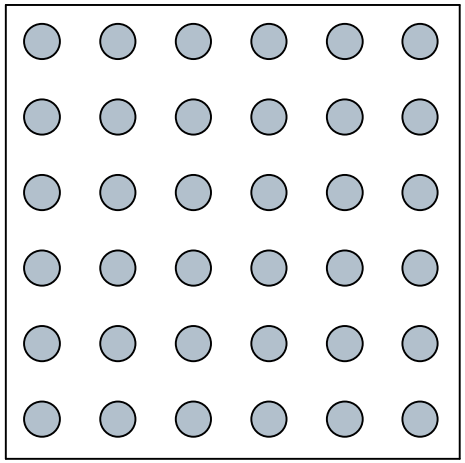
Finite Lattices

The present way in ALPS:



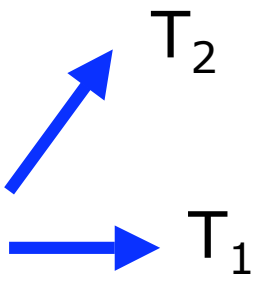
Extent is given by multiples of the Bravais vectors T_1 and T_2

For the square lattice:
Extent =6x6
$\Rightarrow$ 36 sites



Finite Lattices

In the near future in ALPS:



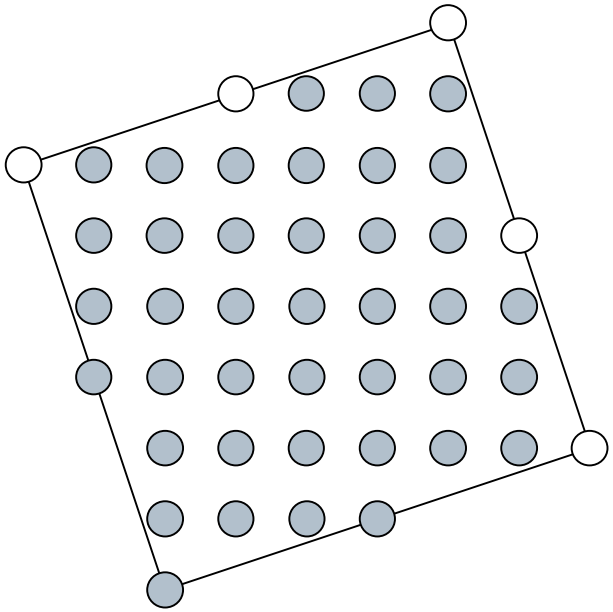
Extent is given by non-collinear spanning vectors.

For the square lattice:

$F_1=(6,2)=6T_1+2T_2$

$F_2=(-2,6)=-2T_1+6T_2$

$\Rightarrow$ 40 sites



Models

- Many Body Lattice Models
- Single Particle Lattice Models
- Constrained Models

Many-Body Hamiltonians

- Spin models:
  - Heisenberg Couplings (any S):

$$\mathbf{S}_1 \bullet \mathbf{S}_2$$

  - Modifications:

$$J_{xy}(S_1^x S_2^x + S_1^y S_2^y) + J_z\, S_1^z S_2^z$$

easy plane, easy axis anisotropies

$$D\,(S_1^z)^2$$

single ion anisotropy

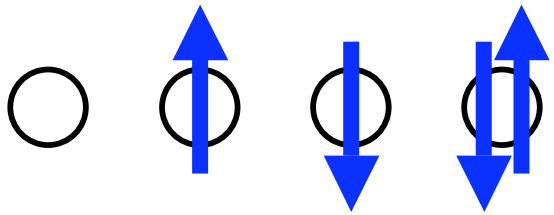
$$J_n(\mathbf{S}_1 \bullet \mathbf{S}_2)^n, \qquad K(\mathbf{S}_1 \bullet \mathbf{S}_2)(\mathbf{S}_3 \bullet \mathbf{S}_4)$$

higher order spin interactions
(biquadratic, Ring exchange,....)

Many-Body Hamiltonians

- Fermionic models:
  - Hubbard model:

$$-t\left(c^{+}_{1,\sigma}c_{2,\sigma}+c^{+}_{2,\sigma}c_{1,\sigma}\right)+U\,n_{1,\uparrow}n_{1,\downarrow}$$



Many-Body Hamiltonians

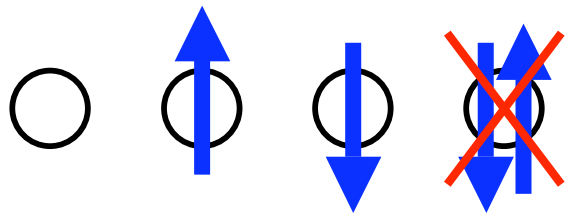
- Fermionic models:
  - Hubbard model:

$$-t\left(c^{+}_{1,\sigma}c_{2,\sigma}+c^{+}_{2,\sigma}c_{1,\sigma}\right)+U\,n_{1,\uparrow}n_{1,\downarrow}$$

  - t-J model: (≈large U limit of the Hubbard model)

$$-t\,\wp\left(c^{+}_{1,\sigma}c_{2,\sigma}+c^{+}_{2,\sigma}c_{1,\sigma}\right)\wp$$

$$+J\left(\mathrm{S}_1\bullet\mathrm{S}_2-1/4n_1n_2\right)$$



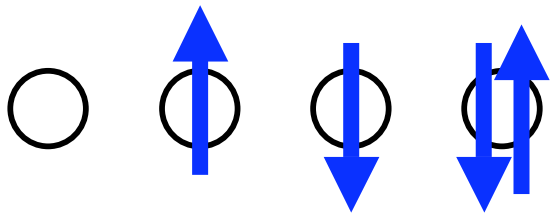
Many-Body Hamiltonians

- Fermionic models:
  - Kondo lattice model:

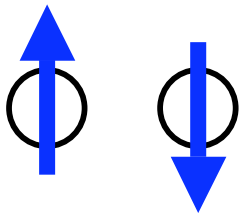
$$-t\, c^{+}_{1,\sigma} c_{2,\sigma} + c^{+}_{2,\sigma} c_{1,\sigma}$$

$$+ J\,(\sigma_1 \bullet \mathrm{S_f})$$

Kondo coupling



Conduction electrons site



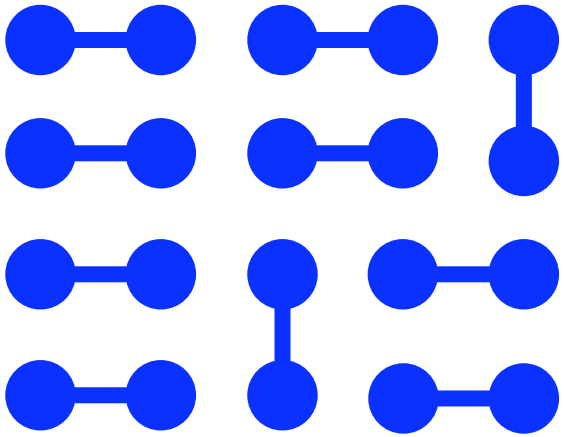
f-electrons site

Single Particle Models

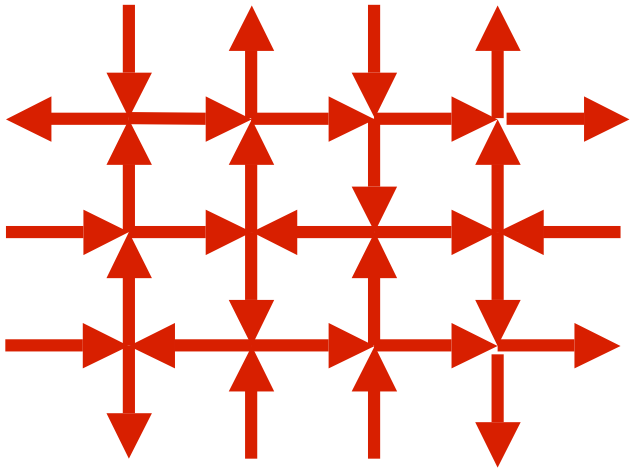
- Disordered potentials and hoppings
  - ⇒ Anderson Localization
- Hopping phases
  - ⇒ Hofstadter Butterfly
- Jordan-Wigner transformation
  - ⇒ Disordered XX-spin chains

Constrained Models (not yet in ALPS)

- Hardcore-dimer models:



- Vertex / Ice models:



Exact Diagonalization

$$H\left|\Psi\right\rangle = E\left|\Psi\right\rangle$$

Exact Diagonalization

- Solve the Schrödinger equation for a many body Hamiltonian on a finite system ⇒ Standard Eigenvalue problem:

$$H\left|\Psi\right\rangle = E\left|\Psi\right\rangle$$

- Within this approach we can basically simulate any model.

- However due to the exponentially growing computational effort it is most useful where more powerful methods fail:

  - Fermionic Models in 1D and 2D (no sign problem)
  - Frustrated Quantum Magnets in 1D/2D/(3D)
  - Quantum number resolved quantities
  - Calculation of basically any observable, i.e. complicated dynamics
  - Benchmark for all other methods

Exact Diagonalization – present day limits

- Spin S=1/2 models:
  40 spins square lattice, 39 sites triangular, 42 sites star lattice
  Dimension: **up to 1.5 billion basis states**

- t-J models:
  32 sites checkerboard with 2 holes
  32 sites square lattice with 4 holes
  Dimension: **up to 2.8 billion basis states**

- Hubbard models
  20 sites square lattice at half filling, 20 sites quantum dot structure
  Dimension: **up to 3 billion basis states**

- Holstein models
  14 sites on a chain + phonon pseudo-sites
  Dimension: **up to 30 billion basis states** **(needs a supercomputer on its own)**

Exact Diagonalization – Ingredients of a code

- Hilbert space
  - Site-Basis represention
  - Symmetries
  - Lookup techniques
- Hamiltonian Matrix
  - Sparse Matrix representation (memory/disk)
  - Matrix recalculation on the fly
- Linear Algebra / Eigensolver backend
  - LAPACK full diagonalization (in ALPS)
  - Lanczos type diagonalization (IETL, in ALPS)
  - More exotic techniques
- Observables
  - Static quantities
  - Dynamic observables

Coding of Basis states

- Representation of basis states in terms of binary numbers (or generalizations thereof):

$$|\uparrow_1\downarrow_2\ldots\rangle = 1_1 0_2 \ldots$$

- In more complicated models like t-J there is no unique or best way to represent the states:

$$|\uparrow_1\downarrow_2 O_3\ldots\rangle = 1_{1,\uparrow}\ 0_{1,\downarrow}\ 0_{2,\uparrow}\ 1_{2,\downarrow}\ 0_{3,\uparrow}\ 0_{3,\downarrow}\ \ldots$$

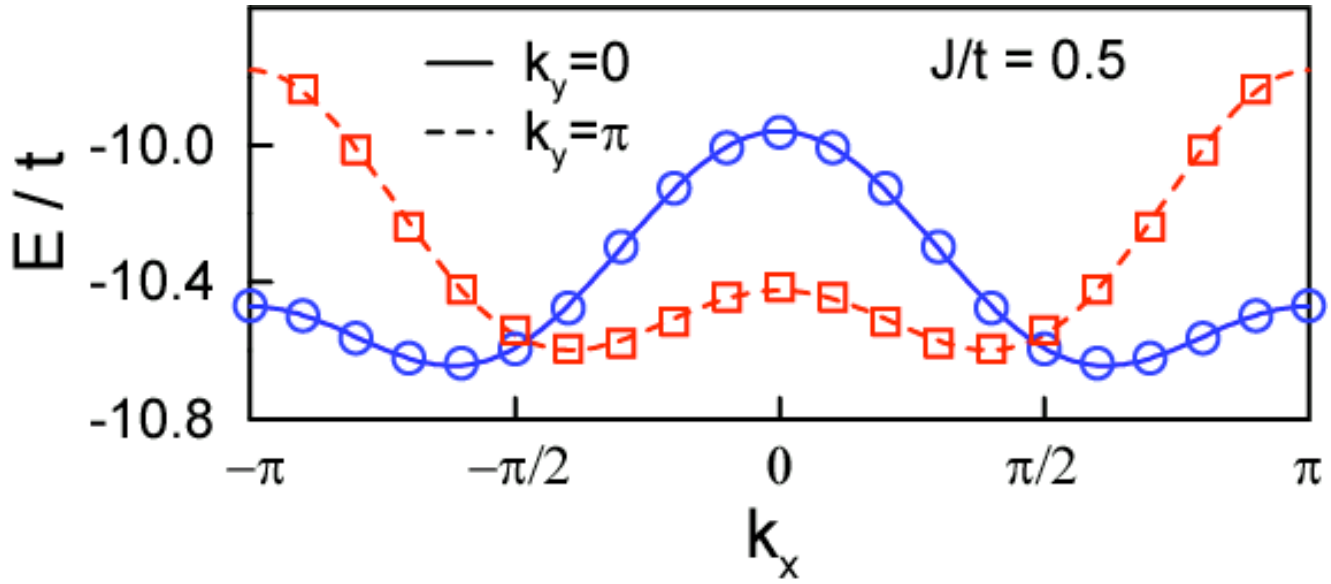
$$|\uparrow_1\downarrow_2 O_3\ldots\rangle = |1_1 1_2 0_3 \ldots.| \otimes |1_{1'} 0_{2'} \ldots|$$

charge spin on occ. sites

Symmetries in ED I

The inclusion of symmetries in an ED code has two major advantages:

1. Quantum number resolved energies and states.
2. Reduction of the Hilbert space to be diagonalized.



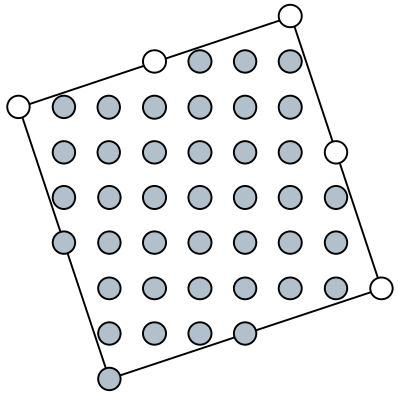
Symmetries in ED II

- U(1) related symmetries:
  - Conservation of particle number(s)
  - Conservation of total Sz
- Spatial symmetry groups:
  - Translation symmetry (abelian symmetry, therefore 1D irreps)
  - Pointgroup symmetries (in general non-abelian)
- SU(2) symmetry
  - Difficult to implement together with spatial symmetries
  - For Sz=0 an operation called “spin inversion” splits the Hilbert space in even and odd spin sectors.

Symmetries in ED III

An example of the symmetry reduction factor:
40 sites square lattice S=1/2 Heisenberg model

- The complete Hilbertspace : Dim=2^{40} = 10^{12}
- By constraining to Sz=0 : Dim=$138*10^9$
- Using spin inversion: Dim=$69*10^9$
- Implementing 40 translations Dim=$1.7*10^9$
- Using all 4 rotations Dim=430'909'650



Linear Algebra in Exact Diagonalization I

Z. Bai, J. Demmel, J. Dongarra, A. Ruhe and H. van der Vorst (eds), Templates for the solution of Algebraic Eigenvalue Problems: A Practical Guide . SIAM, Philadelphia, 2000
http://www.cs.ucdavis.edu/~bai/ET/contents.html

- Lanczos algorithm:
  C. Lanczos, , J. Res. Natl. Bur. Stand. 45, 255 (1950).

  Iterative "Krylov"-space method which brings matrices into tridiagonal form. Method of choice in many large-scale ED programs.
  - Very rapid convergence.
  - Memory requirements between 2 and 4 vectors.
  - Numerically unstable, but with suitable techniques this is under control (Cullum and Willoughby).
  - Easy to implement.

Linear Algebra in Exact Diagonalization II

- Jacobi-Davidson Algorithm:
  E. R. Davidson, Comput. Phys. 7, 519 (1993).
  - Rapid convergence, especially for diagonally dominant matrices (Hubbard model).
  - Varying number of vectors in memory.
  - Often used in DMRG programs as well.
- "modified Lanczos" algorithm:
  E. Gagliano, *et al*. Phys. Rev. B 34, 1677 (1986).
  - actually more like a Power-method, therefore rather slow convergence.
  - needs only two vectors in memory.
  - At each step the approximate groundstate wavefunction is available.
  - Difficult to get excited states.

Lanczos Algorithm I

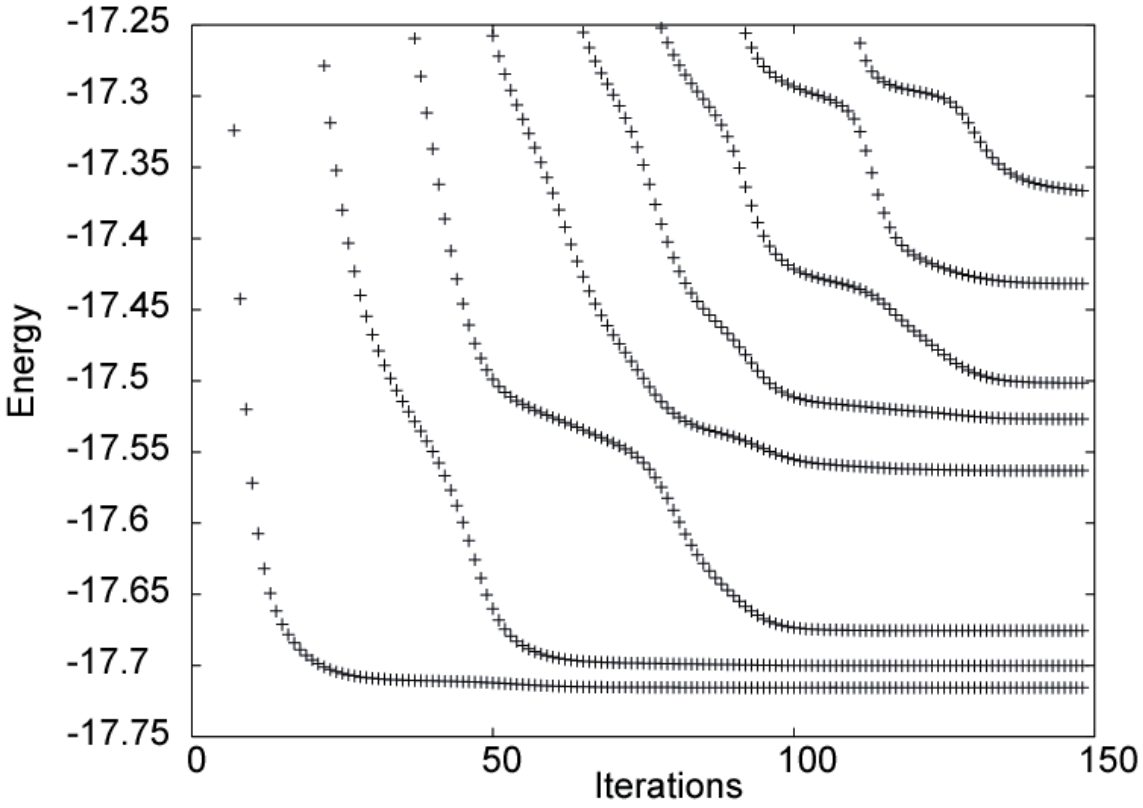
1. Start with a normalized vector $|\phi_1\rangle$
2. Apply the Hamiltonian *H:*
   $a_1 := \langle\phi_1|H|\phi_1\rangle$, $b_1|\phi_2\rangle := H\,|\phi_1\rangle - a_1\,|\phi_1\rangle$
3. $a_n := \langle\phi_n|H|\phi_n\rangle$,
   $b_n|\phi_{n+1}\rangle := H\,|\phi_n\rangle - a_n\,|\phi_n\rangle - b_{n-1}|\phi_{n-1}\rangle$

After n steps:

$$T_n = \begin{pmatrix} a_1 & b_1 & & \\ b_1 & a_2 & b_2 & \\ & b_2 & a_3 & \dots \\ & & \dots & a_n \end{pmatrix}$$

Lanczos Algorithm II

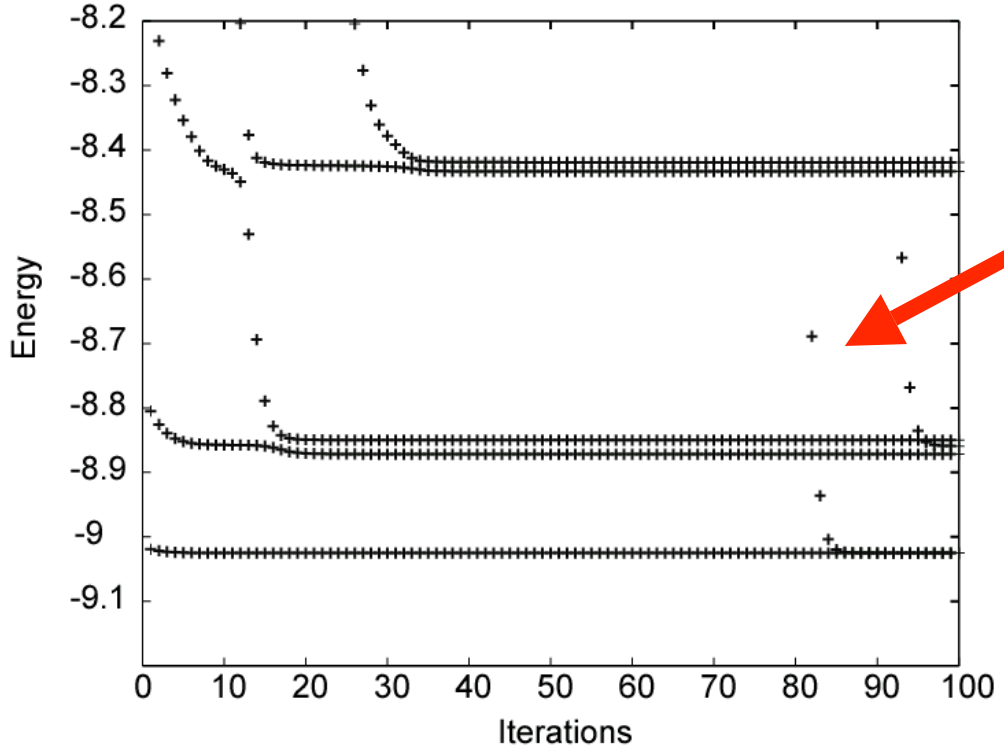
Let's monitor the evolution of $\sigma(T_n)$:



- Eigenvalues start to converge from the extremal eigen-values.
- While converging for excited states one has to be careful as approximate eigenvalues can remain stuck for some time.

Lanczos Algorithm III

What happens once the ground state energy has converged?



Fake eigenvalues called "ghosts" or "spurious eigen-values" appear!

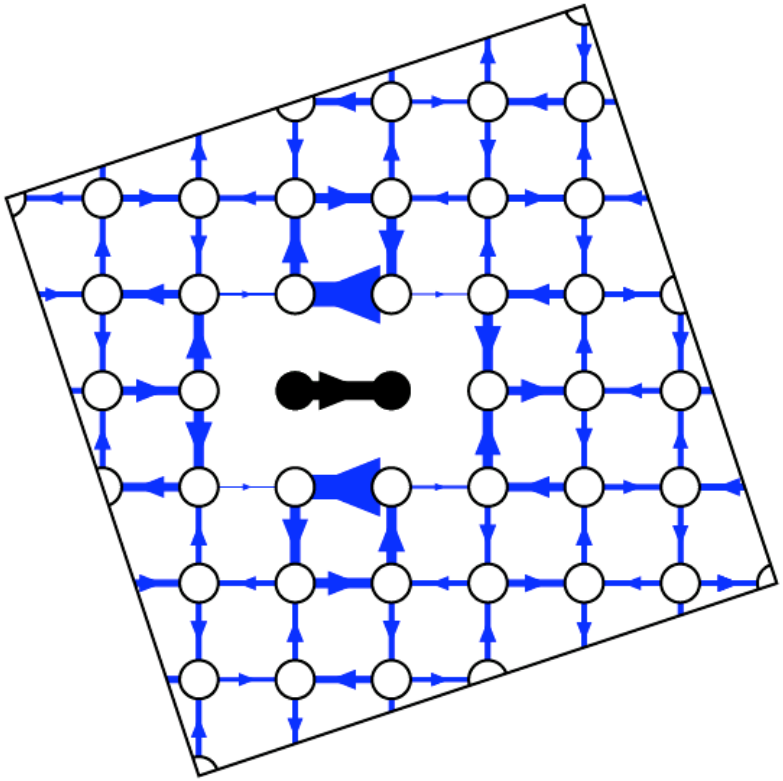
Heuristic techniques to deal with this phenomenon have been investigated by Cullum & Willoughby and are in IETL

Observables in ED

- Energy, as function of quantum numbers!
- "Diagonal" correlation functions:
  easy to calculate in the chosen basis, i.e. S^z-correlations, density correlations, string order parameter,...
- Off-diagonal correlations: S^x-S^x, kinetic energy
- Higher order correlation functions:
  dimer-dimer correlations, vector chirality correlation functions, pairing correlations,...
- Dynamical correlations of all sorts ($\Rightarrow$ talk by D. Poilblanc)
- Note that evaluation of complicated observables can become as important as obtaining the groundstate!
- Note also that in general the precision on correlation functions is not as high as the energy!

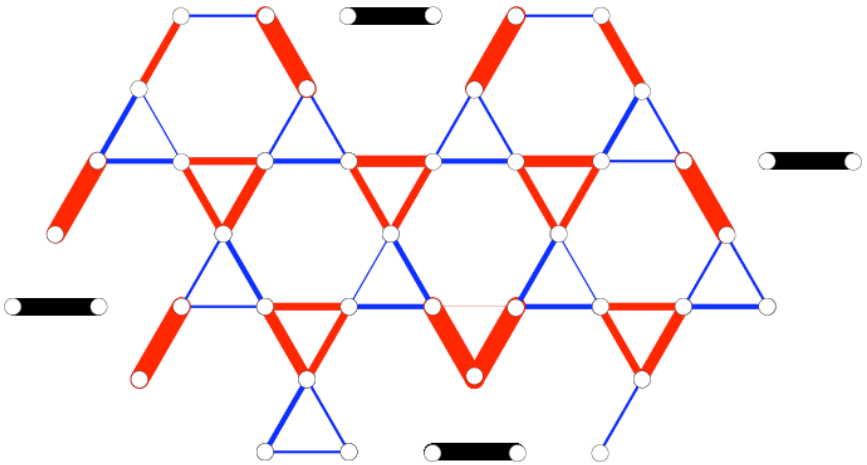
Observables in ED, example pictures

Vector chirality correlations:



$$\langle (S_1 \times S_2)(S_3 \times S_4) \rangle - \langle S_1 \times S_2 \rangle \langle S_3 \times S_4 \rangle$$

Kinetic energy correlations:



$$\langle (c_1^+ c_2 + \text{h.c.})(c_3^+ c_4 + \text{h.c.}) \rangle - \langle c_1^+ c_2 + \text{h.c.} \rangle \langle c_3^+ c_4 + \text{h.c.} \rangle$$

Available ED Codes (to my knowledge)

- ALPS ED Codes (many models, but no symmetries yet)
  - `Fulldiag`: complete diag. with thermodynamics
  - `Sparsediag`: sparse matrix Lanczos, only energies.

- Jörg Schulenburgs Spinpack, written in C/C++,
  can do large-scale calculations
  http://www-e.uni-magdeburg.de/jschulen/spin/

- Nishimori's TITPACK, Fortran implementation,
  widely used in Japan, "cite me" licence.
  http://www.stat.phys.titech.ac.jp/~nishi/titpack2_new/index-e.html

Extensions of Exact Diagonalization

- Finite Temperature Lanczos Methods:

- Contractor Renormalization (CORE):

Extensions of Exact Diagonalization

- Finite Temperature Lanczos Methods:
  - J. Jaklic and P. Prelovsek, Adv. Phys. 49, 1 (2000).
  - M. Aichhorn *et al*., Phys. Rev. B 67, 161103 (2003).

Finite Temperature Lanczos Methods

- These methods (FTLM,LTLM) combine the Lanczos method and random sampling to go to larger systems.
- For high to moderate temperatures these methods can obtain results basically in the thermodynamic limit.
- The Low Temperature Lanczos Method can also go to low temperatures to get correct results on a given sample. Finite size effects however persist.

- Like the T=0 ED method it is most useful, where QMC or T-DMRG etc fail, such as frustrated and fermionic models.

- Possibly in ALPS in the not so distant future...

Extensions of Exact Diagonalization

- Contractor Renormalization (CORE):
  - C.J. Morningstar and M. Weinstein, Phys. Rev. D 54 4131 (1996).
  - E. Altman and A. Auerbach, Phys. Rev. B 65, 104508 (2002).
  - S. Capponi, A. Läuchli and M. Mambrini, cond-mat/0404712, to be published in PRB

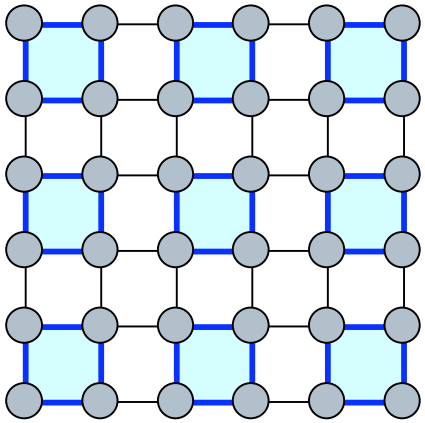
CORE – Basic Idea

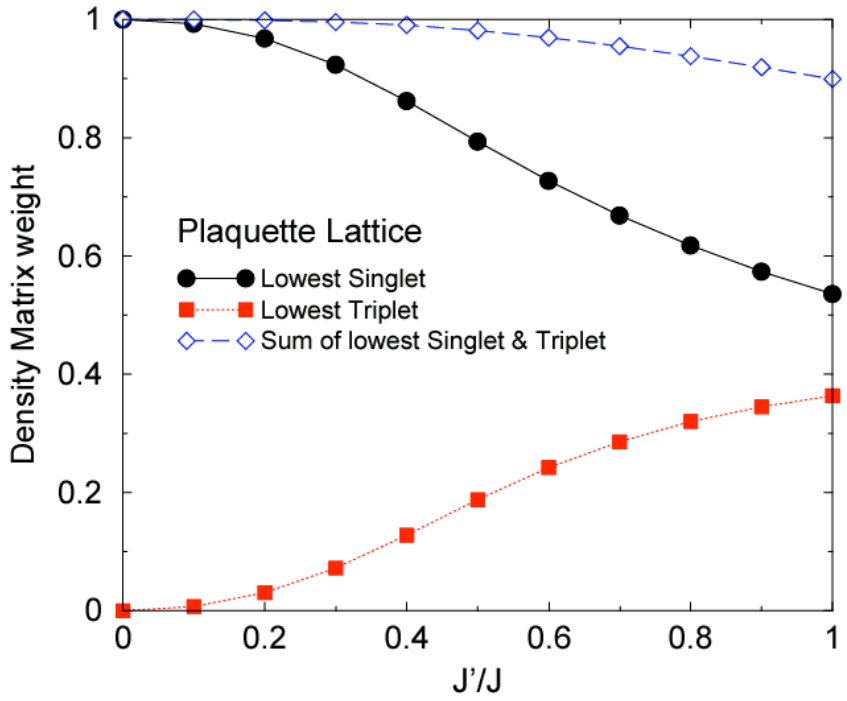
- Choose a suitable decomposition of your lattice and keep a certain number of suitable states
- Determine the effective Hamiltonian by requiring to reproduce the low energy spectrum of the non-truncated system on small clusters.
- Simulate (or treat analytically) the new effective Hamiltonian.

Contractor Renormalization

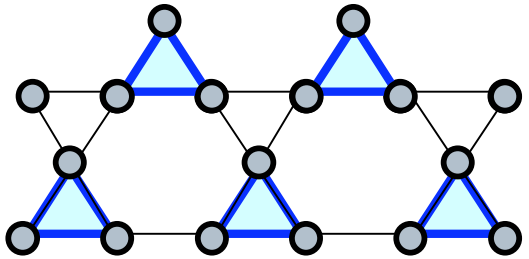
How to choose the states to keep?

- Low energy states of the local building block
- States with the highest weight in the local density matrix





CORE, some results



Kagome antiferro-magnet, keeping only the two doublets of the up-triangles (4 out of 8 states)

The number of non-magnetic excitations before the first magnetic excitation is drastically increasing with system size. Semi-quantitative agreement ED⇔CORE