Exact Diagonalization Techniques on Distributed Memory Machines and the Quest for Identifying Spin Liquid Phases


from de.wikipedia.org

from http://vsc.ac.at

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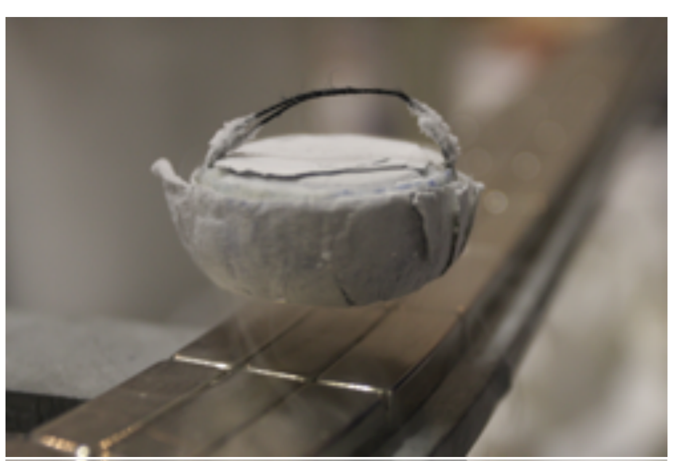
Strongly Correlated Quantum Systems

Some Problems:

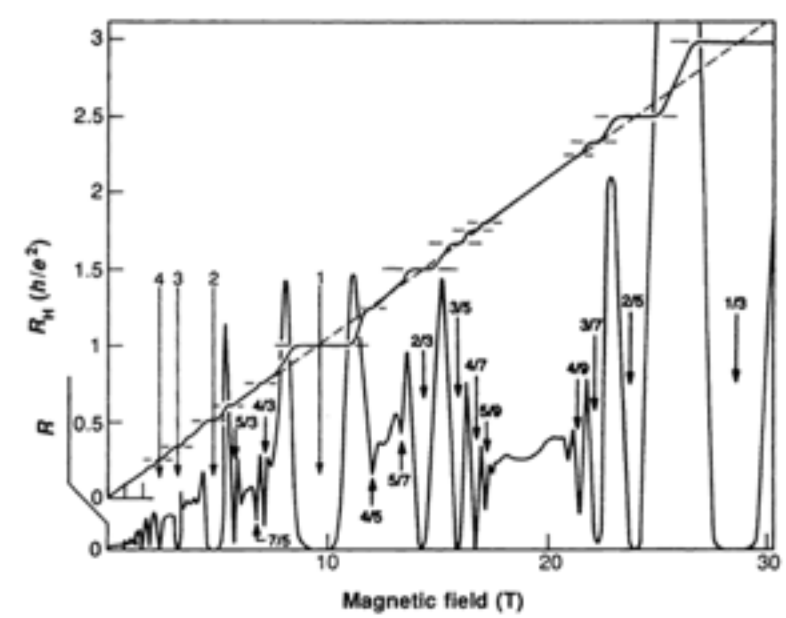
- High temperature superconductivity
- Frustrated magnetism / **Quantum Spin Liquids**
- Fractional Quantum Hall Effect
- …



from de.wikipedia.org

Some Numerical methods:

- Quantum Monte Carlo
- DMRG / Tensor Network Algorithms
- **Exact Diagonalization**
- …



from www.nobelprize.org

Method:
Exact Diagonalization for Distributed Memory Machines

Exact Diagonalization

- Solution of Schrödinger Equation

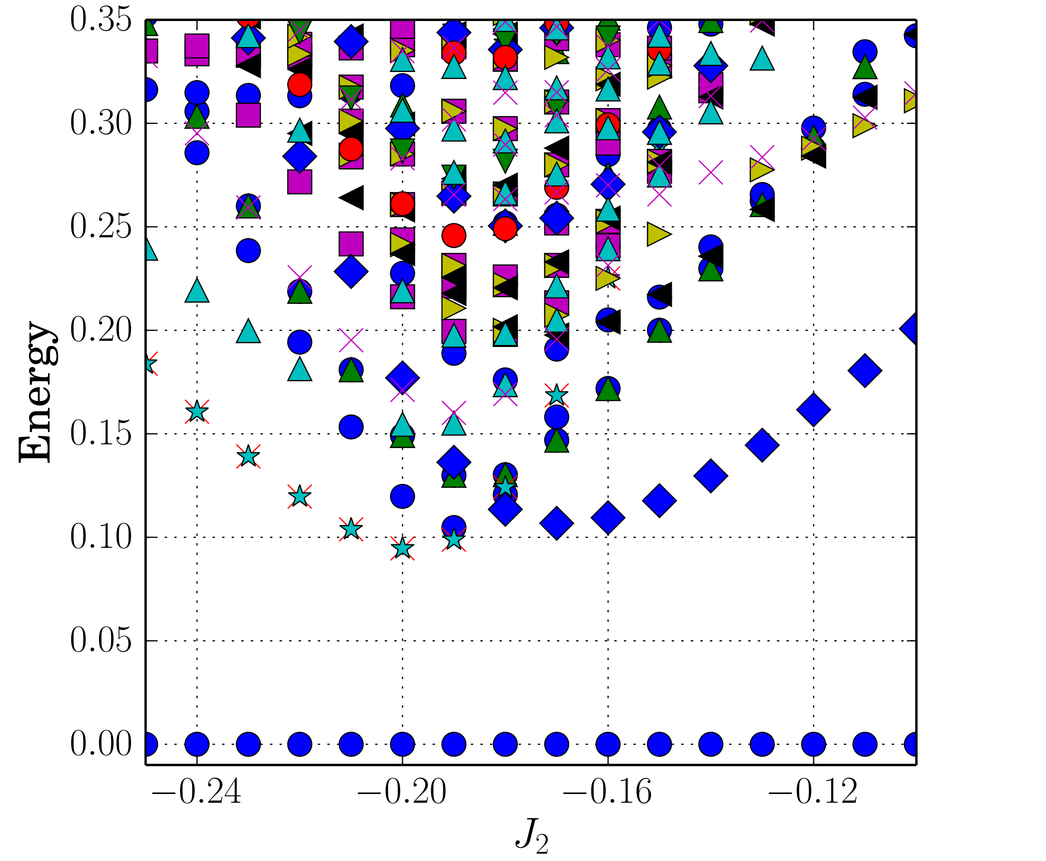
$$H\left|\psi\right\rangle = E\left|\psi\right\rangle$$

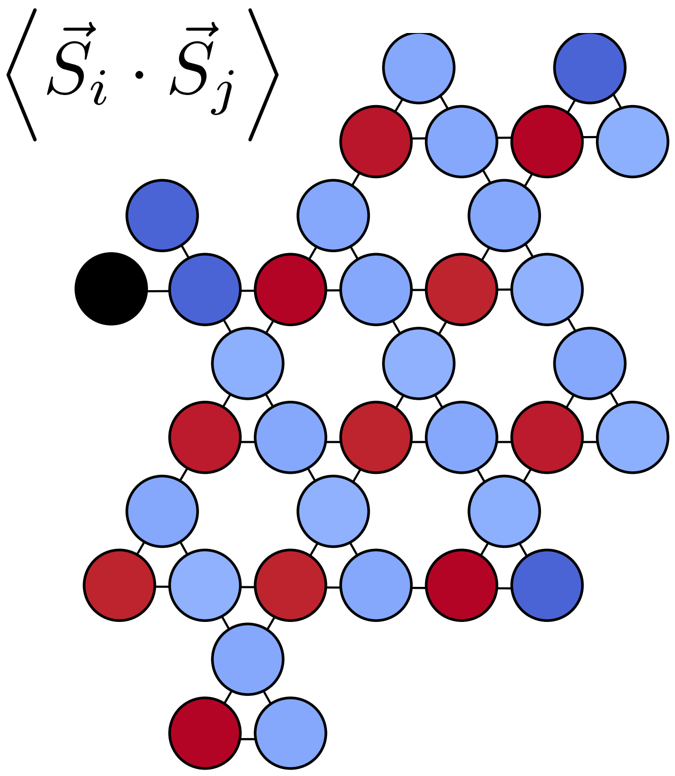
- Straightforward numerical method:
  a) Choose a Basis for the Hilbertspace
  b) Build up Hamiltonian Matrix
  c) Diagonalize it

- eigenstates and spectra of the Hamiltonian can be analyzed

- Typical exponential scaling of computational resources in system size

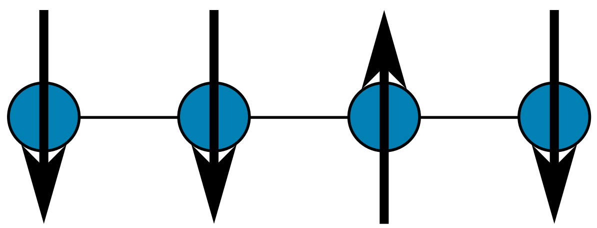
- How can we go to larger system sizes?





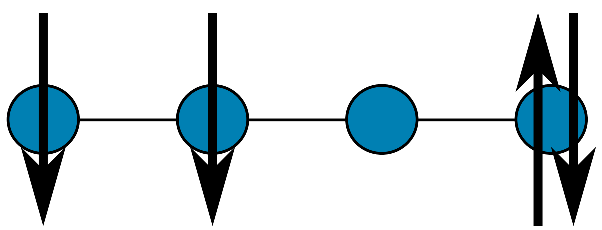
Choosing a basis for the Hilbertspace:

Spin-1/2 models:



$$\longrightarrow \quad [0,0,1,0]_2$$

Hubbard-like models:



$$\longrightarrow \quad [01,01,00,11]_2$$

Example: 40 site Heisenberg Spin 1/2 n.n. model

$$\dim(\mathcal{H}) = 2^{40} = 1099511627776$$

Full Hamiltonian is $2^{40} \times 2^{40}$

Sparse format: $\simeq 40 \cdot 2^{40} \cong 351 \text{ TB}$

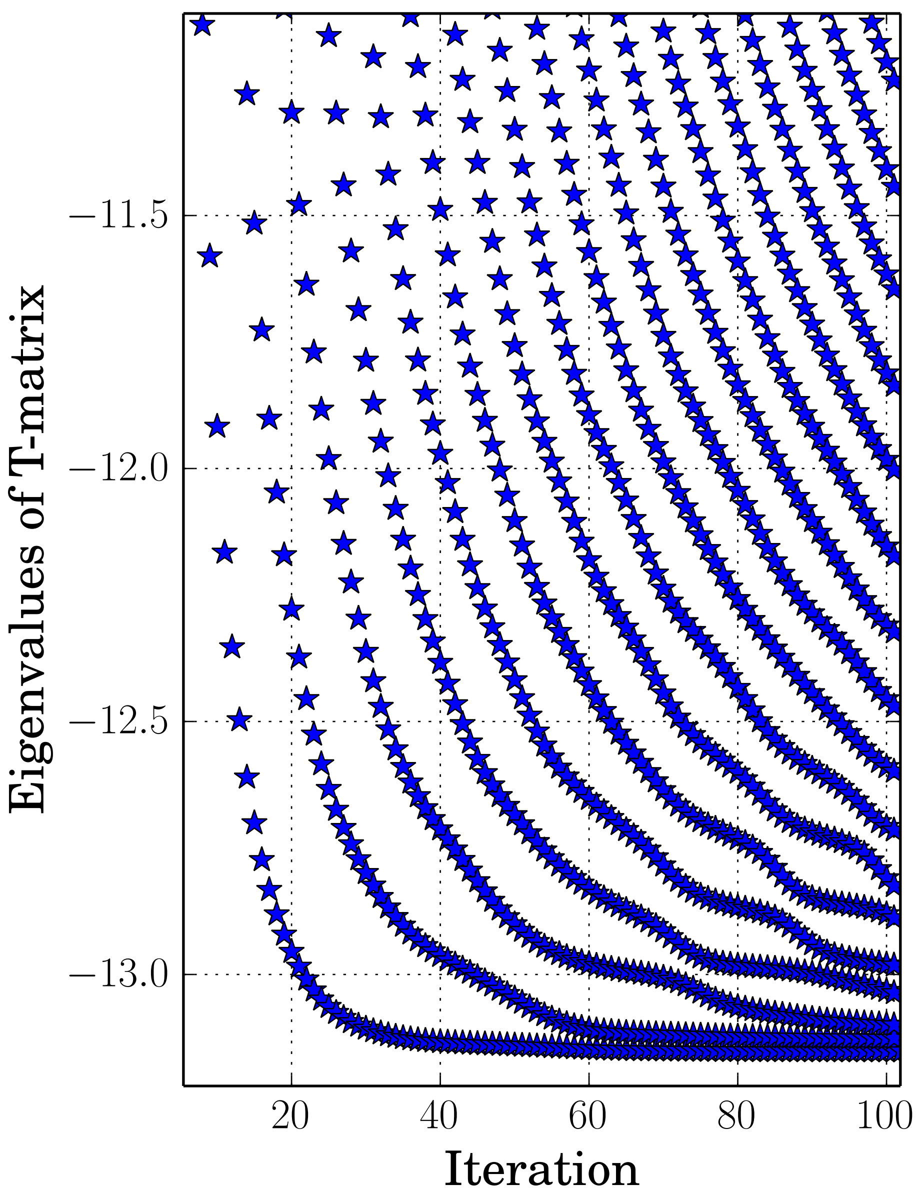
Still such systems can be diagonalized!

- Often one is only interested in low lying eigenstates and energies of the Hamiltonian:
  Lanczos algorithm

- uses only Matrix-Vector multiplications to produce a converging series of eigenvalues and eigenstates

- the Matrix-Vector multiplication can be implemented without storing the Hamiltonian

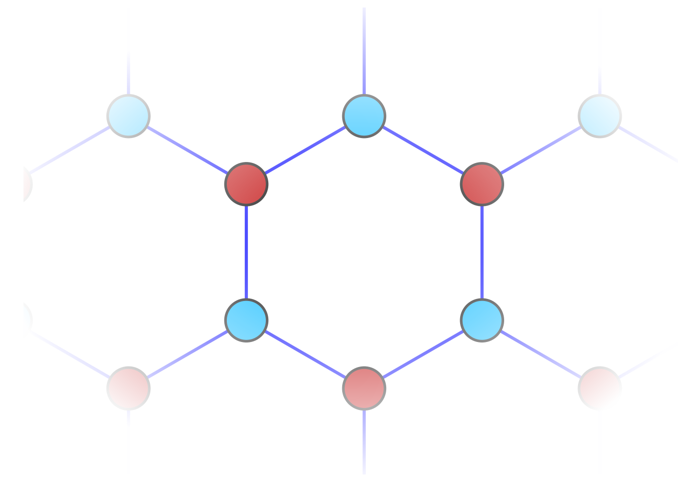
- only 2-4 so-called **Lanczos vectors** are needed. Same dimension as Hilbertspace

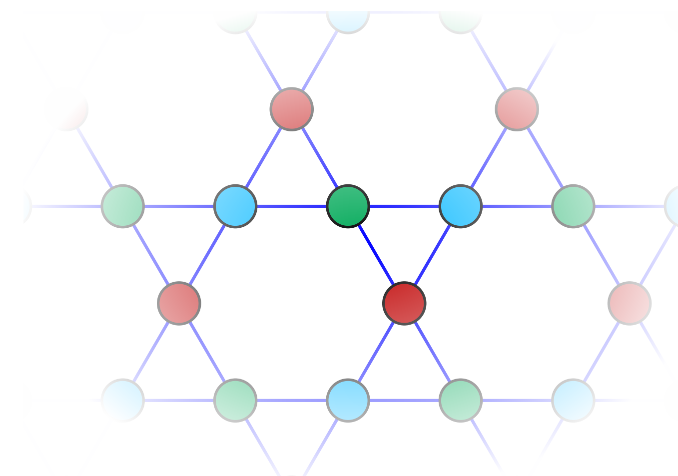


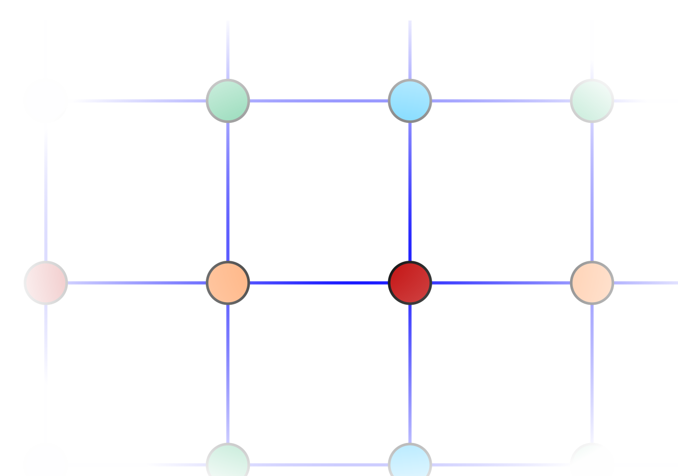
Symmetries:

$$[H, S] = 0$$

- can be used to block diagonalize the Hamiltonian
- space group symmetries, particle number conservation,
  spin-flip symmetry
- gain further physical insight to the system
- Calculations are done in a symmetrized basis
- in order to compute fast and memory efficient in this basis so-called **sublattice coding** techniques are applied.
- concepts by H.Q. Lin, *Phys. Rev. B* (1990) and A. Weiße, *Phys. Rev. E.* (2013)
- extended these concepts for 3 and 4 sub lattices in two arbitrary dimension

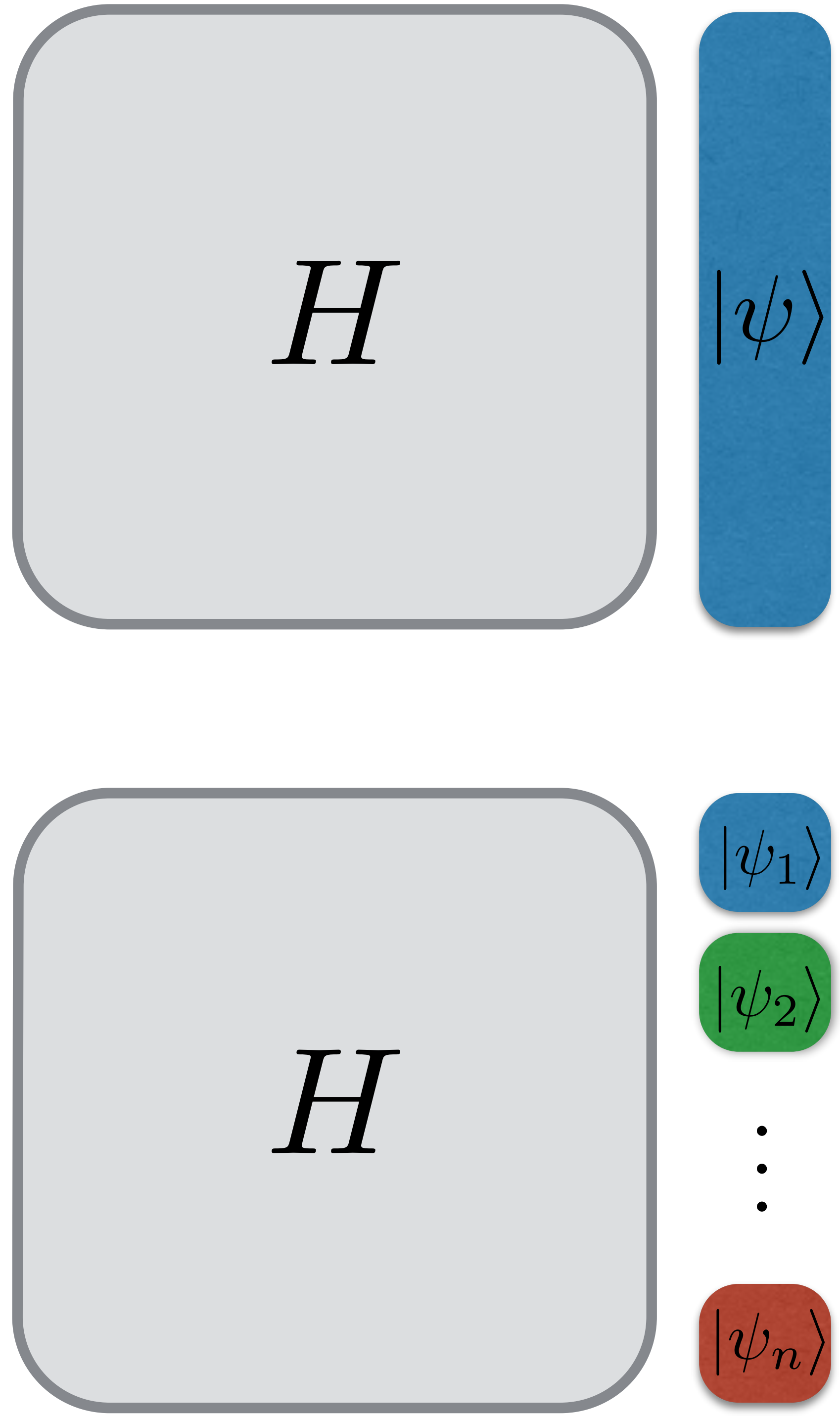






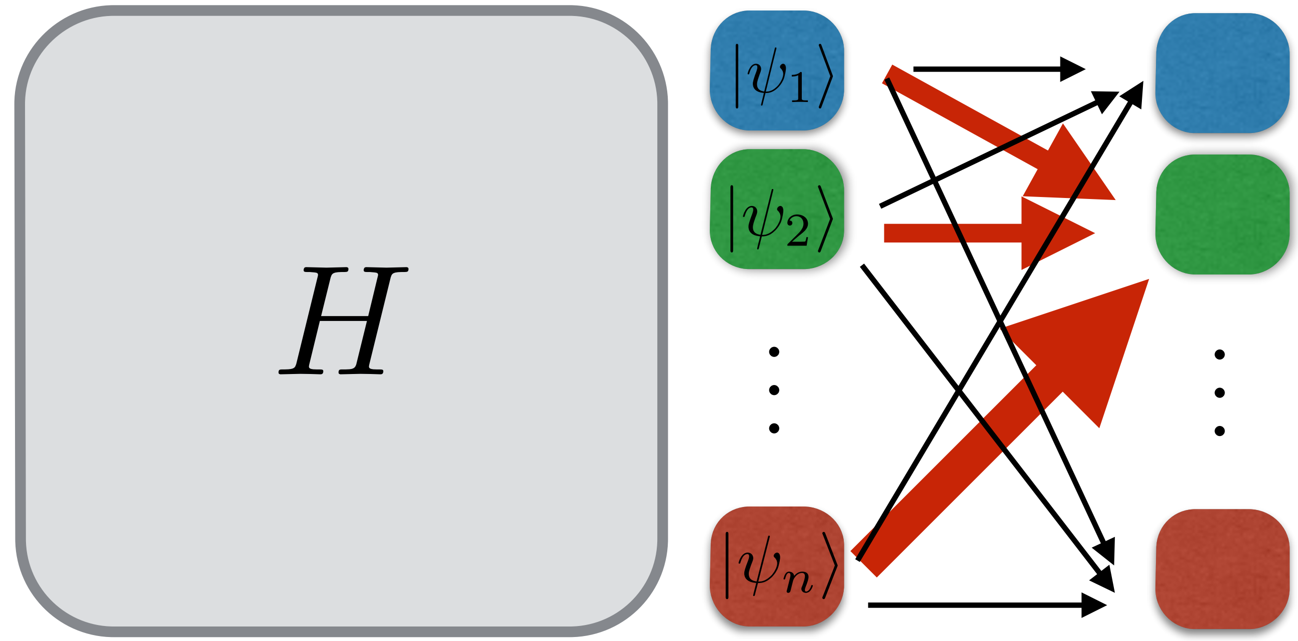
Parallelization:

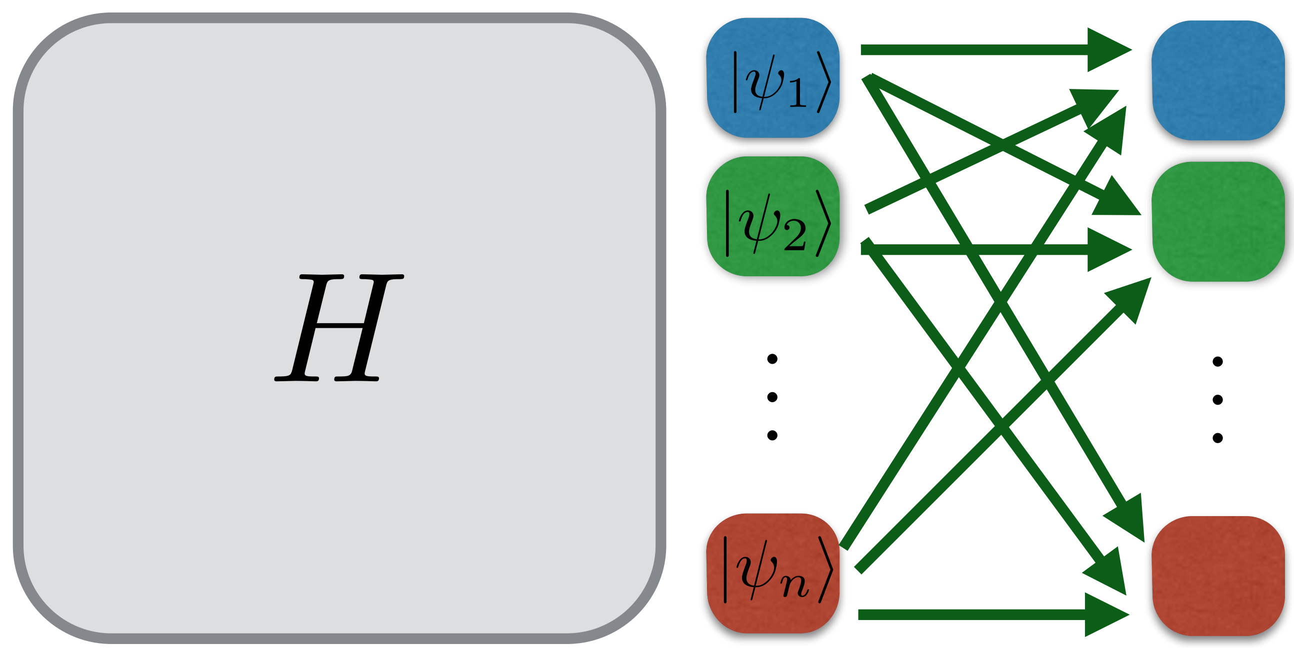
- main part in the whole computation is the Matrix-Vector multiplication of the Hamiltonian with a Lanczos vector
- this has to be parallelized efficiently
- easy on shared-memory machines with OpenMP
- for distributed-memory machines we split up the Lanczos vectors amongst the processes
- Communication between the processes using MPI is necessary



Parallelization:

- processes have to send other processes parts of the Lanczos vector
- once once messages are received the new coefficients are added to the output vector
- timing in this send-receive procedure is of paramount importance if we want our code to scale to large system sizes
- randomly distributing the Hilbertspace among the processes and buffering the communication yields good results



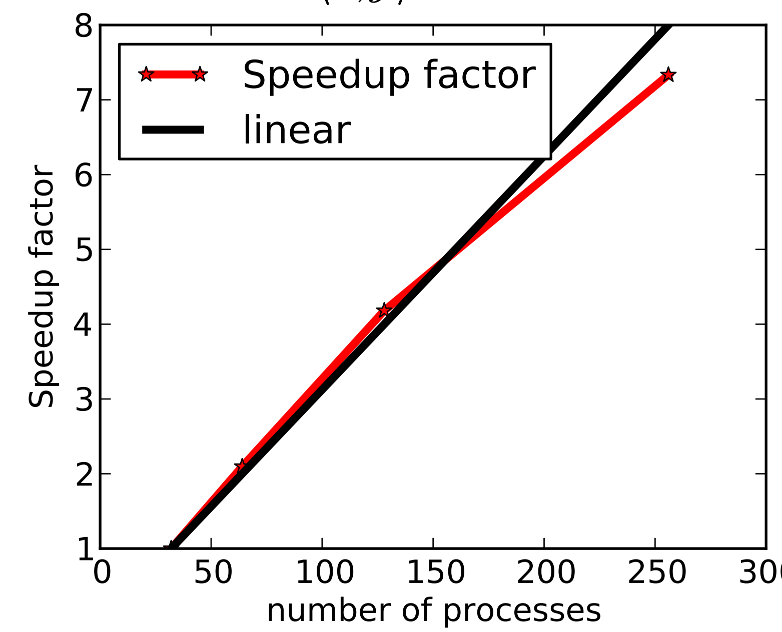


Benchmarks:

Scaling:

- performed on leo3
  (local university supercomputer)
- 40 site Heisenberg nearest neighbor model on square lattice

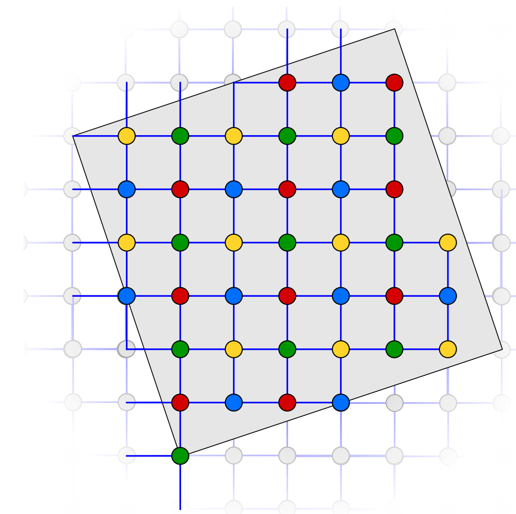
$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$



Big system 1:

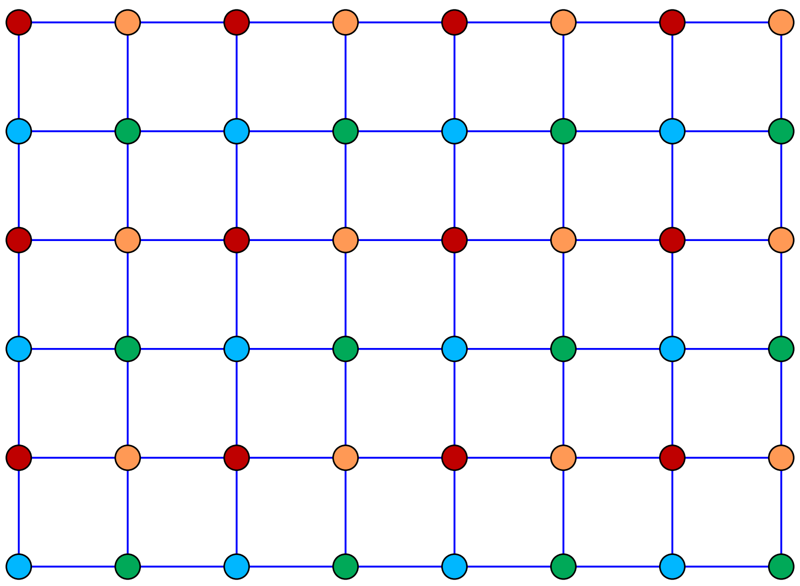
- Transverse field Ising model on 40 site Square lattice
- Dimension of g.s. block: 3.436.321.976
- 512 processes on VSC3
- 2m 30s secs per Lanczos iteration

$$H = J \sum_{\langle i,j \rangle} S_i^z S_j^z + h \sum_k S_k^x$$



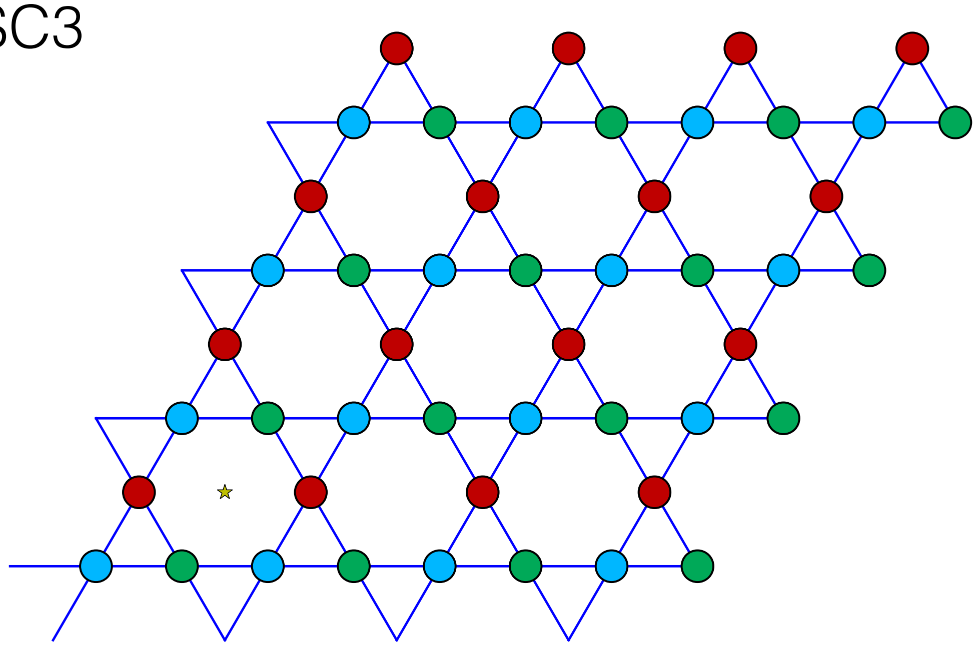
Benchmarks:

Big system 2:



- Heisenberg nearest neighbor model on a 48 site square lattice
- Dimension of g.s. block: 83.986.162.605
- 8192 processes on Vienna Scientific Cluster VSC3
- 20m 40s per Lanczos iteration

Big system 3:



- Heisenberg nearest neighbor model on a 48 site Kagome lattice
- Dimension of g.s. block: 83.979.009.353
- 8192 processes on VSC3
- 20m 10s per Lanczos iteration

- 10240 processes on RZG Hydra in Garching
- 4m 15s per Lanczos iteration

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Application: *Identifying Spin Liquid Phases*

A. Wietek, A. Sterdyniak, A. M. Läuchli, (in preparation)

Chiral Spin Liquids

- X.G. Wen, F. Wilczek, A. Zee, Phys.Rev. B 39, 17 (1989) proposed a class of states called ***Chiral Spin Liquid***

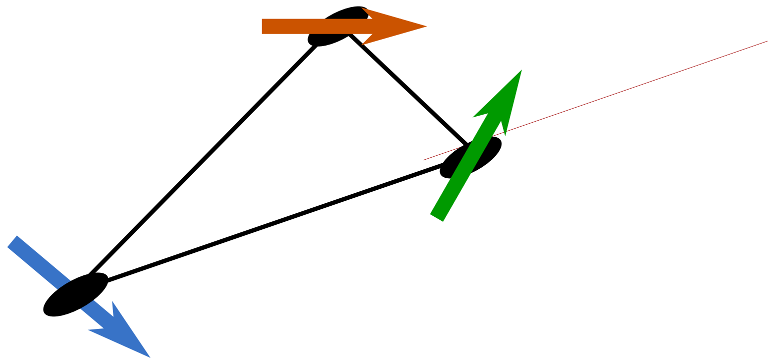
- break parity (reflection) and time reversal symmetry

- Scalar Chirality $\vec{S}_1 \cdot \left(\vec{S}_2 \times \vec{S}_3\right)$ as an order parameter for time-reversal symmetry

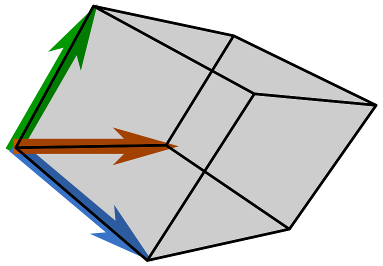
- anyonic fractional excitations -> Spin Liquid

- chiral edge states

- historically first considered as a Laughlin wave function on a lattice

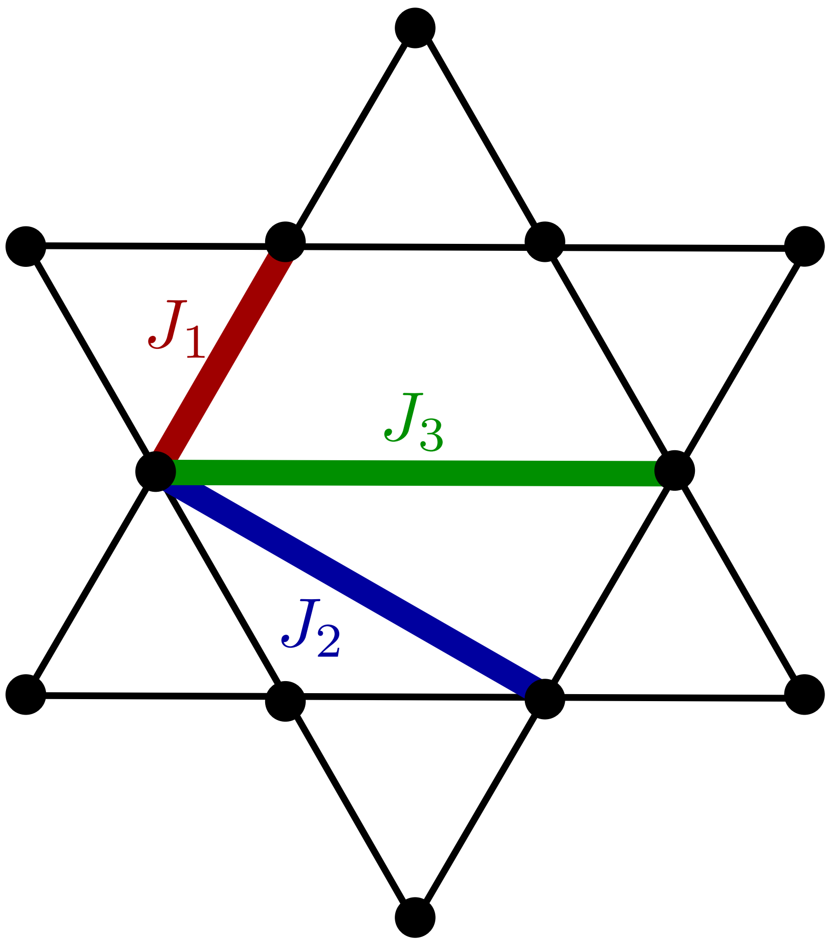


$$\vec{S}_1 \cdot \left(\vec{S}_2 \times \vec{S}_3\right)$$



- S. Gong, W. Zhu & D. N. Sheng, Nature *Scientific Reports* **4**, 6317 (2014) found a realistic model realizing a CSL groundstate

- Heisenberg Model on the Kagome Lattice with up to third nearest neighbor interactions



$$H = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \cdot \vec{S}_j + J_3 \sum_{\langle\langle\langle i,j \rangle\rangle\rangle} \vec{S}_i \cdot \vec{S}_j$$

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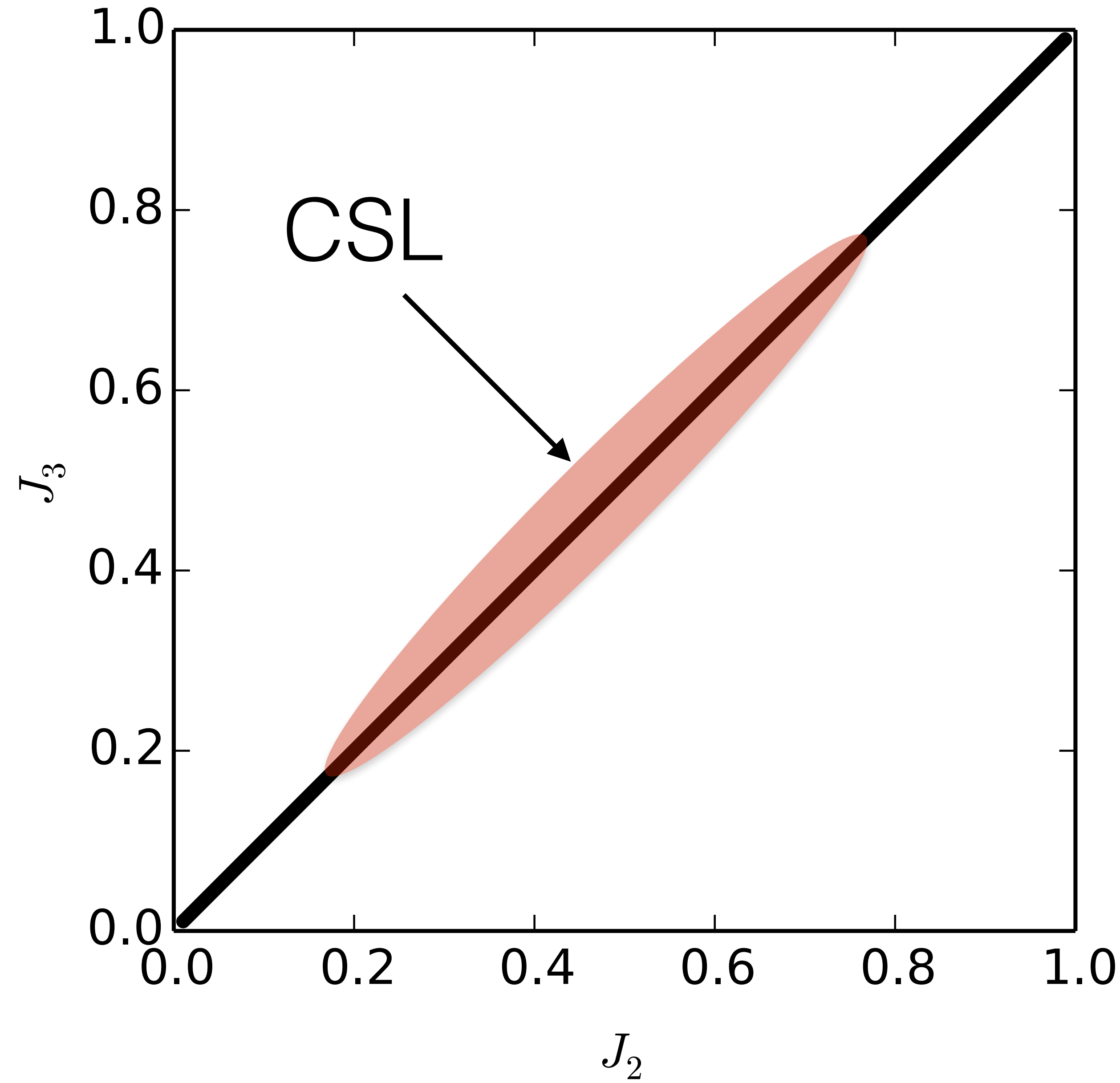


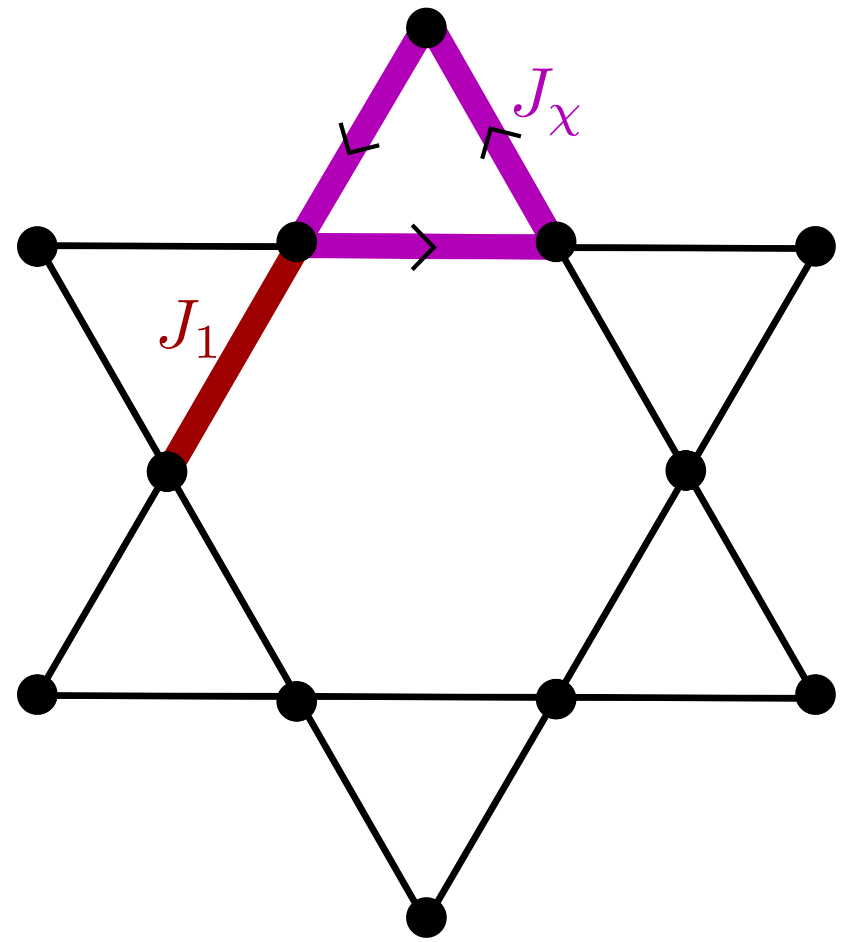
$$H = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \cdot \vec{S}_j + J_3 \sum_{\langle\langle\langle i,j \rangle\rangle\rangle} \vec{S}_i \cdot \vec{S}_j$$

- CSL phase detected for

$$0.2 \lesssim J_2 = J_3 \lesssim 0.7 \qquad J_1 = 1$$

- B.Bauer et al., *Nature Communications* **5**, 5137 (2014) proposed a different model also on the Kagome lattice

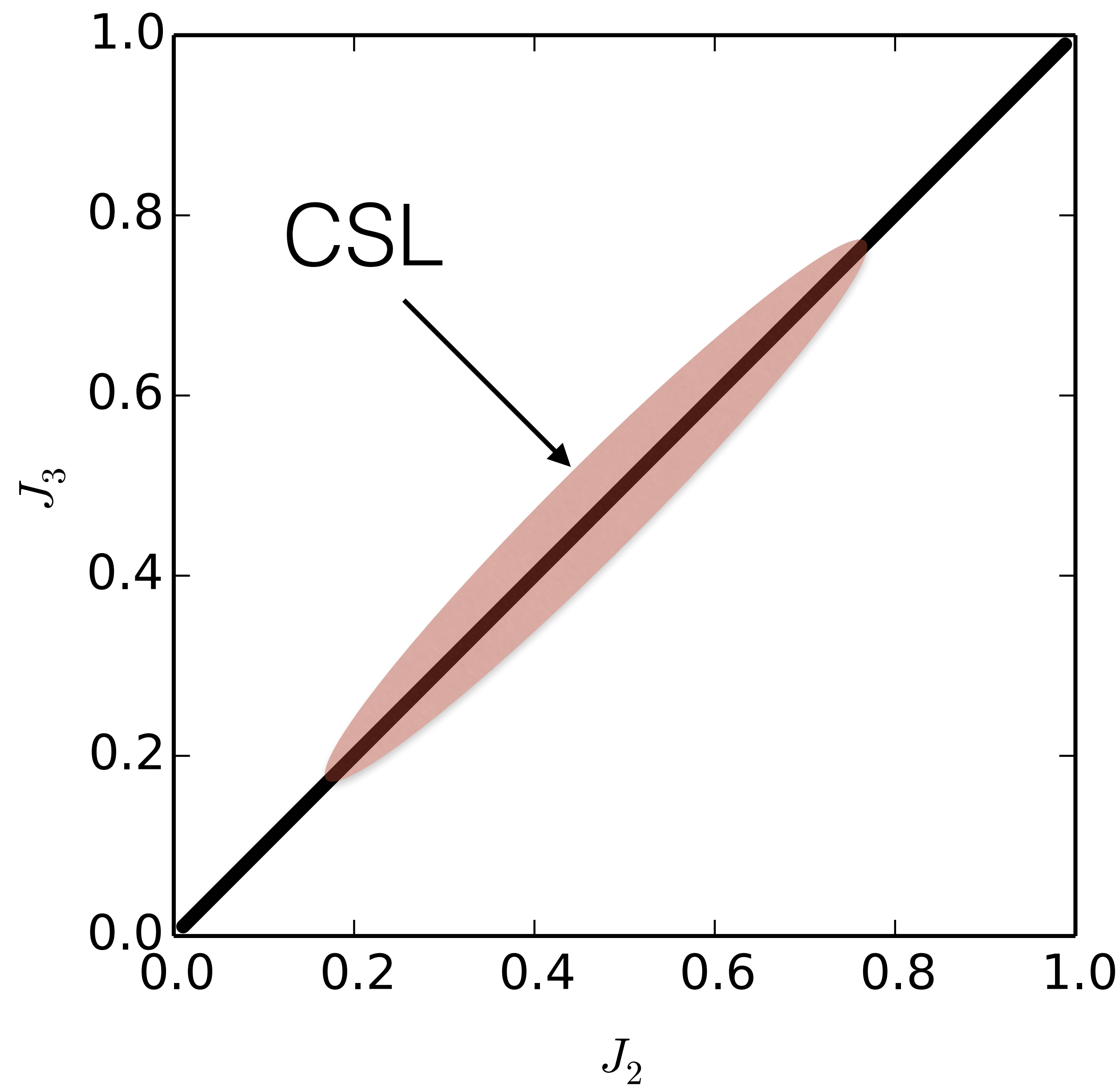
- Heisenberg nearest neighbour Model with additional Scalar Chirality term



$$H = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J_\chi \sum_{i,j,k \in \triangle} \vec{S}_i \cdot \left(\vec{S}_j \times \vec{S}_k \right)$$

Unanswered Questions:

- Are these two CSL phases related ?
- Is there a simple physical picture or a variational wave function that describes this CSL phases ?
- Can we come up with guiding principles that allow us to stabilize on other lattices ?
- questions adressed by A. Wietek, A. Sterdyniak, A. M. Läuchli, (in preparation)



Gutzwiller projected wave functions:

- X.G.Wen (see e.g. Quantum Field Theory of Many-Body Systems, Oxford Graduate Texts) proposed a construction method for several kinds of spin liquids

- Introduce *parton operators:*

$$\vec{S}_i = \frac{1}{2} f_{i\alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} f_{i\beta}$$

- Rewrite original Hamiltonian in terms of these new operators and apply mean-field theory

- This leads to a mean field Hamiltonian

$$H_{\text{mean}} = \frac{1}{2} \sum_{i,j,\sigma} \left(\chi_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.} \right) .$$

- choose mean field parameters χ_{ij}

- compute groundstate of this mean field Hamiltonian

- lives on a different Hilbertspace. Double occupancies and vacancies of sites possible

- Gutzwiller projection to obtain physical Spin wave function

$$\begin{array}{ccc} |\downarrow, \downarrow\uparrow, \emptyset, \uparrow\rangle & \overset{\mathcal{P}}{\Rightarrow} & 0 \\ |\downarrow, \uparrow, \downarrow, \uparrow\rangle & & |\downarrow, \uparrow, \downarrow, \uparrow\rangle \end{array}$$

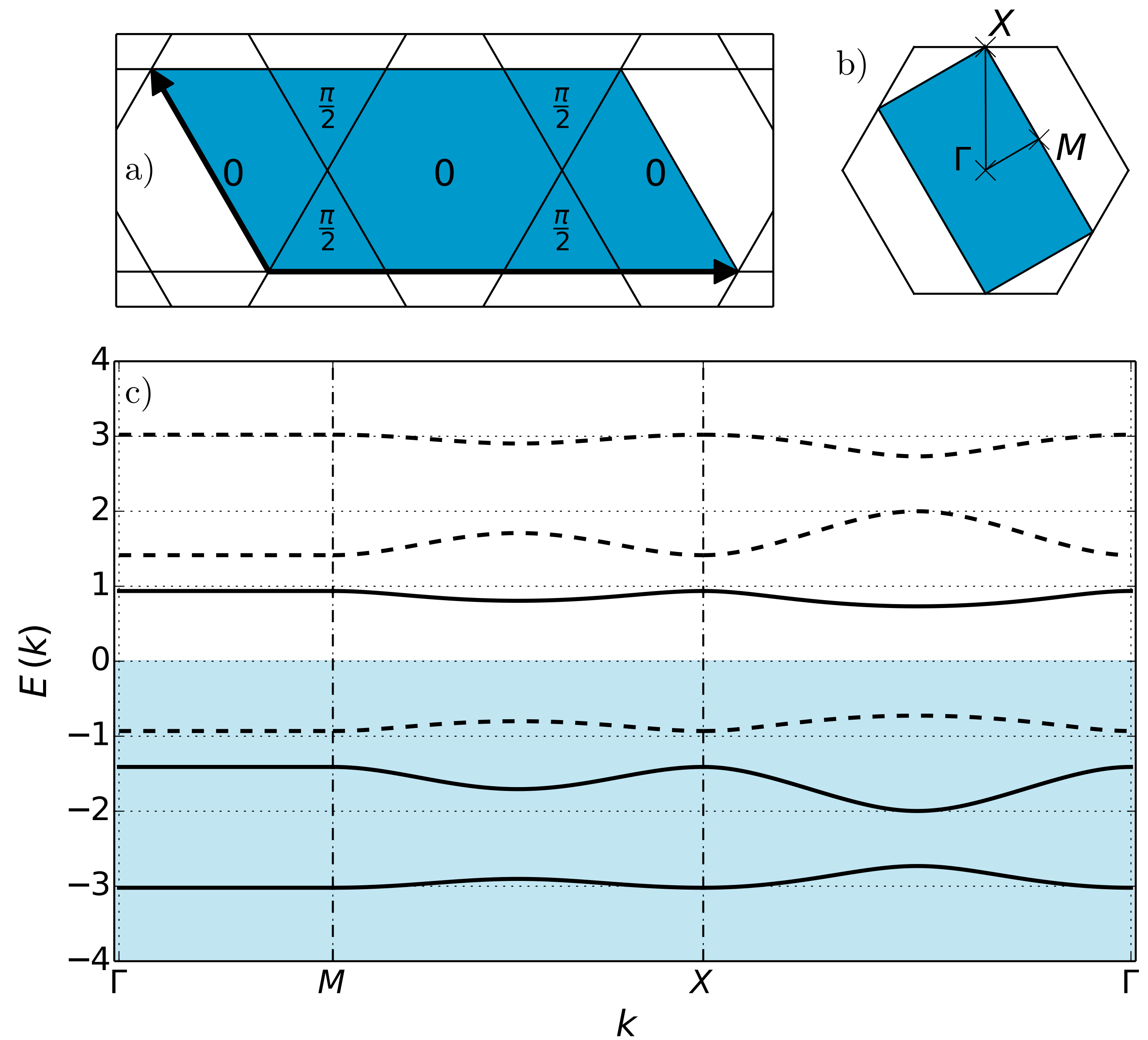
Gutzwiller projected wave functions:

- Choose mean field parameters such that we have $\pi/2$ flux through triangles and zero flux through hexagons

- Gutzwiller project this ground state and compare it to groundstates from Exact diagonalization

- Comparision by computing overlaps of the wave functions

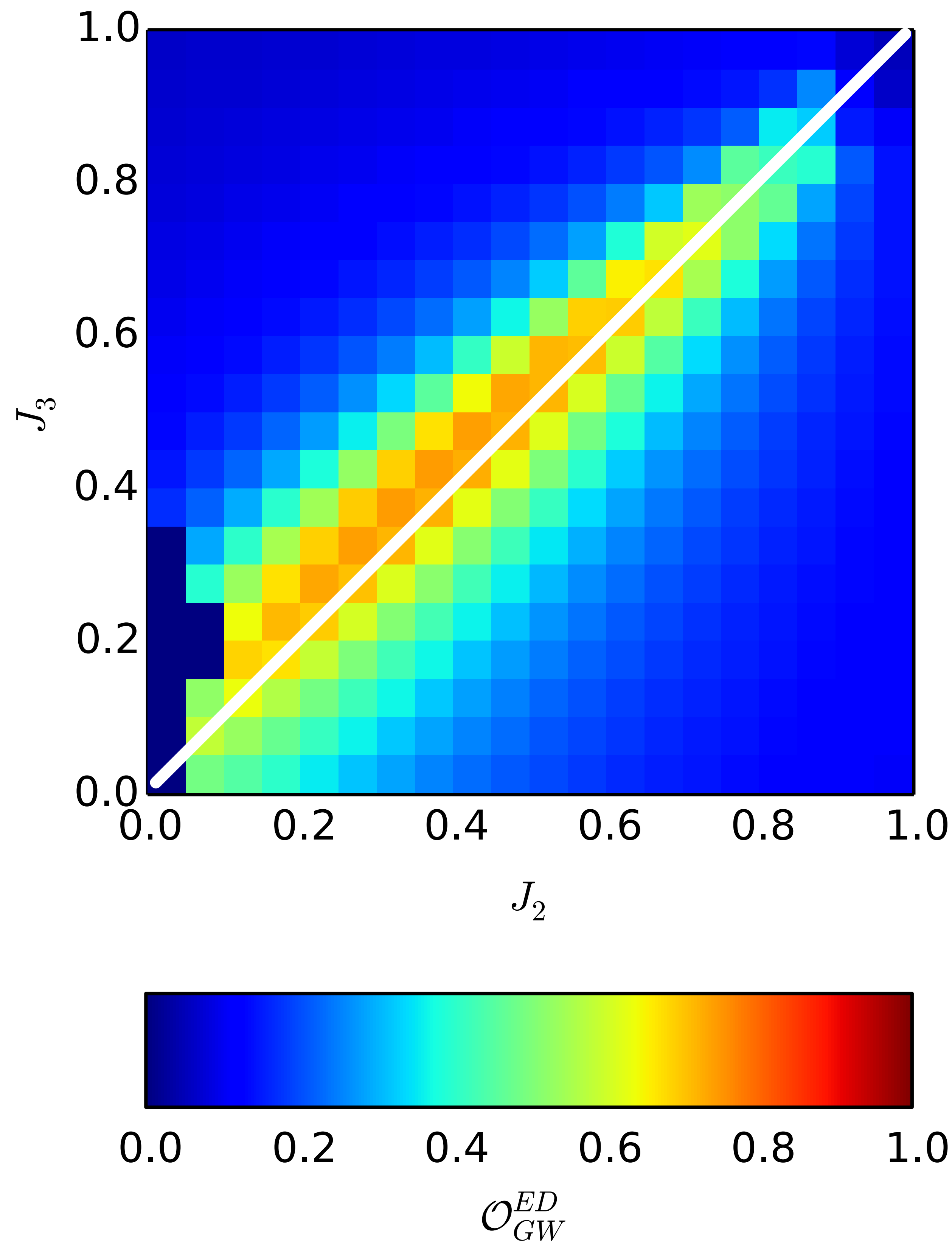
$$\mathcal{O}_{\mathrm{GW}}^{\mathrm{ED}} \equiv \sqrt{|\langle\psi_{\mathrm{ED}}|\psi_{GW}\rangle|^2}$$



- Comparision by computing overlaps of the wave functions

$$\mathcal{O}_{\mathrm{GW}}^{\mathrm{ED}} \equiv \sqrt{|\langle\psi_{\mathrm{ED}}|\psi_{GW}\rangle|^2}$$

- Groundstate wave functions computed on a 30 site kagome cluster
- overlaps again on the critical line for $0.2 \lesssim J_2 = J_3 \lesssim 0.7$
- very good overlap of up to 80%
- the ground state wave function is a dressed version of our variational Gutzwiller projected Wavefunction in this region

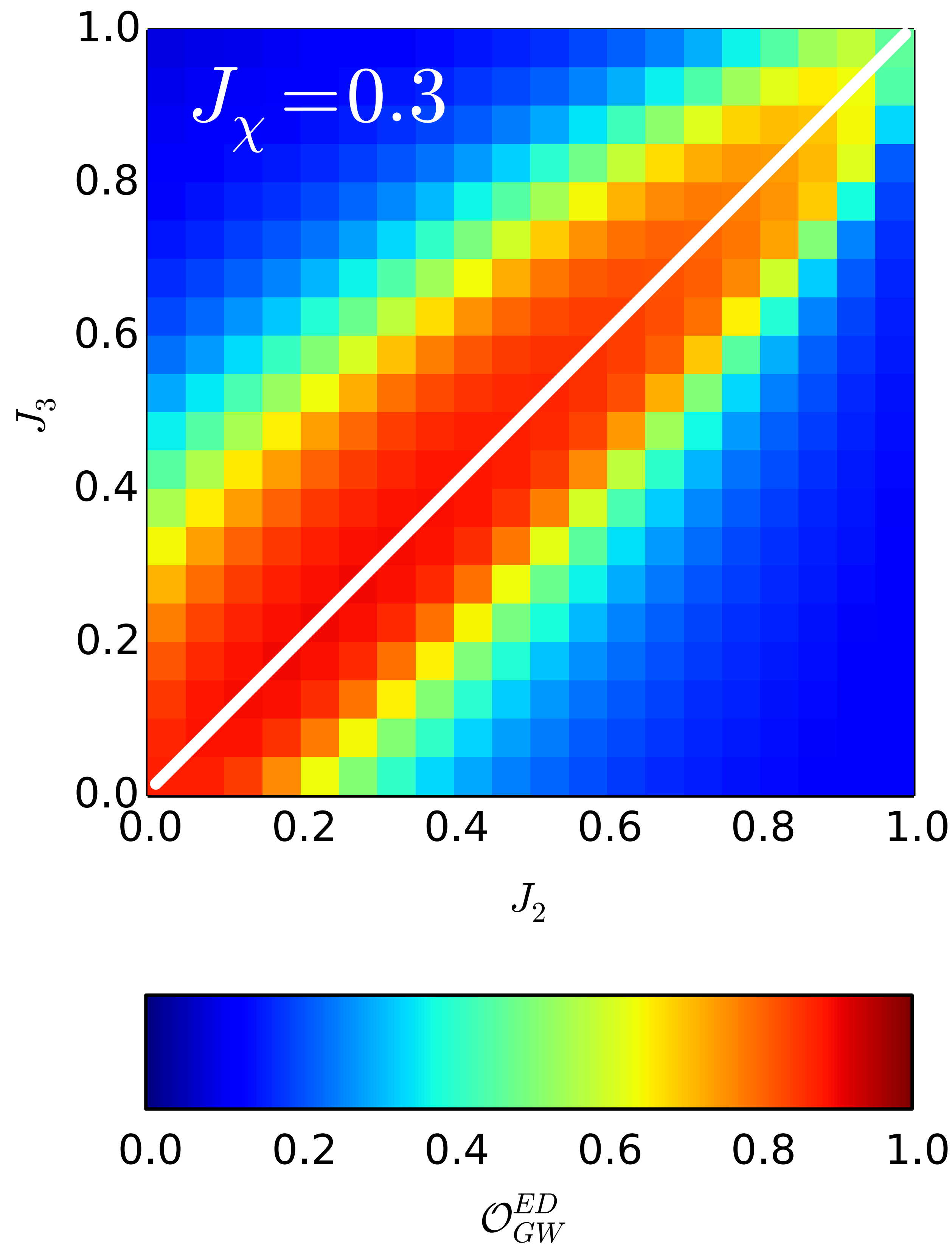


- Adding an additional scalar chirality term

$$J_\chi \sum_{i,j,k\in\triangle} \vec{S}_i \cdot \left(\vec{S}_j \times \vec{S}_k\right)$$

  to the Hamiltonian increases the overlap

- overlaps of up to 95%
- Overlaps with the $J_1 - J_\chi$ model were also computed
- again very good overlaps of up to 96%
- the CSL phase found on the kagome is described by our variational wave function



Conclusion:

- Developed new methods to efficiently use symmetries in Exact Diagonalization
- Developed a state-of-the-art ED Code for distributed memory machines which scales very well up to biggest system sizes
- With this code we are able to investigate models in frustrated magnetism and understand phases occurring in these models

- Investigated a Chiral Spin Liquid phase in the phase diagram of the Heisenberg model on the kagome lattice with up to third nearest neighbor interactions
- found a variational wave function explaining this phase
- showed by computing overlaps with the ground state wave function from ED that the CSL phase is described by our variational wave function

Thank you for your attention!

Supplementary material

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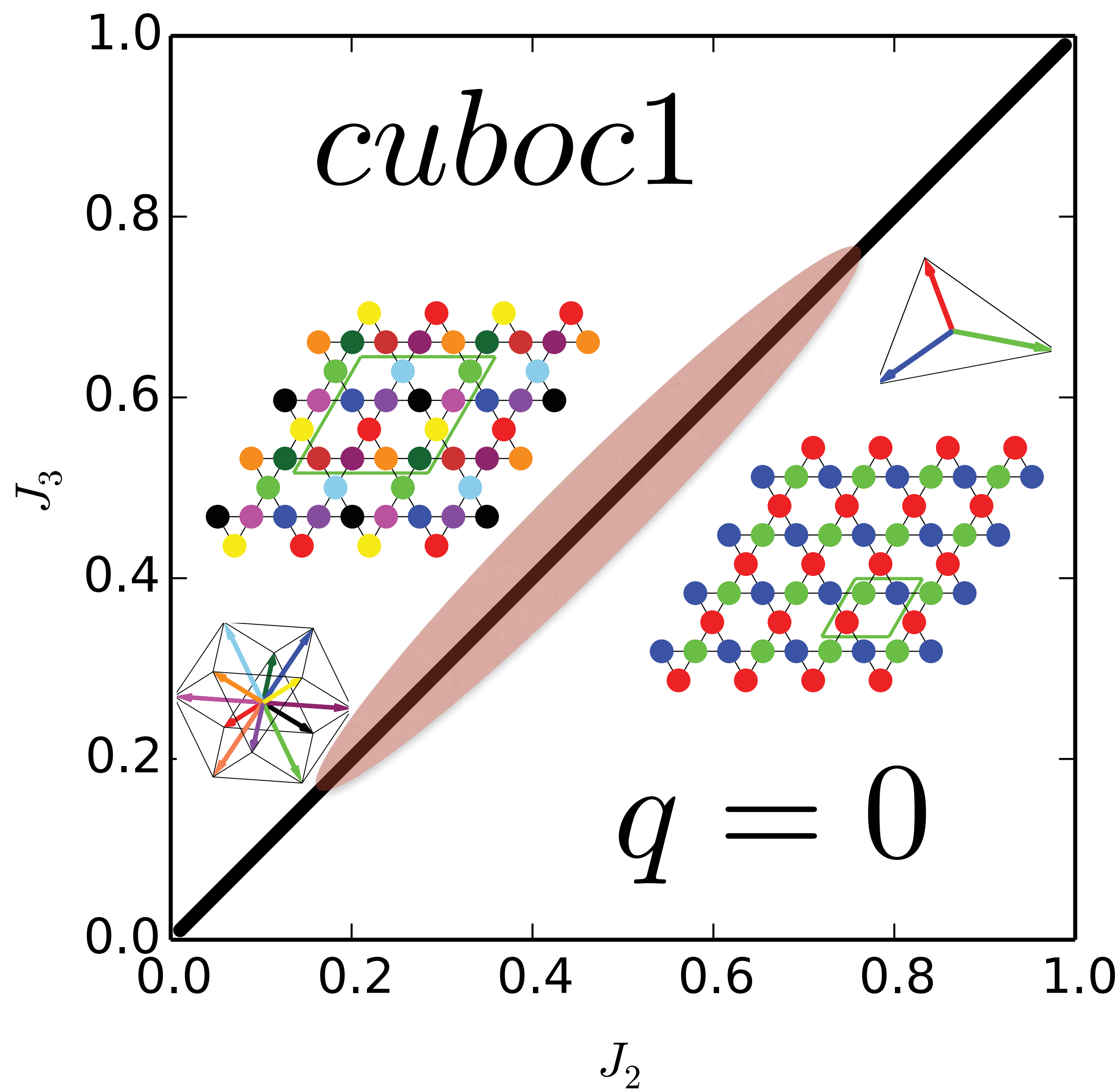
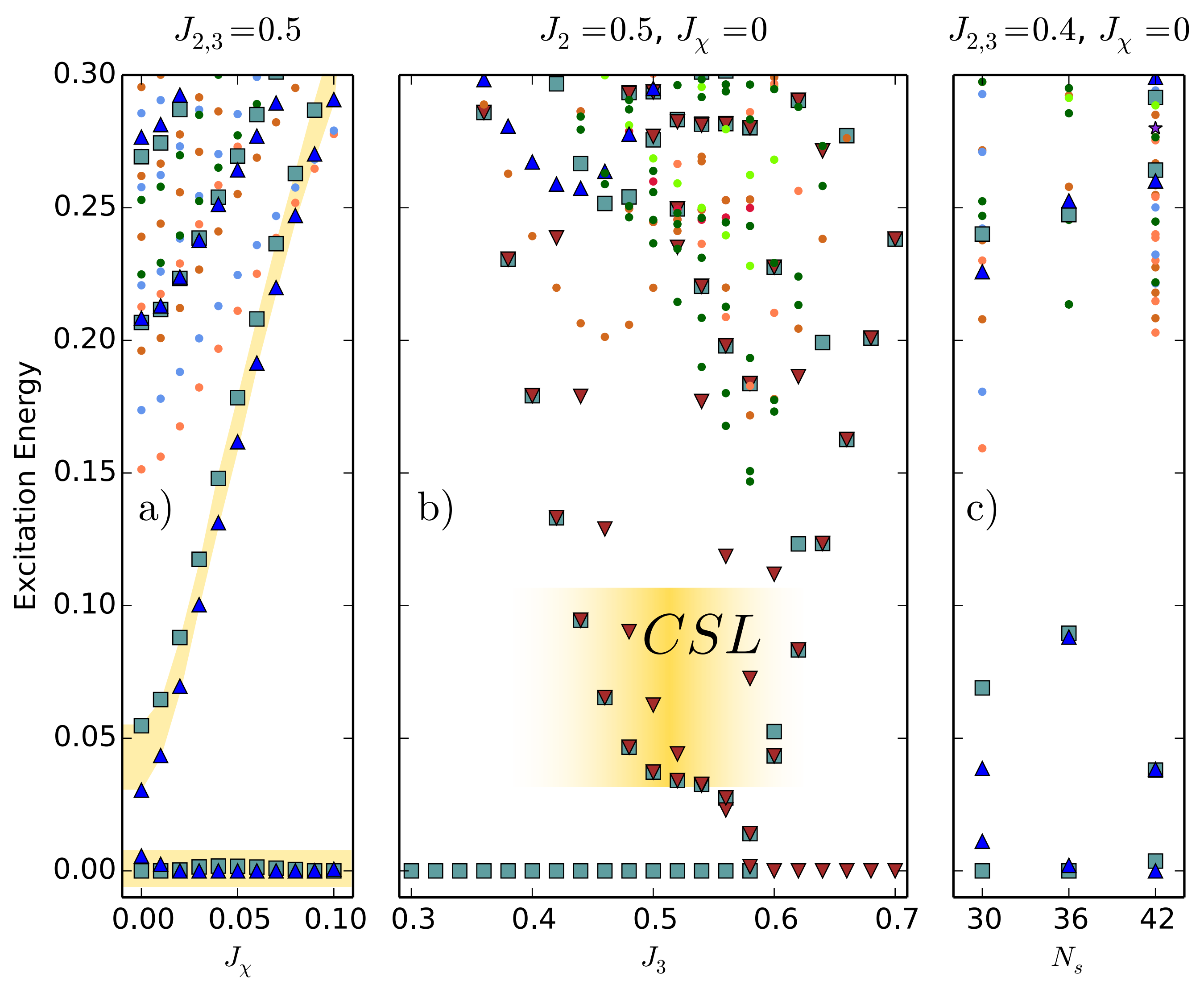
- Classical phase diagram was investigated by Messio et al., *PRL* 108, 207204 (2012)

- CSL is on the critical line between the classical cuboc1 and $q = 0$ order

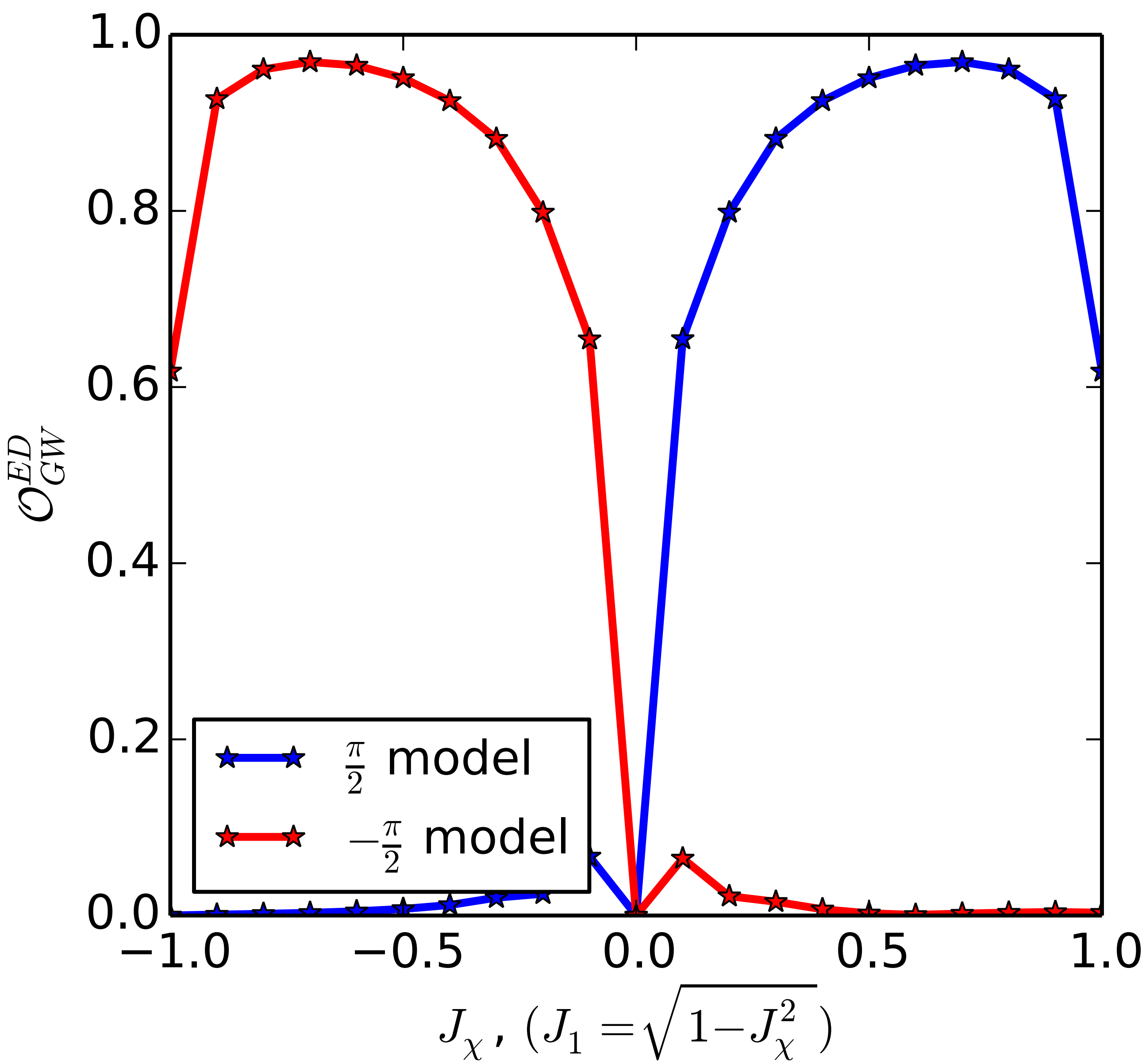
- cuboc1 order has a finite expectation value of scalar chirality $\vec{S}_1 \cdot \left(\vec{S}_2 \times \vec{S}_3\right)$



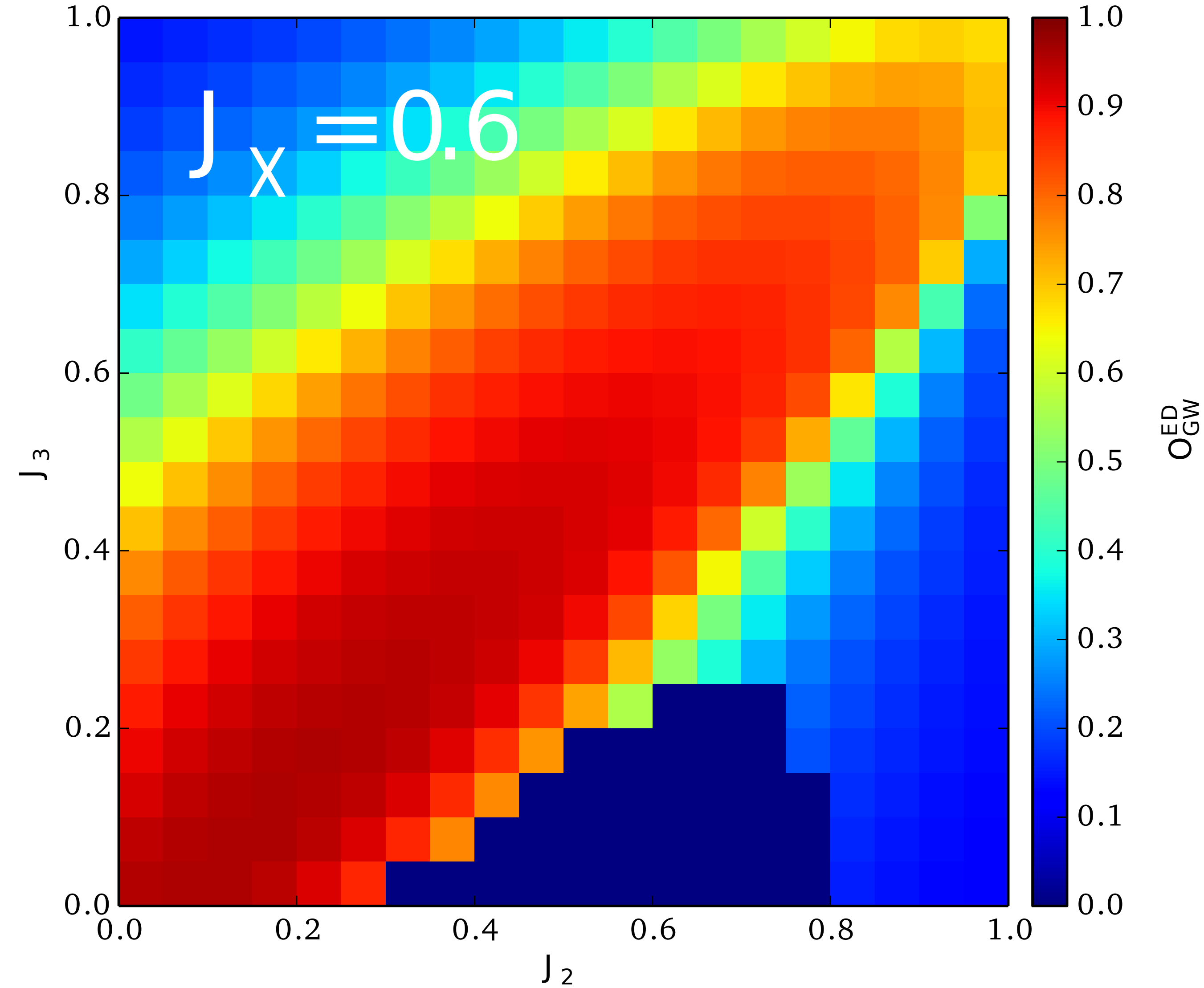
from Messio et al., *Phys. Rev. B* 83, 184401 (2011)



$J_{2,3}=0.5$
$J_2=0.5,\ J_\chi=0$
$J_{2,3}=0.4,\ J_\chi=0$
Excitation Energy
a)
b)
c)
CSL
J_χ
J_3
N_s



$\mathcal{O}^{ED}_{GW}$
$\frac{\pi}{2}$ model
$-\frac{\pi}{2}$ model
J_χ, $(J_1 = \sqrt{1-J_\chi^2})$



$J_\chi = 0.6$
J_3
J_2
O^{ED}_{GW}