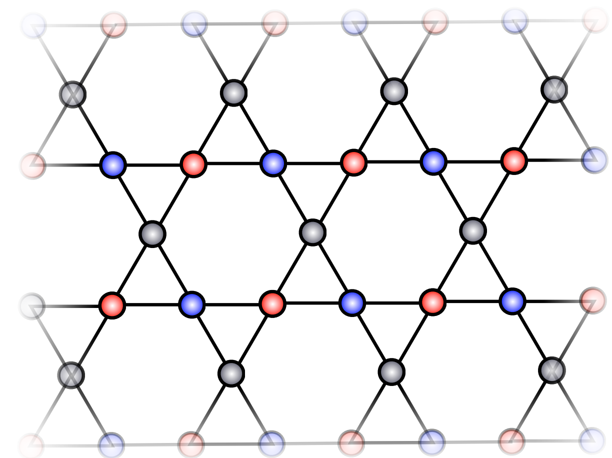

An Exact Diagonalization Perspective on the S=1/2 Kagome Heisenberg Antiferromagnet

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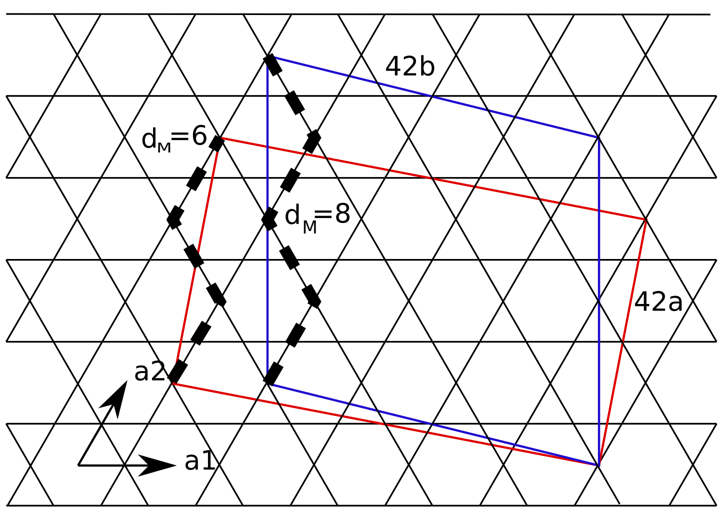
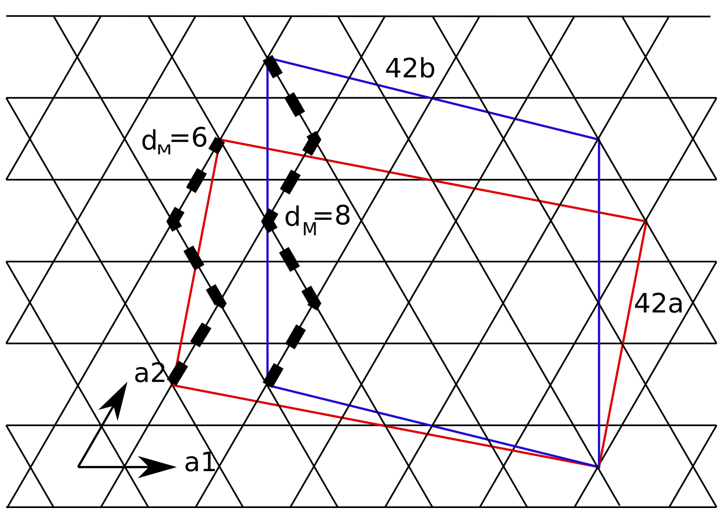
KITP Fragnets12 Program, Santa Barbara, 10/31/2012

Motivation(s)



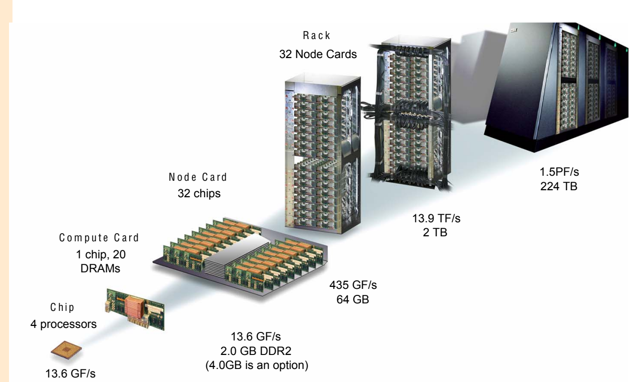
- Why still ED for Kagome ? (DMRG did it all ...)
- Benchmark results
- Spectral evidence for topological degeneracy ?
- Compare recently suggested scenarios with actual (exact) low-energy spectrum

Motivation(s)



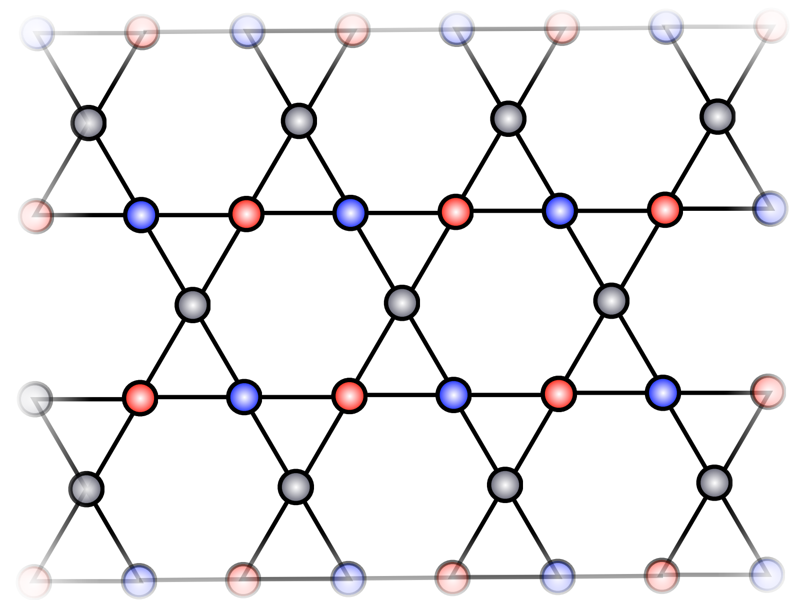
- Why still ED for Kagome ? (DMRG did it all ...)
- Benchmark results
- Spectral evidence for topological degeneracy ?
- Compare recently suggested scenarios with actual (exact) low-energy spectrum

- MPI parallel Exact Diagonalizations are challenging but feasible in other domains (Full CI Quantum Chemistry, Nuclear structure)
- How far can we go with spin models (~ 50 spins) ?
- How fast is the hardware (demanding all to all communication) ?



MPI Parallel Kagome ED Code: Technical Aspects

- Three-sublattice stable symmetry implementation for fast lookups



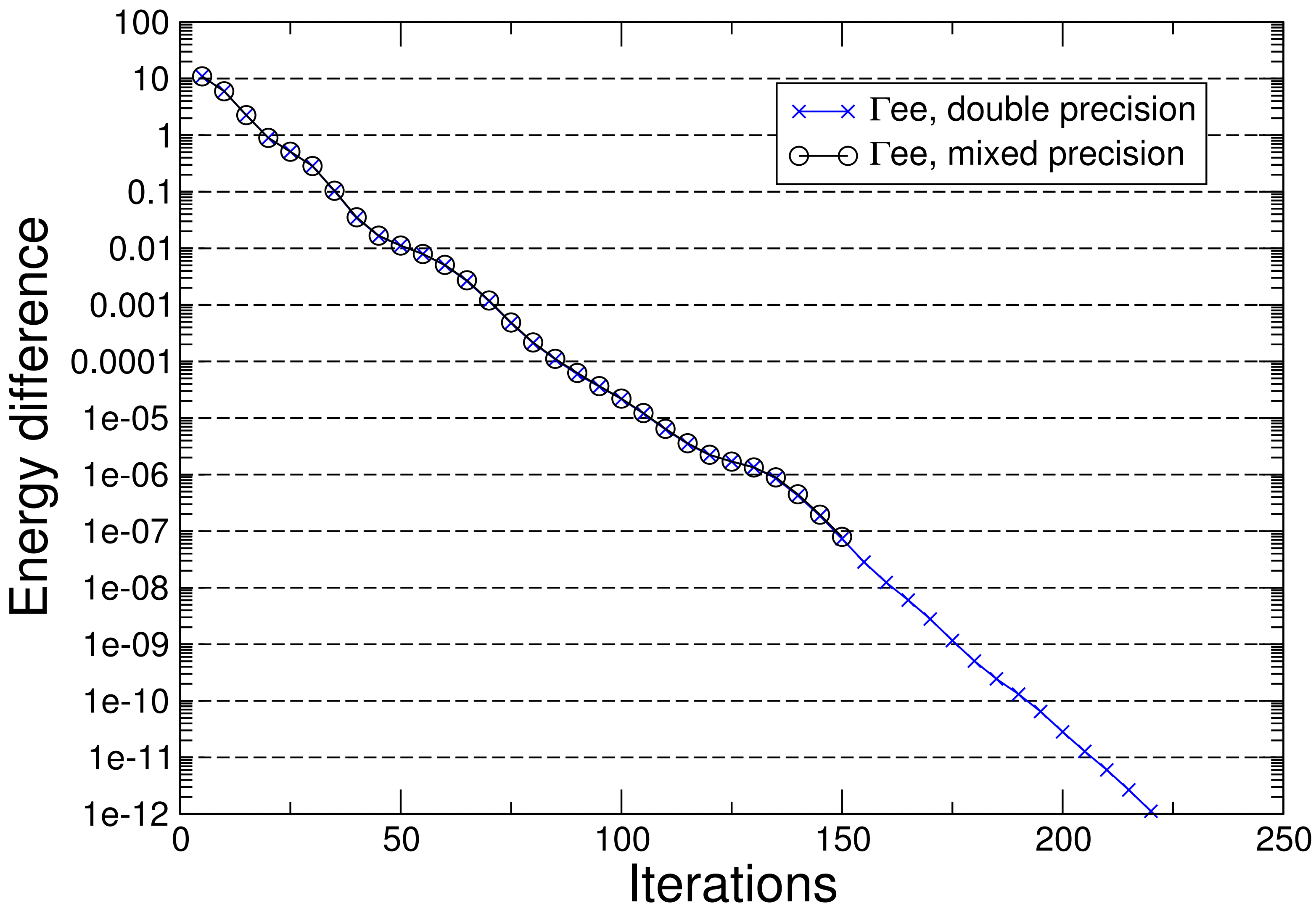
- MPI protocol based implementation for distributed memory architectures

- 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

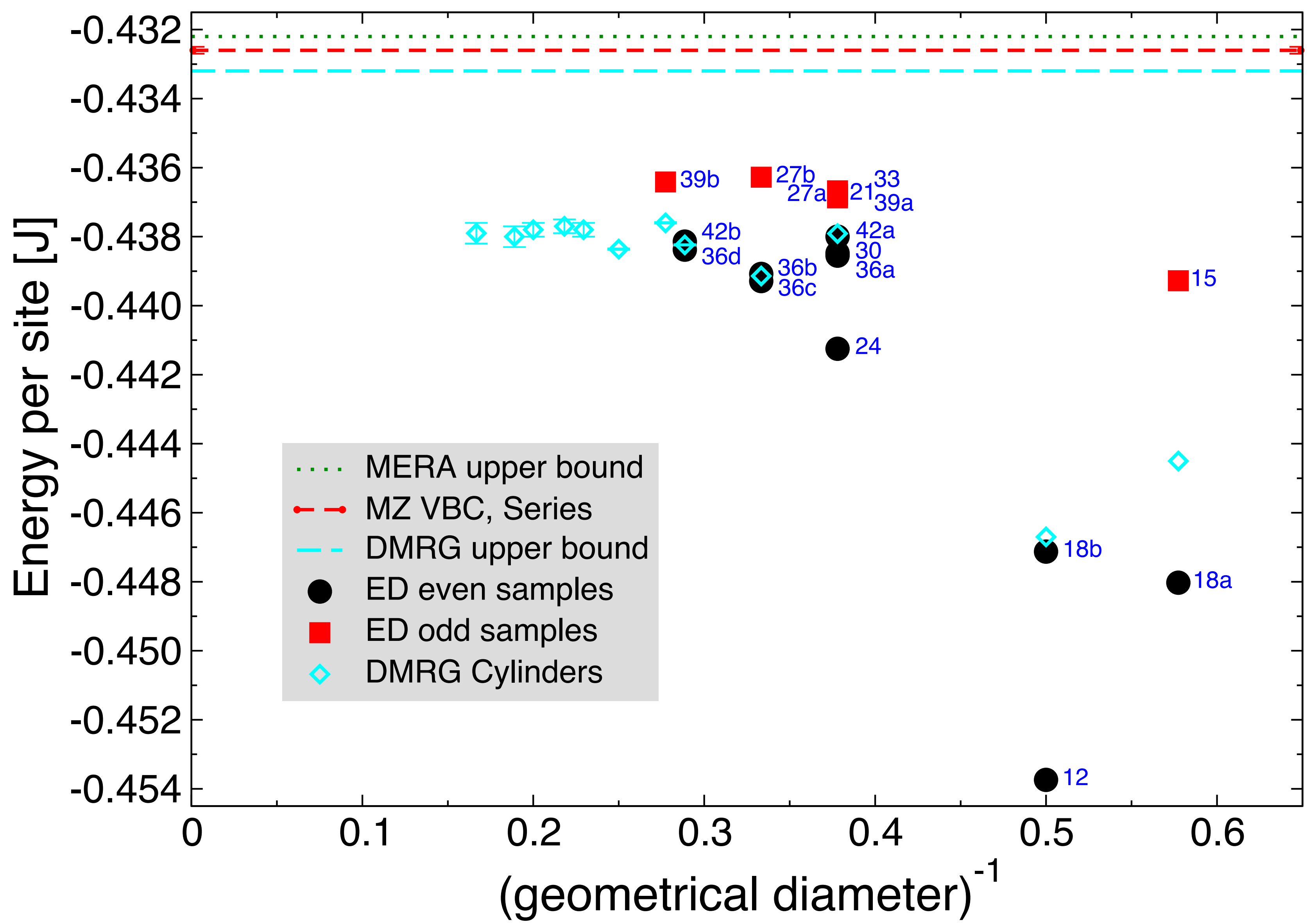
- Convergence for such large Hilbert spaces ? Finite precision arithmetic ?
  Seems ok



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

Kagome S=1/2 Heisenberg model: Energy per site: earlier ED results

- ED Energy per site as a function of diameter (**N up to 42 sites**).



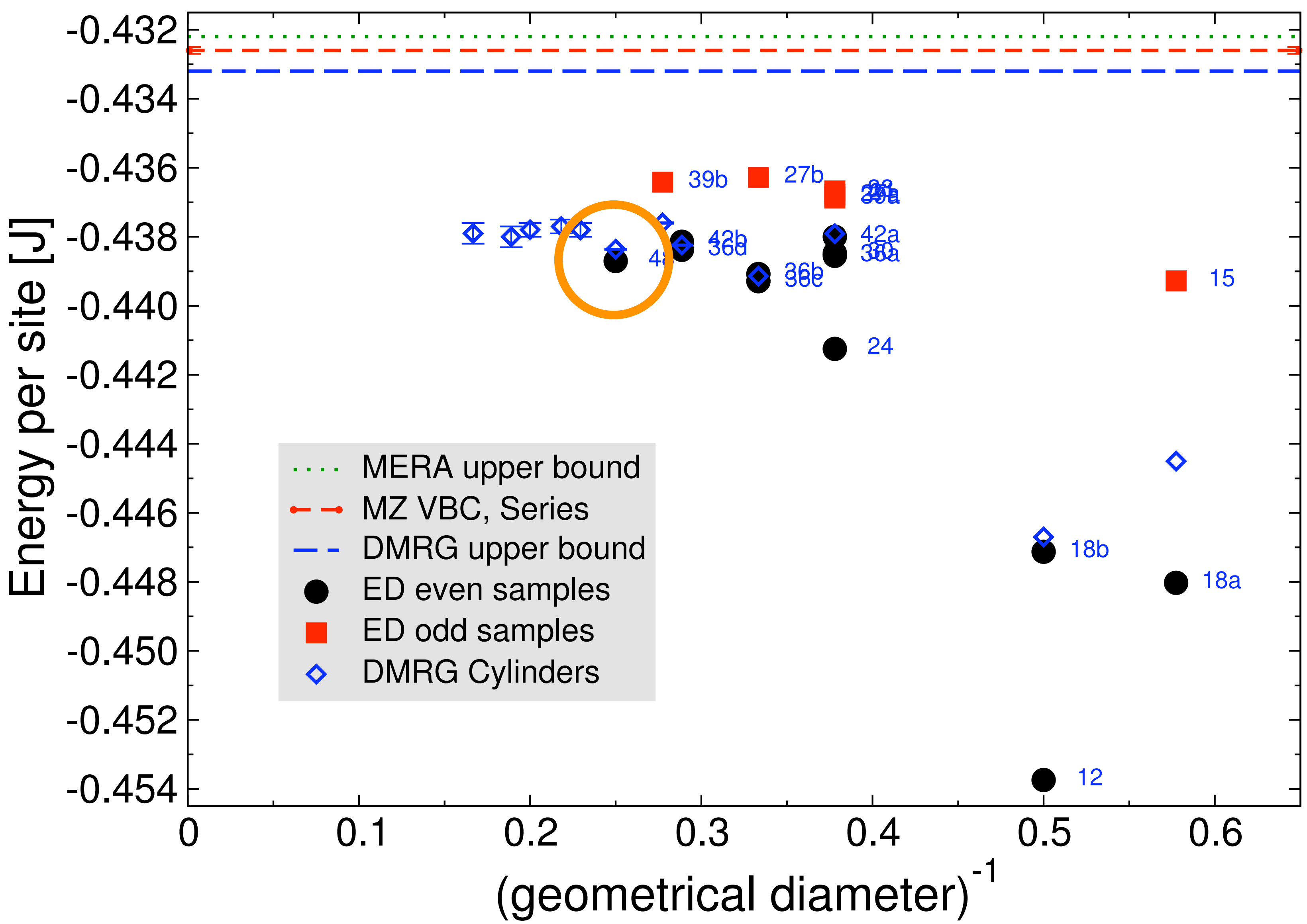
AML, J. Sudan and E. Sorensen, PRB **83**, 212401 (2011)

DMRG Results:
S. Yan *et al.*, Science 2011

- Good agreement between ED and DMRG at same diameter.

Now with 48 sites:

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



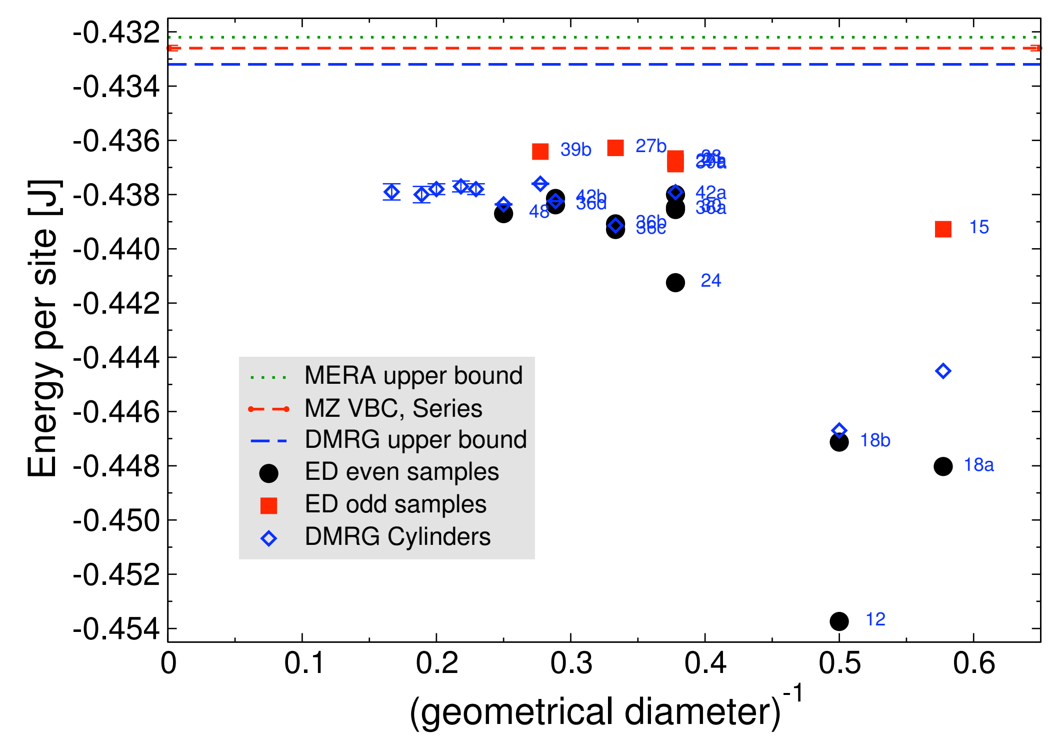
ED 48 sites:

- Ground state energy per site:

$$E/NJ = -0.4387$$

- upper bound on spin gap

$$\Delta/J = 0.168$$



- substantially lower GS energy than early 48 site torus DMRG estimate (HC Jiang *et al.*, PRL 2008) and slightly lower than Depenbrock *et al.*

$$E/NJ = -0.43663$$

Torus	4	$-0.4383(2)$	0.151

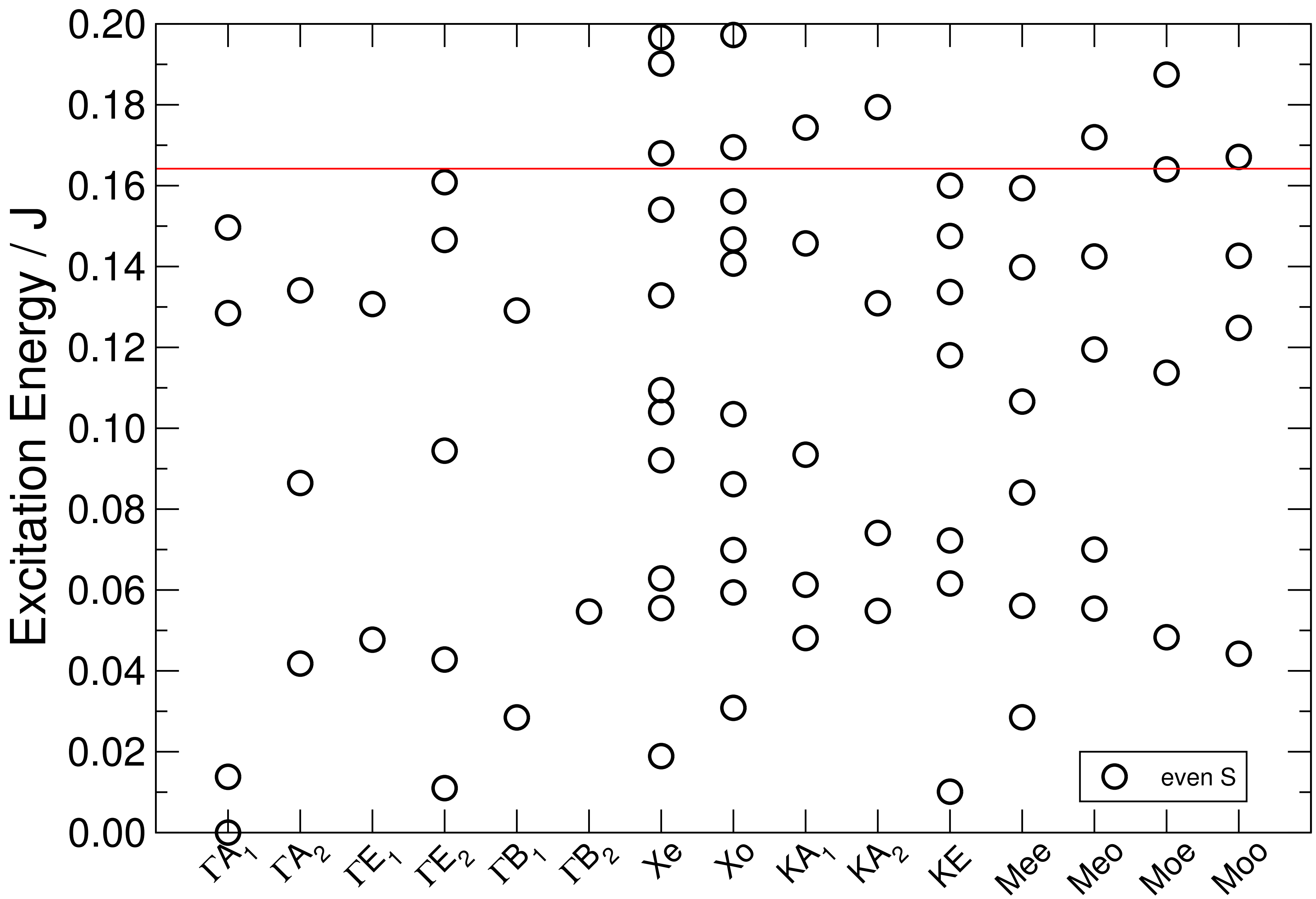
- good agreement with S. Yan *et al.*, Science 2011 and Depenbrock *et al*, PRL 2012 cylinder DMRG results at the same diameter.

- still a bit lower than variance extrapolated VMC results by Y. Iqbal *et al,* arXiv:1209

$$E/J = -0.437845(4)$$

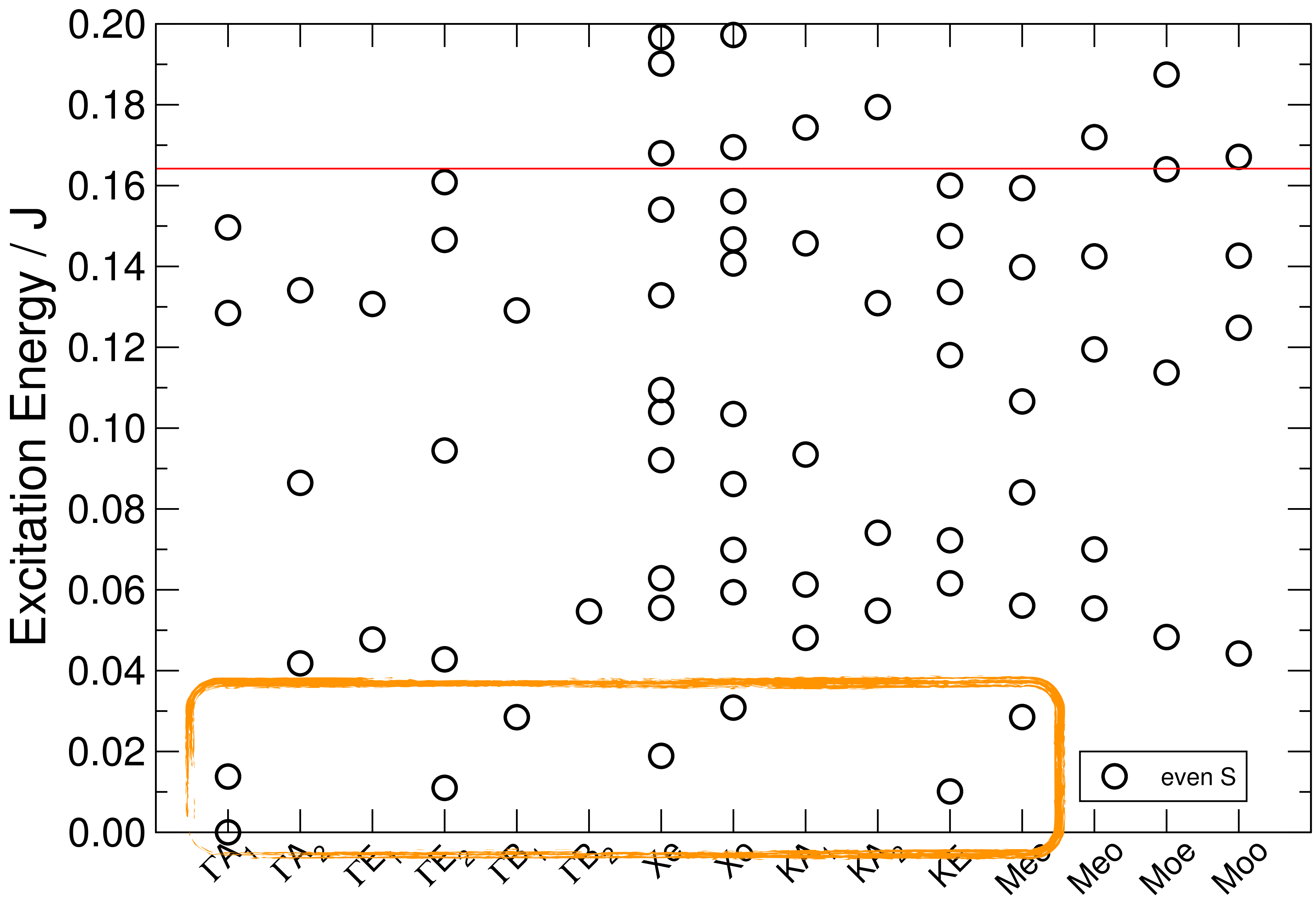
Low Energy Spectrum (N=36)

- C. Lhuillier *et al.*, PRB 1997, EPJB 1998, EPL 2009



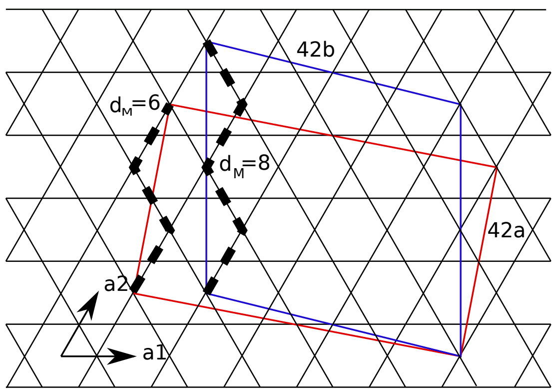
Low Energy Spectrum (N=36)

- C. Lhuillier *et al.*, PRB 1997, EPJB 1998, EPL 2009

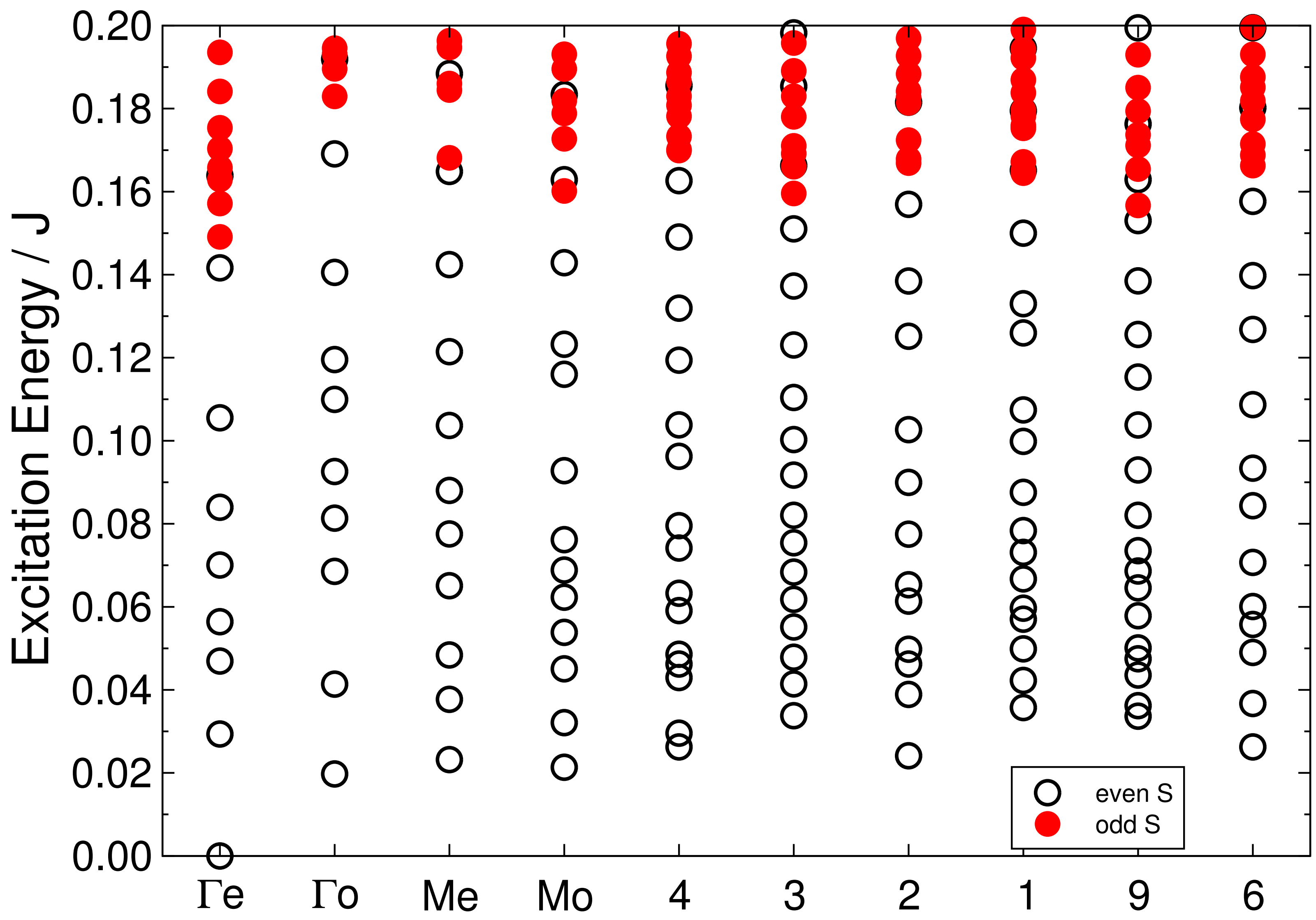


many low-lying singlet states !

Low Energy Spectrum (N=42b)

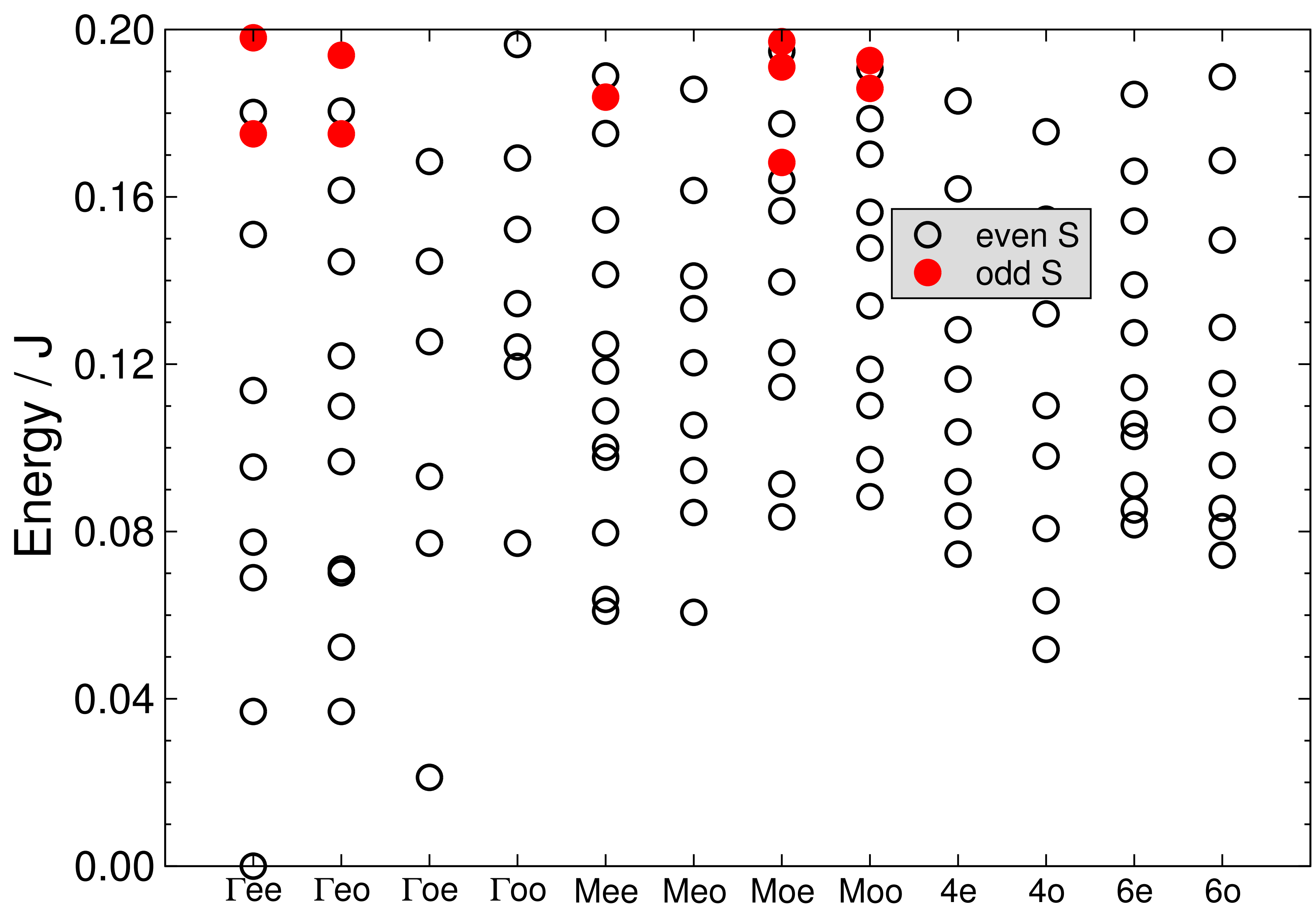


- AML, R. Johanni, R. Moessner



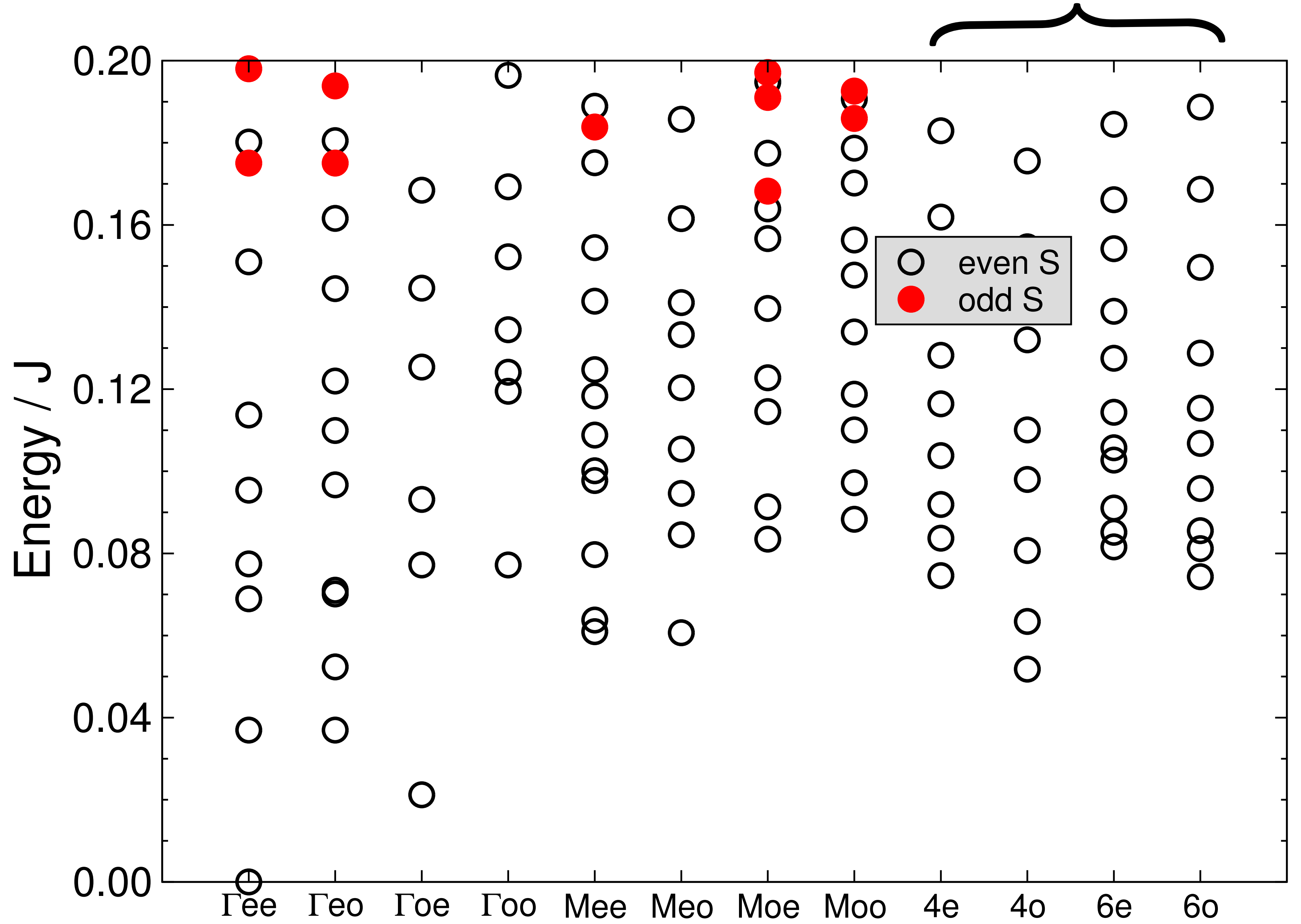
- still rather dense spectrum !

Low Energy Spectrum (N=48)

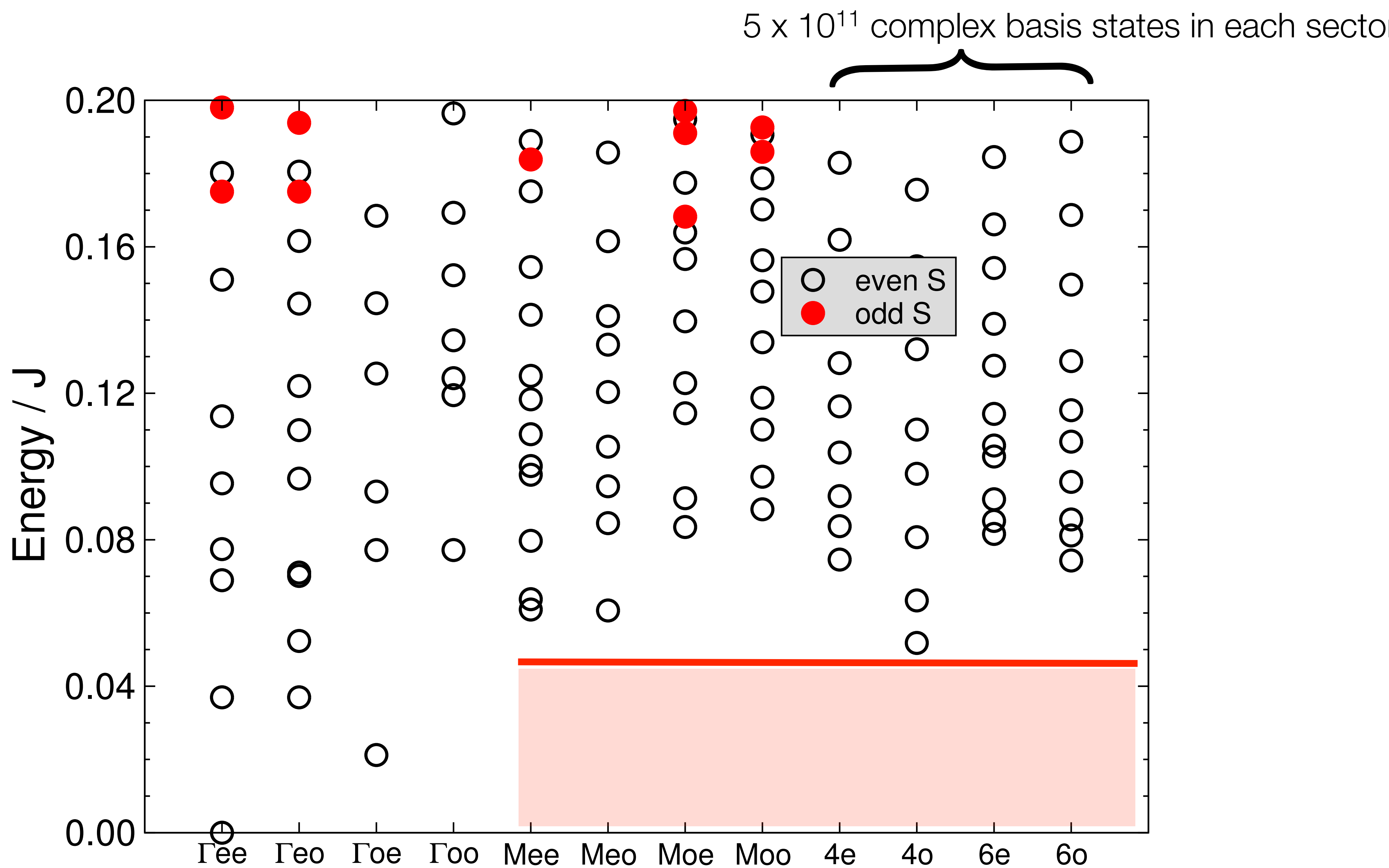


Low Energy Spectrum (N=48)

5 x 10^{11} complex basis states in each sector

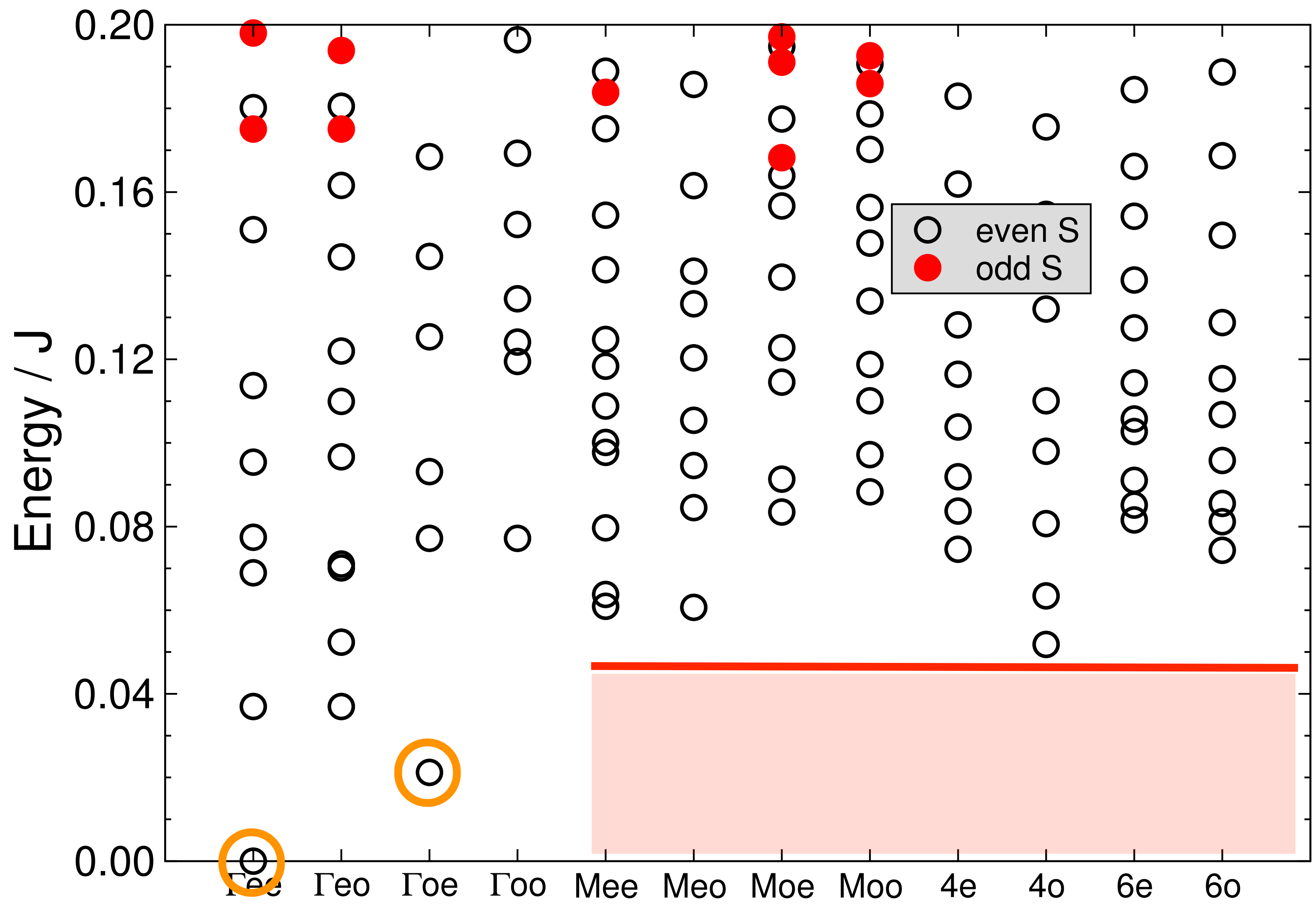


Low Energy Spectrum (N=48)



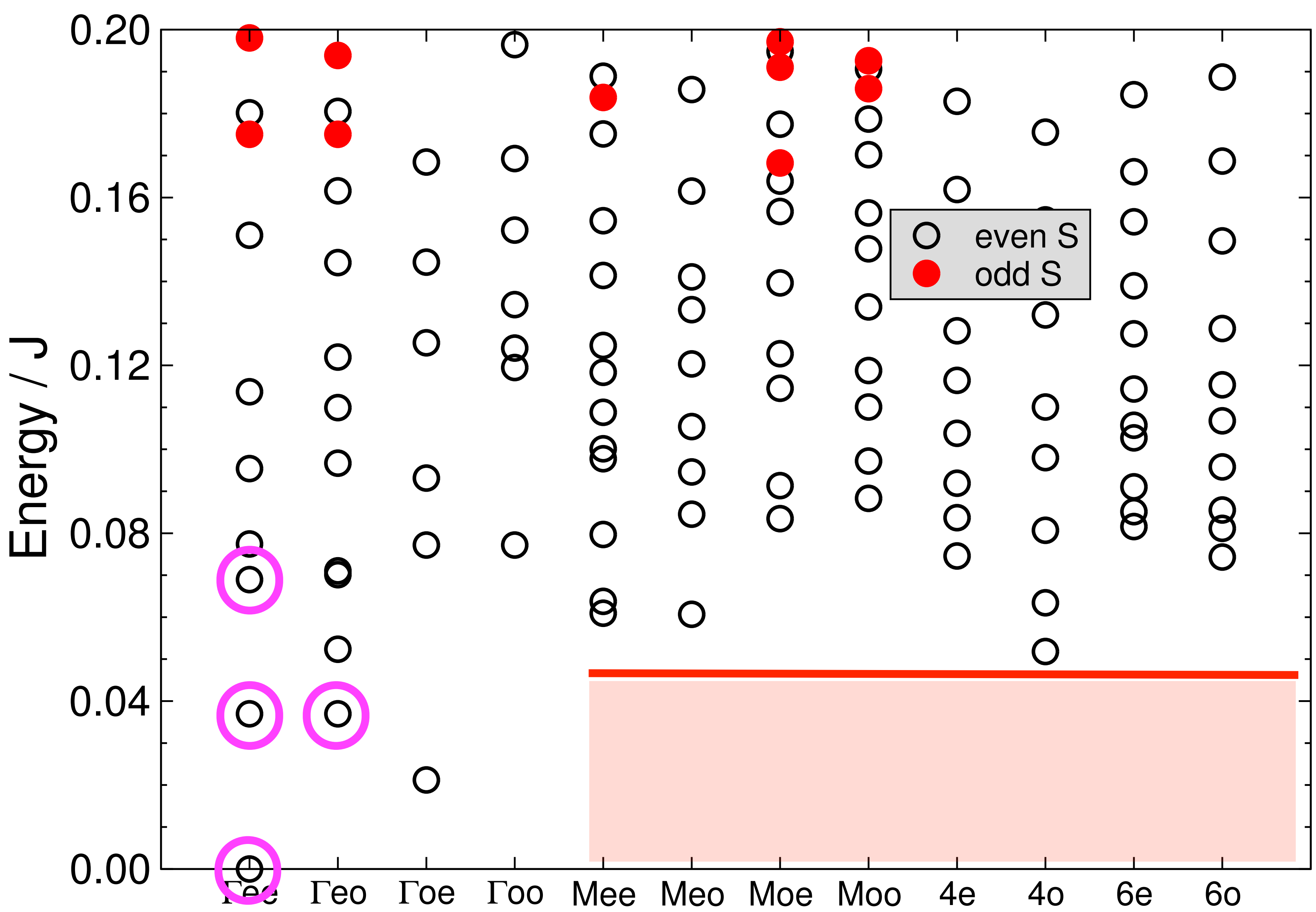
translation symmetry breaking unlikely

Low Energy Spectrum (N=48)



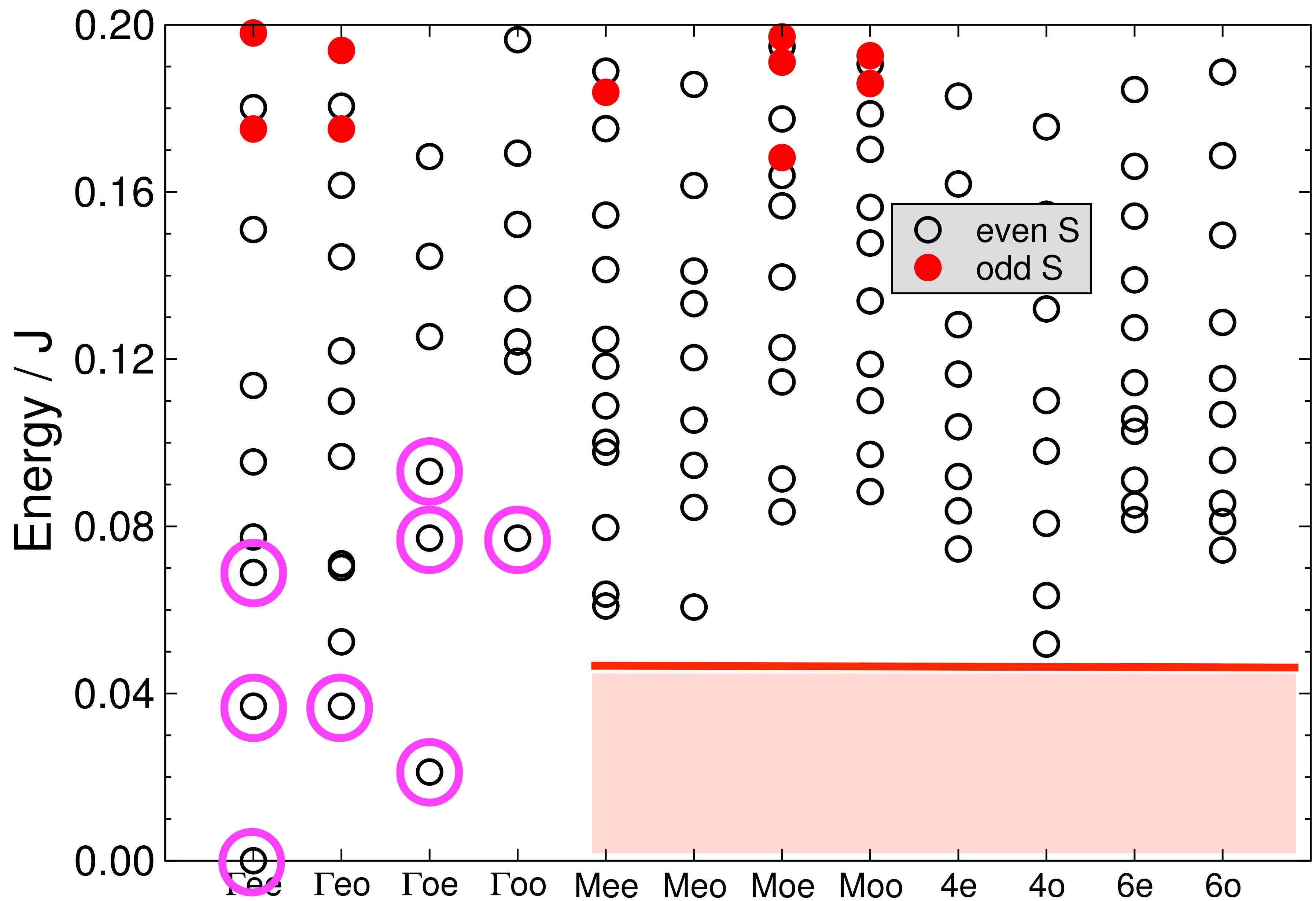
Inversion symmetry breaking ?

Low Energy Spectrum (N=48)



Z_2 topological degeneracy ?

Low Energy Spectrum (N=48)

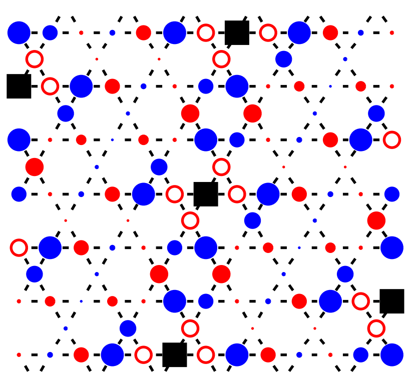


Z_2 topological times Z_2 spatial symmetry breaking ?

Real space spin-spin correlations

- spin correlations are small, but strongest and staggered on paths which wrap around the sample

- Is this a feature of a spin liquid ?



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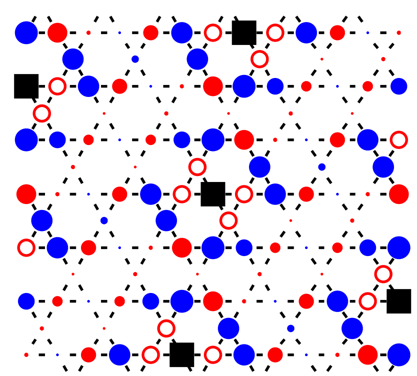

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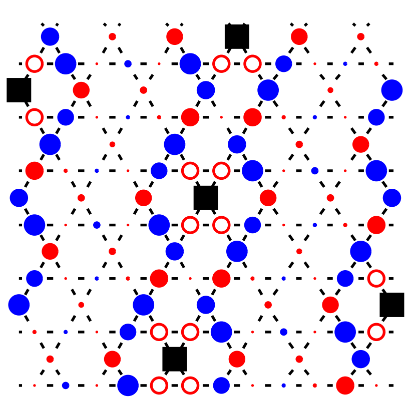

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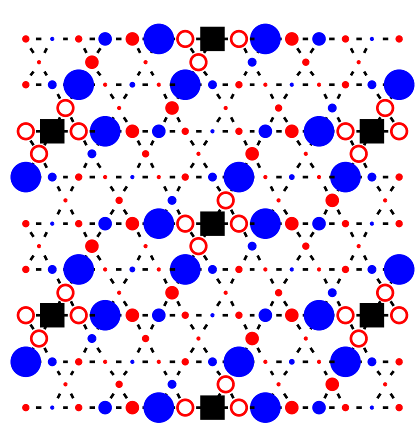
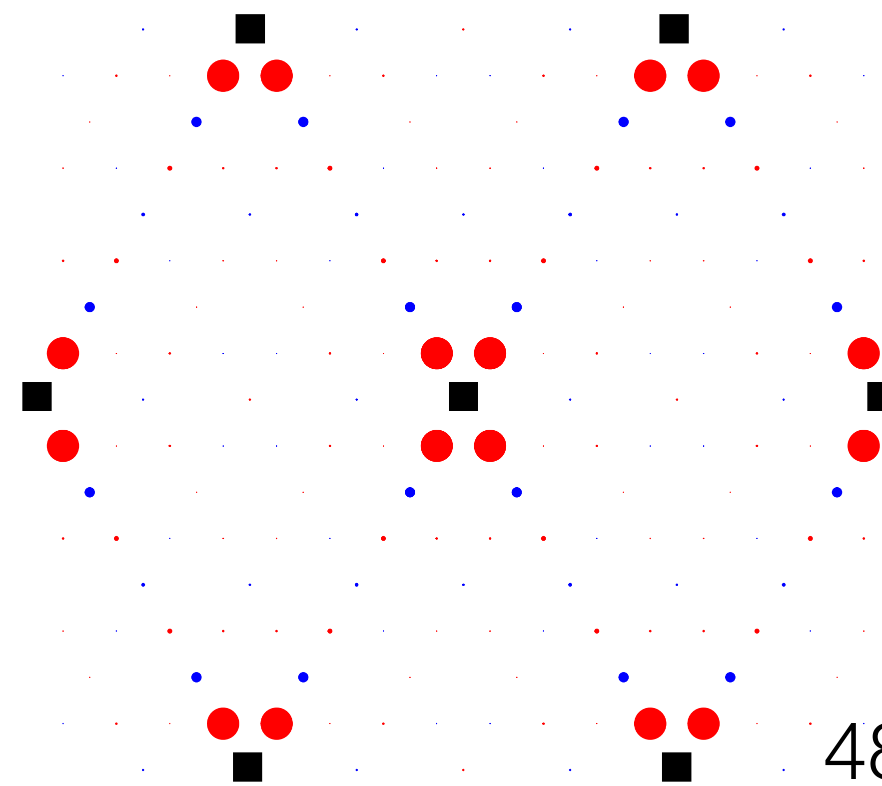


36d

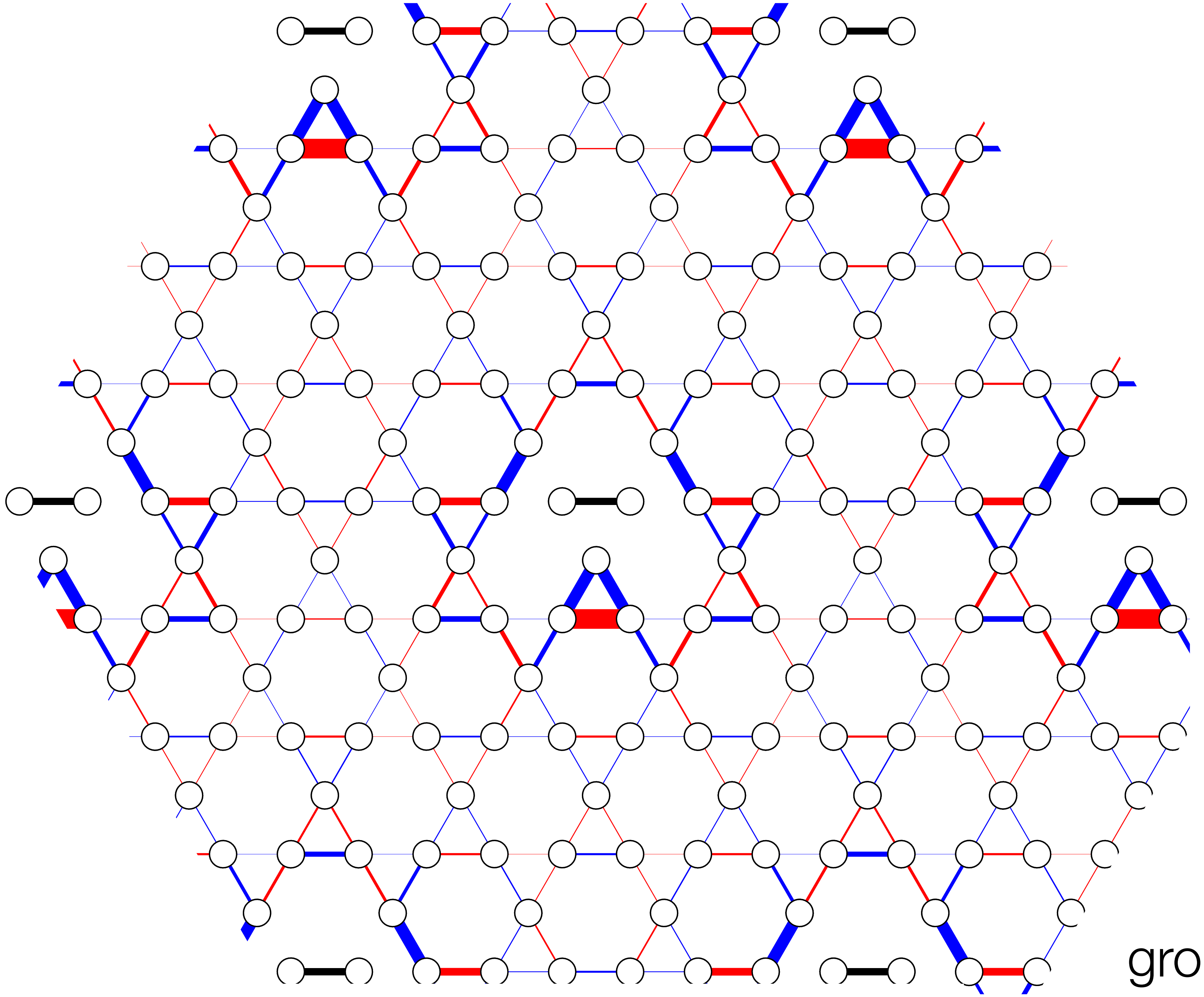


48

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

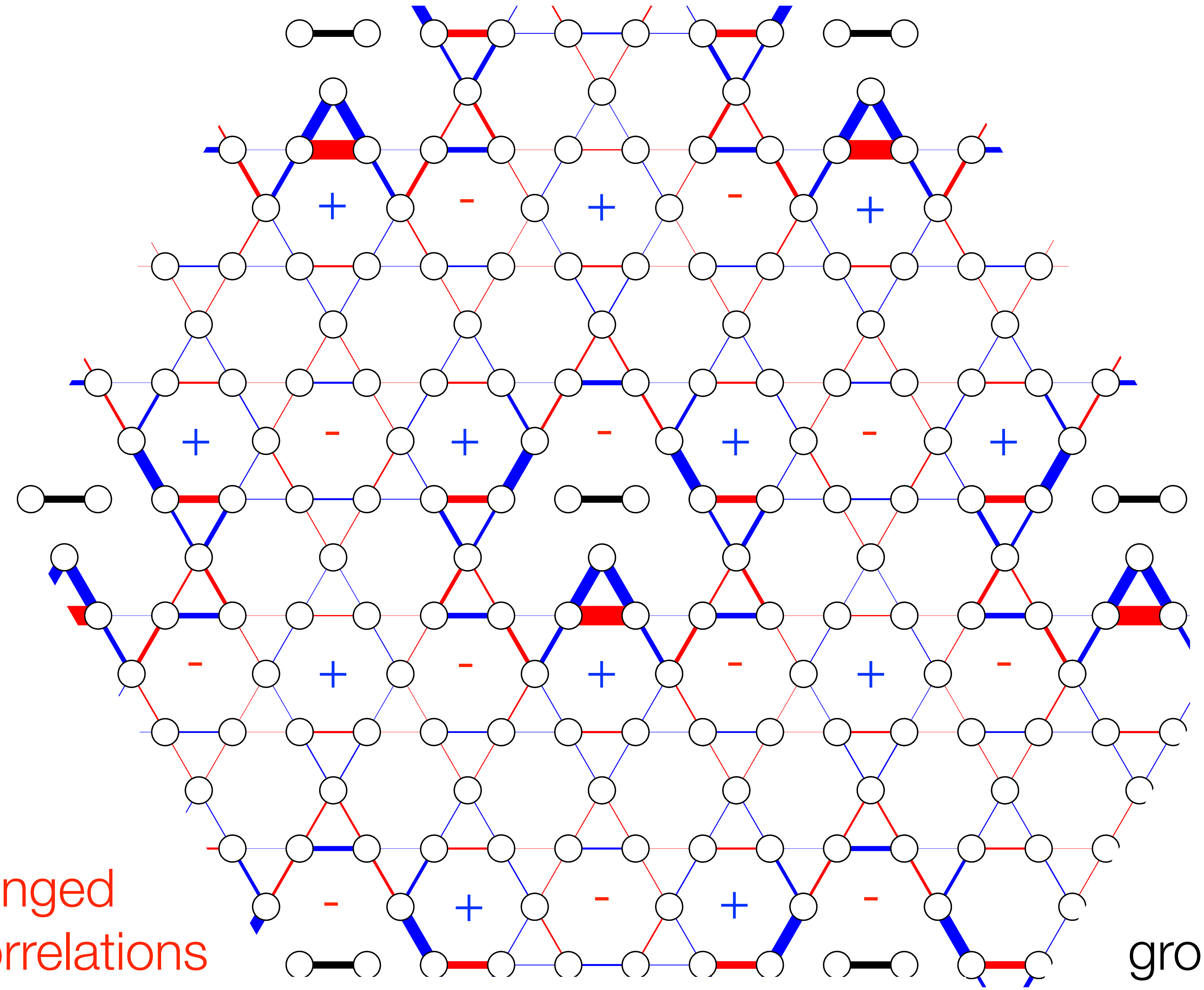
AML, R. Johanni, R Moessner

Dimer-Dimer correlations



N=48
ground state

Dimer-Dimer correlations

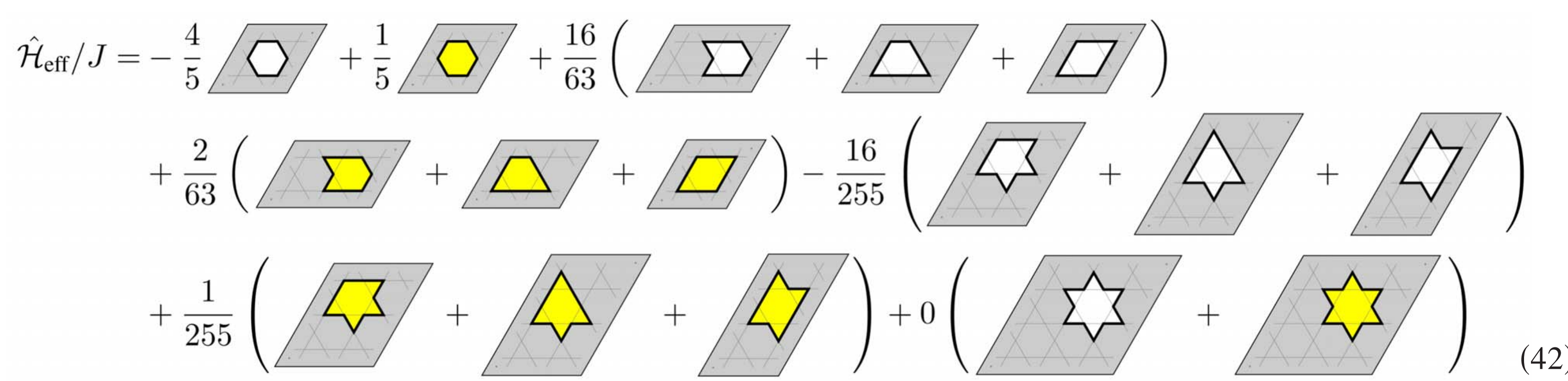


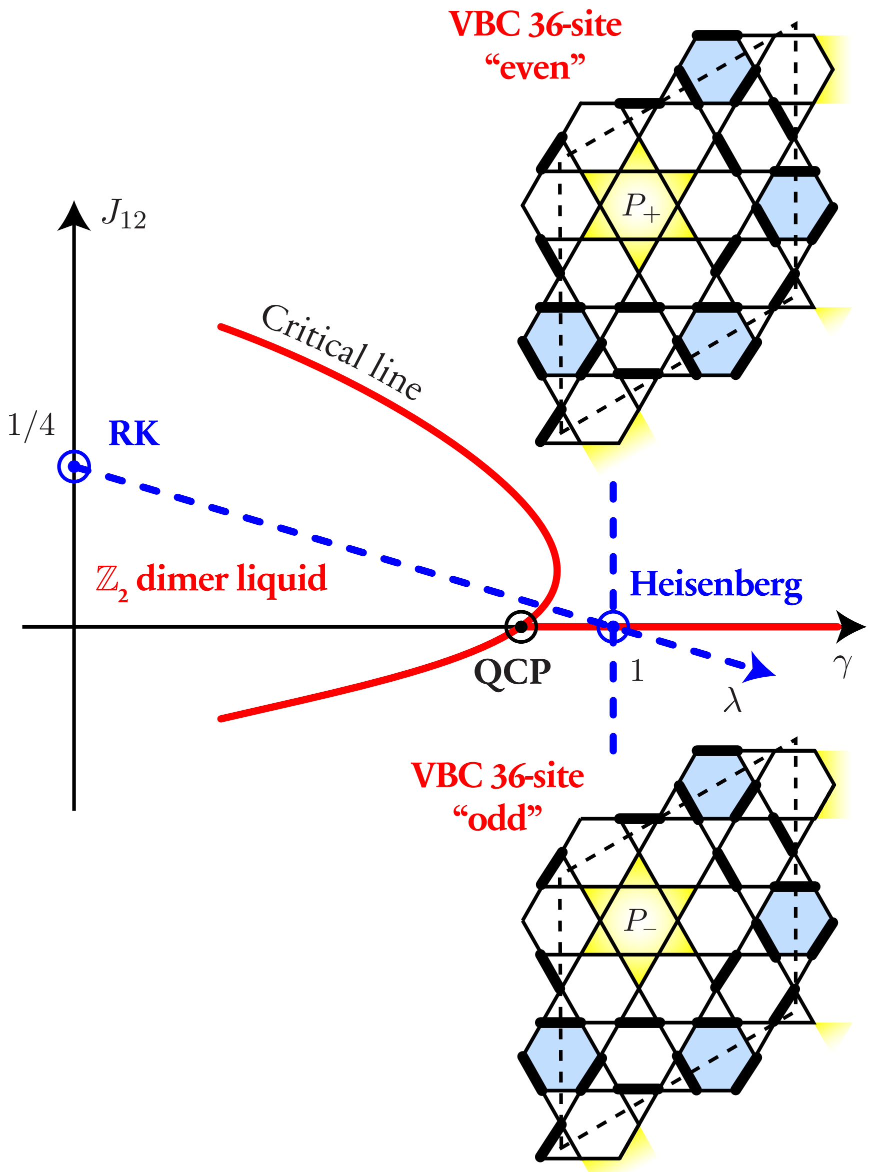
short ranged
diamond correlations

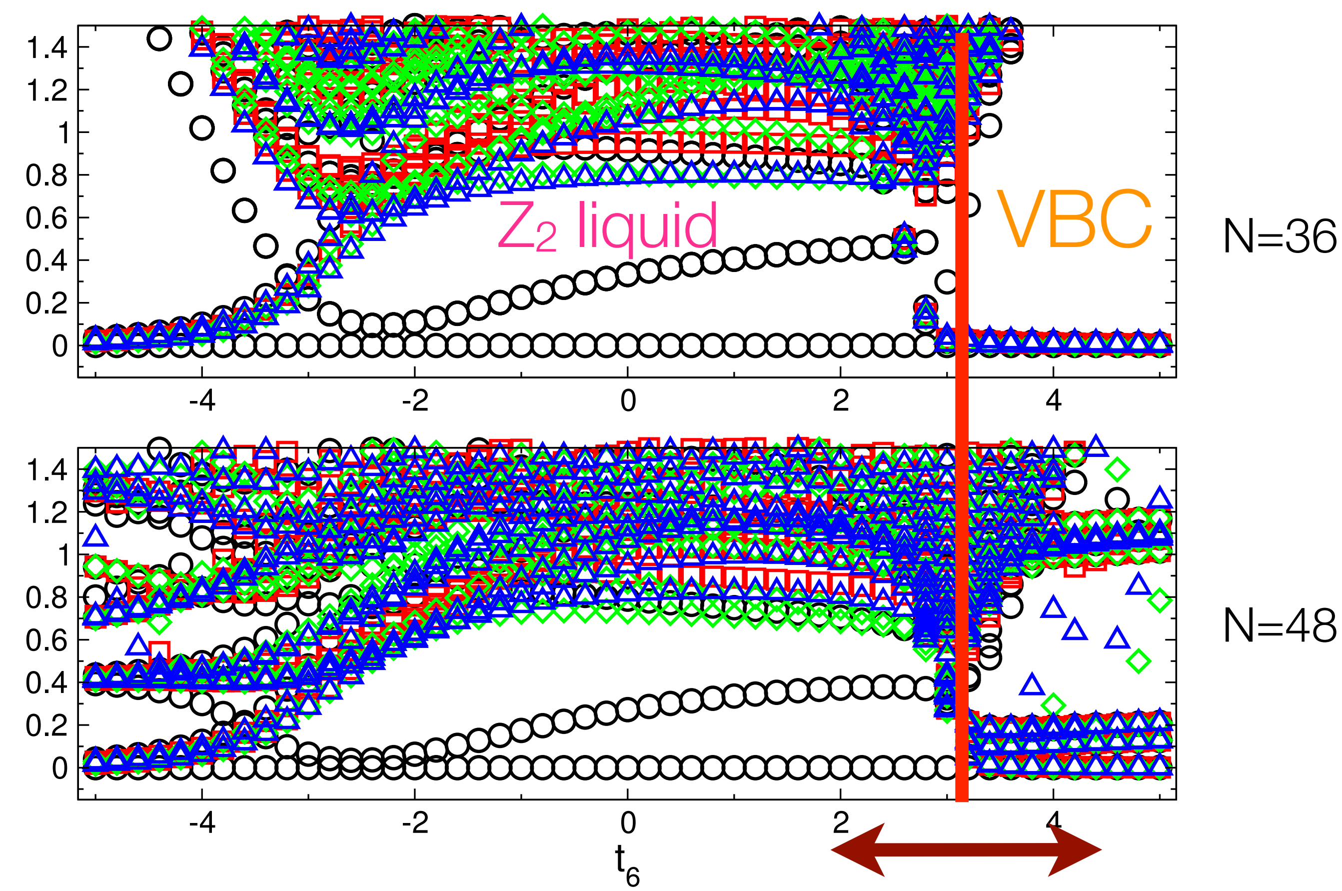
N=48
ground state

Effective Quantum Dimer Model

C. Zeng & V. Elser, PRB 95
D. Poilblanc *et al.*, PRB 2010
D. Schwandt *et al.*, PRB 2010





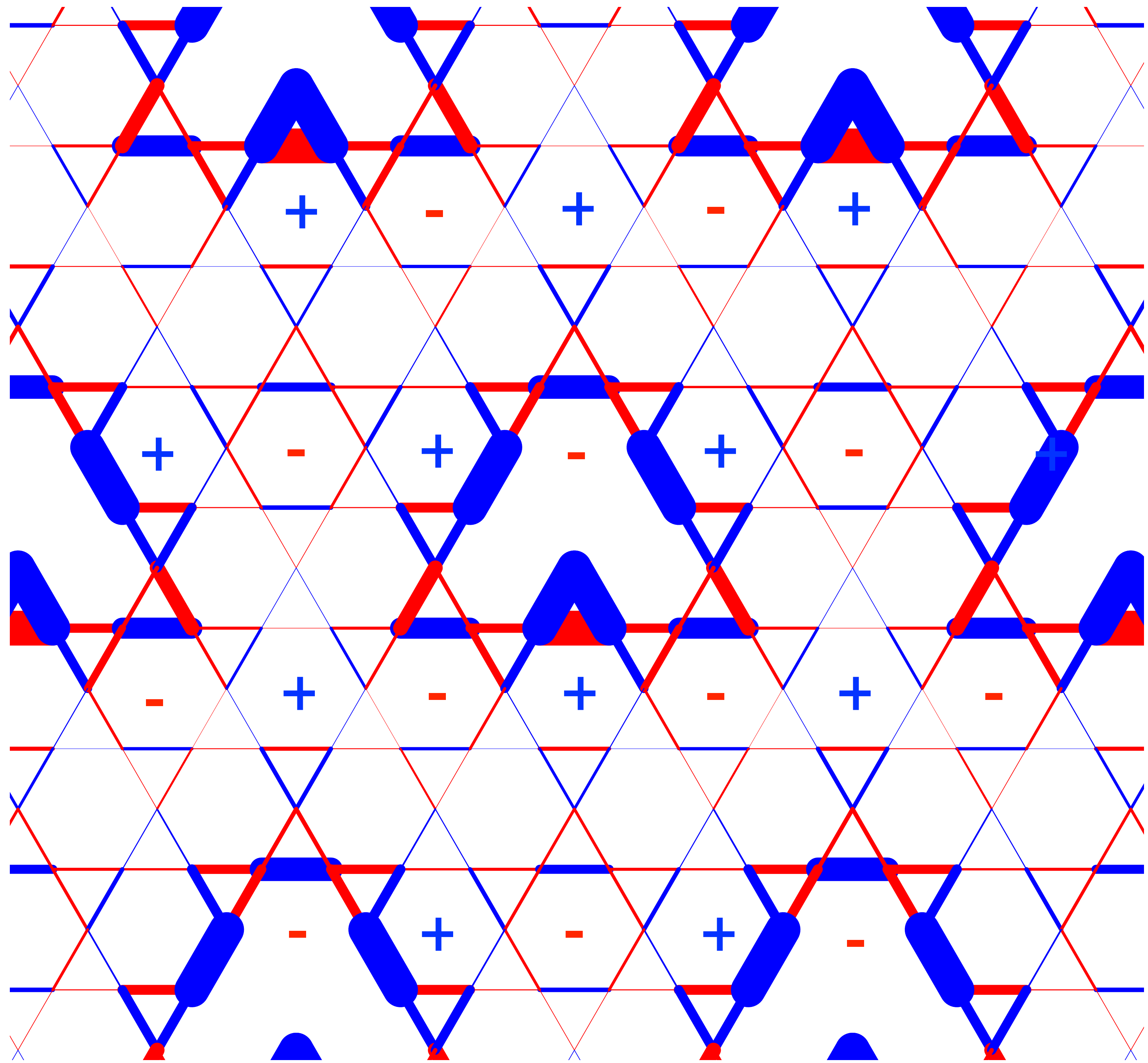


effect of increasing t_6 relative to t_8

AML, R. Johanni & R. Moessner

Quantum Dimer Model

- QDM with slightly enhanced length-8 resonance amplitude
- Now in the Z_2 liquid region !
- Displays short-ranged diamond VBC correlations
- Can explain quantum numbers of Z_2 liquid + finite size splitting of topo levels
- But inversion symmetry breaking level(s) not explained

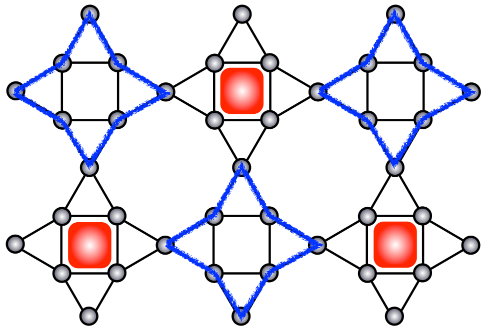


AML, R. Johanni & R. Moessner

Conclusions & Outlook

- Highly parallel MPI exact diagonalization for S=1/2 spin systems up to 48 sites
- Low energy spectrum reveals *no* sign of translational symmetry breaking
- Possible inversion symmetry breaking and / or Z_2 topological degeneracy ?
- Short range diamond VBC correlations, as in DMRG.

- Correlation functions in excited states (ongoing)
- Square kagome ? Valence bond crystal or spin liquid ?



Thank you for your attention !