SU(4) materials: emergence and developments

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Collaborators



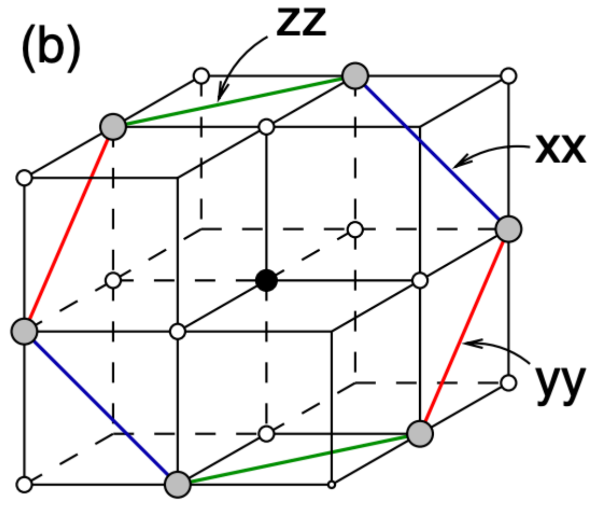
- Satoshi Fujimoto (Osaka Univ.)
- Karlo Penc (Wigner Research Centre for Physics, Hungary)
- Frank Pollmann (TUMunich)
- Based on: M.G.Y., and S. Fujimoto, arXiv:2111.14470 (accepted in PRB Letter with Editors' suggestion).
  M.G.Y., K. Penc, and F. Pollmann, in preparation.

Outline

- Introduction
- Finite-temperature results (cTPQ)
- Ground-state properties (DMRG)
- Summary

Kitaev materials

- Quantum spin liquids had long been a “vague” notion even theoretically. The first “rigid” foundation was given by Kitaev (2003/2006). This is the theory of Kitaev spin liquids.



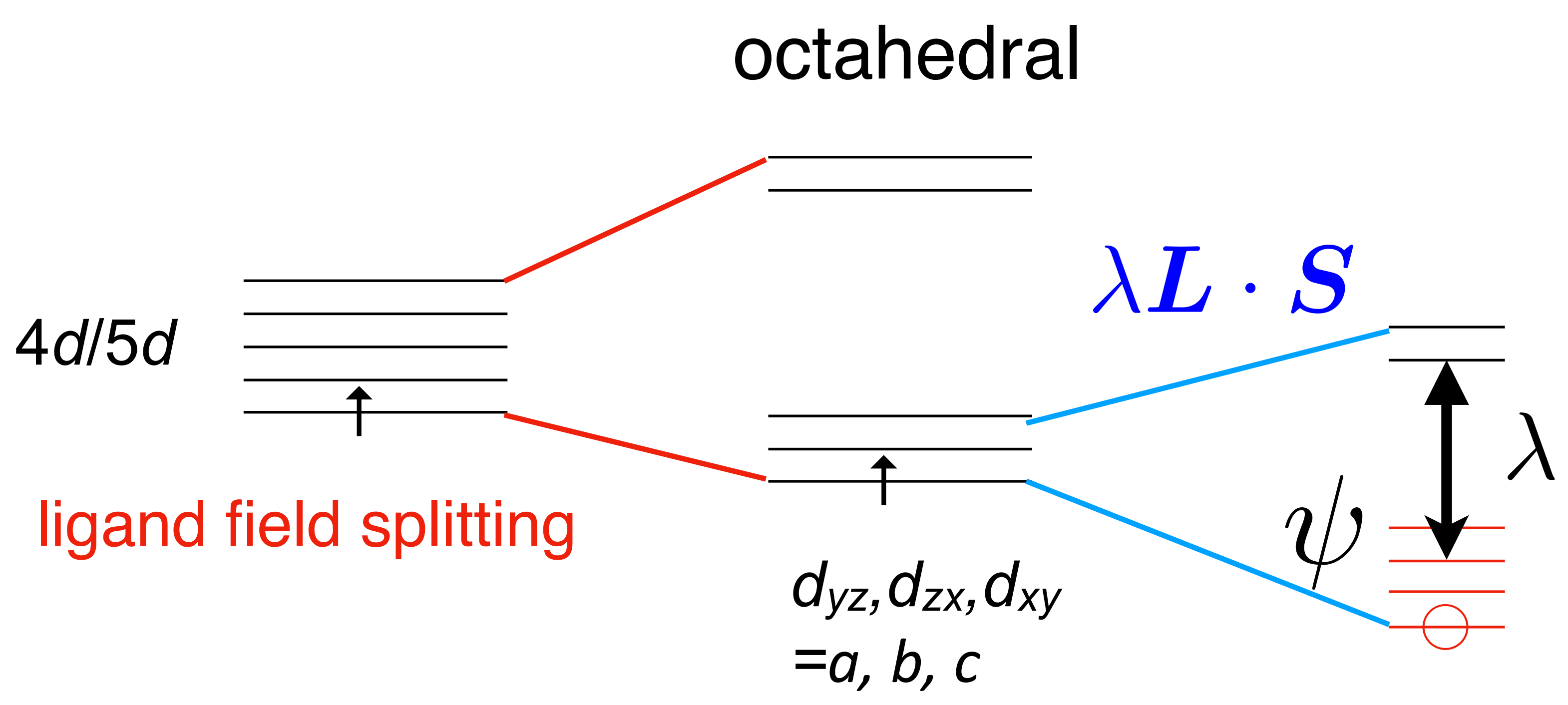
$$H = -J_x \sum_{\langle jk \rangle \in x} \sigma_j^x \sigma_k^x - J_y \sum_{\langle jk \rangle \in y} \sigma_j^y \sigma_k^y - J_z \sum_{\langle jk \rangle \in z} \sigma_j^z \sigma_k^z$$

- After the discovery of candidate materials like α-$RuCl_3$, this is one of the most important fields in condensed matter physics.

- What is the next Kitaev?

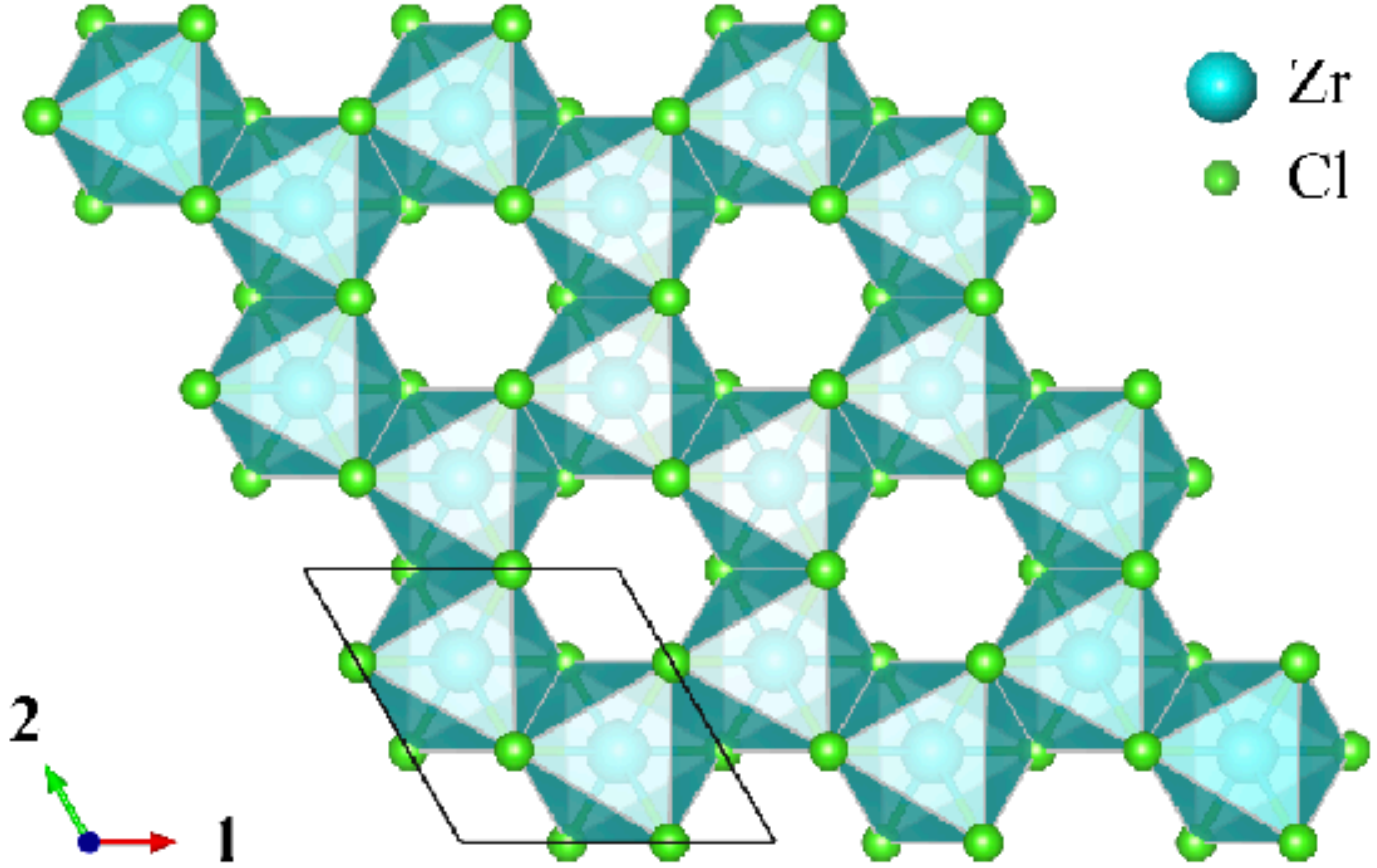
SU(4) materials: α-$ZrCl_3$

The next Kitaev would be d¹!



Ti^{3+}, Zr^{3+}, Hf^{3+} d^1 S=1/2, L=1

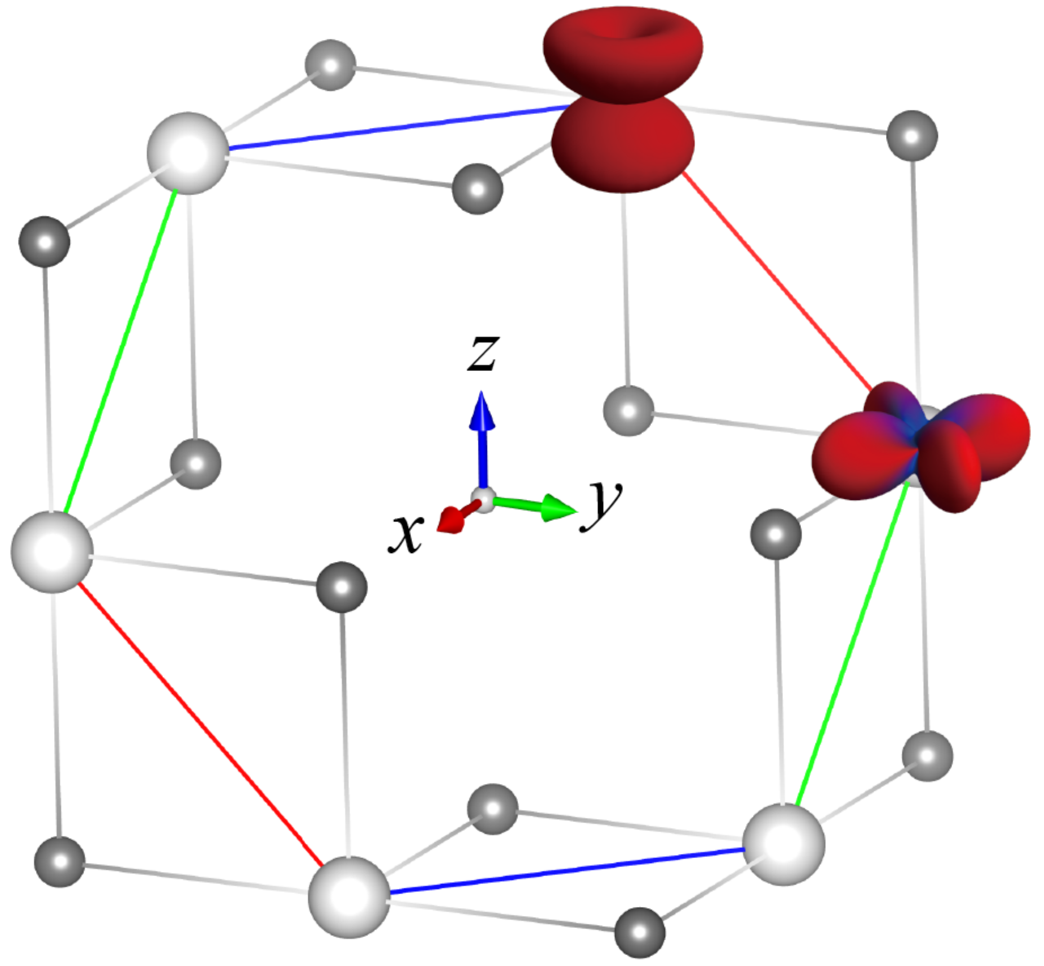
$3ZrCl_4$ (gas) + Zr(solid) → $4ZrCl_3$ (solid)



M.G.Y. *et al.*, PRL **121**, 097201 (2018).

- In 2018, we proposed that a d^1 electronic system will be another QSL.

SU(4) Heisenberg model



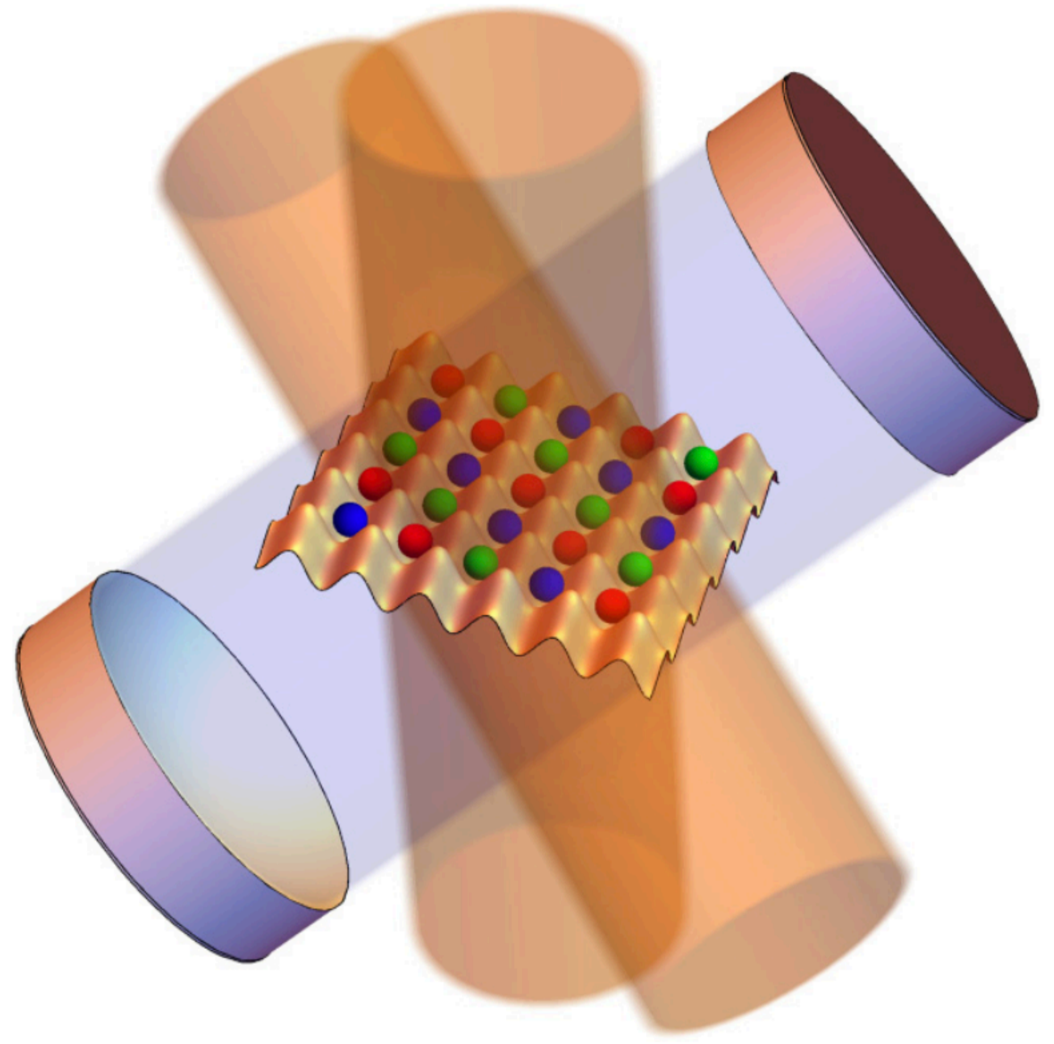
- The Hamiltonian looks like this:
- $$H = \sum_{\langle ij \rangle} P_{ij} = \sum_{\langle ij \rangle} \left(2S_i \cdot S_j + \frac{1}{2} \right) \left(2T_i \cdot T_j + \frac{1}{2} \right).$$
- A simple form is a swapping operator P_{ij} of SU(4).
- If you separate four states into two spin d.o.f. and two orbital d.o.f., then the model can also be written as the right hand side.

Connection to “organics”

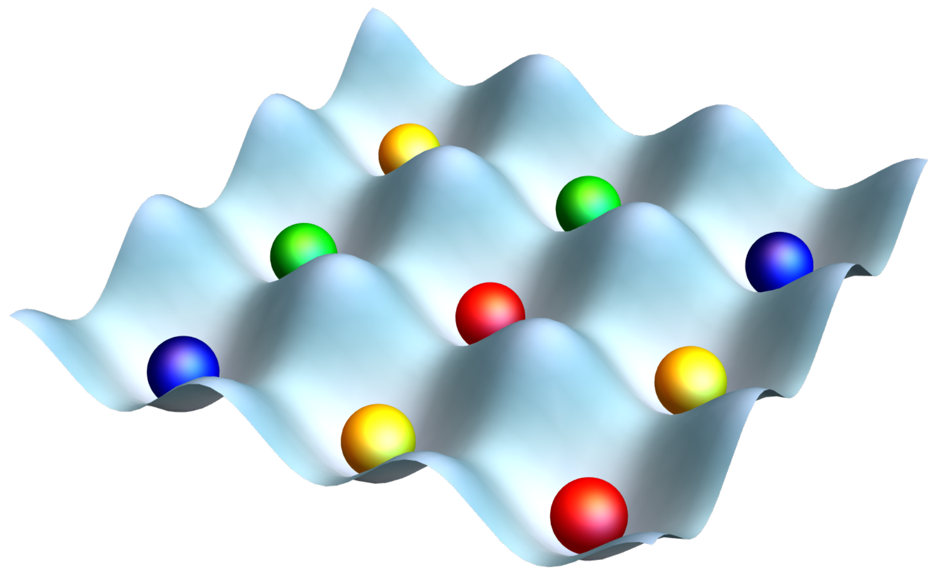
- Twisted bilayer graphene:
  - Some SU(4) models are thought to be related to twisted bilayer graphene with spin&valley degrees of freedom.
- Metal-organic framework realization:
  - d^1 metal-organic frameworks with Zr^{3+}, Hf^{3+} are also SU(4) candidates.
  - cf. M.G.Y. et al., Phys. Rev. Lett. **121**, 097201 (2018).

Even if the d[1] material does not exist,
Cold atomic realization will help.

- Even if d^1 honeycomb materials do not exist, cold atomic realization will help.
- Cold atoms with a nuclear spin F has the SU(2F+1) symmetry.
- SU(6) and SU(10) has been realized. SU(4) may be realized, too.
- By trapping in the optical lattice we may realize QSOL.



S. F. Caballero-Benitez, G. Mazzucchi, and I. B. Mekhov, PRA **93**, 063632 (2016).



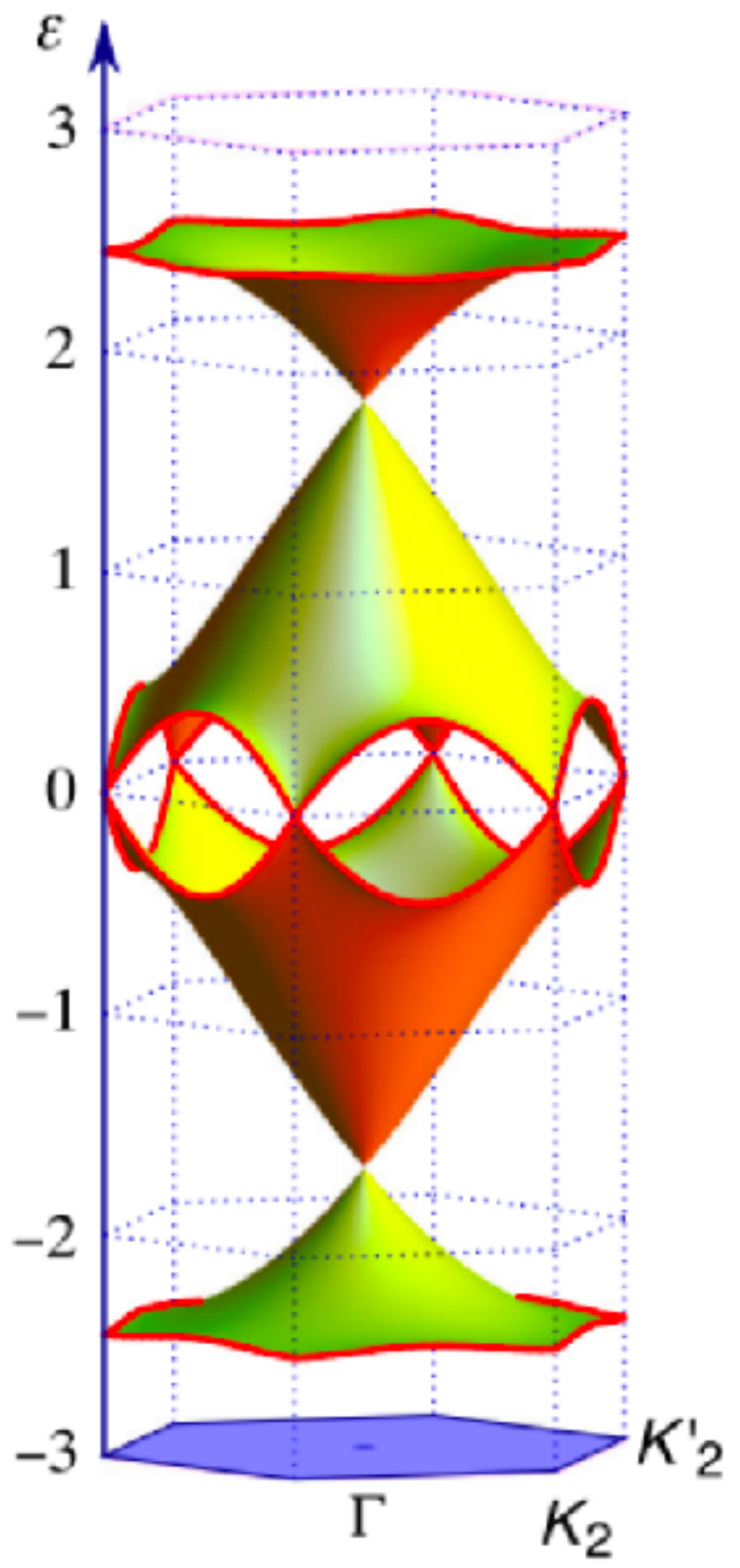
Long-standing unsolved problem

Can SU(4) models realize a quantum spin-orbital liquid?

- Wang-Vishwanath (2009) proposed a quantum spin-orbital liquid (QSOL) ground state for the SU(4) Heisenberg model on the square lattice.
- Later, the square lattice was found to be ordered, the honeycomb lattice became another candidate. (P. Corboz et al. 2012)
- However, the real ground state (and finite-temperature) properties have still been illusive for more than a decade. We give a (partial) answer to the problem using cTPQ and DMRG methods.

Previous work on SU(4) honeycomb

- The combination of iPEPS/ED/VMC calculation by P. Corboz et al. suggested a scenario of a gapless Dirac spin liquid for the ground state, while there was no unbiased numerical evidence for the gap or its absence.
- Today I will propose another scenario (a gapped scenario) from the cTPQ and DMRG calculations. These methods are believed to be less biased.



P. Corboz *et al.*, PRX **2**, 041013 (2012).

Finite-temperature results (brief overview)

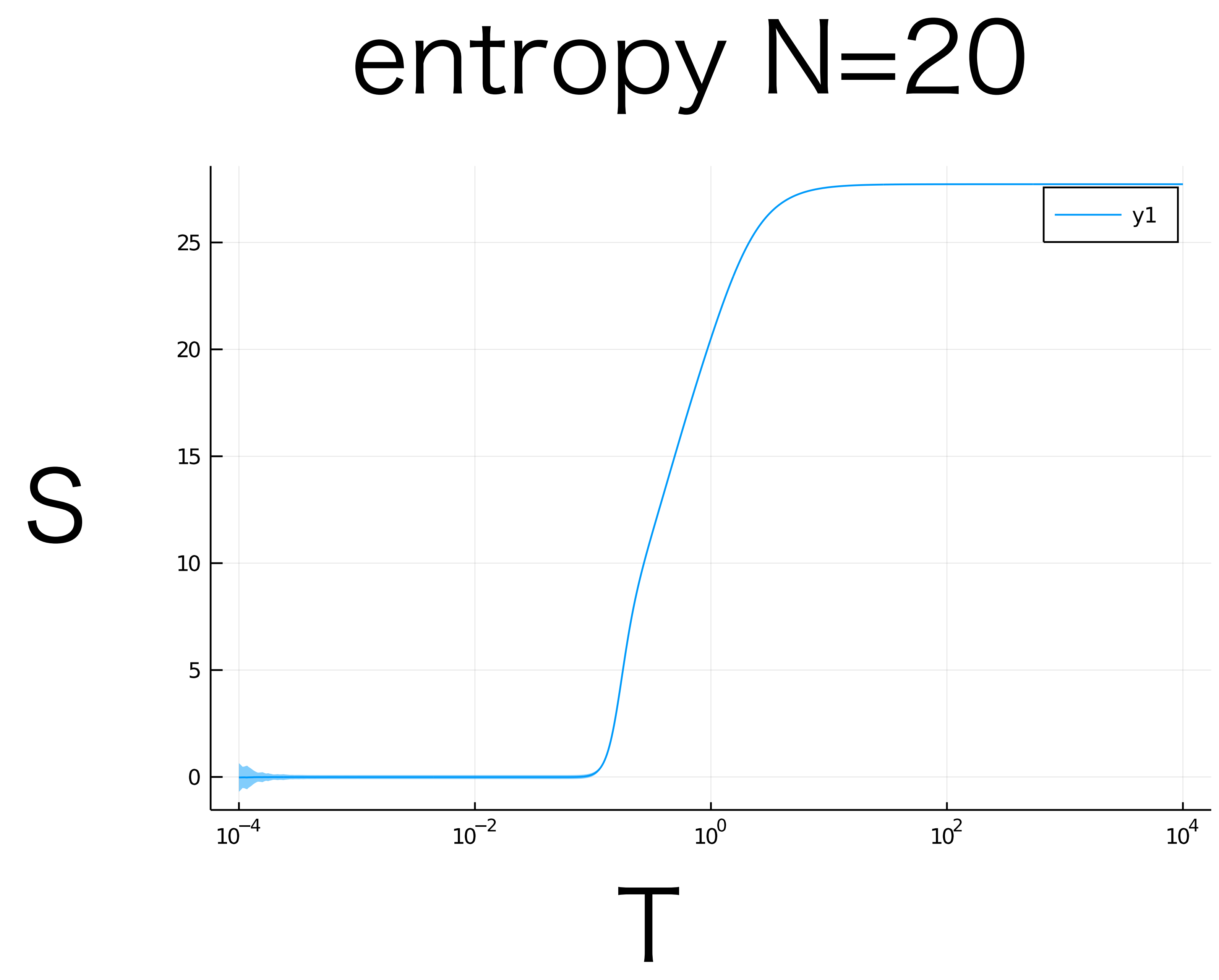
Canonical thermal pure quantum states

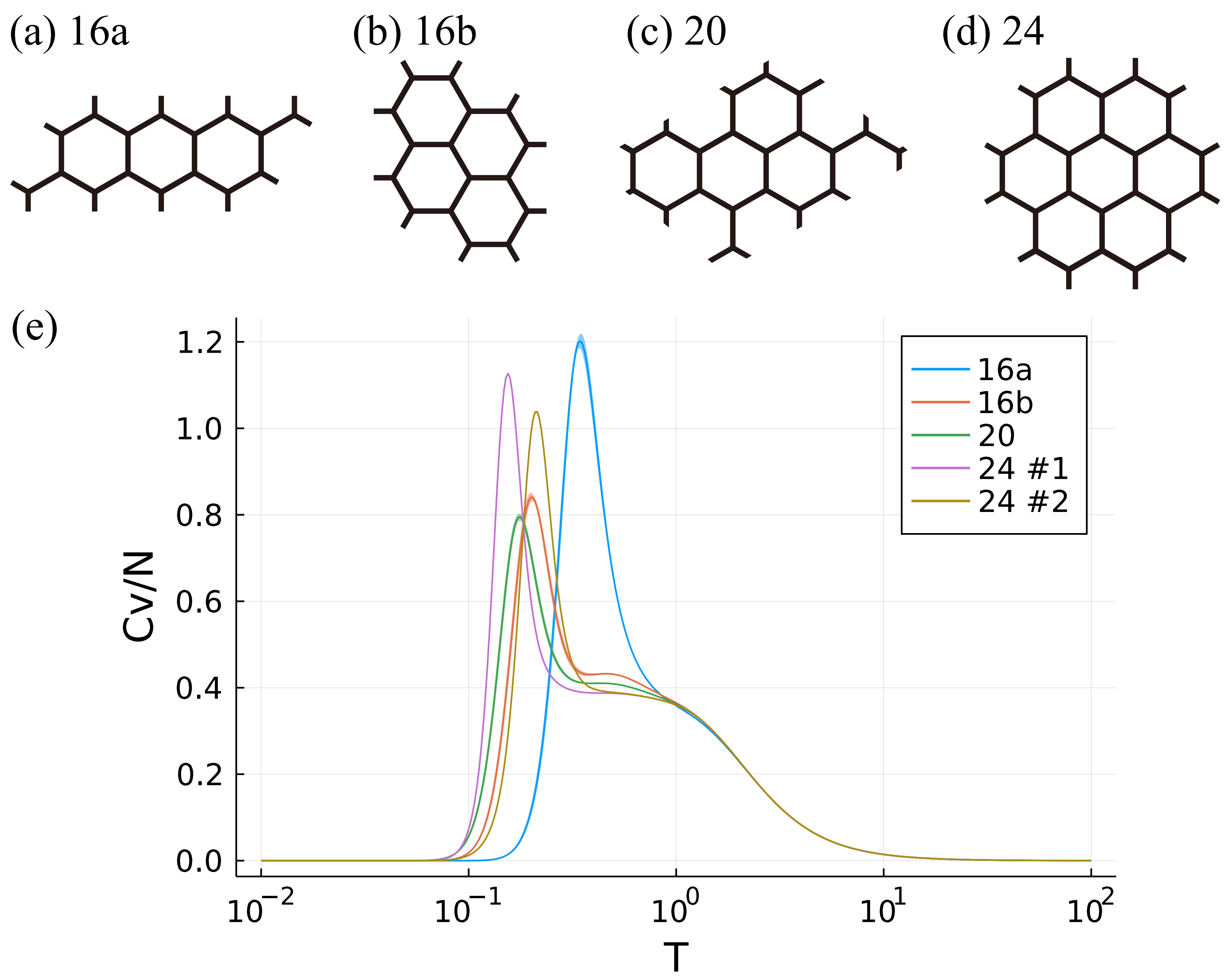
Heat capcity at finite temperature

- The canonical thermal pure quantum (cTPQ) state method is a powerful method to calculate the heat capacity at finite temperature.
- Based on Nataf and Mila, we newly implement the SU(N) symmetry in the cTPQ method, allowing the first finite-temperature calculation for the SU(4) Heisenberg model on the honeycomb lattice.
- Using the supercomputer, we can compute the heat capacity of the SU(4) Heisenberg model up to 24 sites.
  - ISSP supercomputer: AMD EPYC 7702 x 288 = 18432 cores.

Calculation up to 24 sites

Peak and shoulder structure



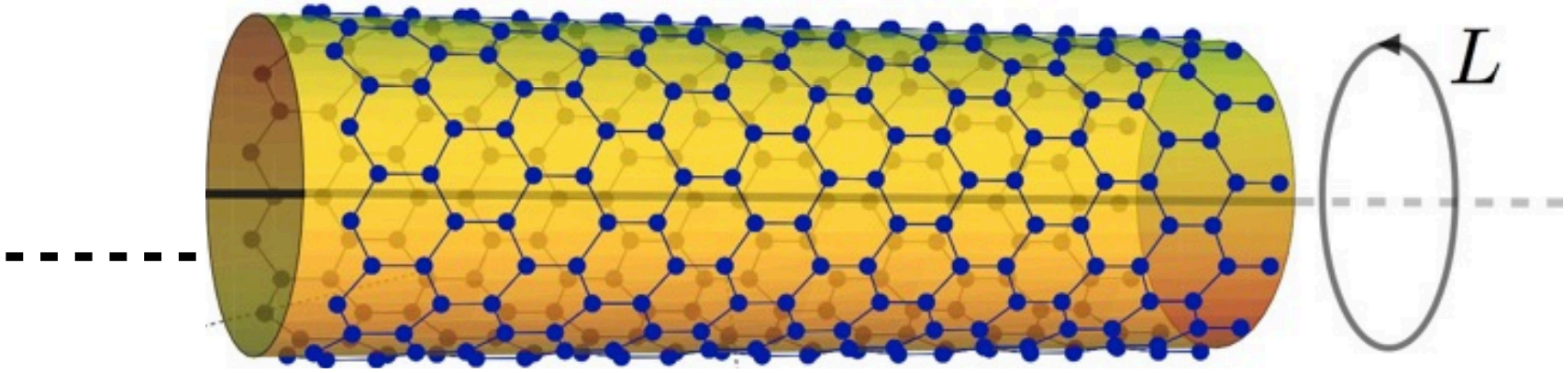


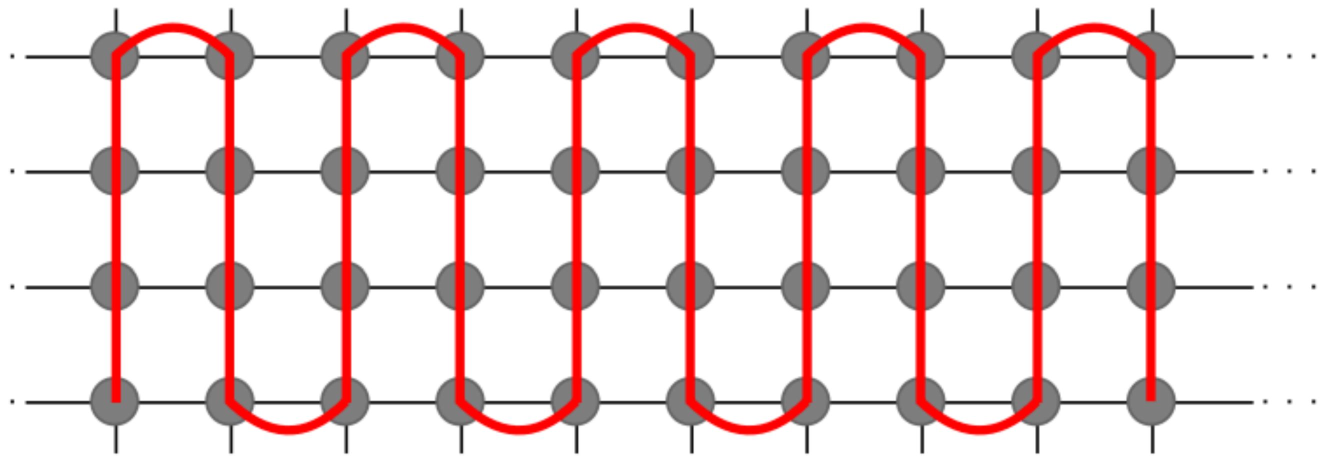
- *cTPQ method is randomized, i.e. results differ slightly for each shot, but the peak&shoulder structure is stable.

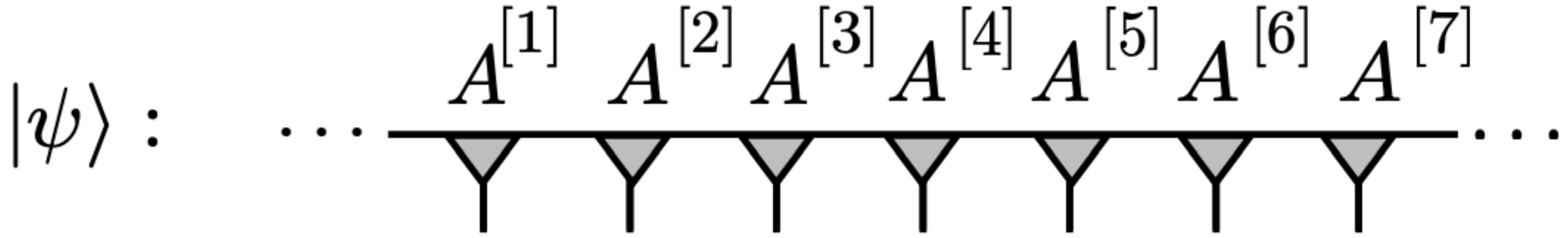
Ground-state properties (DMRG simulation)

2D DMRG
Cylinder geometry

- In 2D, we use the cylinder geometry.
- The cost grows rapidly about Ly.
- Finally, we extrapolate over Ly.







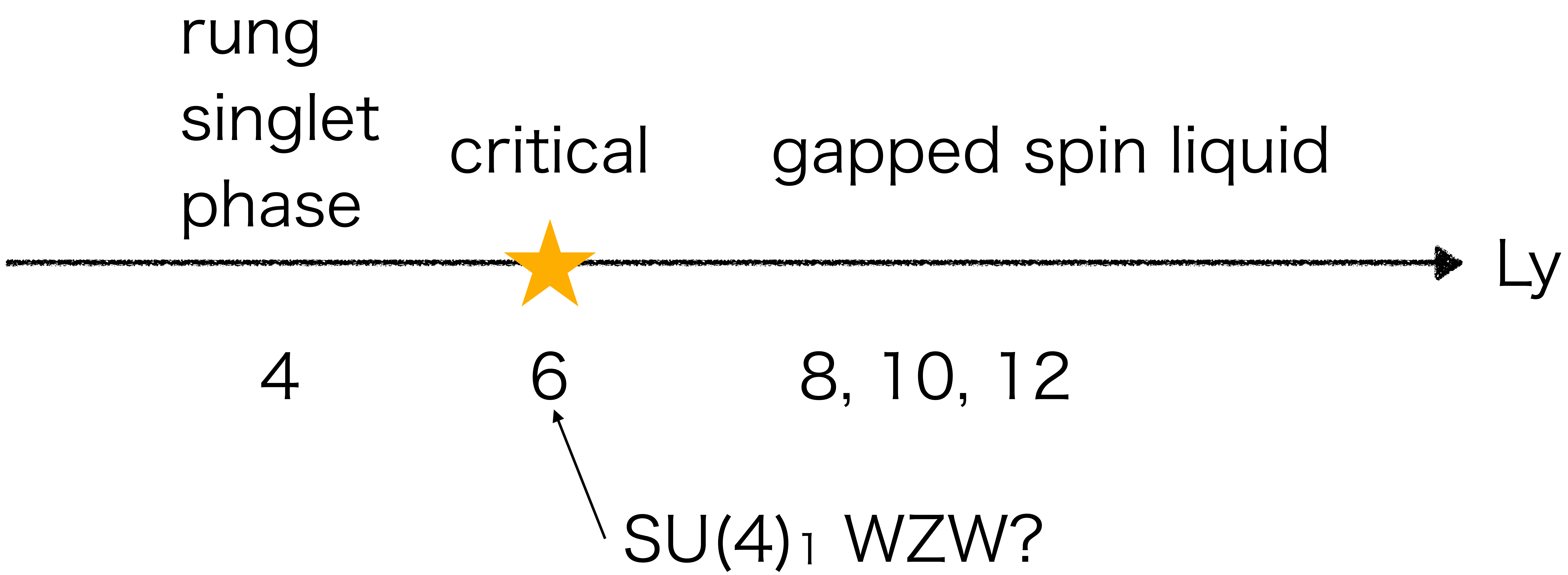
http://quantumtensor.pks.mpg.de/wp-content/uploads/2016/06/slides_1.pdf

Calculation details

- Fully exploiting the SU(4) symmetry (New!).
- Calculation on Intel Xeon Gold 6238R x 2 + NVIDIA A100 (40GB) x 2.
- 384GB main memory & 8TB working SSD with RAID0, allowing the calculation up to 400 sites. This spec is actually overkill.
- Keeping up to m = 12800 SU(4) states equivalent to more than a million U(1) states. Truncation error down to $<10^{-5}$ (Ly = 12).
- Keeping M = 220 irreducible representations of SU(4).

Observation

- Phase diagram for Ly:



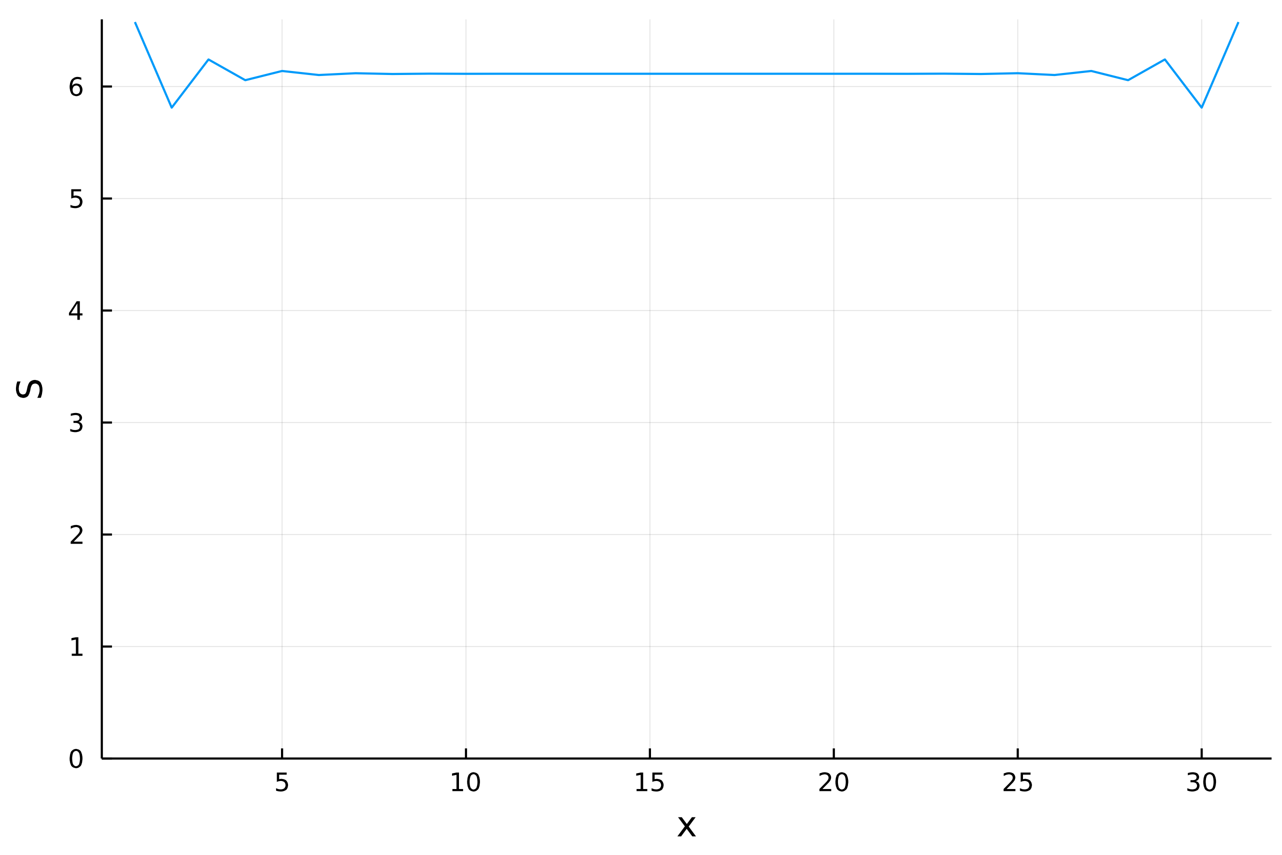
- Somehow it gets critical when Ly=6.

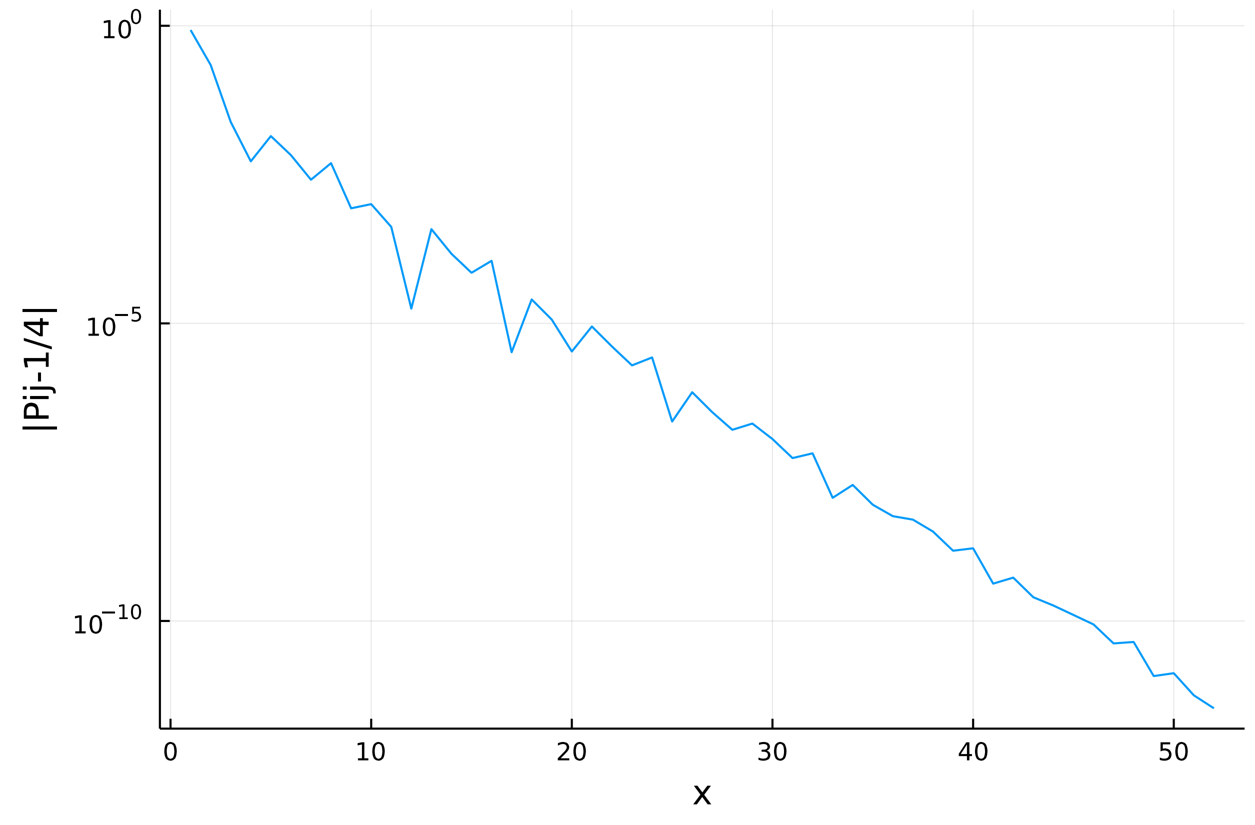
Ly = 12 (gapped spin liquid)

Gapped state
Ly=12 case

m=12800
M=220 for SU(4)

- In order to check a gap, we checked the entanglement entropy and the spin correlation for the 32x12 cylinder.
- It is gapped because the entanglement entropy is constant.
- It is gapped because the correlation decays exponentially.
- We already saw the signature of gapped SL.



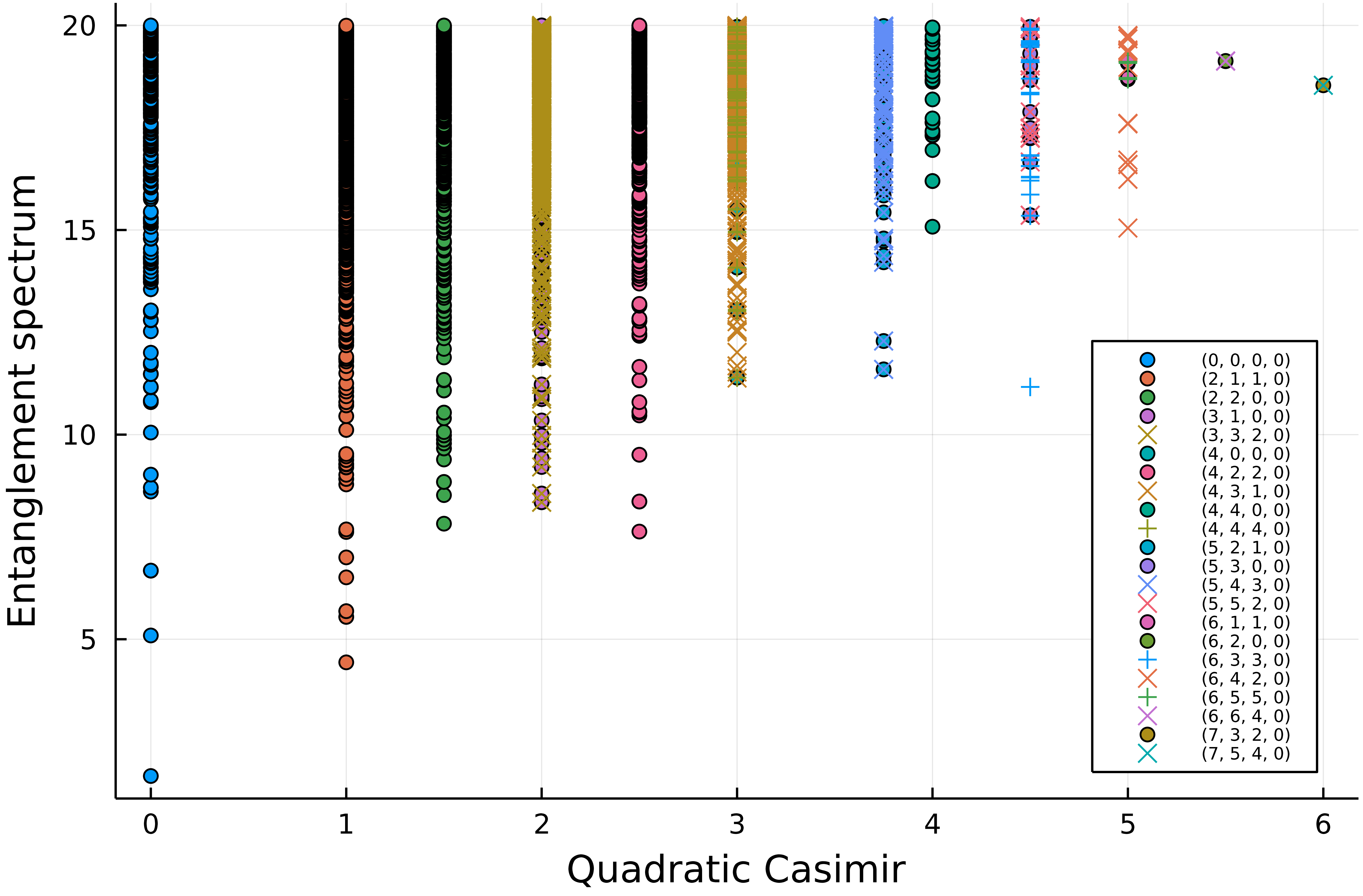


Entanglement spectroscopy

Absence of Anderson’s tower of states

m=12800
M=**220** for SU(4)

- We also checked the entanglement spectrum for the 32x12 cylinder.
- SU(4) symmetry is not broken.

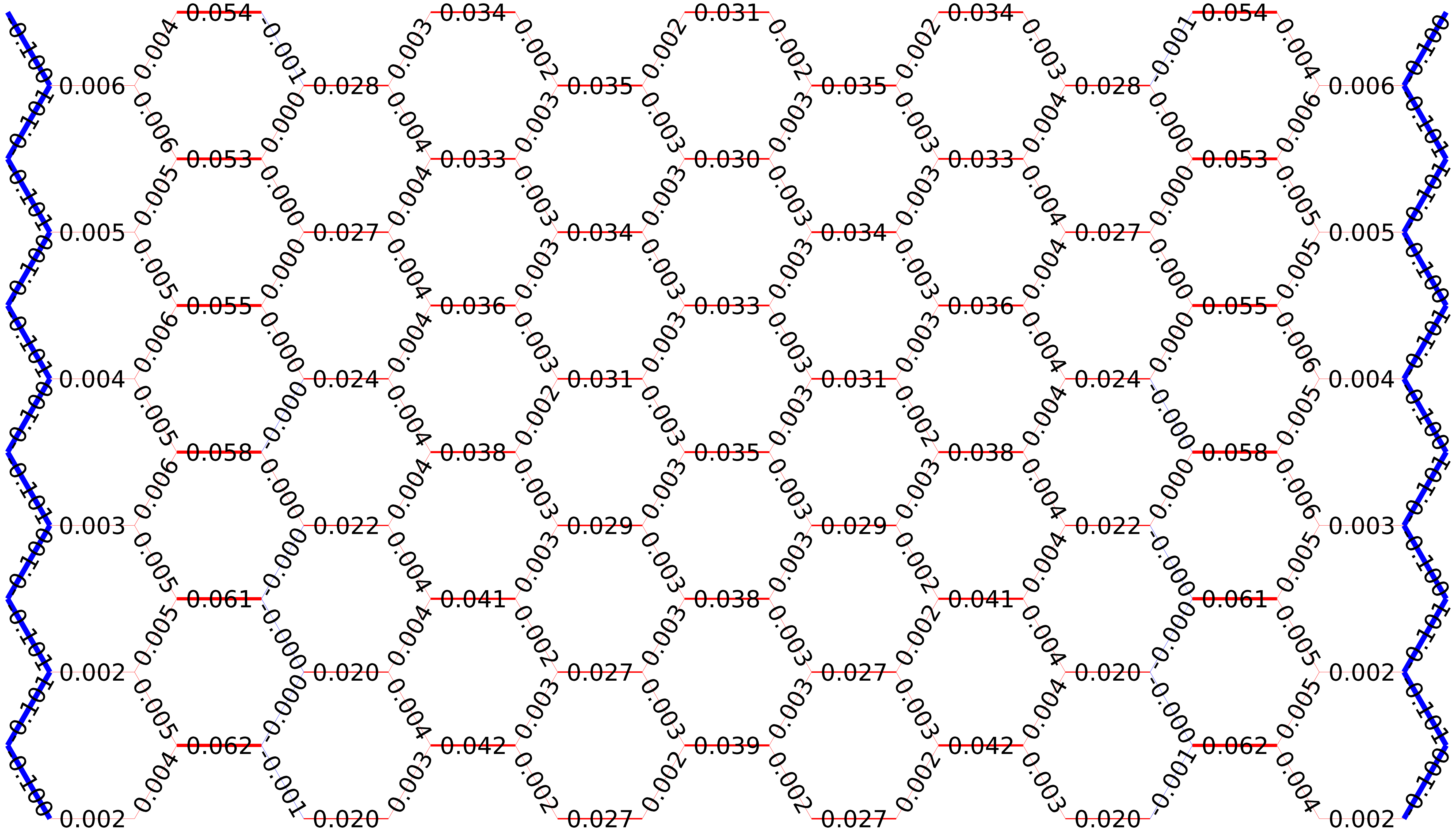


Absence of tetramerization

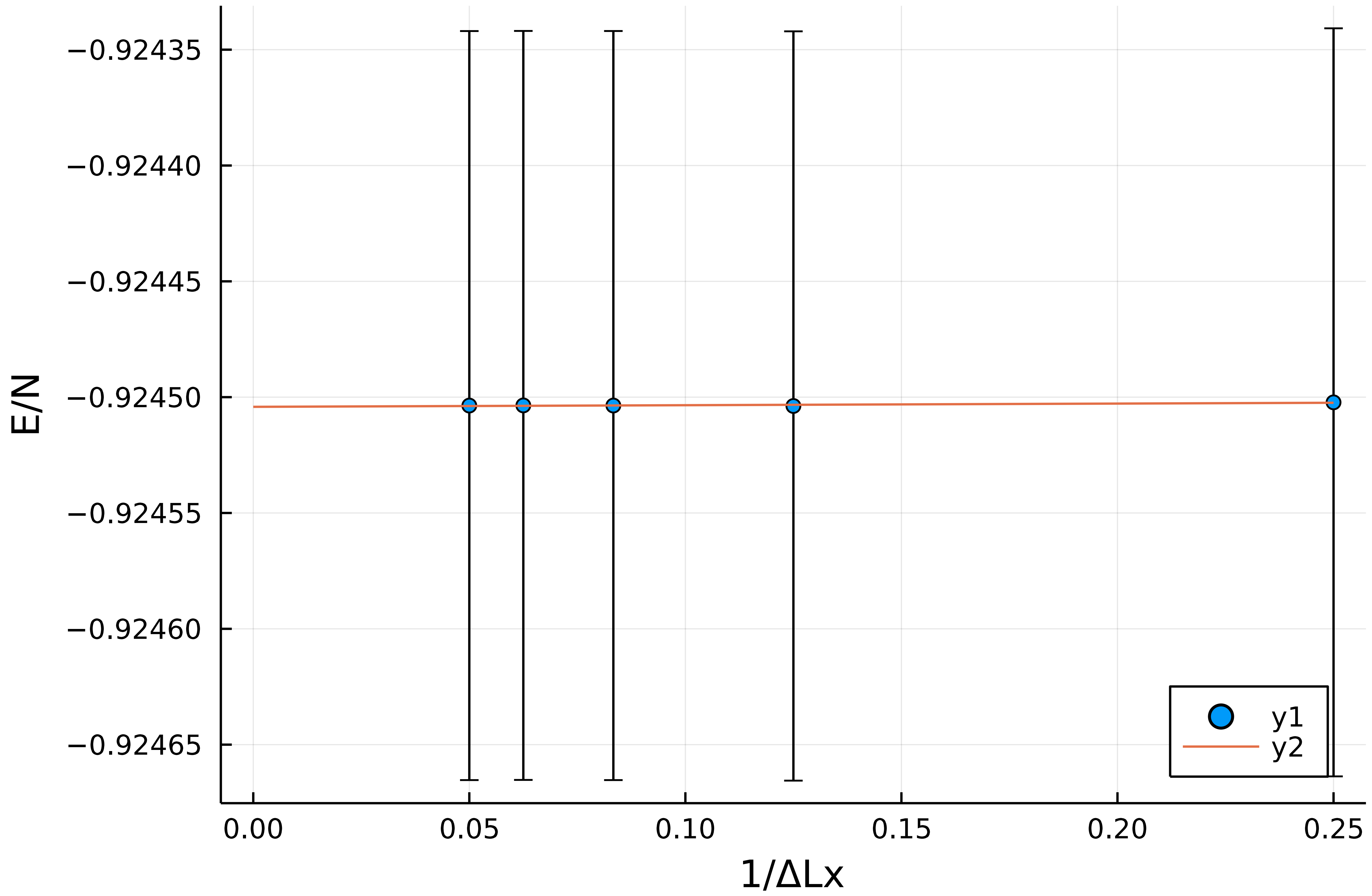
Expectation values of bond operators

m=12800
M=**220** for SU(4)

- Plot of P_{ij}-<P_{ij}>:
- 12x12 cylinder
- The rung singlet state is suppressed more.

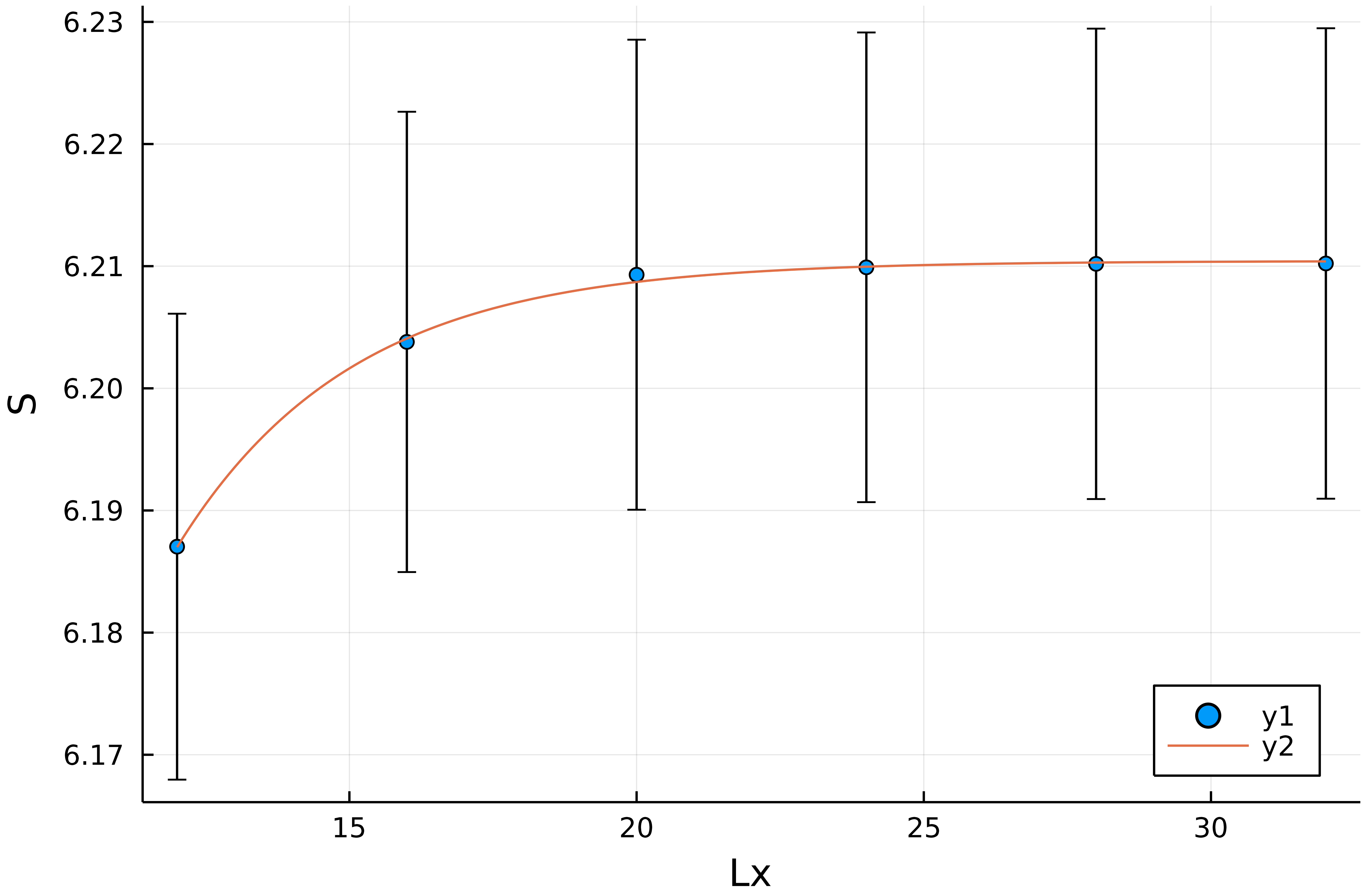


Ground state energy



- E(Ly=12)/N = -0.9245(1)

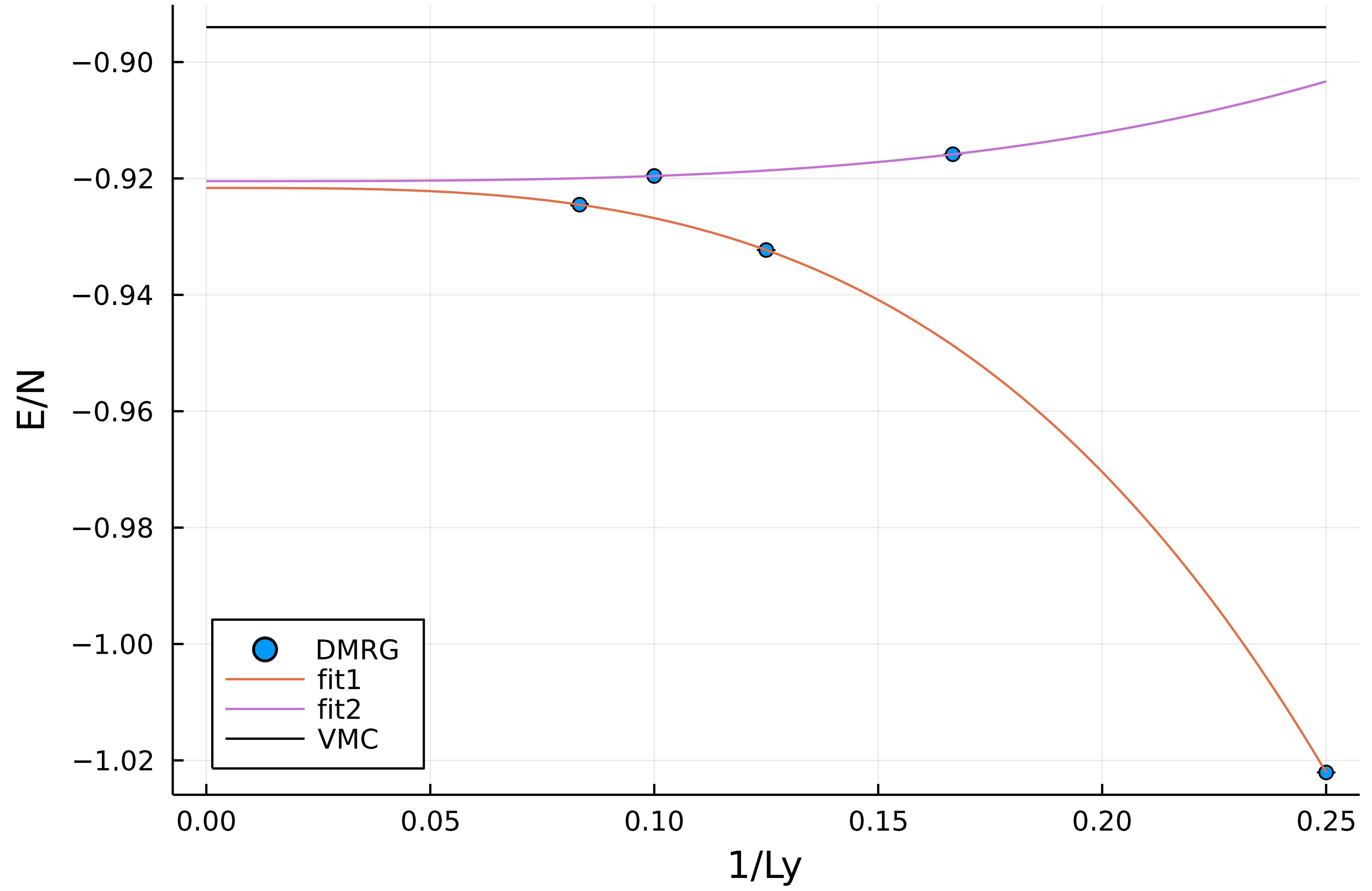
Entanglement entropy



- S(Ly=12) = 6.21(1)
- Exponential fit.

Energy comparison

- By power-law (p ~ 3.235) fitting E/N = -0.9210(6)



- It is much lower than that of the previous work (VMC) E/N=-0.894, so the Dirac SL observed in the previous work may not be a true g.s.

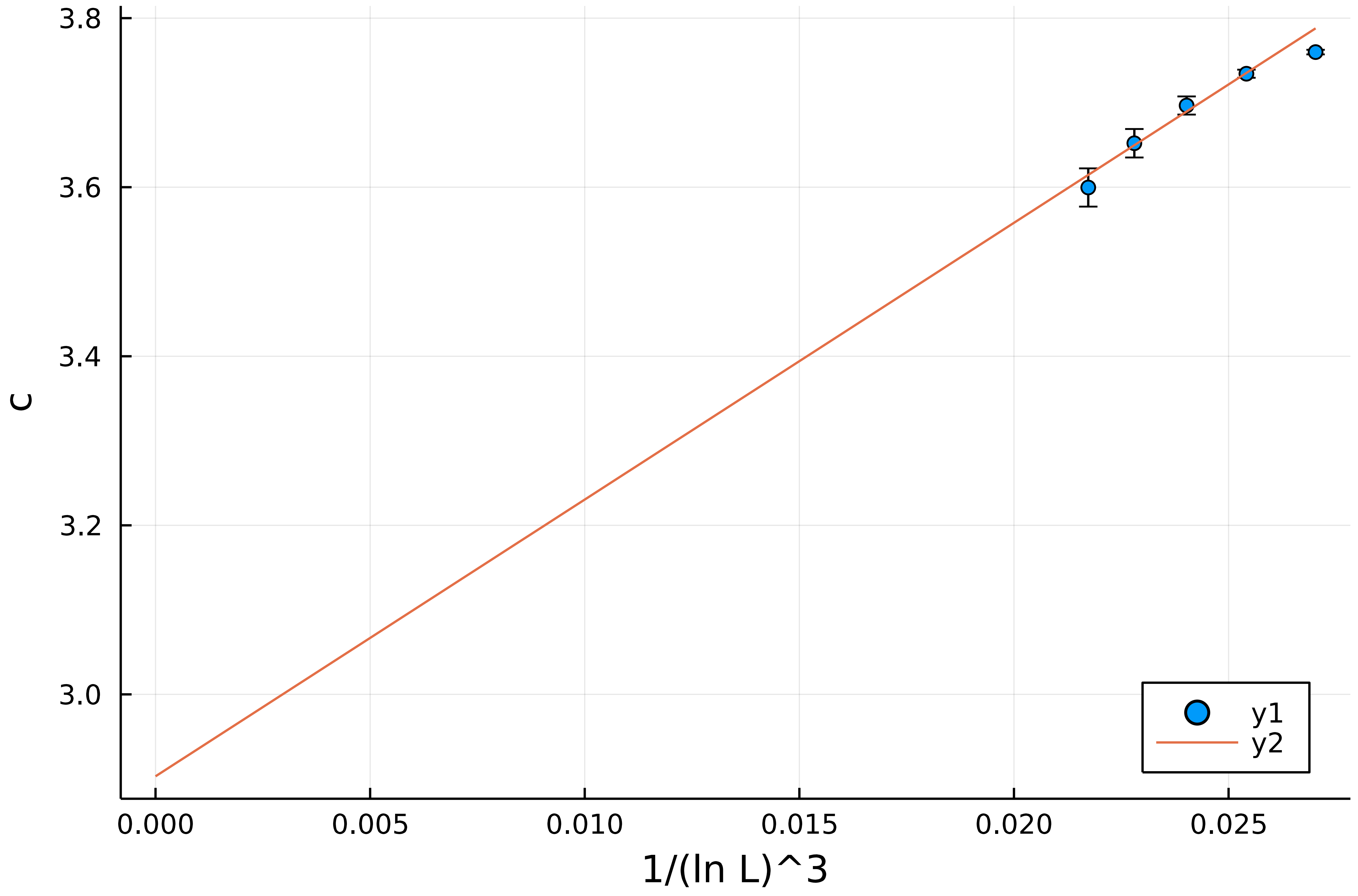
[Supplementary] Central charge

Ly=6 seems to have $SU(4)_1$ Wess-Zumino-Witten criticality

- From the fitting of the 28x6 to 36x6 central charge, we get the central charge for the infinite cylinder: c = 2.90(11)

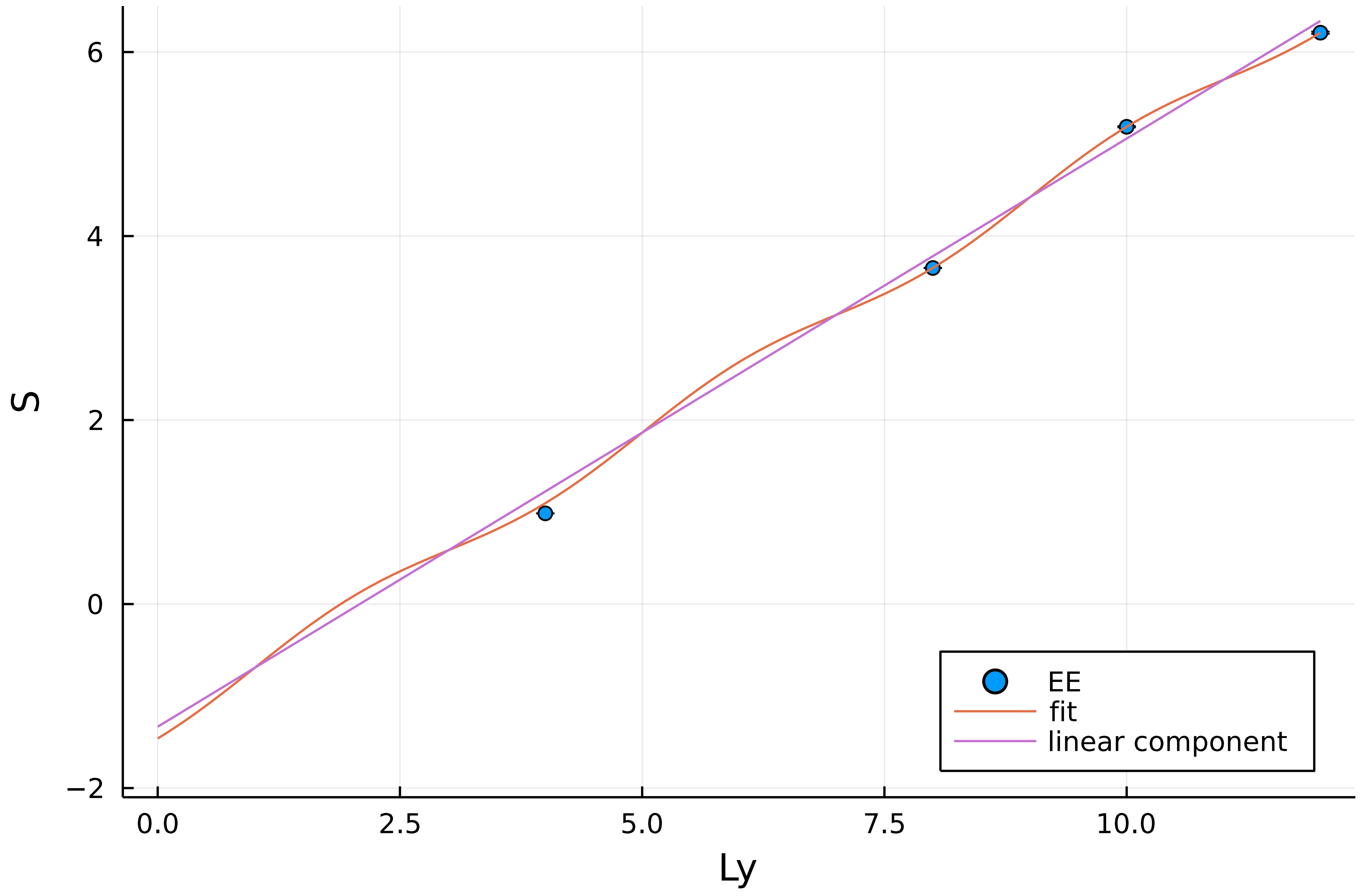
- Consistent with $SU(4)_1$ WZW.

- The finite size scaling follows
  T. Ziman and H. J. Schulz PRL 59, 140 (1987).



Topological entanglement entropy

$$S = a + bL_y + c\cos\left(\frac{\pi}{2}L_y\right)$$



- γ =-a=1.33(3)
- close to ln(4) = 1.3862943611198906 ?

Summary

- SU(4) physics contains:
  - Nice candidate materials, as well as cold atom realization.
  - Very nice ground-state properties.
  - New route towards quantum spin liquids.
- About the realization:
  - Collaboration with experimentalists has just begun.