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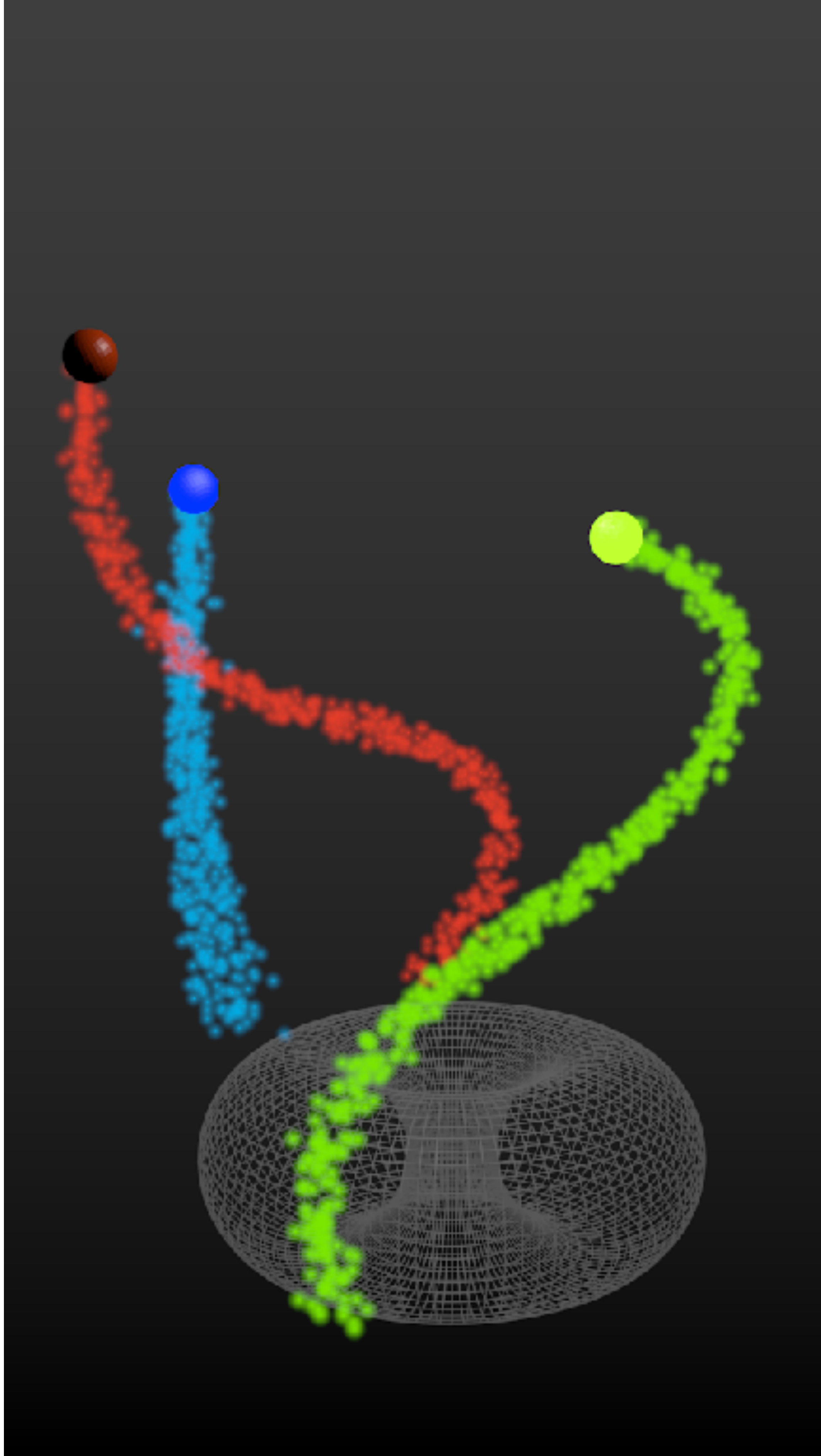
NUMERICAL IDENTIFICATION OF QUANTUM SPIN LIQUIDS

Alexander Wietek
University of Innsbruck
TopMat Workshop, IPhT Paris-Saclay
27/6/2018



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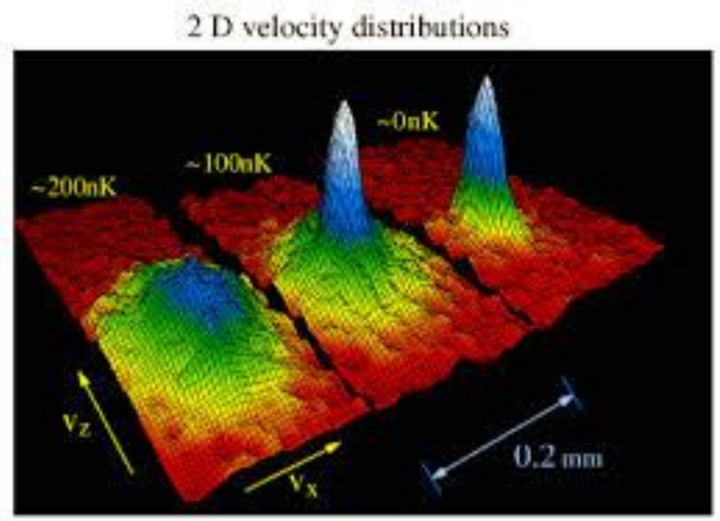
Andreas M. Läuchli

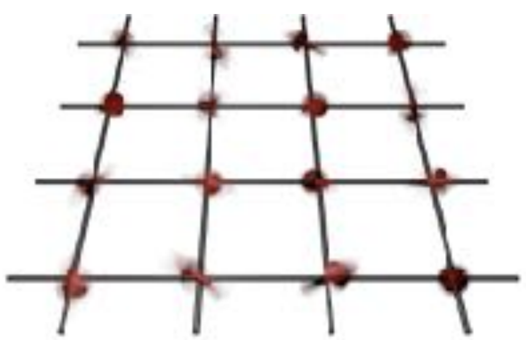
Antoine Sterdyniak

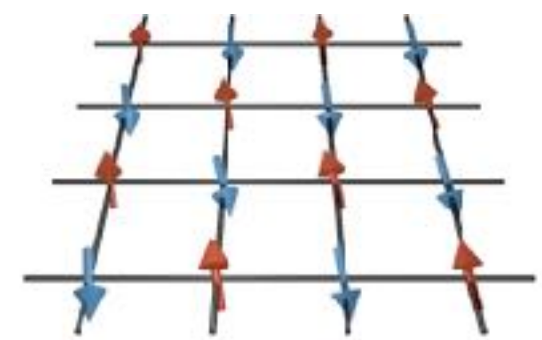
PHASES OF MATTER

High symmetry

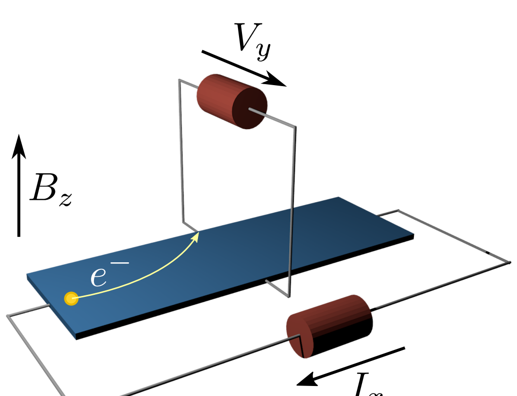
Lower symmetry

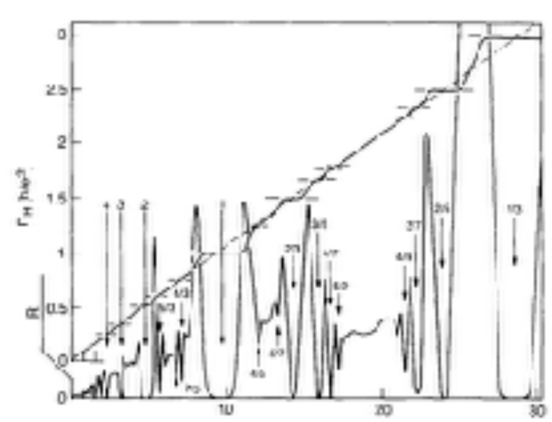


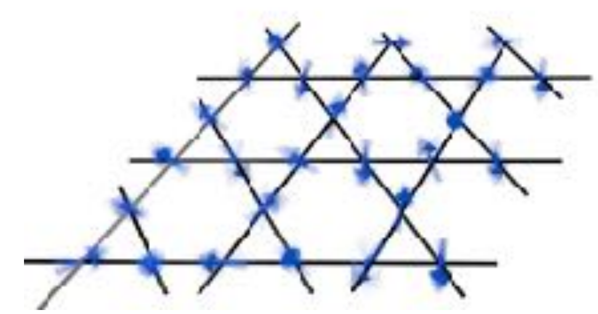




„Higher“ symmetry





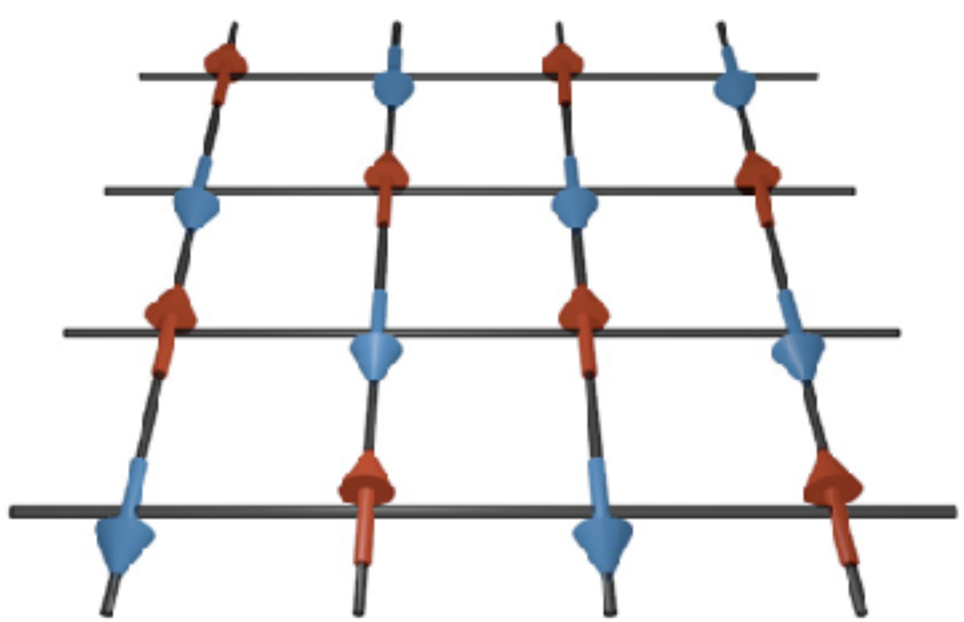


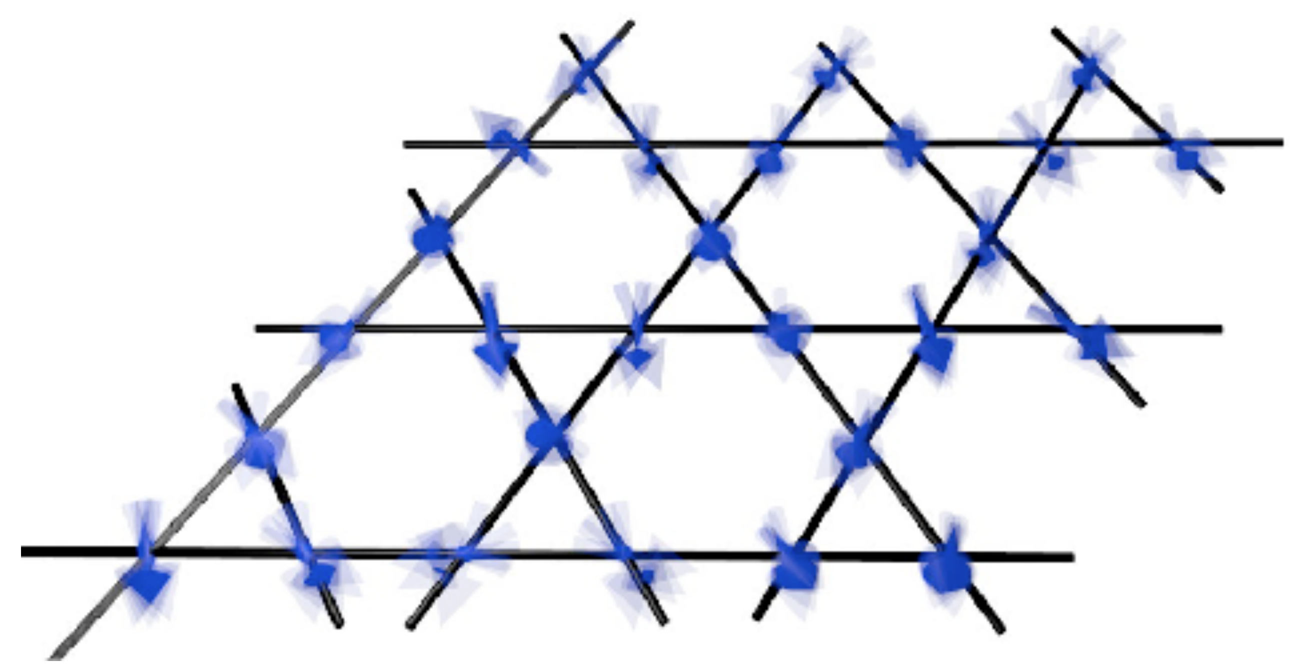
NOVEL STATES OF MATTER IN FRUSTRATED MAGNETISM

- Study of low-dimensional quantum spin models

$$H = \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j ,$$

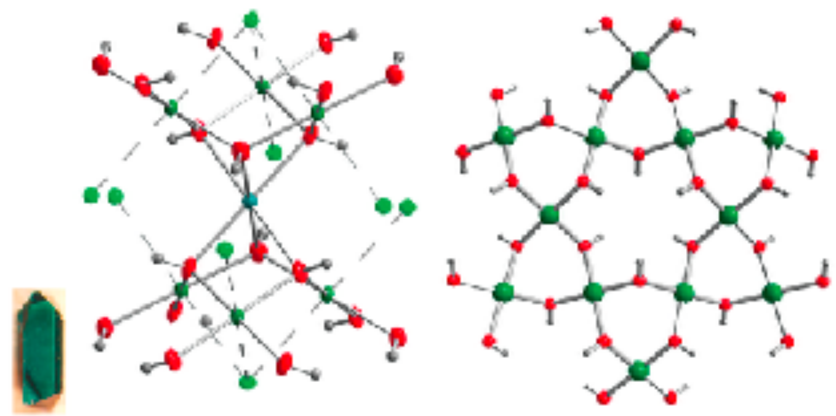
- Complex behavior if local energy constraints cannot be minimized simultaneously

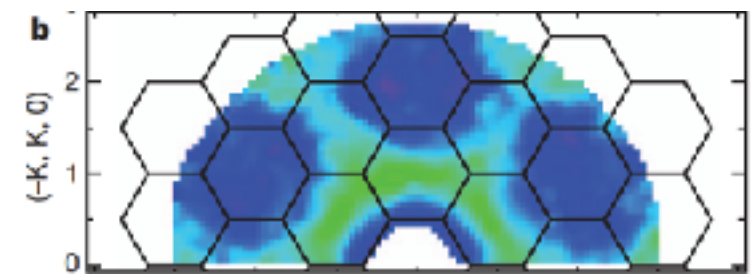




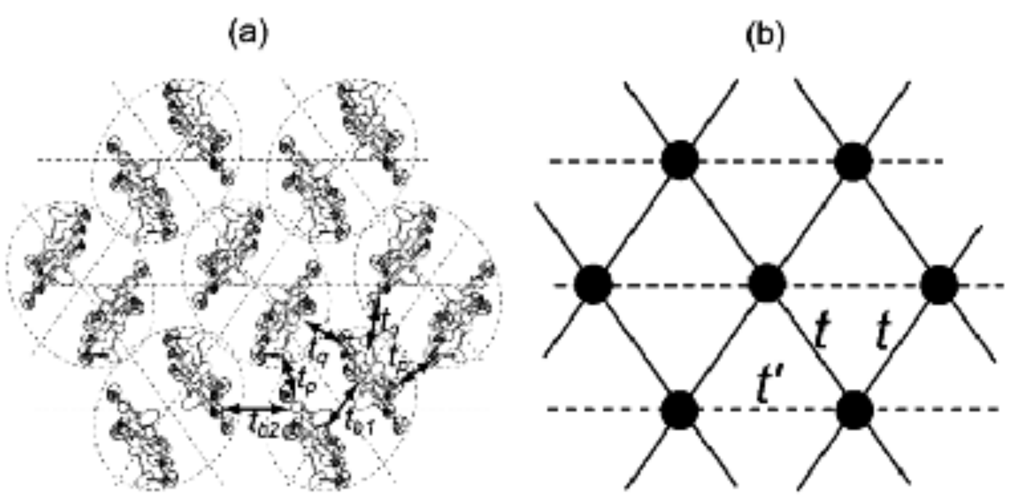
NOVEL STATES OF MATTER IN FRUSTRATED MAGNETISM

- Various experimental systems



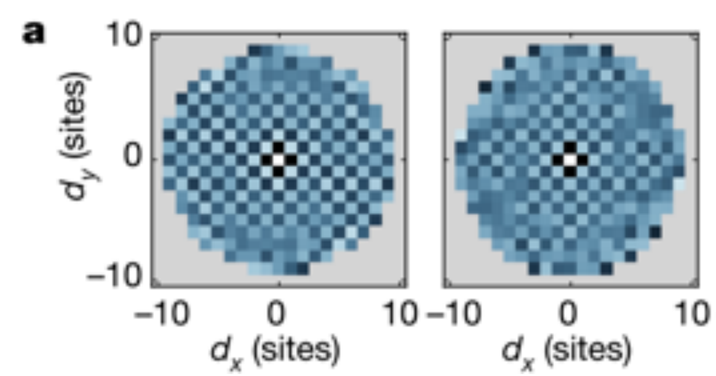


[Han et al. Nature (2012) 11659]



$\kappa-(\mathrm{BEDT-TTF})_2\mathrm{Cu}_2(\mathrm{CN})_3$

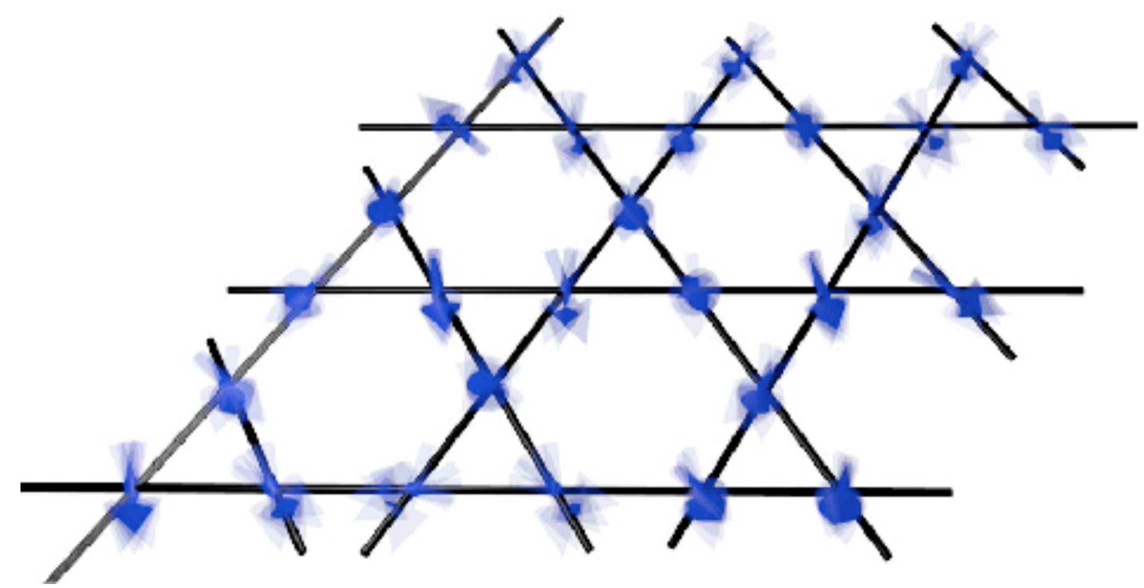
[Shimizu et al, Phys. Rev. Lett (2003)]



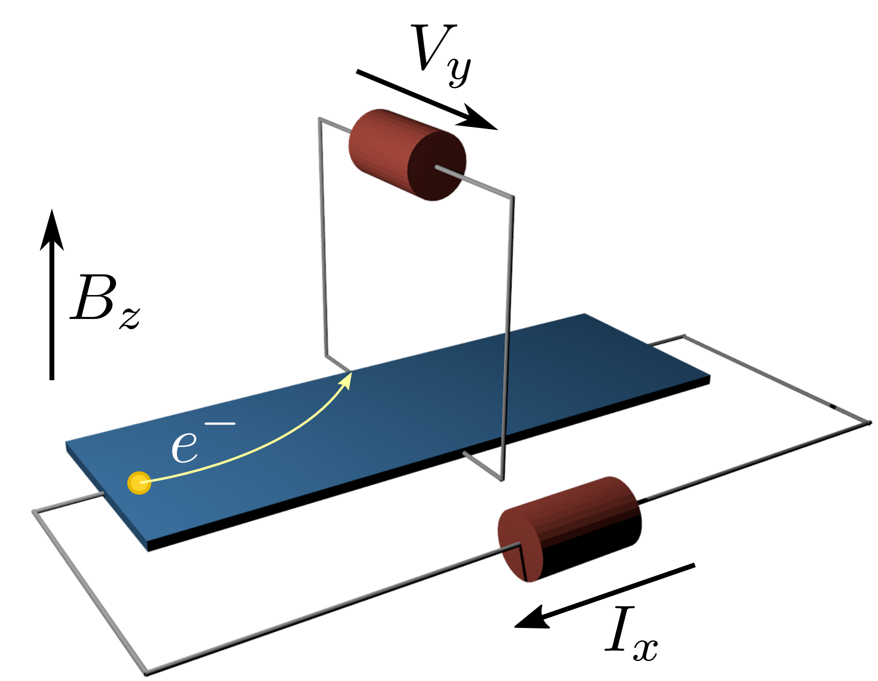
[Mazurenko et al., Nature 545, 462–466 (2017)]

NOVEL STATES OF MATTER IN FRUSTRATED MAGNETISM

- Ordering is suppressed by low dimension, quantum fluctuations and frustration
- Exotic non-trivial paramagnetic phases can emerge
  Quantum Spin Liquids
- Confinement / deconfinement of emergent quasiparticles
- e.g. Z_2 spin liquids, Dirac spin liquids
- Chiral spin liquids
  spin version of fractional quantum Hall effect



QUANTUM HALL EFFECTS



- At low temperatures and high magnetic fields several plateaux appear in the Hall resistivity

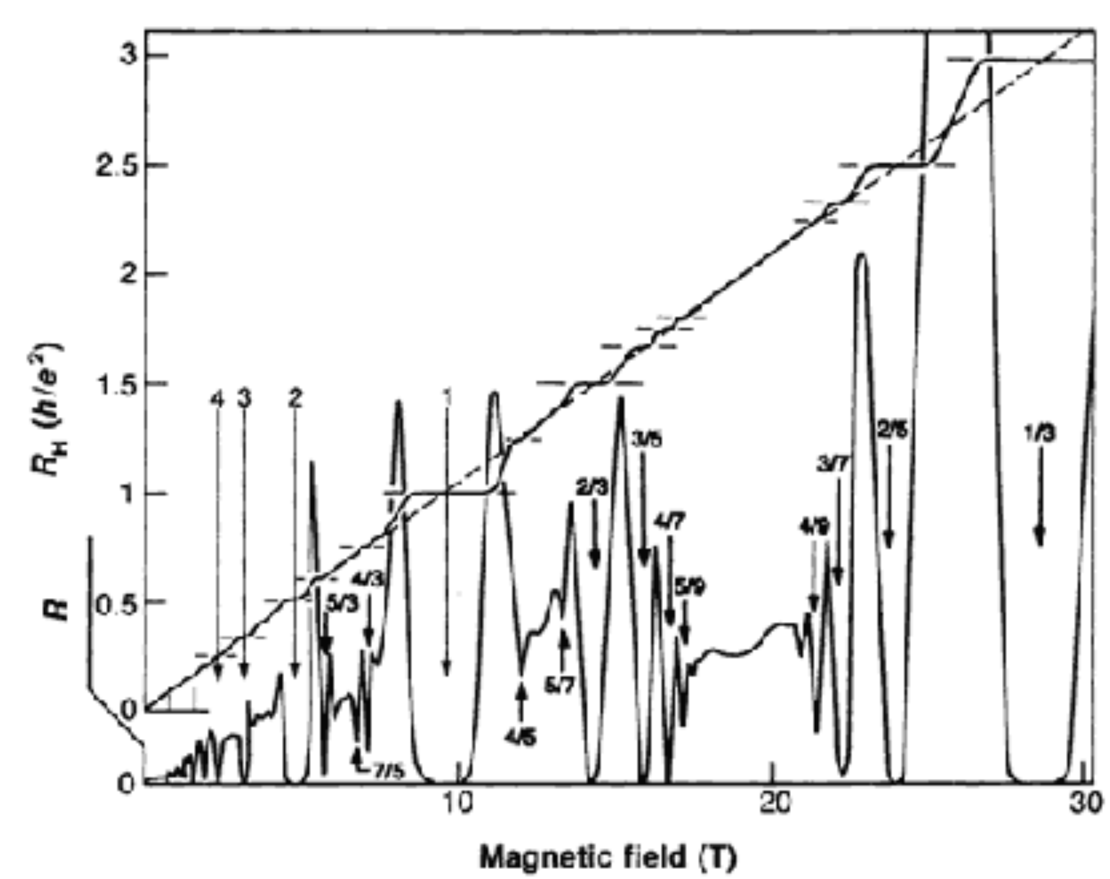
$$R_H \equiv \frac{V_y}{I_x} \qquad\qquad R_H = \frac{1}{\nu}\frac{h}{e^2}$$

- $\nu = 1, 2, \ldots$ -> integer QHE
- $\nu = \frac{1}{3}, \frac{2}{5} \ldots$ -> fractional QHE

- Pure quantum mechanical effect

[Klitzing, Dorda, Pepper, Phys. Rev. Lett. 45, 494 (1980)]

[Tsui, Stormer, Gossard. Phys. Rev. Lett. 48.22 (1982)]



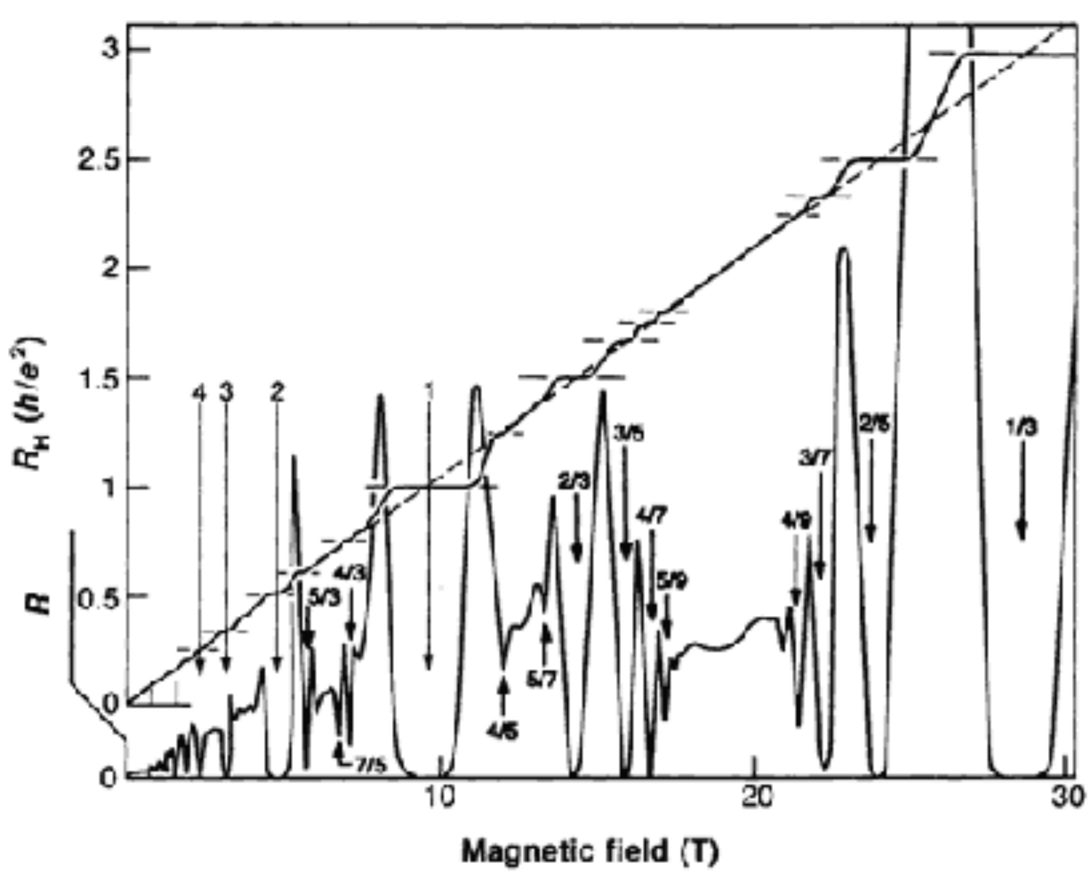
FRACTIONAL QUANTUM HALL EFFECT

- Strongly interacting electrons in 2D limit at low temperatures, high magnetic fields and pure samples
- ground state at filling fractions $\nu = 1/(2p+1)$ described by Laughlin wave function

$$\psi_p(z_1, \ldots, z_n) = \prod_{i<j} (z_i - z_j)^{2p+1} \prod_k e^{-|z_k|^2}$$

[R. B. Laughlin, Phys. Rev. Lett. 50, 1395 (1983)]

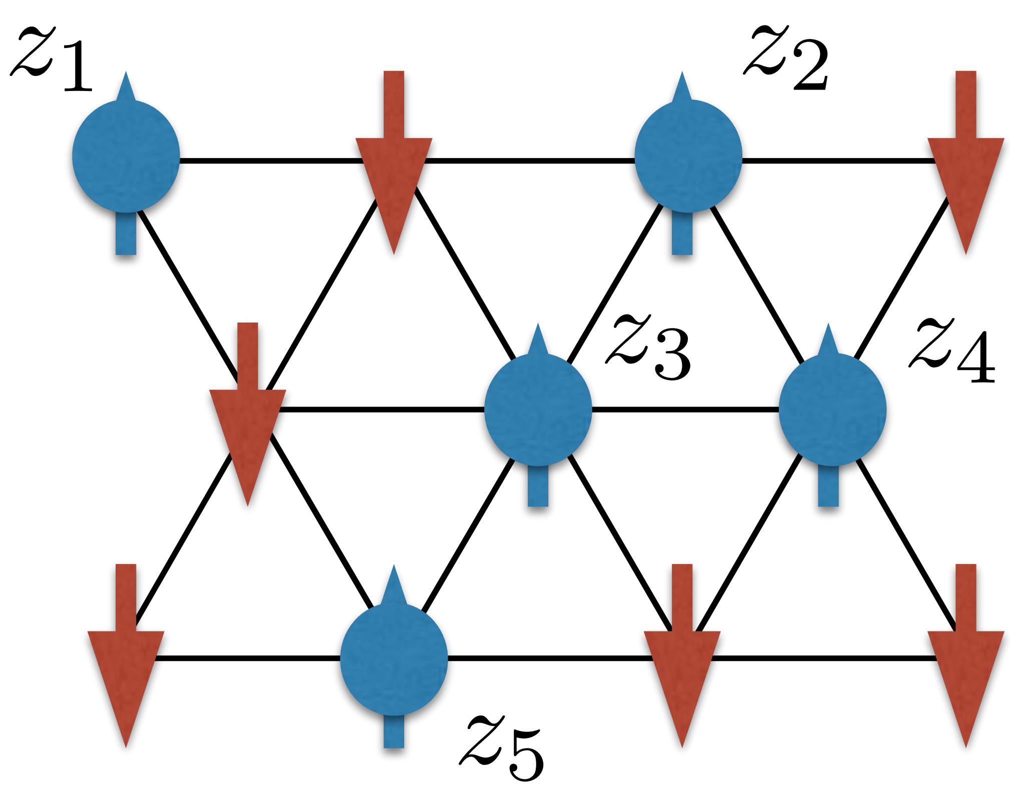
- phase transitions between different filling fractions without breaking a symmetry



CHIRAL SPIN LIQUIDS

[V. Kalmeyer, R.B. Laughlin, Phys. Rev. Lett. 59 (1987)]

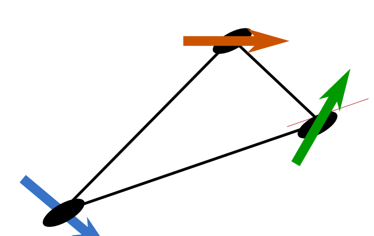
- translate fractional QHE physics for spins
- mapping continuum wave function for bosonic $\nu = 1/2$ Laughlin state to hard-core bosons (i.e. spins) on a lattice

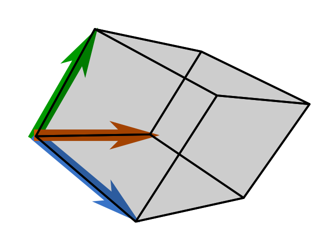


$$\Psi_{2,N}(z_1,\ldots,z_N) = \prod_{j<k}(z_j - z_k)^2 \prod_k \mathrm{e}^{-\frac{1}{4l_0^2}|z_k|^2}$$

- Spin singlet state, time-reversal and reflection symmetry broken

$$\mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)$$





CHIRAL SPIN LIQUIDS

[X.G. Wen, F. Wilczek, A. Zee, Phys. Rev. B 39 (1989)]

- Consider a generic spin Hamiltonian

$$H = \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j ,$$

- Introduce fermionic parton operators

$$\mathbf{S}_i = \frac{1}{2} c^\dagger_{i\alpha} \sigma_{\alpha\beta} c_{i\beta}$$

- Equivalent fermionic model with local gauge symmetry $c^\dagger_{i\alpha} \to e^{i\theta_i} c^\dagger_{i\alpha}$

$$H_{\text{parton}} = -\frac{1}{2} \sum_{i,j,\alpha,\beta} J_{ij} c^\dagger_{i\alpha} c_{j\alpha} c^\dagger_{j\beta} c_{i\beta}$$

if subject to single-particle per site constraint: $c^\dagger_{i\uparrow} c_{i\uparrow} + c^\dagger_{i\downarrow} c_{i\downarrow} = 1$

- Introduce mean-field decoupling

$$\chi_{ij} \equiv c^\dagger_{i\alpha} c_{j\alpha} \to \chi_{ij} = \langle c^\dagger_{i\alpha} c_{j\alpha} \rangle$$

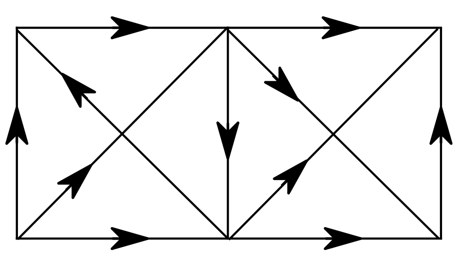
CHIRAL SPIN LIQUIDS

[X.G. Wen, F. Wilczek, A. Zee, Phys. Rev. B 39 (1989)]

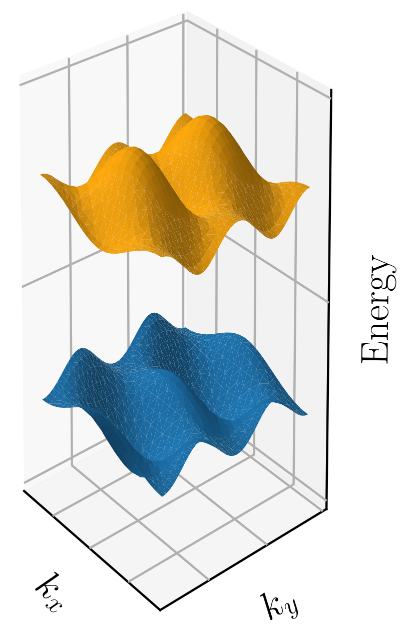
- Mean-field parton Hamiltonian

$$H_{\text{mean}} = \sum_{i,j,\alpha} (\chi_{ij} c^\dagger_{i\alpha} c_{j\alpha} + \text{H.c.}) + \sum_i \mu_i (n_i - 1)$$

- Choose ansatz $\chi_{ij} = \bar{\chi}_{ij} e^{i a_{ij}}$ such that band structure has Chern bands



$\chi_{i\to j} = e^{i\pi/2}$



- Taking continuum limit and integrating out partons gives effective action for gauge fields: Chern-Simons field theory

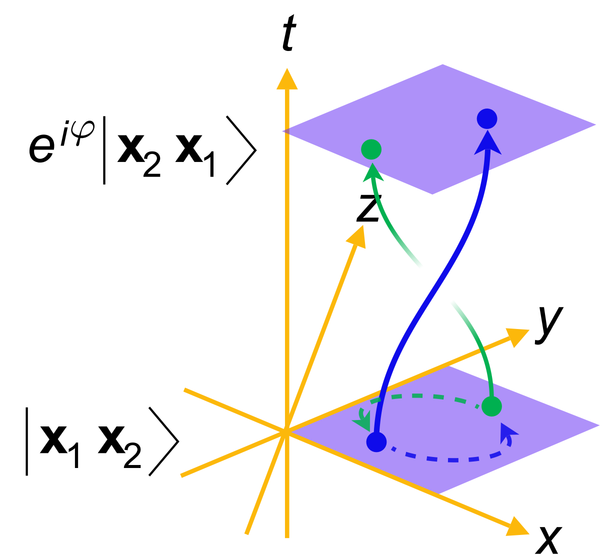
$$S = \int \mathrm{d}^3 x \frac{1}{2} \sigma_{xy} a_\mu \partial_\nu a_\lambda \epsilon_{\mu\nu\lambda} + \mathcal{O}(1/g^2), \quad \mu = 0, 1, 2$$

CHIRAL SPIN LIQUIDS

[X.G. Wen, F. Wilczek, A. Zee, Phys. Rev. B 39 (1989)]

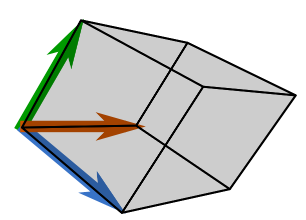
- Chern-Simons field theory

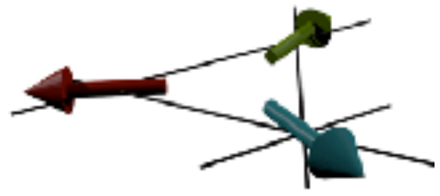
$$S = \int \mathrm{d}^3x \frac{1}{2} \sigma_{xy} a_\mu \partial_\nu a_\lambda \epsilon_{\mu\nu\lambda} + \mathcal{O}(1/g^2), \quad \mu = 0, 1, 2$$



- Non-zero (spin) Hall conductivity
- gapless chiral edge modes
- semionic statistics (exchange phase $\pi/2$)
- twofold degenerate ground state with periodic boundary
- time-reversal and reflection symmetry broken
- Proposed as ground state of triangular lattice Heisenberg antiferromagnet, that is actually 120° ordered

$\mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)$





[Bernu et al., Phys Rev B, 50, 10048 (1994)]

NUMERICAL IDENTIFICATION OF CHIRAL SPIN LIQUIDS

THE QUEST FOR THE CHIRAL SPIN LIQUID

- The Chiral Spin Liquid was proposed end of the 80s
- Is there any model realizing this phase?
- Analytically solvable models proposed by

  [D. F. Schroeter, E. Kapit, R. Thomale, M. Greiter, Phys. Rev. Lett. 99, 097202 **(2007)**]

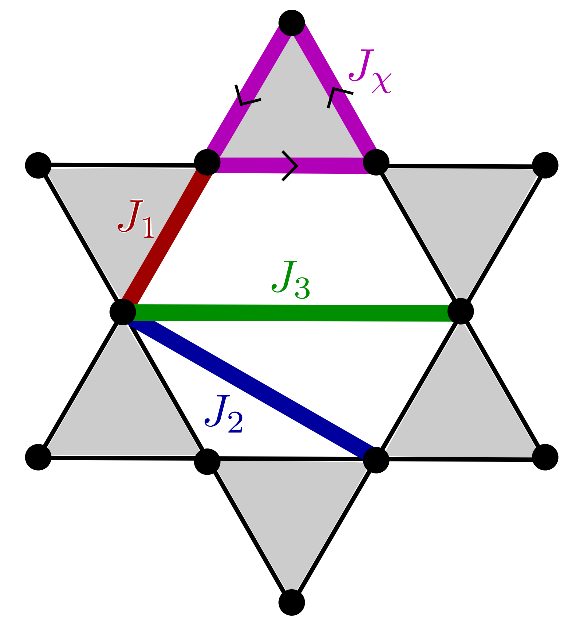
  [A. Nielsen, J. Cirac, and G. Sierra, Nature Commun. 4,2864 **(2013)**]

- Long-range, many spin interactions, barely experimentally relevant
- Hints for emergence in simpler models given by

  [Laura Messio, Bernard Bernu, and Claire Lhuillier, Phys. Rev. Lett. 108, 207204 **(2012)**]

NUMERICAL DISCOVERY OF EMERGENT CSL

- DMRG and Exact Diagonalization studies showed emergence of several CSL phases in various models
- Kagome lattice systems



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

[S. Gong, W. Zhu, D. N. Sheng, Nature *Sci. Rep.* 4, 6317 **(2014)**]

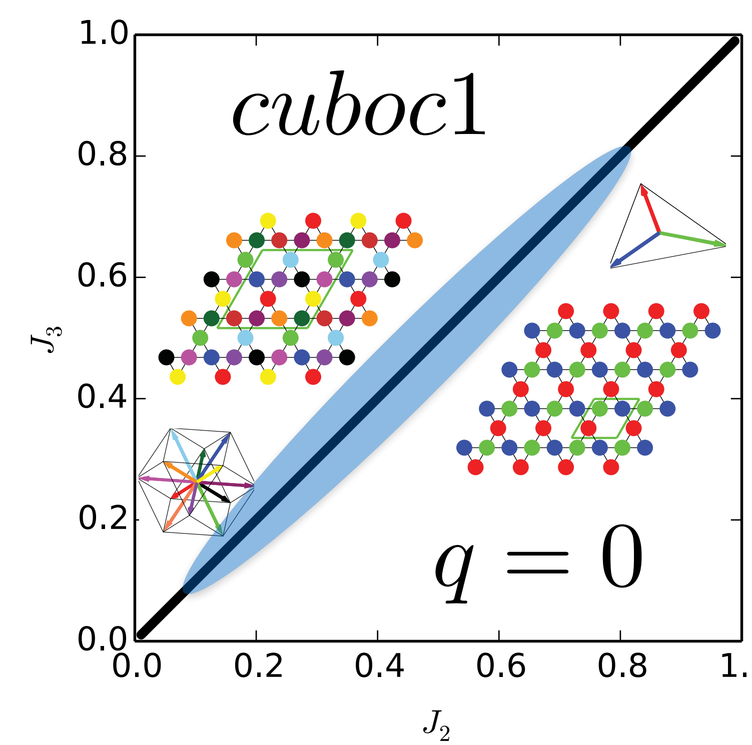
[Yin-Chen He, D. N. Sheng, and Yan Chen, Phys. Rev. Lett. 112, (2014)]

[A. Wietek, A. Sterdyniak, A. M. Läuchli, Phys. Rev. B 92, 125122 (2015)]

$$H = J_\chi \sum_{(i,j,k) \in \triangle} \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)$$

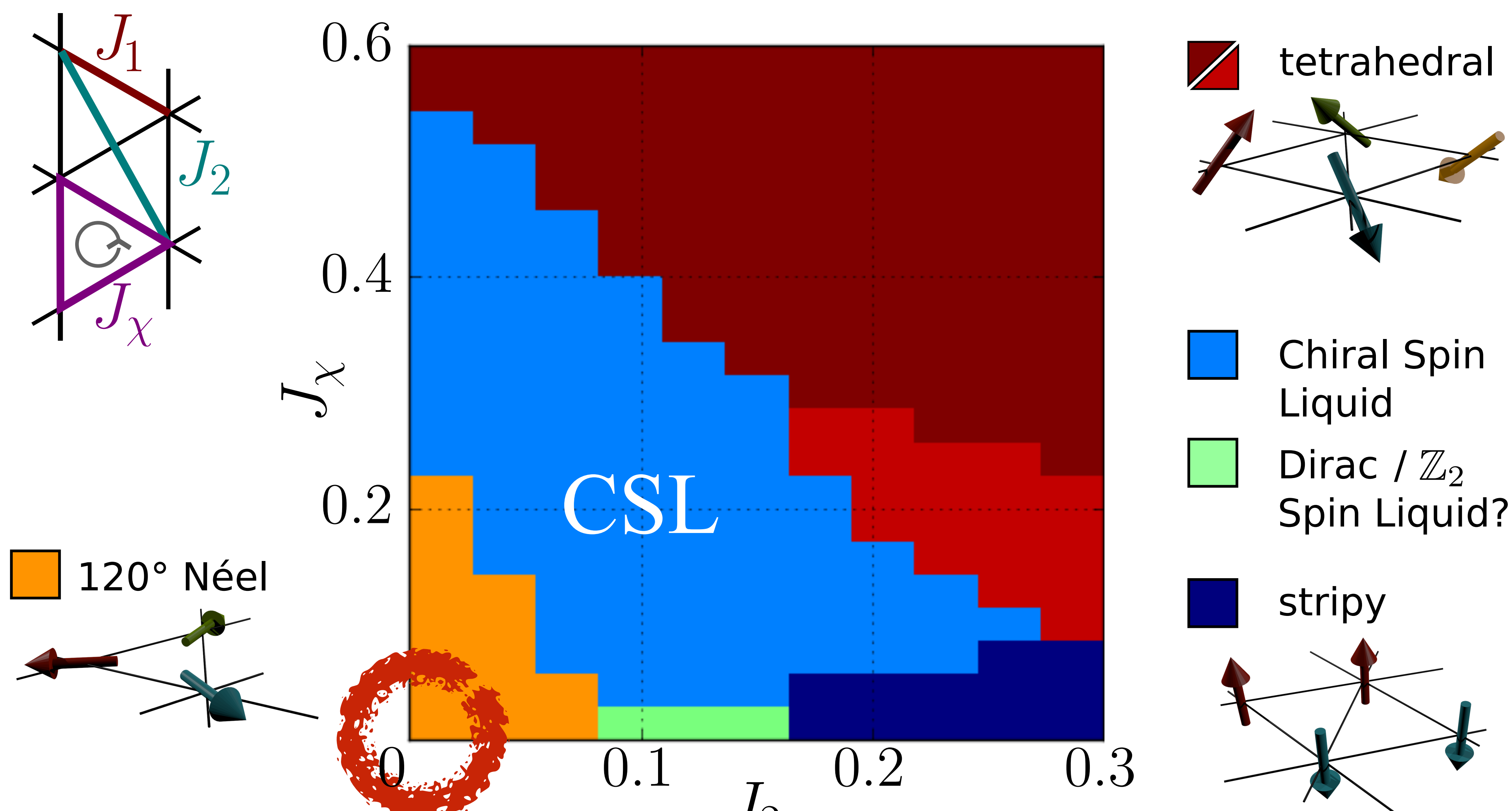
[B. Bauer et al., Nature *Comm.* 5, 5137 (2014)]

[A. Wietek, A. Sterdyniak, A. M. Läuchli, Phys. Rev. B 92, 125122 (2015)]



CHIRAL SPIN LIQUID ON THE TRIANGULAR LATTICE

[A. Wietek, A. M. Läuchli, Phys. Rev. B 95, 035141 (2017)]



[V. Kalmeyer, R.B. Laughlin (1987)]

$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_\chi \sum_{i,j,k \in \triangle} \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)$$

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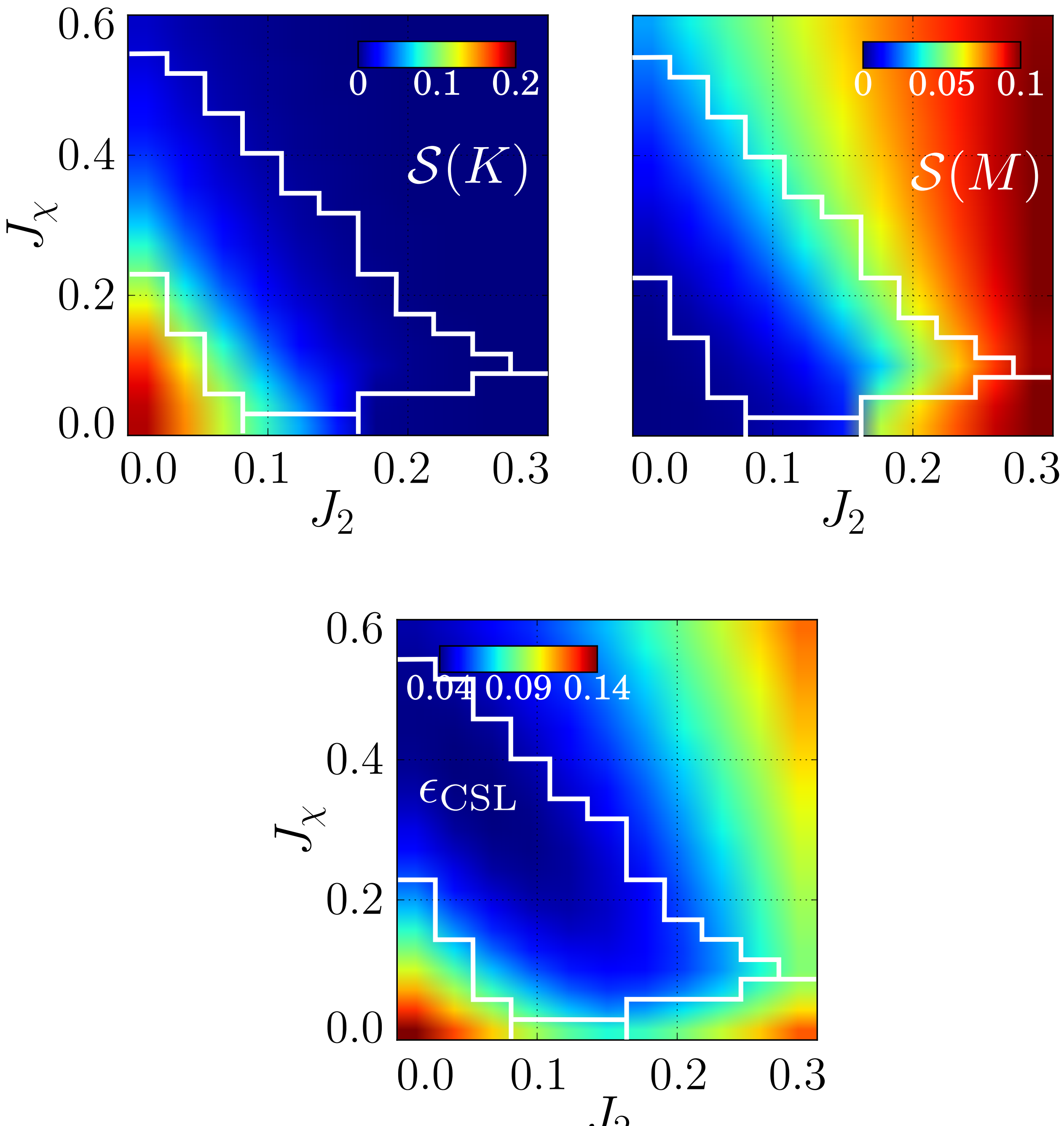
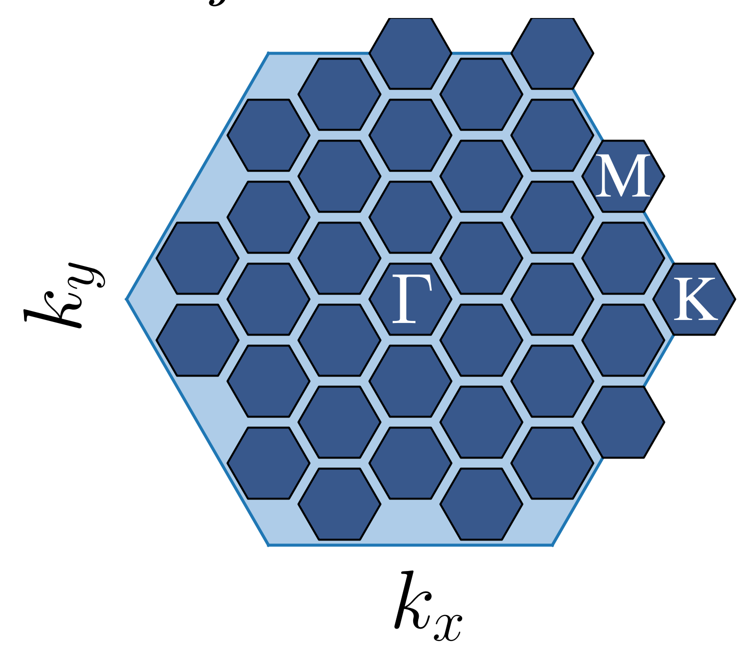
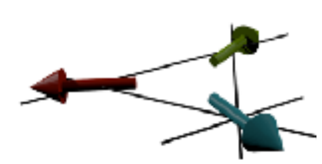


Spin structure factor

$$\mathcal{S}(q) = |\sum_j e^{iq(\mathbf{r}_j - \mathbf{r}_0)} \langle \mathbf{S}_j \cdot \mathbf{S}_0 \rangle|^2$$



$q = K:$



$q = M:$

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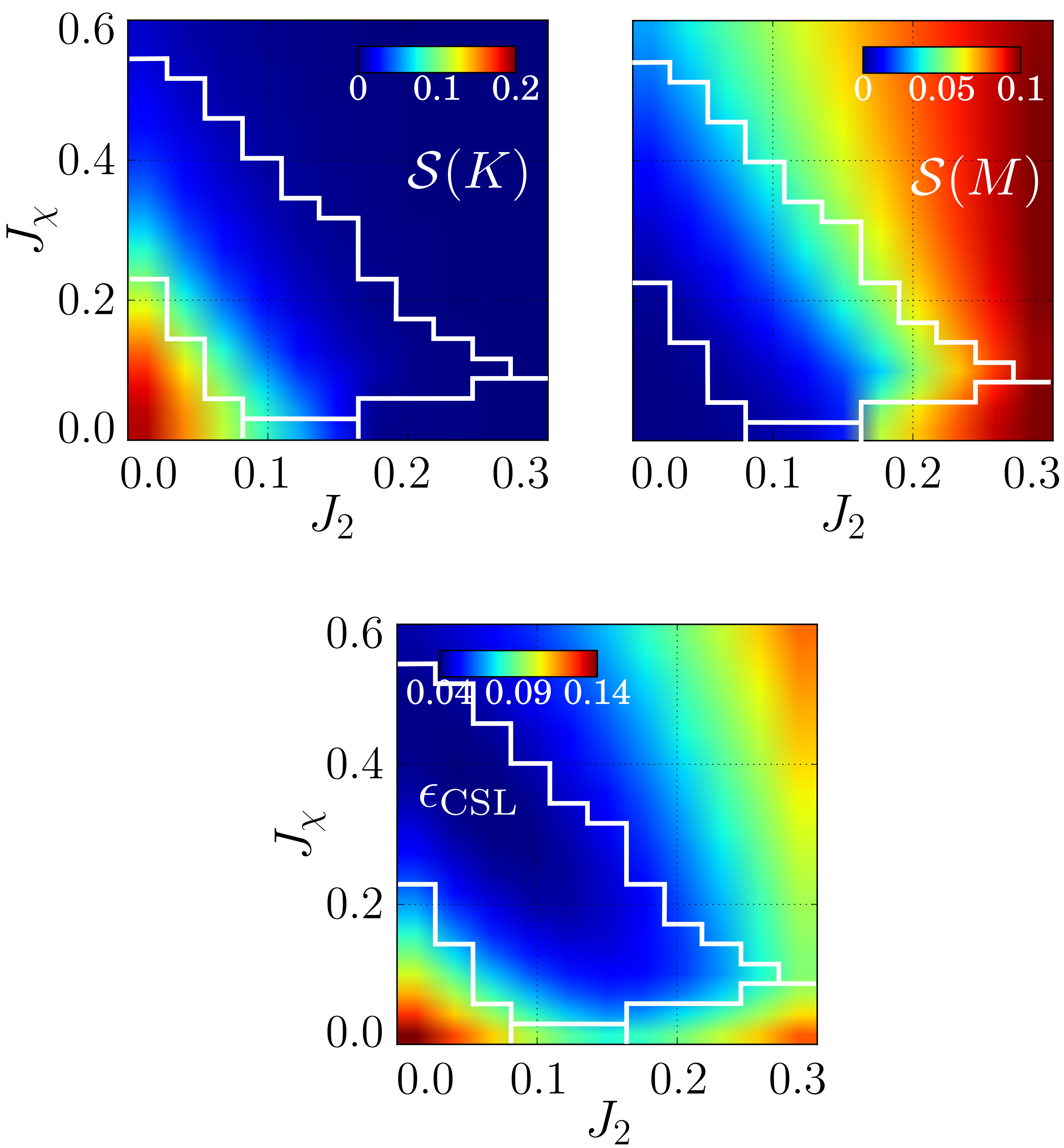
[A. Wietek, A. M. Läuchli, Phys. Rev. B 95, 035141 (2017)]



Energy of model CSL

$$\epsilon_{\mathrm{CSL}} = (E_{\mathrm{CSL}} - E_0)/E_0$$

- variational energy of model CSL wave function
- Gutzwiller projected w.f. similar to Laughlin w.f.
- low energy in the spin disordered region

GUTZWILLER PROJECTED CHIRAL SPIN LIQUIDS

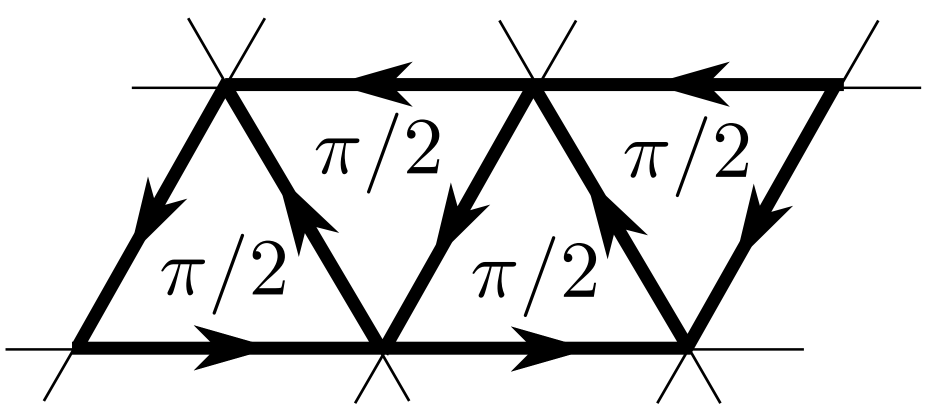
- Introduce fermionic parton operators

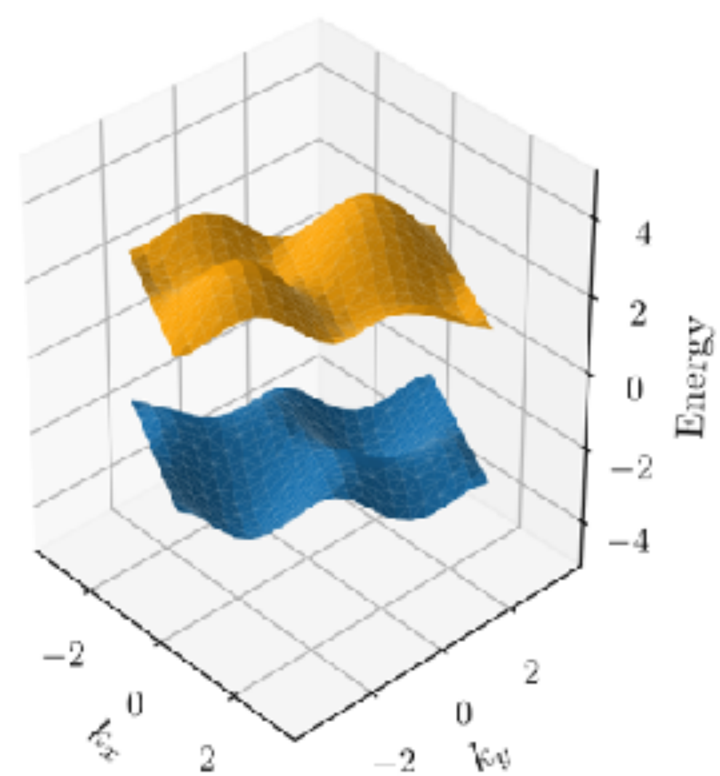
$$\mathbf{S}_i = \frac{1}{2} c^\dagger_{i\alpha} \sigma_{\alpha\beta} c_{i\beta}$$

- Mean-field ansatz for Parton operators $\chi_{ij} \equiv c^\dagger_{i\alpha} c_{j\alpha} \to \chi_{ij} = \langle c^\dagger_{i\alpha} c_{j\alpha} \rangle$

$$H_{\text{mean}} = \sum_{i,j,\alpha} (\chi_{ij} c^\dagger_{i\alpha} c_{j\alpha} + \text{H.c.}) + \sum_i \mu_i (n_i - 1)$$

- Choose ansatz to form bands with Chern numbers +/- 1





GUTZWILLER PROJECTED CSL

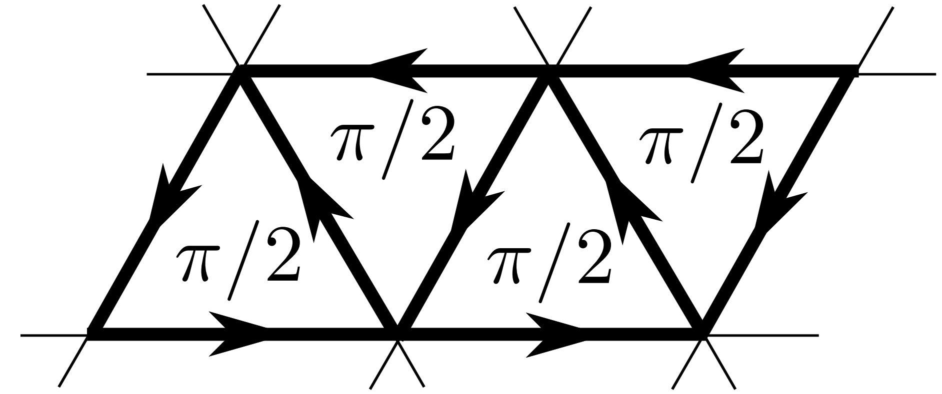
- Filled lower Chern band is mean-field ground state
- Perform Gutzwiller projection to obtain spin wave function

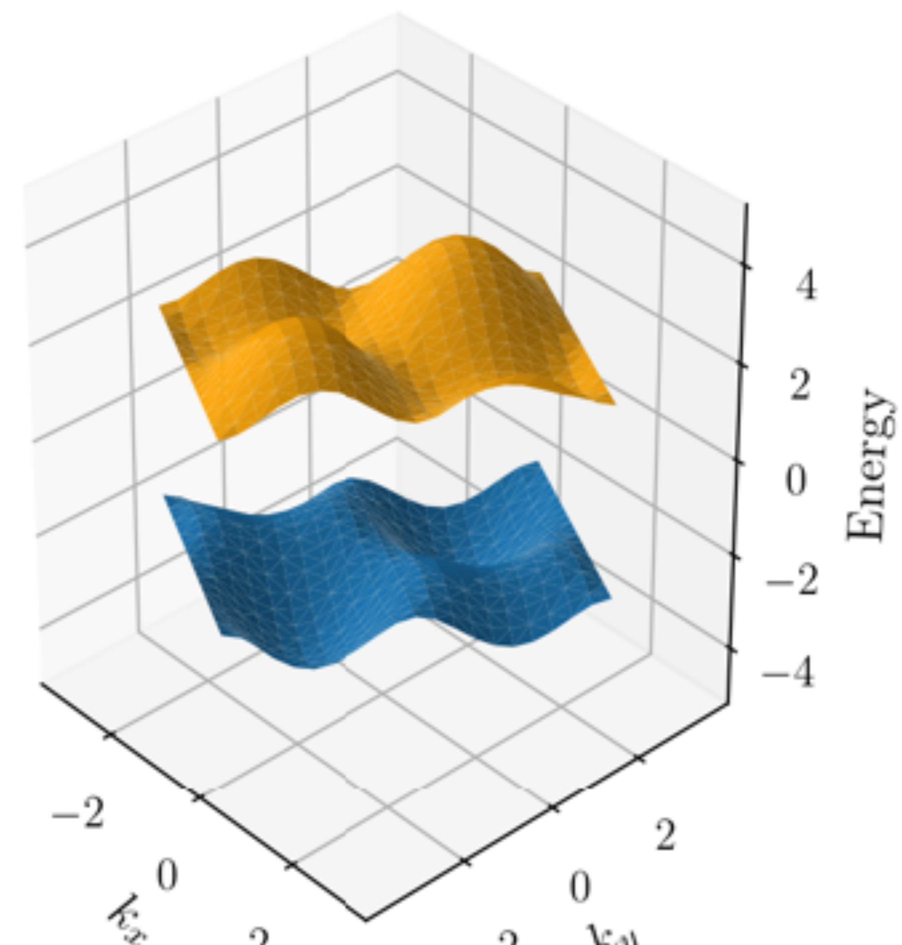
$$|\downarrow, \downarrow\uparrow, \emptyset, \uparrow\rangle \overset{\mathcal{P}}{\Rightarrow} 0$$

$$|\downarrow, \uparrow, \downarrow, \uparrow\rangle \Rightarrow |\downarrow, \uparrow, \downarrow, \uparrow\rangle$$

- Different flux choices through torus generate different states
- Only two-dimensional space spanned by arbitrary flux choices, spanned by

$|\psi_{\text{CSL-I}}\rangle$ $|\psi_{\text{CSL-II}}\rangle$





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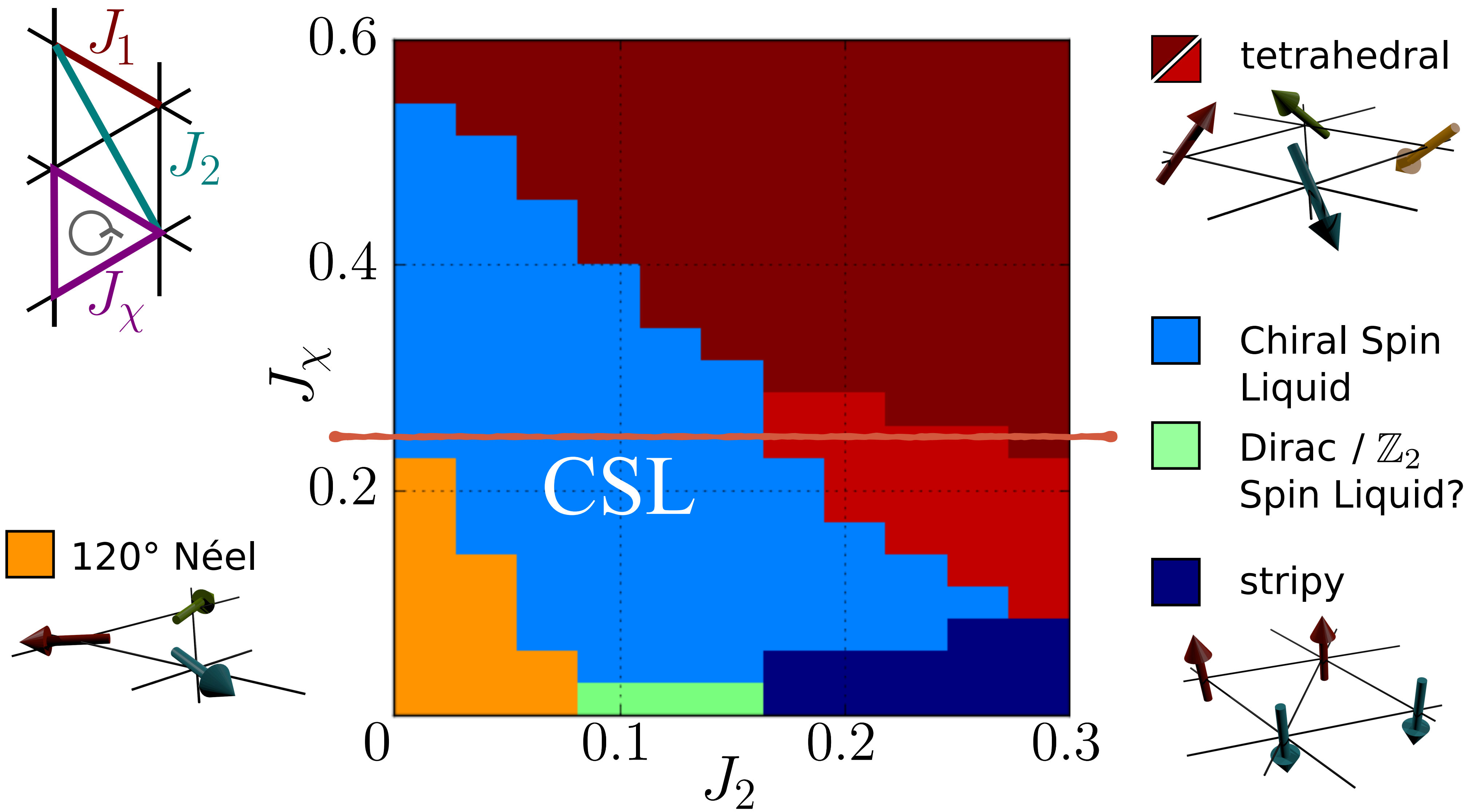
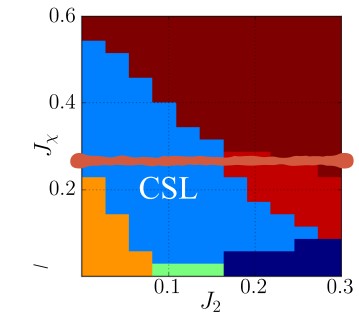
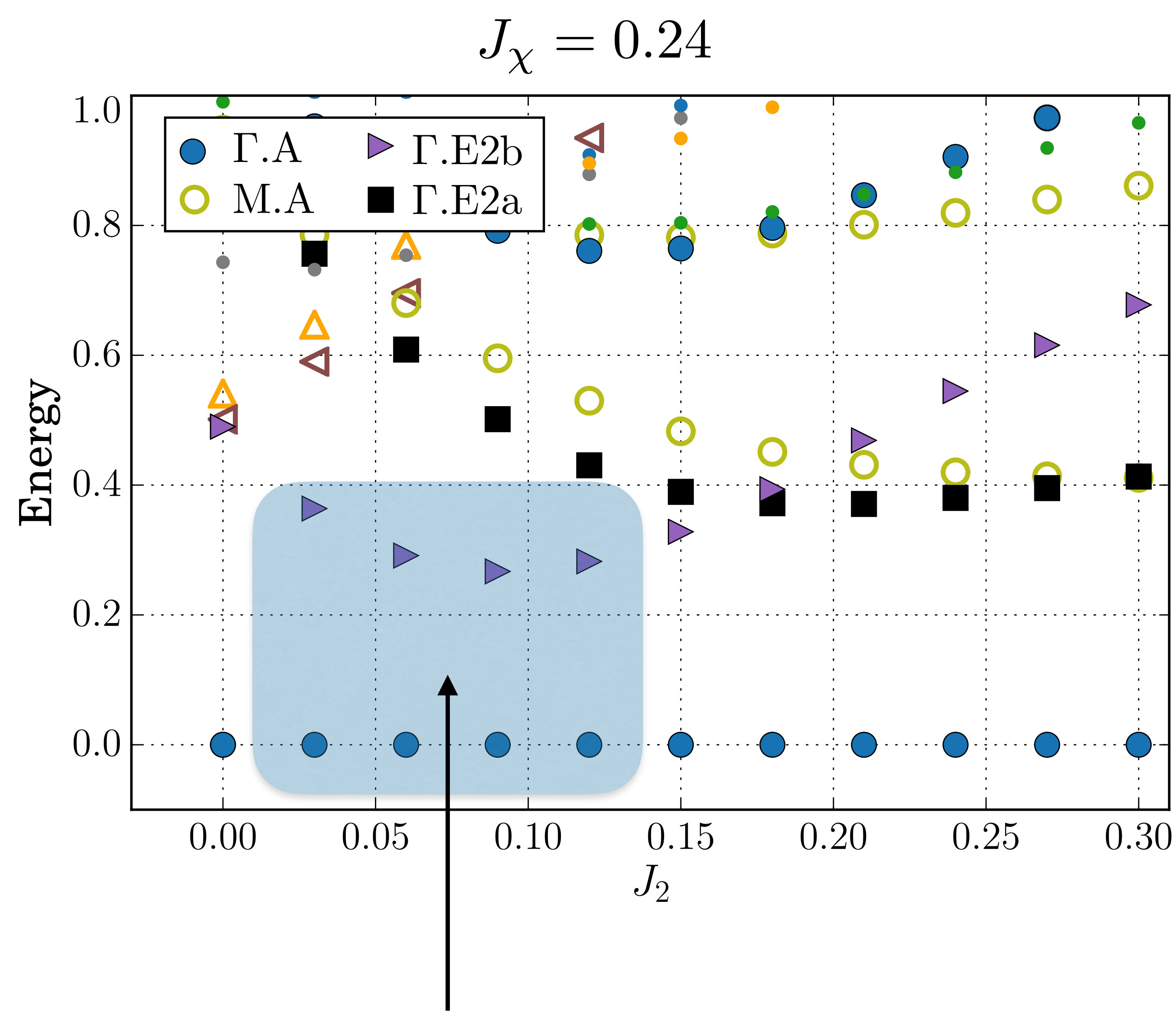


$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_\chi \sum_{i,j,k \in \triangle} \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)$$

CHIRAL SPIN LIQUID ON THE TRIANGULAR LATTICE

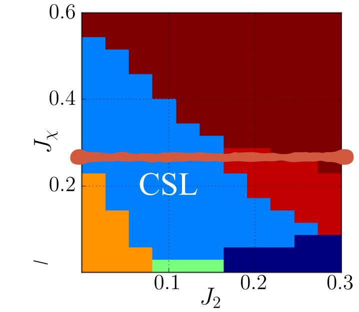


- many-body energy spectrum computed with Exact Diagonalization on 36 sites with periodic boundaries
- claim:
  two low lying singlet states constitute the two degenerate CSL wave functions on the torus
- numerical evidence:
  compare to two model CSL wave functions



two singlet states

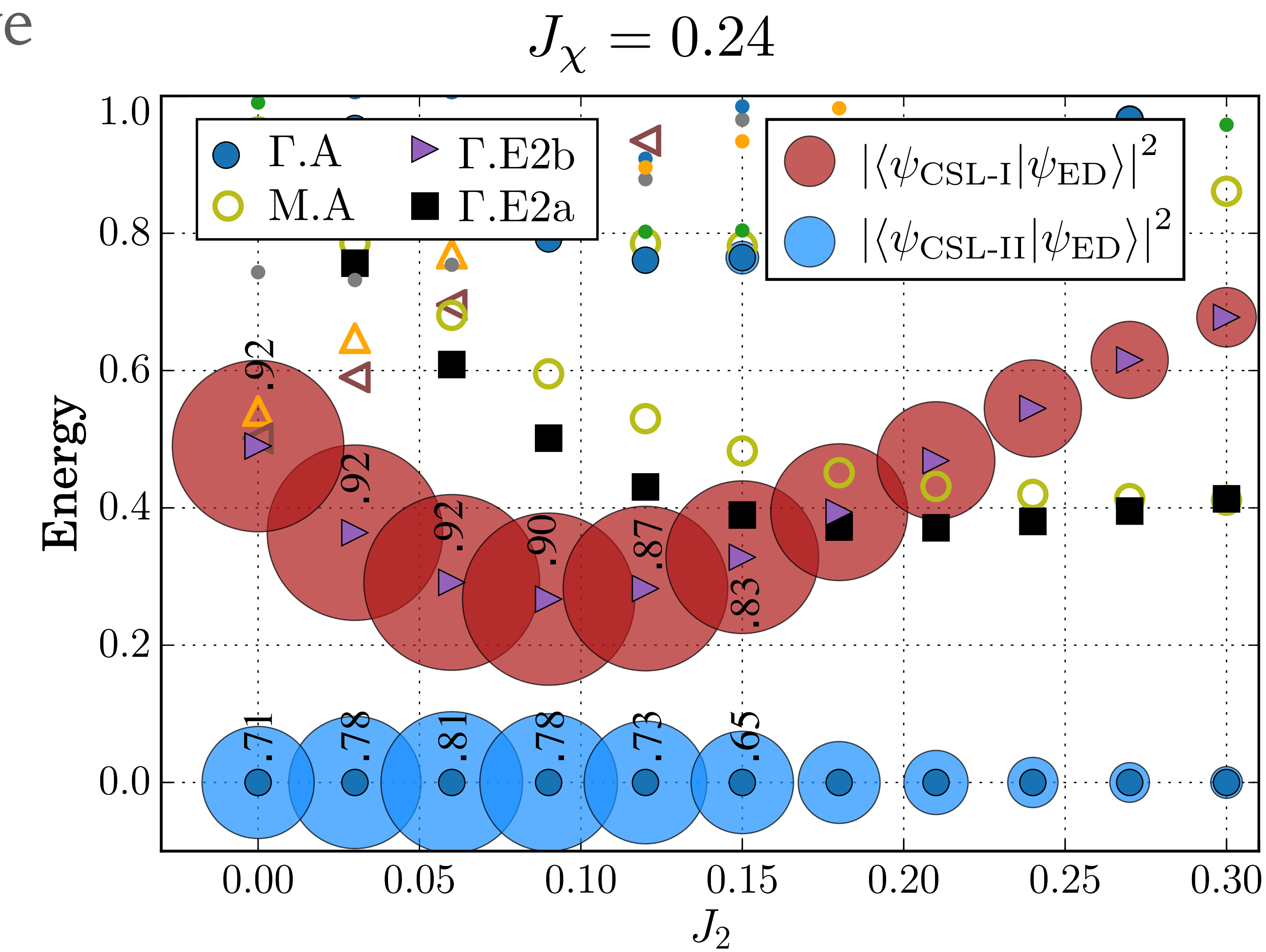
CHIRAL SPIN LIQUID ON THE TRIANGULAR LATTICE



- construct the pair of CSL wave functions on torus from Gutzwiller projection

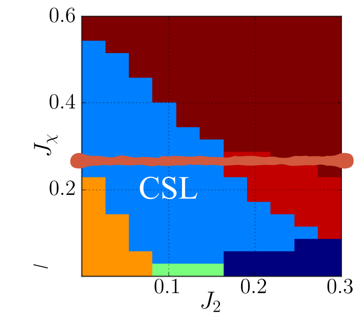
$|\psi_{\text{CSL-I}}\rangle$ $|\psi_{\text{CSL-II}}\rangle$

- linearly independent with comparable low variational energy
- compute overlap with exact numerical eigenvalues



$$\mathcal{O}_{\text{GW-ED}} \equiv \left|\langle\psi^0_{\text{ED}}|\psi_{\text{CSL}}\rangle\right|^2 + \left|\langle\psi^1_{\text{ED}}|\psi_{\text{CSL}}\rangle\right|^2$$

CHIRAL SPIN LIQUID ON THE TRIANGULAR LATTICE

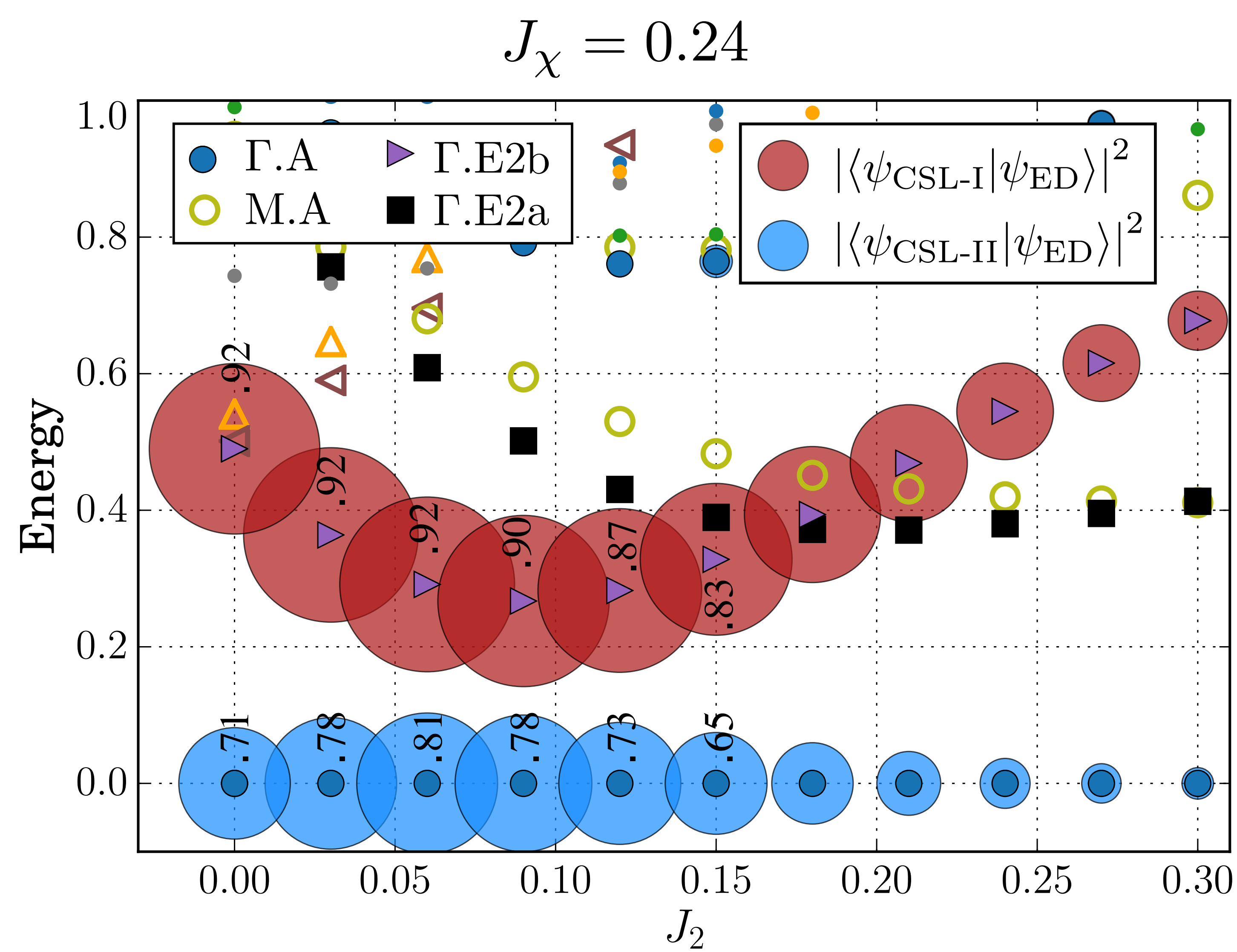


- overlaps of up to 0.92
- dimension of Hilbert space

  $$\dim(\mathcal{H}) = 2^{36} = 68 \text{ billion}$$

- orthogonality catastrophe: overlaps expected to converge to zero exponentially

- Our findings have also recently been confirmed by an independent DMRG study

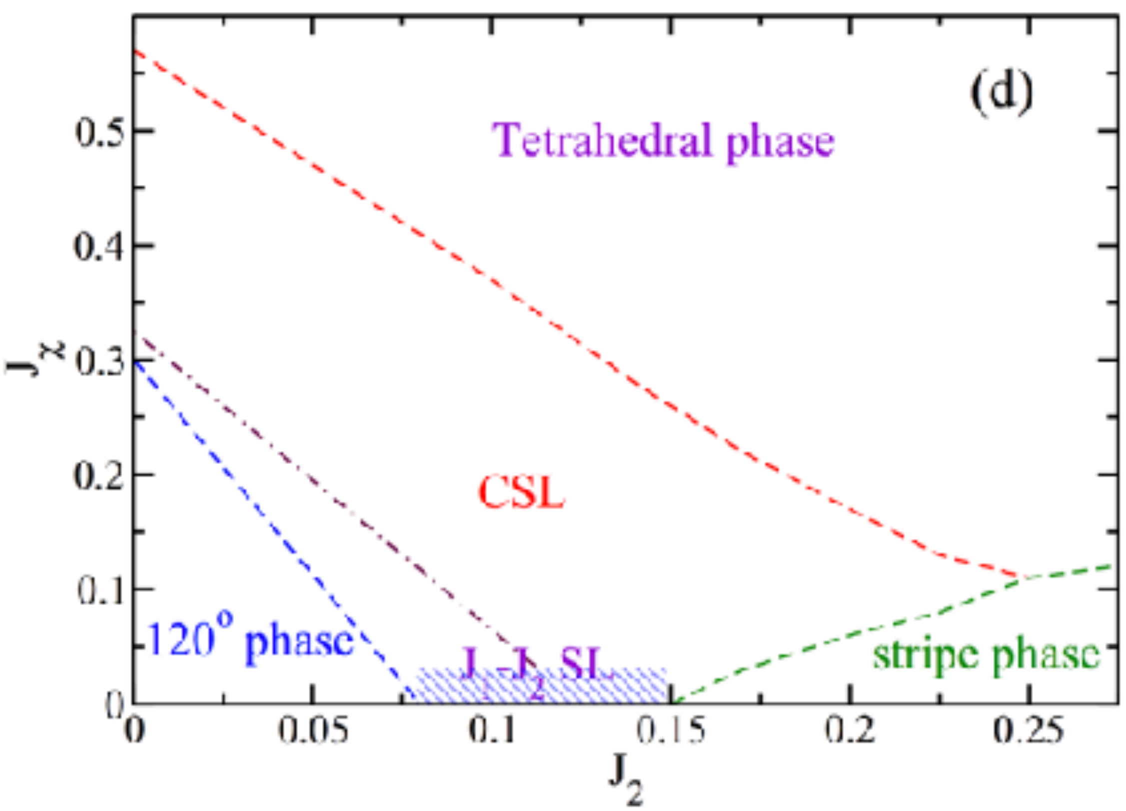


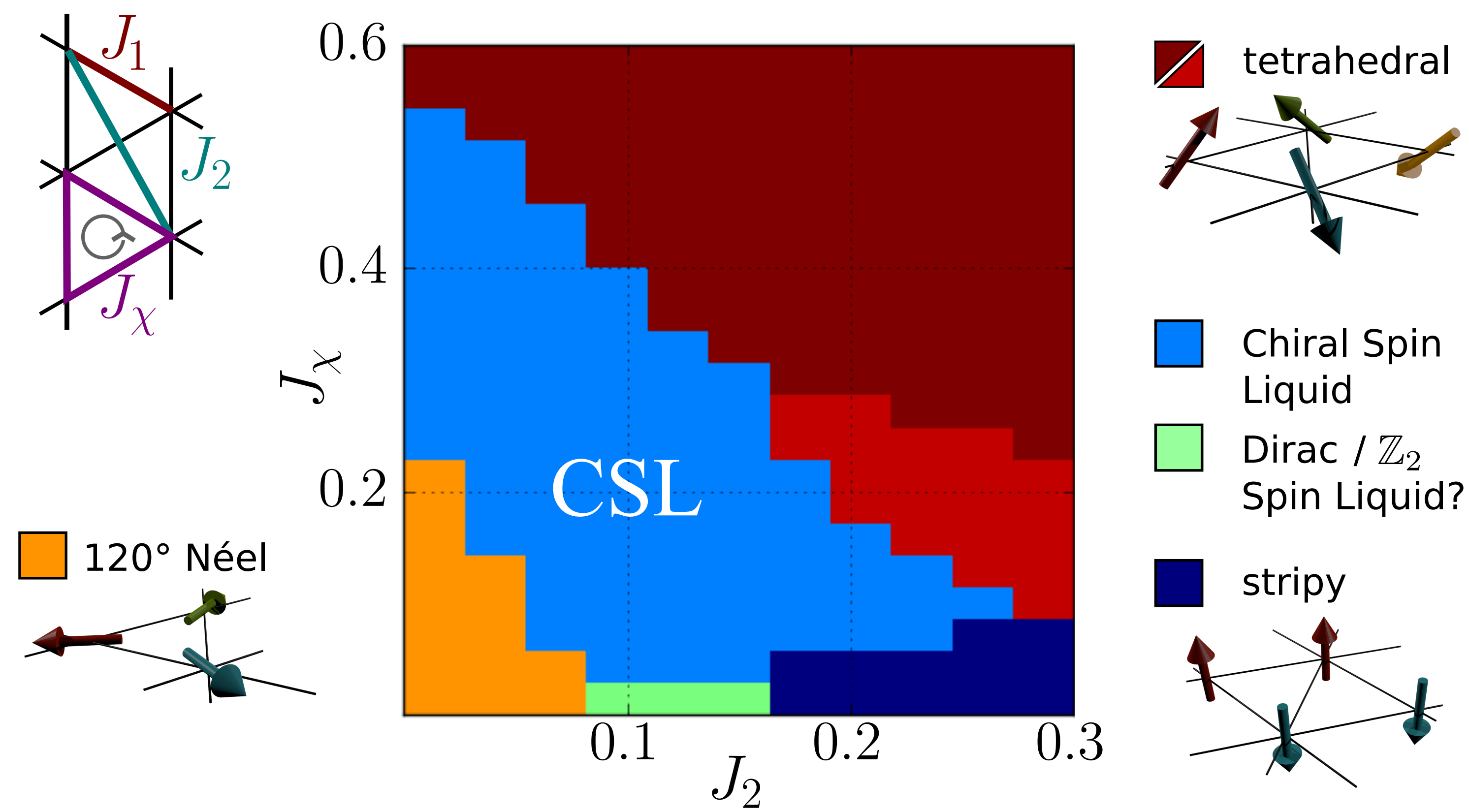
[Shou-Shu Gong et al., Phys. Rev. B 96.7 (2017)]

CHIRAL SPIN LIQUID ON THE TRIANGULAR LATTICE

[A. Wietek, A. M. Läuchli, Phys. Rev. B 95, 035141 (2017)]

[Shou-Shu Gong et al., Phys. Rev. B 96.7 (2017)]





CHIRAL SPIN LIQUID ON KAGOME LATTICE

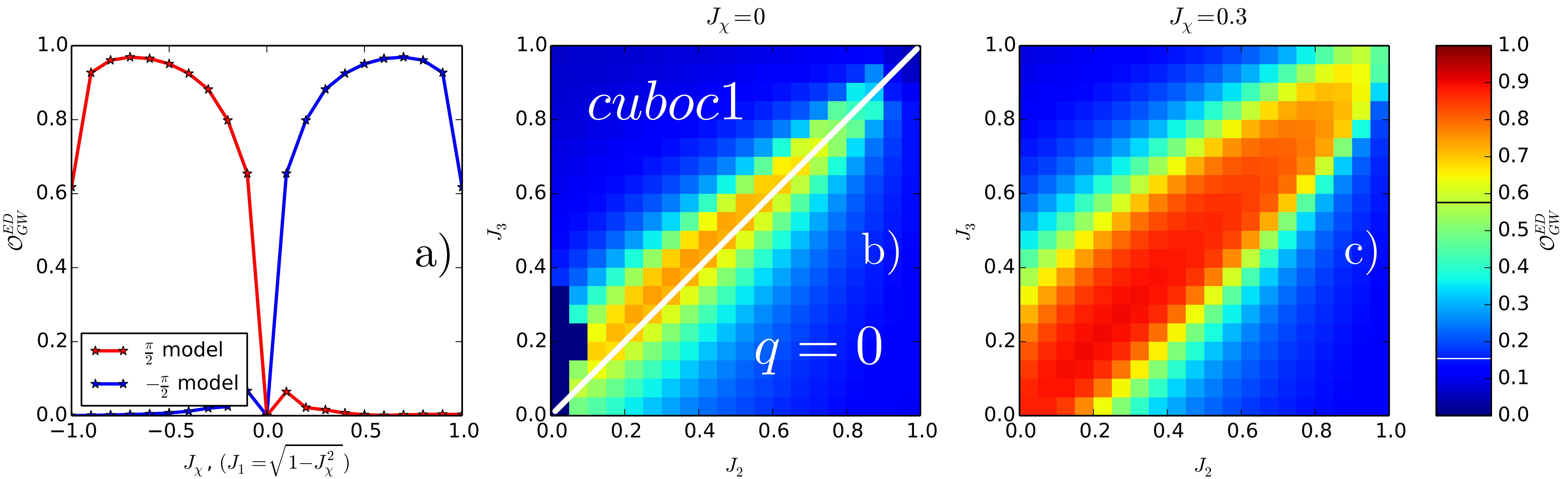
- Extended Heisenberg model on kagome lattice

$$H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_3 \sum_{\langle\langle\langle i,j \rangle\rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_\chi \sum_{i,j,k \in \triangle, \bigtriangledown} \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)$$

[S. Gong, W. Zhu, D. N. Sheng, Nature *Sci. Rep.* 4, 6317 (2014)] [B. Bauer et al., Nature *Comm.* 5, 5137 (2014)]

[Yin-Chen He, D. N. Sheng, and Yan Chen, Phys. Rev. Lett. 112, (2014)]

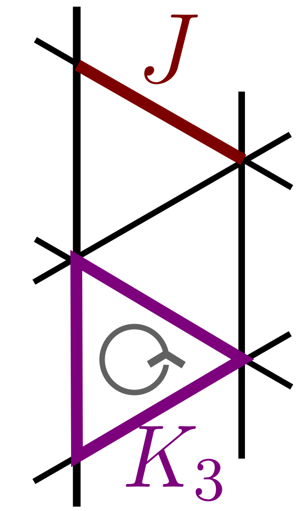
- Computation of overlaps: up to 0.95



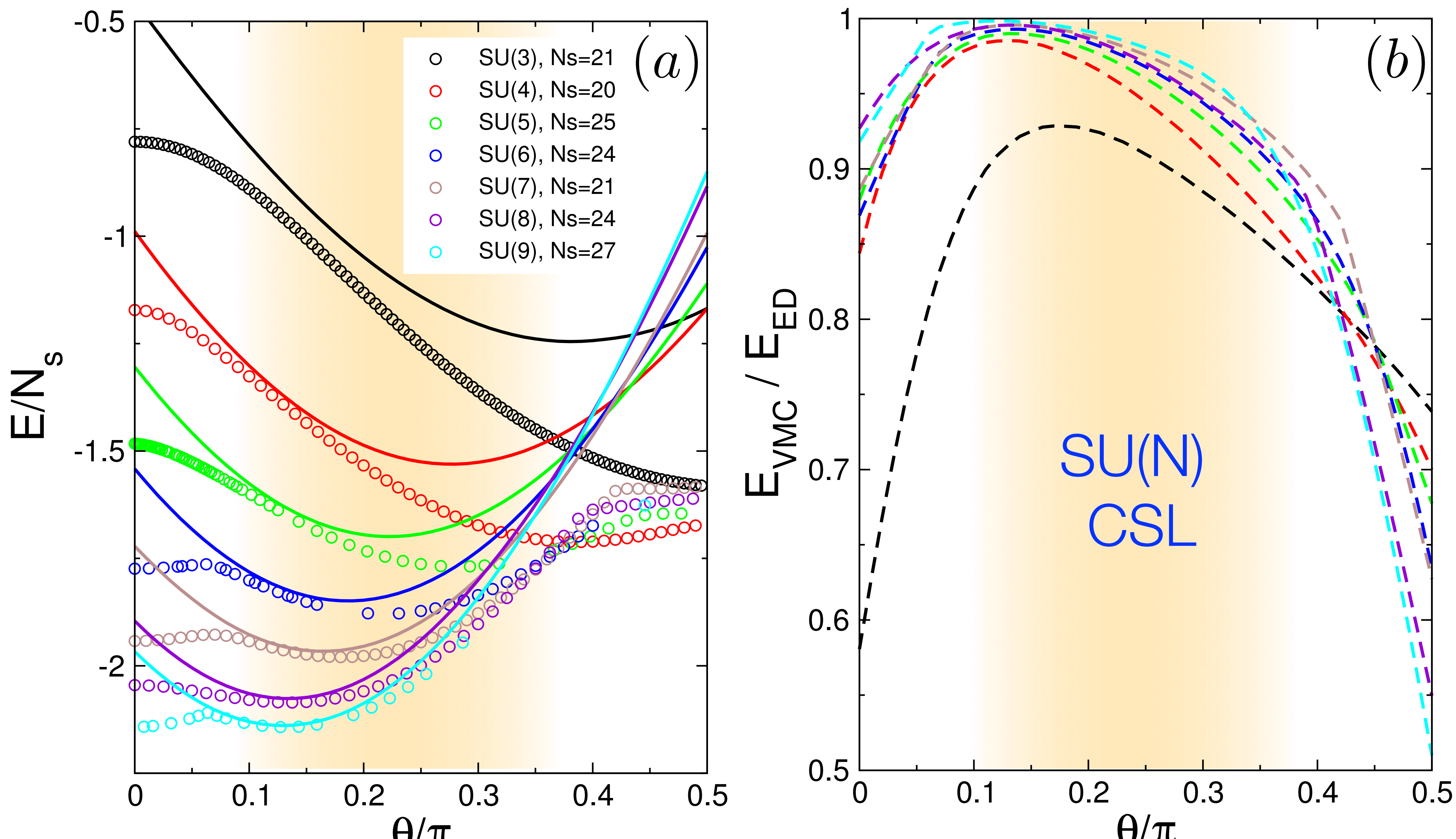
[A. Wietek, A. Sterdyniak, A. M. Läuchli, Phys. Rev. B 92, 125122 (2015)]

CHIRAL SPIN LIQUID IN SU(N) FERMIONIC MOTT INSULATORS

[P. Nataf, M. Lajkó, A. Wietek, K. Penc, F. Mila, A. M. Läuchli, Phys. Rev. Lett. 117, 167202]



$$H = J \sum_{\langle i,j \rangle} P_{ij} + K_3 \sum_{(i,j,k)} (i P_{ijk} + \mathrm{h.c.})$$



$J = \cos(\theta),\ K_3 = \sin\theta$

CHIRAL SPIN LIQUID IN SU(N) FERMIONIC MOTT INSULATORS

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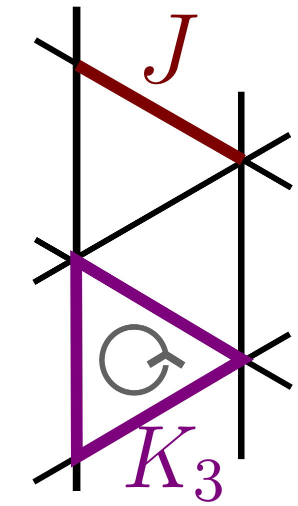
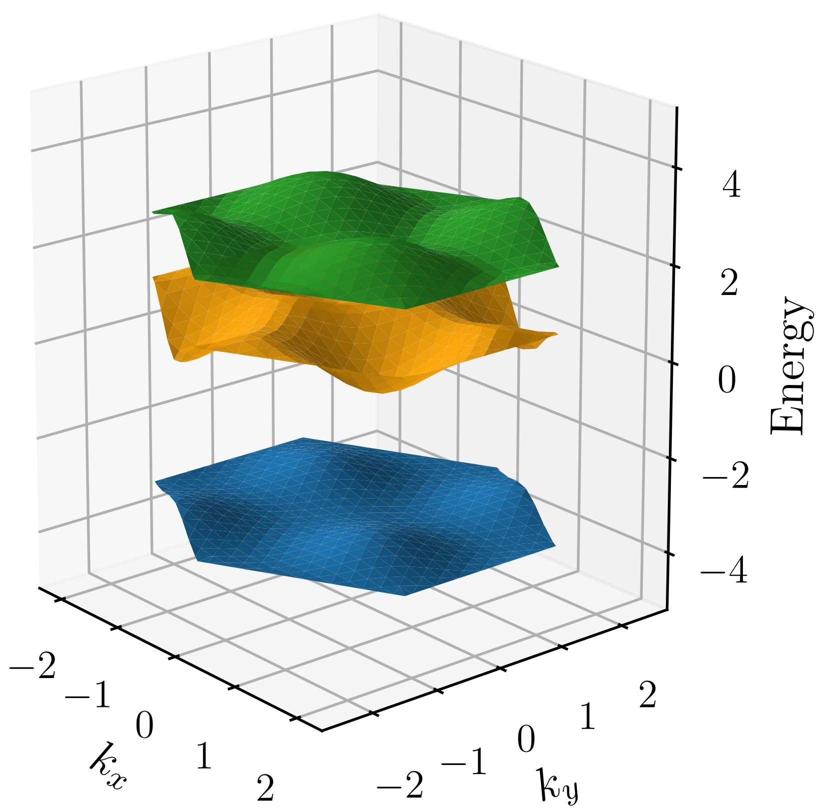
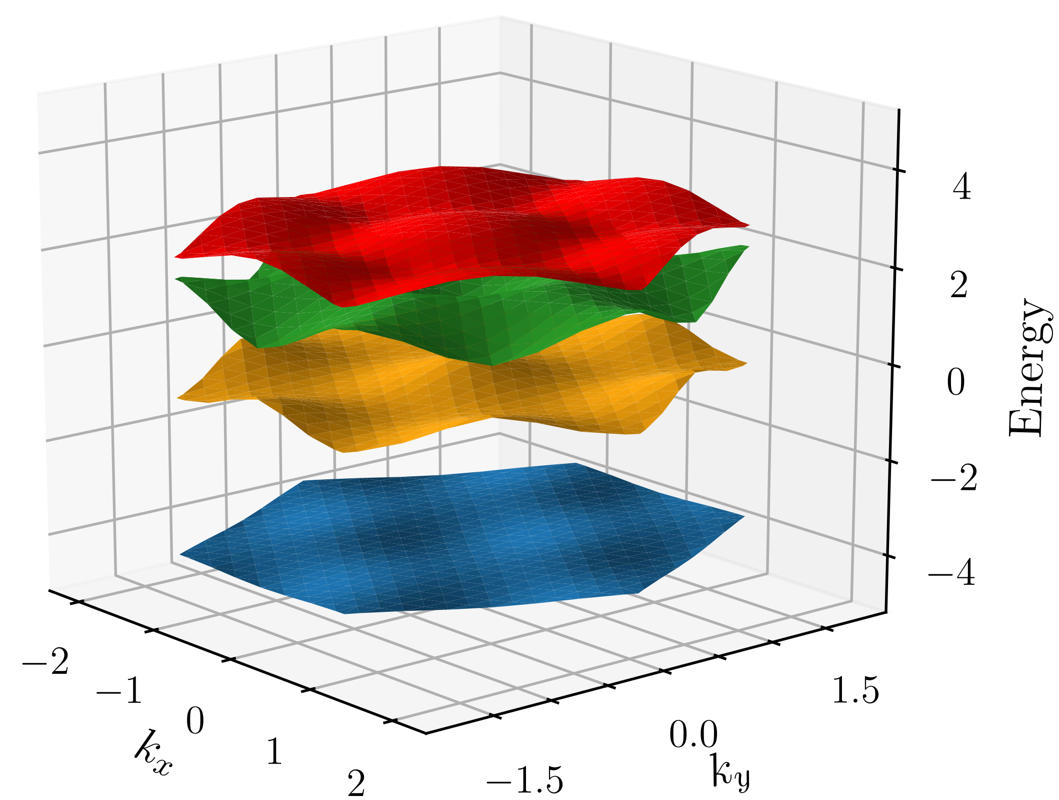




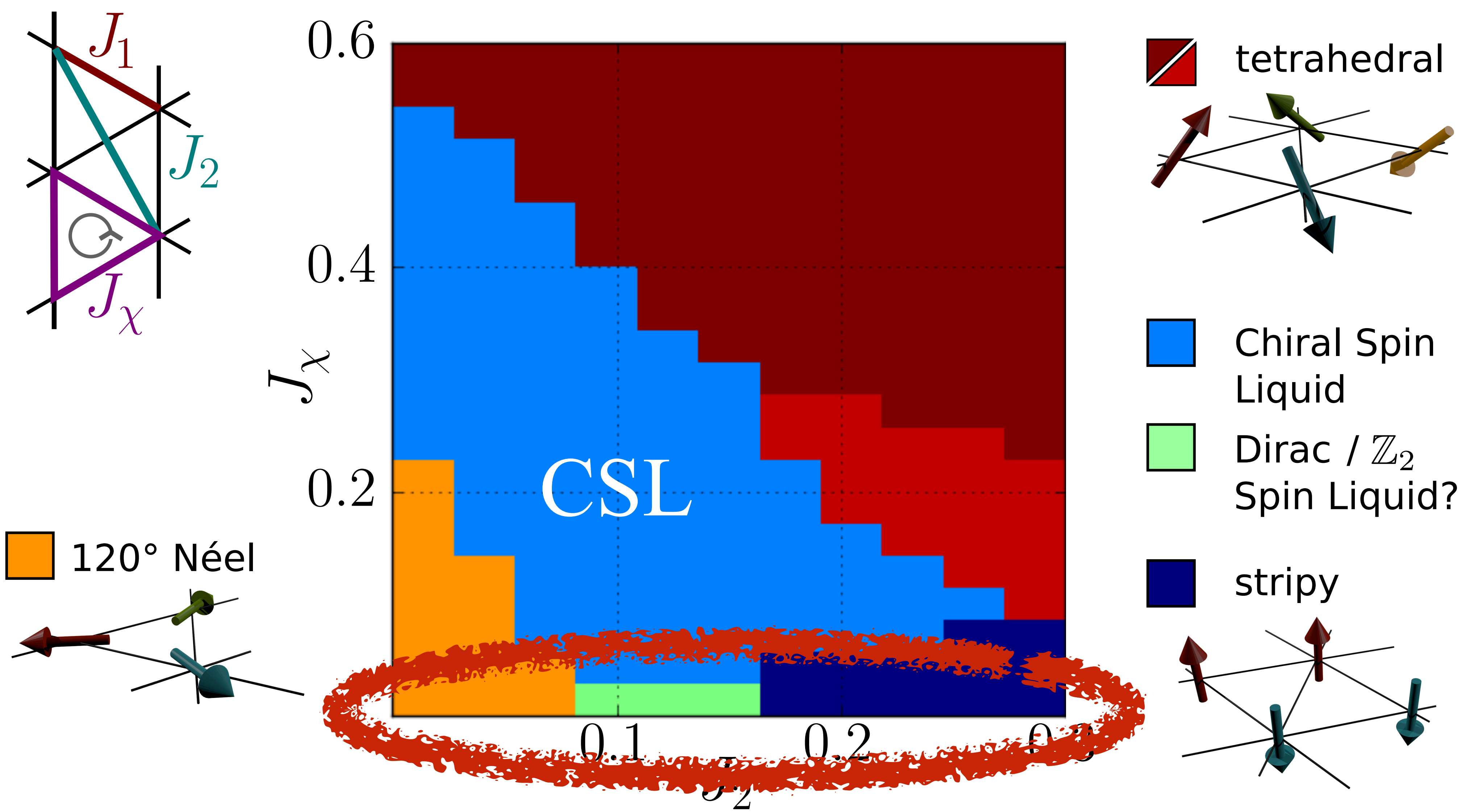
SU(3)



SU(4)

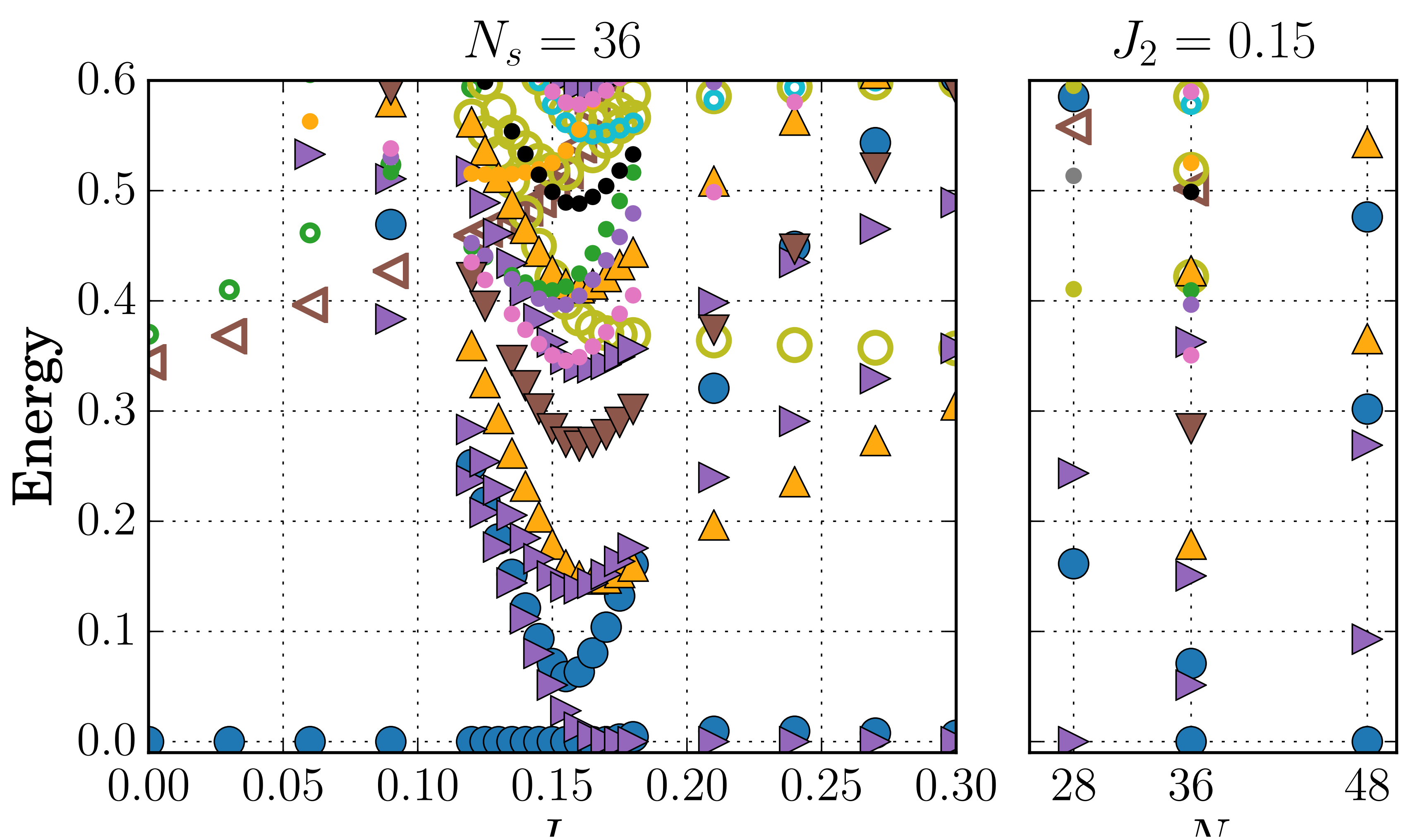
J_1–J_2 MODEL ON THE TRIANGULAR LATTICE

[A. Wietek, A. M. Läuchli, Phys. Rev. B 95, 035141 (2017)]



J_1–J_2 MODEL ON THE TRIANGULAR LATTICE

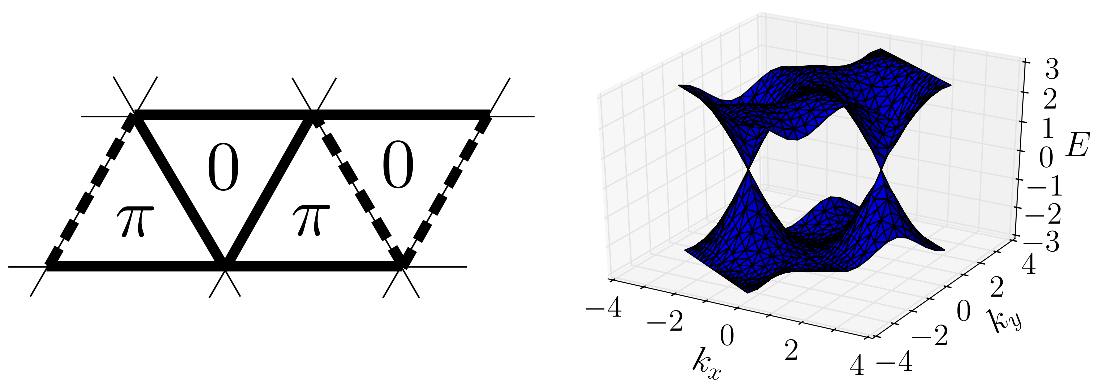
- Debate which kind of phase is realized in the intermediate regime
- Z_2 spin liquid [Zhu, White, PRB (2015)] [Hu, Gong, Zhu, Sheng PRB (2015)] [Saadatmand, Powell, McCulloch PRB (2015)]
- Dirac spin liquid [Kaneko, Morita, Imada, JPSJ 83, 093707 (2014) [Iqbal, Hu, Thomale, Poilblanc, Becca PRB 93 144411 (2016)]

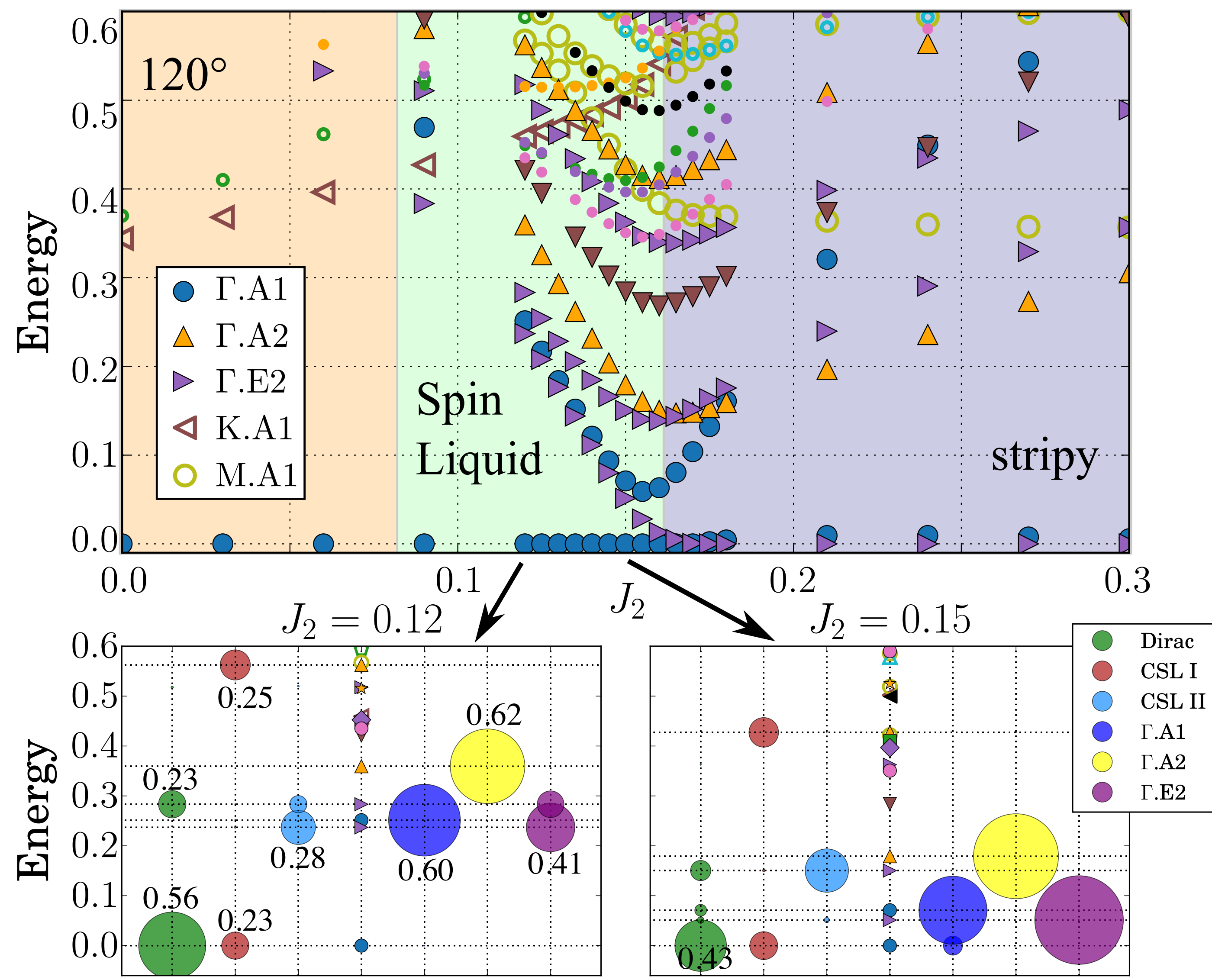


J_1-J_2 MODEL ON THE TRIANGULAR LATTICE

[A. Wietek, A. M. Läuchli, Phys. Rev. B 95, 035141 (2017)]

- Constructed Dirac spin liquid wave function





- Computed overlap of various model wave functions with exact eigenstates

ALGORITHMIC ADVANCES FOR EXACT DIAGONALIZATION

EXACT DIAGONALIZATION

- Solving the Schrödinger equation

$$H\,|\psi\rangle = E\,|\psi\rangle$$

  by numerically computing exact eigenvalues and eigenstates

- Several new developments of the method
- Sparse-matrix algorithms for finite temperature properties,
- Thermodynamics with quantum typicality

  [S. Sugiura and A. Shimizu, Phys. Rev. Lett. 108, 240401 (2012)]

  [Goldstein et al. Phys. Rev. Lett. 96, 050403(2006)]

- Finite temperature dynamics

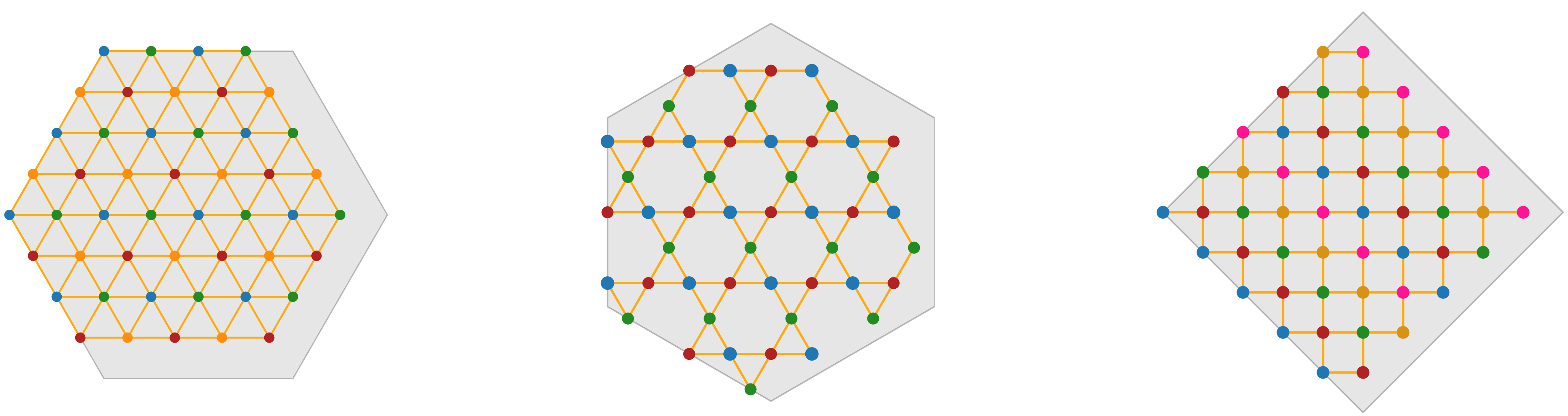
  [Yamaji et al., arXiv:1802.02854 (2018)]

EXACT DIAGONALIZATION

- Simulations of SU(N) symmetric models

  [P. Nataf and F. Mila Phys. Rev. Lett. 113, 127204 (2012)]

- For spin 1/2 systems several interesting simulation clusters exist close to 50 lattice sites



- Developed new algorithms and code allowing for simulating 50 spin-1/2 particles

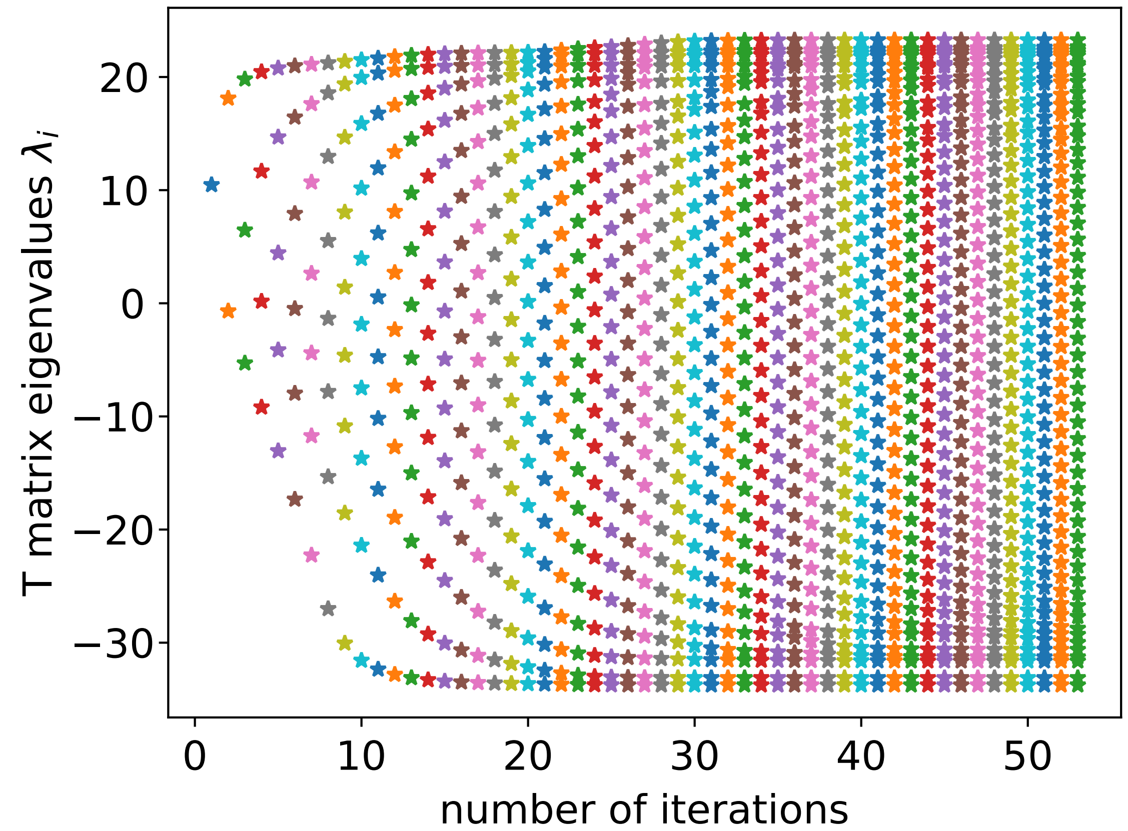
  [A. Wietek and A. Läuchli, arXiv:1804.05028]

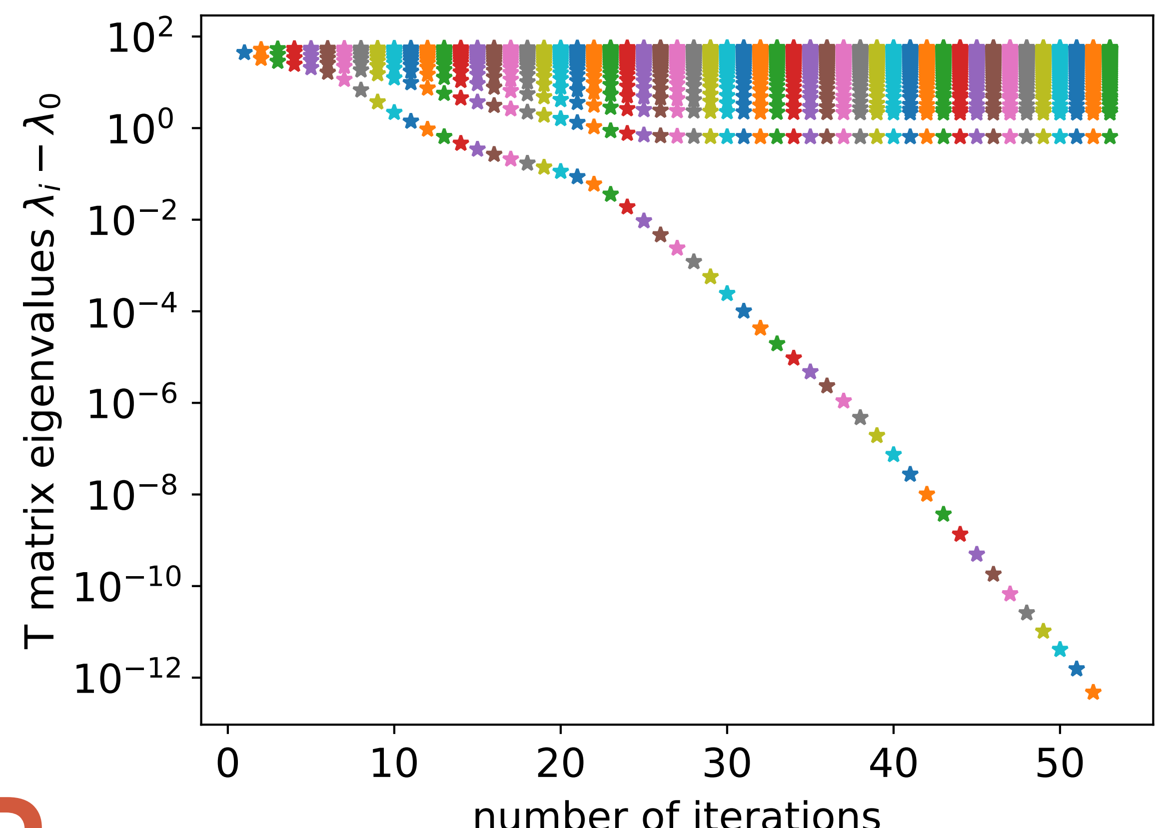
$\sim 10^{22}$ GB

LANCZOS ALGORITHM

[C. Lanczos, J. Res. Natl. Bur. Stand. 45.4 (1950)]

- Iterative method to compute extremal eigenstates
- Only matrix-vector multiplications necessary
- Exponentially fast convergence
- Matrix-vector multiplications can be performed without storing the matrix
- 3-4 Lanczos vectors need to be stored in memory

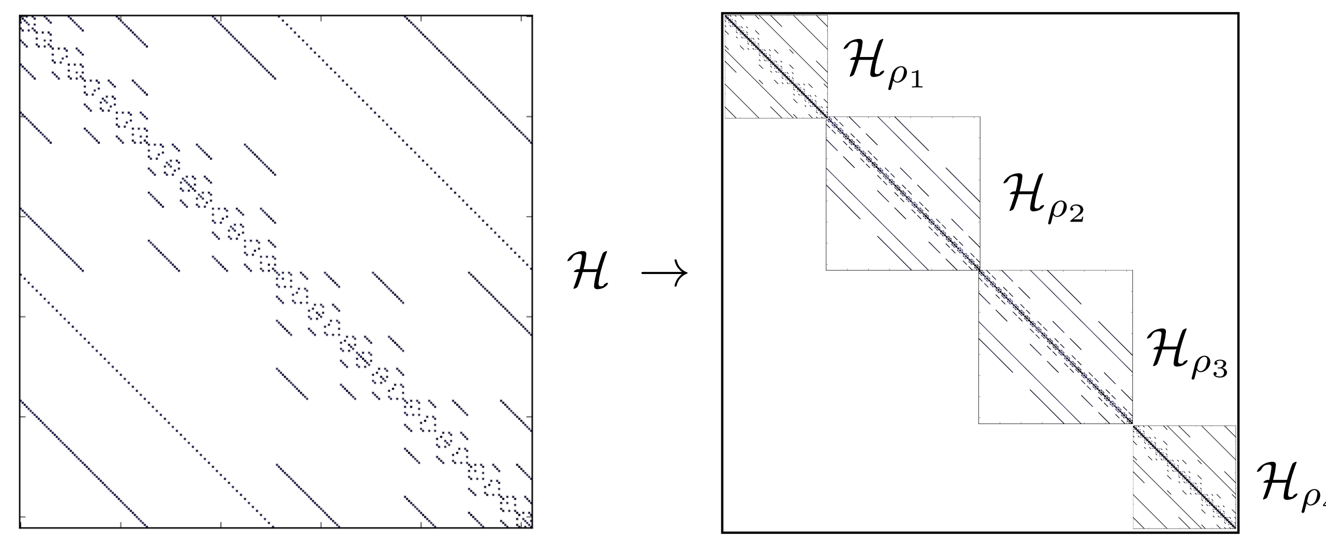


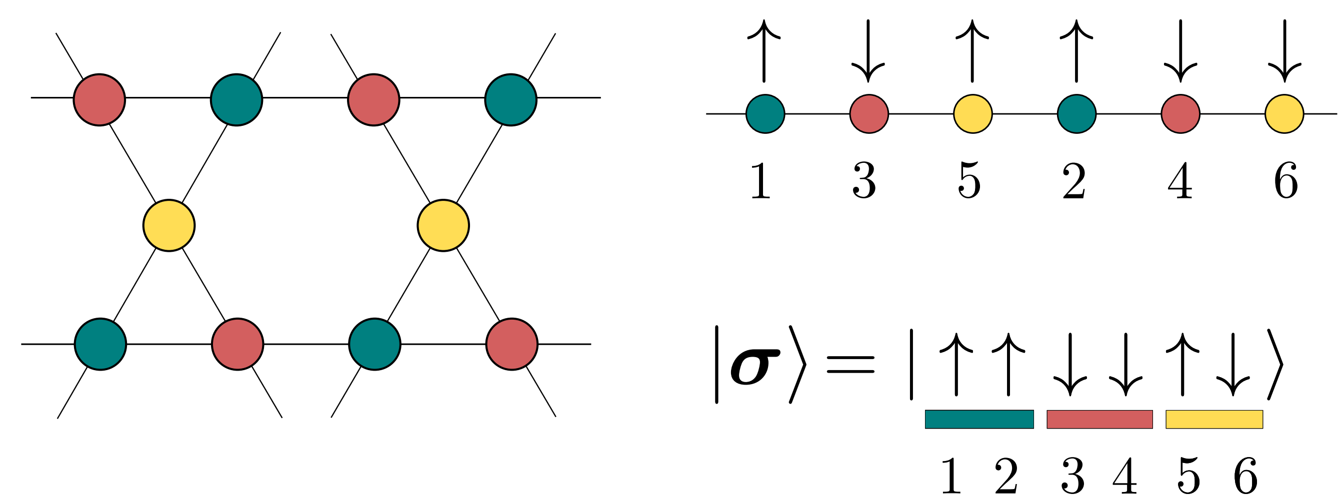


~10^8 GB

IMPLEMENTING SYMMETRIES

- Usage of space group and local symmetries allow for block diagonalization
- Computations in symmetry-adapted basis are challenging
- Developed sublattice coding algorithm for applying symmetries
- Lookup tables for action of symmetries on sublattices
- Allow for fast evaluation of matrix elements in symmetrized basis

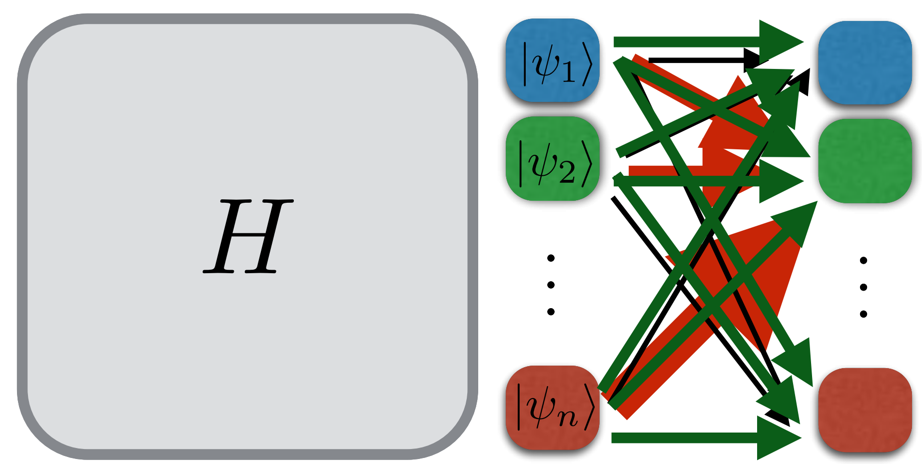




~10^4 GB

LARGE SCALE PARALLELIZATION

- Parallelization for distributed memory machines
- Splitting up the workload between the processes
- Randomly distributing the basis of the Hilbert space solves load balancing problems
- Hybrid implementation using the MPI standard and POSIX shared memory functions for lookup tables
- Benchmarks with up to several 1000 CPU cores



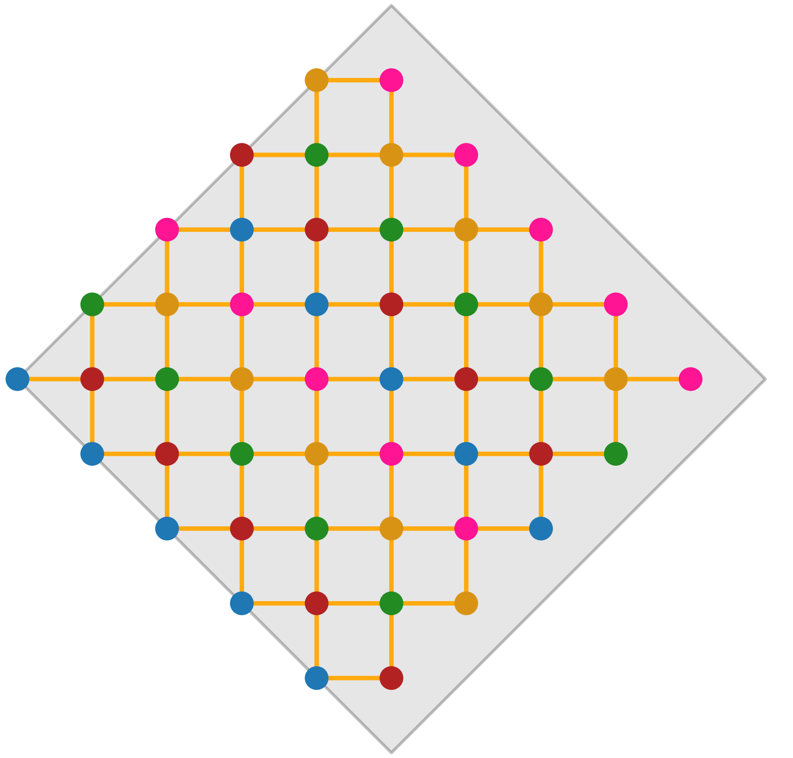
~10 GB

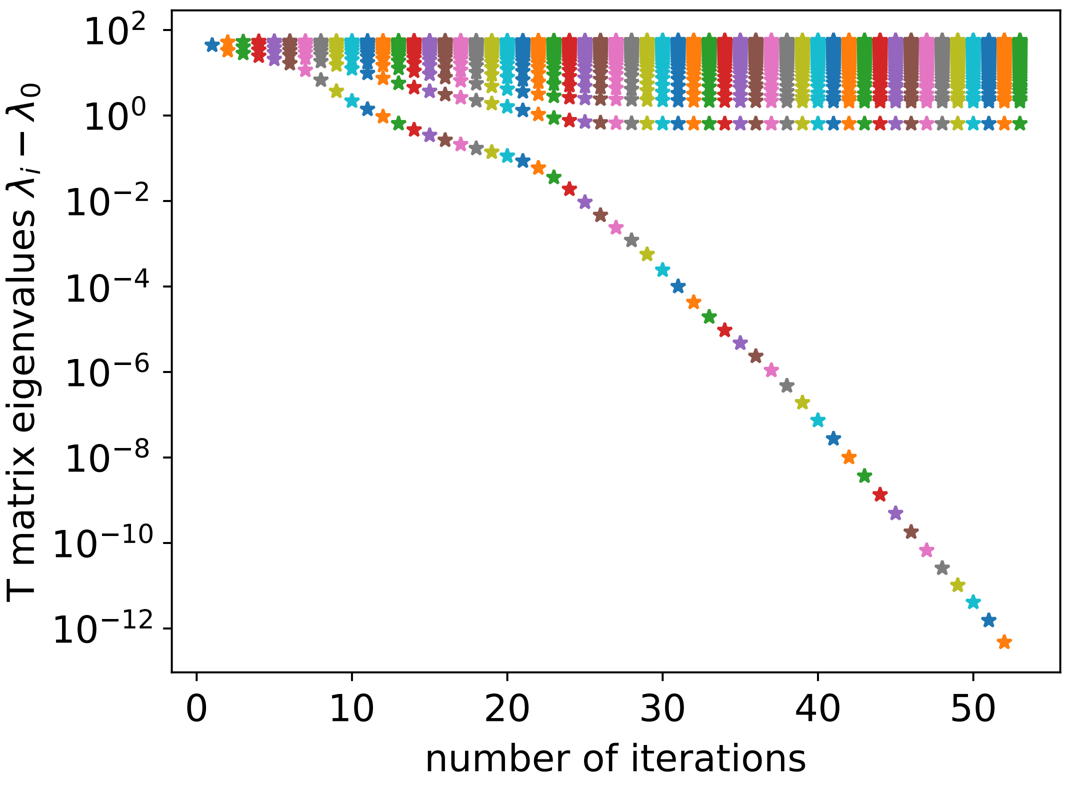
BENCHMARK PROBLEM

- Heisenberg spin 1/2 model

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

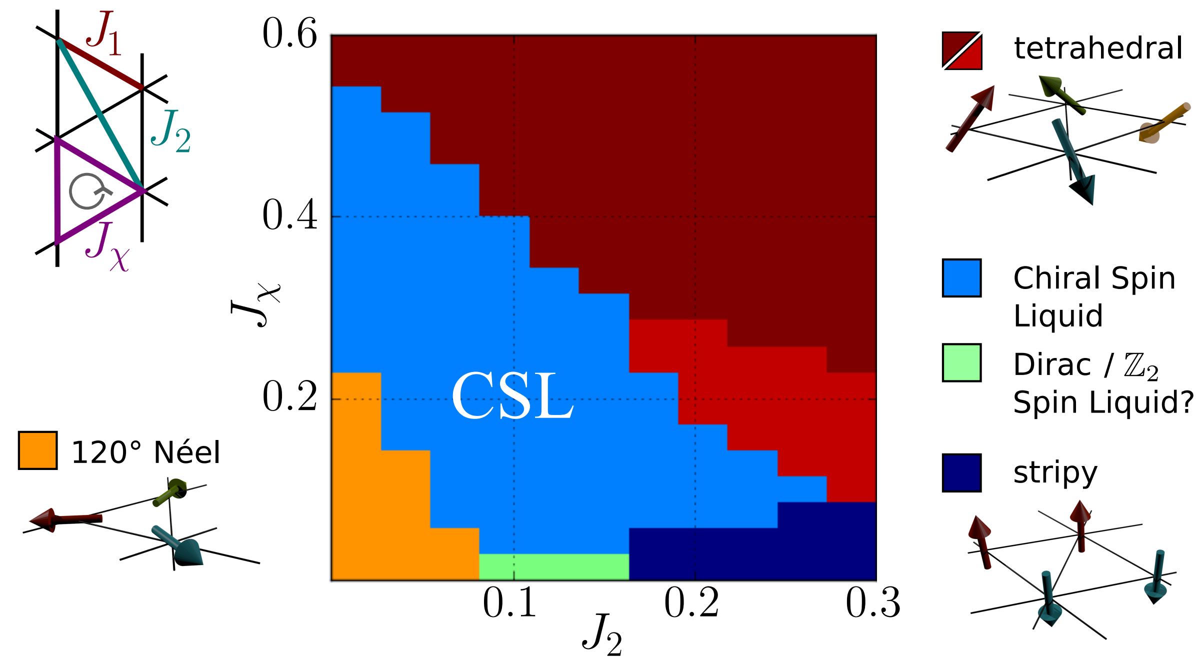
- Dimension of Hilbert space: $3 \cdot 10^{11}$
- Benchmark performed on supercomputer Sekirei at University of Tokyo (3456 cores)
- Total memory usage: 15.5 TB
- Time per Matrix-vector multiplication: 3304 seconds
- Ground state energy: -33.7551019315
- Checked using Quantum Monte Carlo

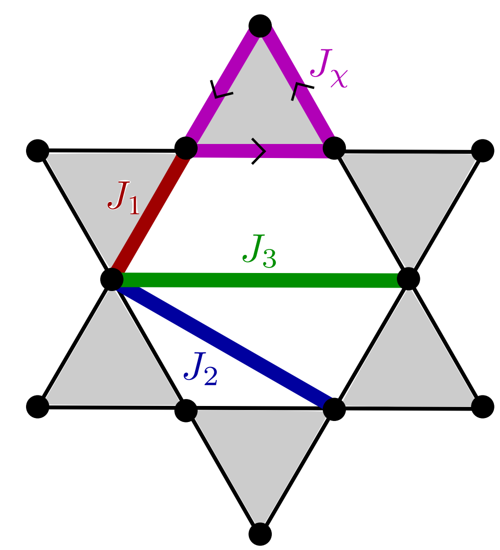


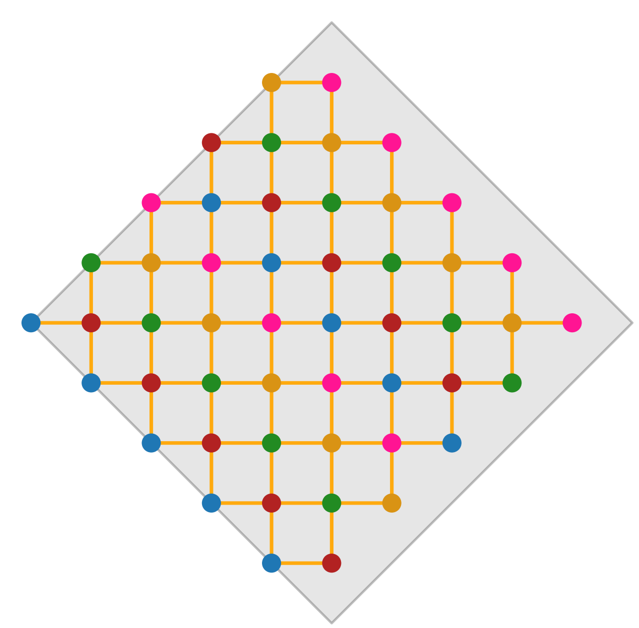


SUMMARY

- Discovery of several chiral spin liquid phases in extended Heisenberg models
- Comparing numerical exact states on small lattices with ansatz CSL wave functions
- Findings are now cross-validated by DMRG and ED
- Novel developments for the ED method now allowing to simulate spin systems up to 50 spin 1/2 particles







THANK YOU FOR YOUR ATTENTION!