Title: Spin-liquid states on the pyrochlore lattice and Rydberg atoms simulator

Speakers: Nikita Astrakhantsev

Series: Machine Learning Initiative

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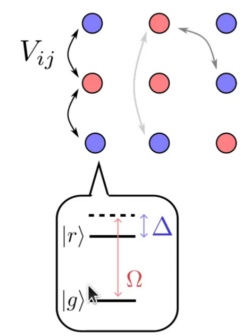
Abstract: The XXZ model on the three-dimensional frustrated pyrochlore lattice describes a family of rare-earth materials showing signatures of fractionalization and no sign of ordering in the neutron-scattering experiments. The phase diagram of such XXZ model is believed to host several spin-liquid states with fascinating properties, such as emergent U(1) electrodynamics with emergent photon and possible confinement-deconfinement transition. Unfortunately, numerical studies of such lattice are hindered by three-dimensional geometry and absence of obvious small parameters.
In this talk, I will present my work [Phys. Rev. X 11, 041021] on the variational study of the pyrochlore XXZ model using the RVB-inspired and Neural-Network-inspired ansätze. They yield energies better than known results of DMRG at finite bond dimension. With these wave functions, we study the properties of frustrated phase at the Heisenberg point, and observe signatures of long-range dimer correlations.

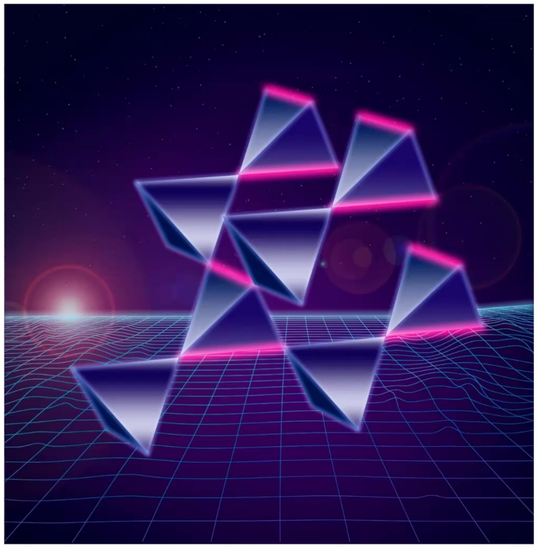
Lastly, I will sketch the prospects of using the Programmable Rydberg Simulator platform for the study of these spin-liquid states. I will construct two possible embeddings of the pyrochlore XXZ model onto the Rydberg atoms simulator, employing the notion of spin ice and perturbative hexagon flip processes.

Zoom link: https://pitp.zoom.us/j/99480889764?pwd=cnY2RHBjeDZvRkM2K3FlYU9OWjgxUT09

Spin liquids on the pyrochlore lattice and Rydberg atoms simulator

Nikita Astrakhantsev
Condensed Matter Theory Group
University of Zurich





Universität Zürich[UZH]

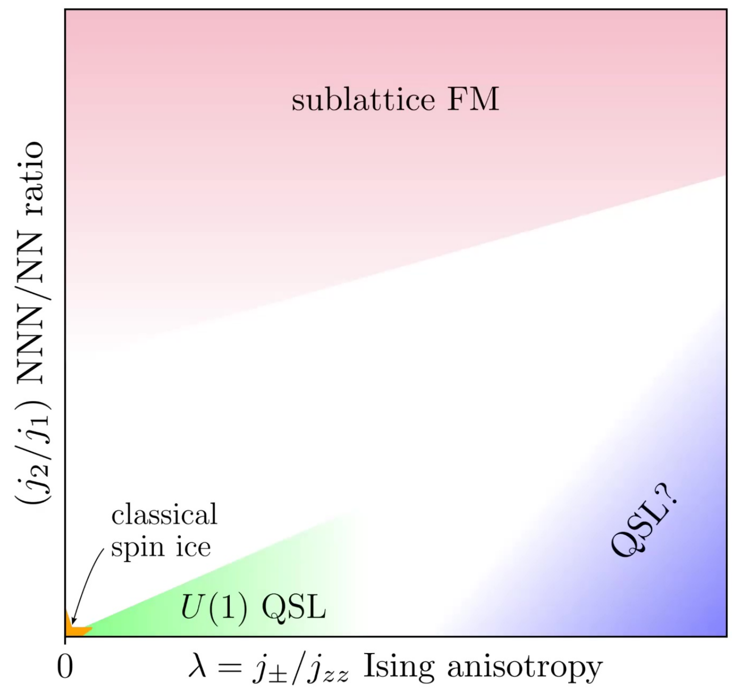
FNSNF
Schweizerischer Nationalfonds
zur Förderung der wissenschaftlichen Forschung

Outline

1. **Intro: QSL states of the pyrochlore lattice**

2. **Classical study: unexpected variational results**
   [***NA*** *et al,* Phys. Rev. X 11, 041021]

3. **Rydberg atoms and pyrochlore**
   [***NA*** *et al,* ongoing]
   a. Rydberg atoms
   b. Two mapping

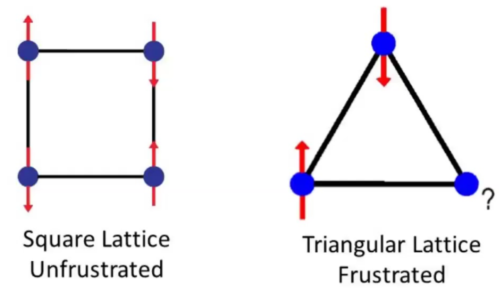


Quantum spin liquids (QSL)

- No characterization by symmetry breaking

- Frustration "melts" simple orders

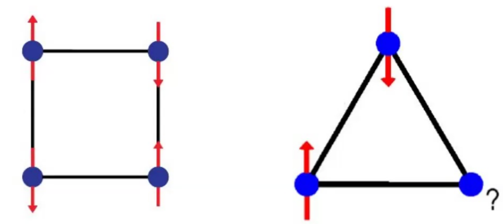
$$\hat{H} = J \sum_{\langle i,j \rangle} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j$$



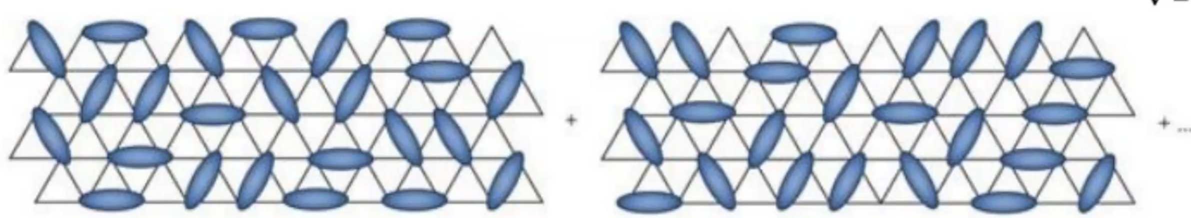
Quantum spin liquids (QSL)

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

- No characterization by symmetry breaking
- Frustration “melts” simple orders
- Resonating Valence Bond (RVB) ansatz
  [PW Anderson 1973]



 $= \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$

$|\Psi\rangle =$ 

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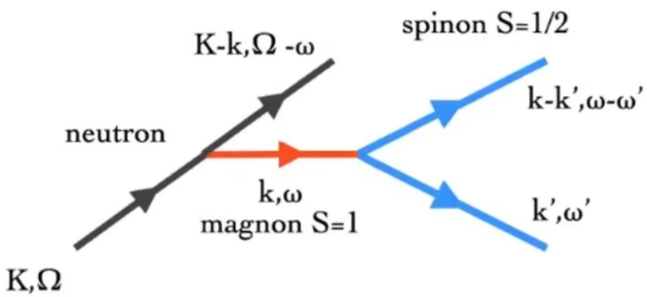
QSL in 3D pyrochlore lattice?

- Magnetic susceptibility and neutron scattering in rare-earth pyrochlores $Tb_2Hf_2O_7$, $Ce_2Sn_2O_7$, ... *[Sibille Nat. Comm. 2017, Sibille PRL 2015]*

Hermele et al., PRB (2004), Savary PRB (2012)

QSL in 3D pyrochlore lattice?



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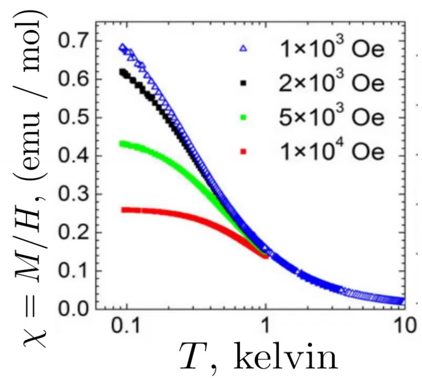
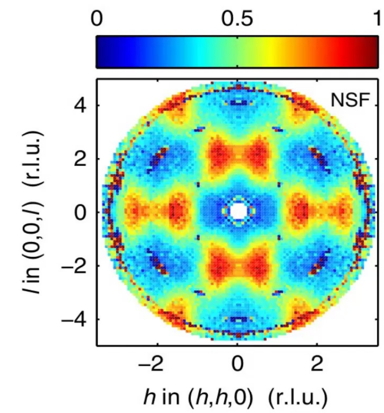
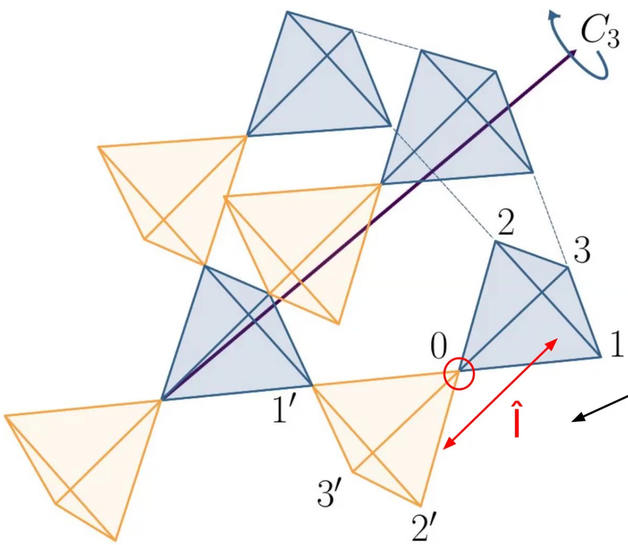




- No ordering T > 0.07 K
- Diffusive pattern (pinch points) – **fractionalization**?

Pyrochlore system

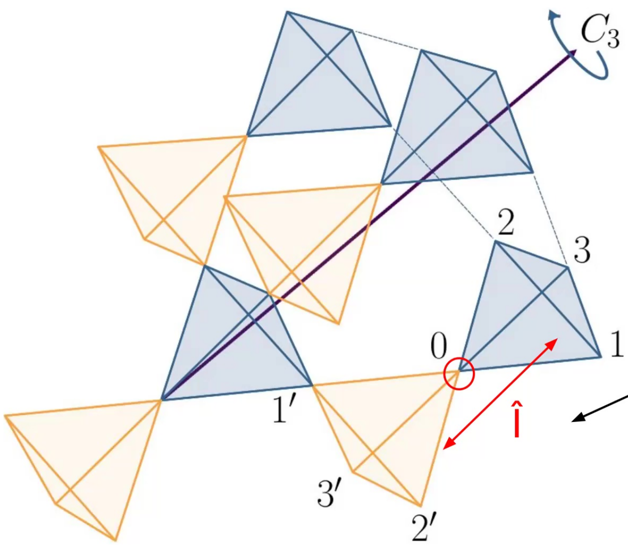


- Cubic arrangement of tetrahedra
- Corner sharing → frustration
- Symmetries include:

  1) rotation (`easy-axis'')

  2) inversion (up ↔ down)

Pyrochlore system



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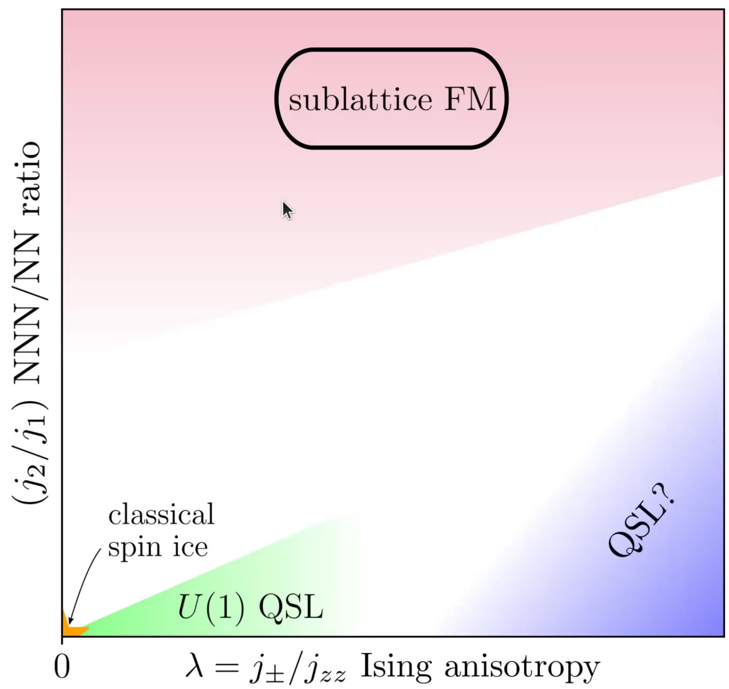
$$\hat{H} = j_1 \sum_{\langle i,j \rangle - \mathrm{NN}} \hat{h}_\lambda(i,j) + j_2 \sum_{\langle\langle i,j \rangle\rangle - \mathrm{NNN}} \hat{h}_\lambda(i,j)$$

$$\hat{h}_\lambda(i,j) = \frac{\lambda}{2}\left(\hat{S}_i^+\hat{S}_j^- + \hat{S}_j^+\hat{S}_i^-\right) + \hat{S}_i^z\hat{S}_j^z,$$

spin anisotropy [SU(2) ↔$U_z(1)$] due to **"easy axis"**


sublattice FM
(j_2/j_1) NNN/NN ratio
classical
spin ice
$U(1)$ QSL
QSL?
0
$\lambda = j_\pm/j_{zz}$ Ising anisotropy

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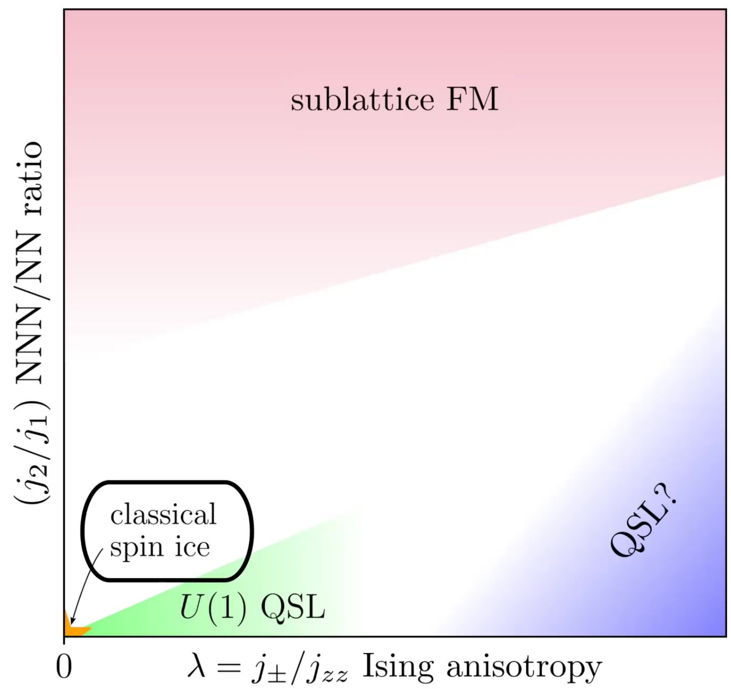
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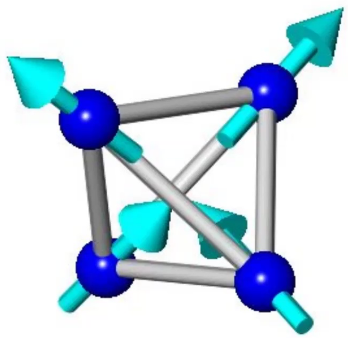
λ = 0: spin ice rule

- Spin-ice: **two up, two down rule**, gap 2 j_{zz}

$$\hat{H}_0 = j_{zz} \sum_{\text{tetr.}} \left(\sum_{i \in \text{tetr.}} \hat{S}_i^z \right)^2$$



Hermele et al., PRB (2004), Savary PRB (2012)

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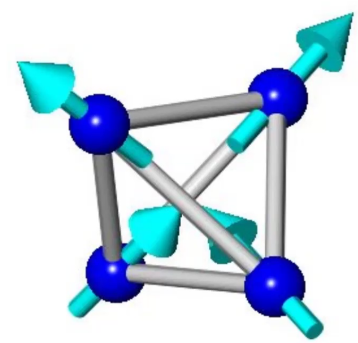


- At λ = 0 residual entropy

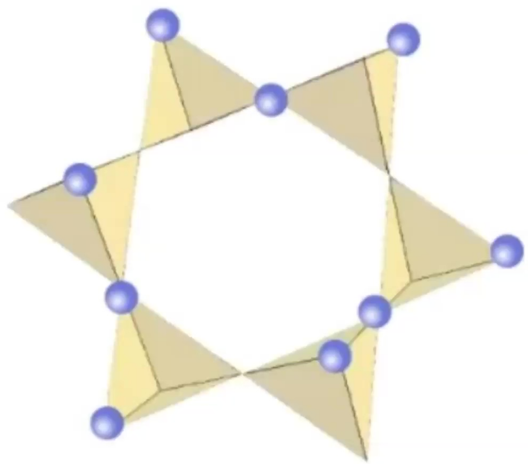
$$S = \frac{k_\mathrm{B}}{2} \log \frac{3}{2}$$

Hermele et al., PRB (2004), Savary PRB (2012)

Low-λ: mapping to EM

$$\hat{H}_0 = j_{zz} \sum_{\text{tetr.}} \left(\sum_{i \in \text{tetr.}} \hat{S}_i^z \right)^2$$

$$\hat{H}_1 = \underbrace{\lambda j_{zz}}_{j_\pm} \sum_{\langle i,j \rangle \in \text{NN}} \left(\hat{S}_i^+ \hat{S}_i^- + \text{h.c.} \right)$$



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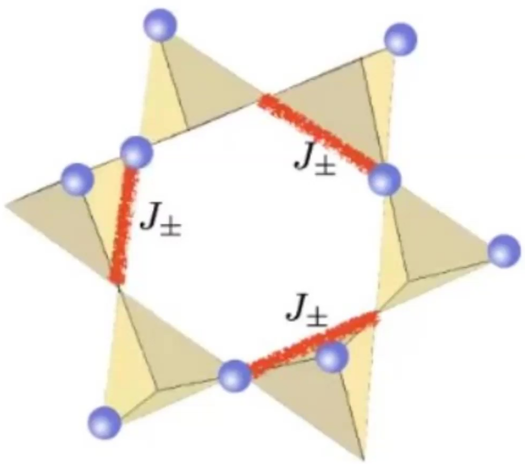
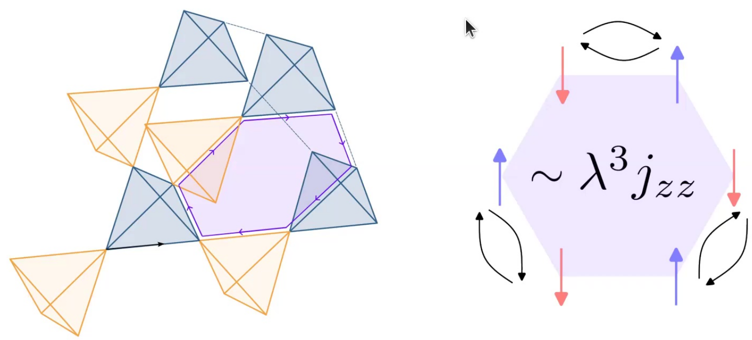


$$\hat{H}_{\text{spin ice}} = K \sum_{\text{hex.}} \left(\hat{S}_1^+ \hat{S}_2^- \hat{S}_3^+ \hat{S}_4^- \hat{S}_5^+ \hat{S}_6^- + \text{h.c.} \right)$$

$$K = \lambda^3 j_{zz}$$

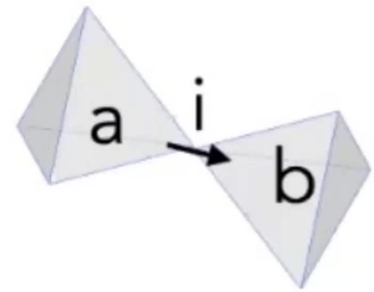


Hermele et al., PRB (2004), Savary PRB (2012)

Compact U(1) gauge theory

- Gauge fields:

$$\hat{S}_i^z = \hat{E}_{ab}$$
$$\hat{S}_i^\pm = e^{\pm i \hat{A}_{ab}}$$



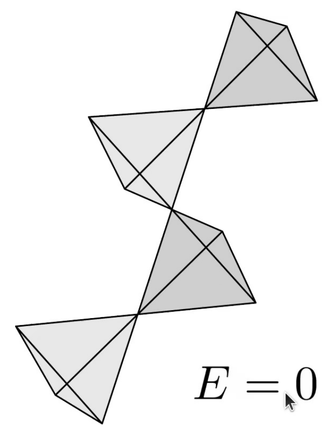
Hermele et al., PRB (2004), Savary PRB (2012)

U(1) QSL

- Deconfined phase: **textbook** Hamiltonian

$$\hat{H}_{\text{EM}} \approx U \sum_{\langle a,b \rangle} (E_{ab}^2 - 1/4) + K/2 \sum_{\text{hex.}} \underbrace{(\text{curl}\vec{A})^2}_{\vec{B}^2}$$

- Quasiparticles:
  - Gapped fractionalized **spinon**



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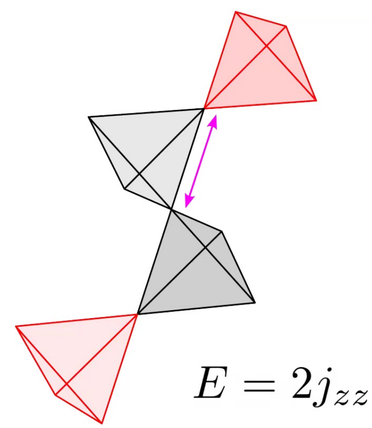

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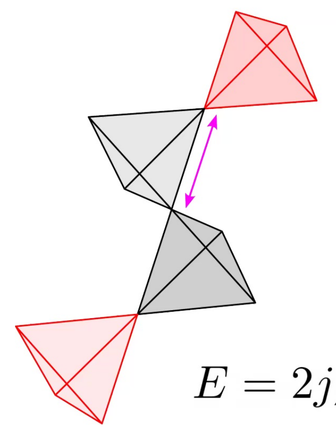
- **Electric flux = topological order**



$E = 2j_{zz}$

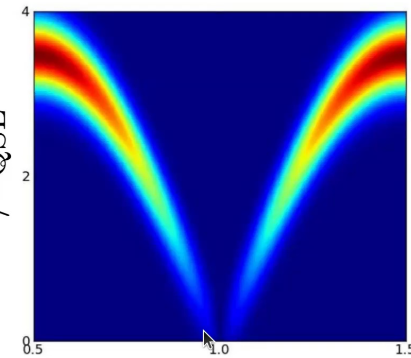
Hermele et al., PRB (2004), Savary PRB (2012)

Expected experimental signatures

- Photon in inelastic neutron scattering (prediction)

$$\langle \hat{S}^z_{\boldsymbol{k}} \hat{S}^z_{-\boldsymbol{k}} \rangle \propto |\boldsymbol{k}| \delta(\omega - c_{\mathrm{QSL}} |\boldsymbol{k}|)$$

- |**k**| weight, **small velocity** $c_{\mathrm{QSL}} \propto \lambda^{3/2}$

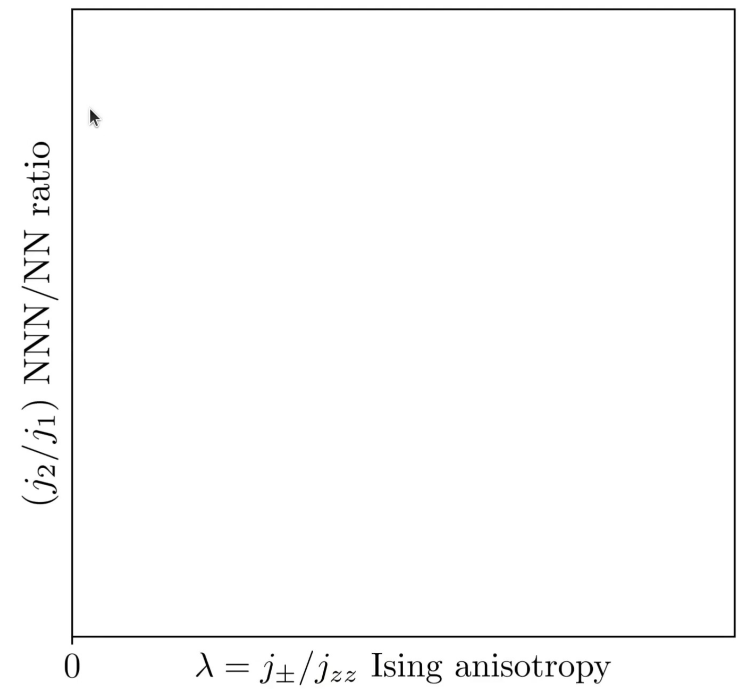


$\omega a / c_{\mathrm{QSL}}$

$\boldsymbol{k} = (h, h, h)$

Owen Benton et al., PRB (2012), K. Ross et al., 2011, Y. Takiwa et. al 2018

Rich phase diagram



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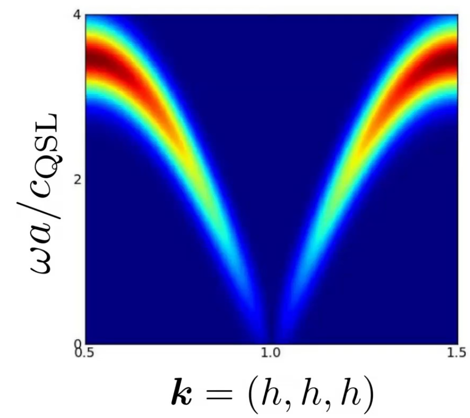
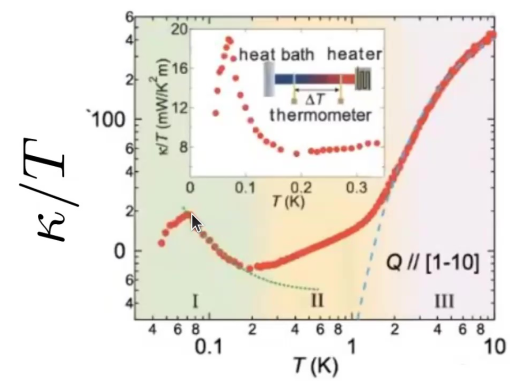
- Specific heat

$$C_{\mathrm{photon}} \propto (T/c_{\mathrm{QSL}})^3$$





Owen Benton et al., PRB (2012), K. Ross et al., 2011, Y. Takiwa et. al 2018

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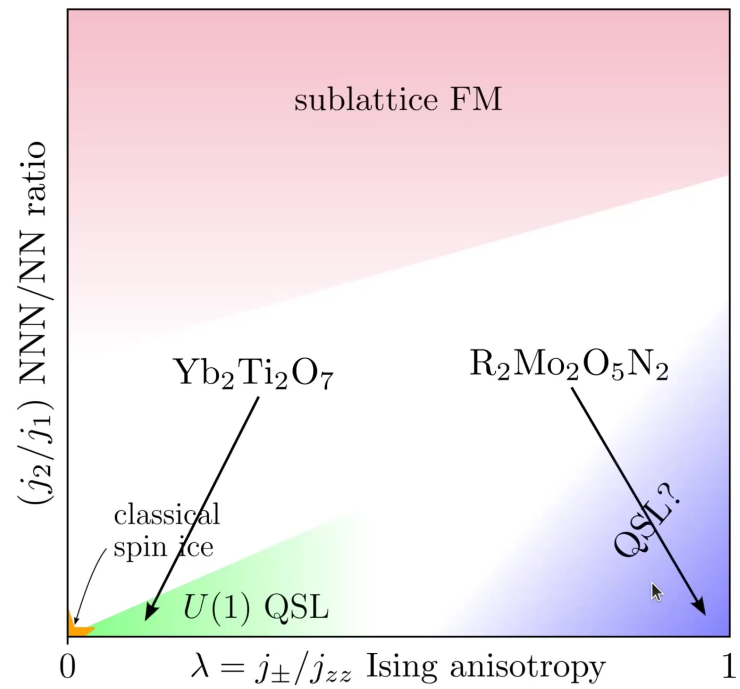
Rich phase diagram

- Large $j_2 / j_1 \longrightarrow$ ordered submattice FM
  [Iqbal PRX 2019]
- $\lambda \ll 1$: U(1) QSL and spin ice
  [Hermele PRB 2004, Savary 2012]
- $\lambda = 1$, $j_2 / j_1 = 0$ — spin liquid?



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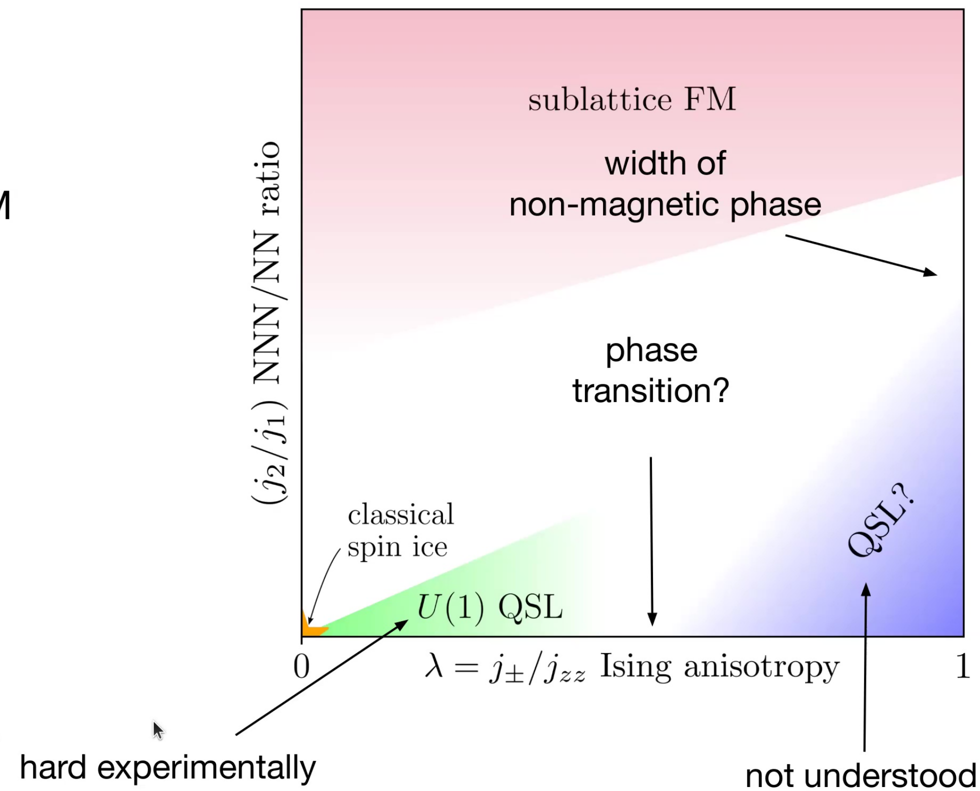

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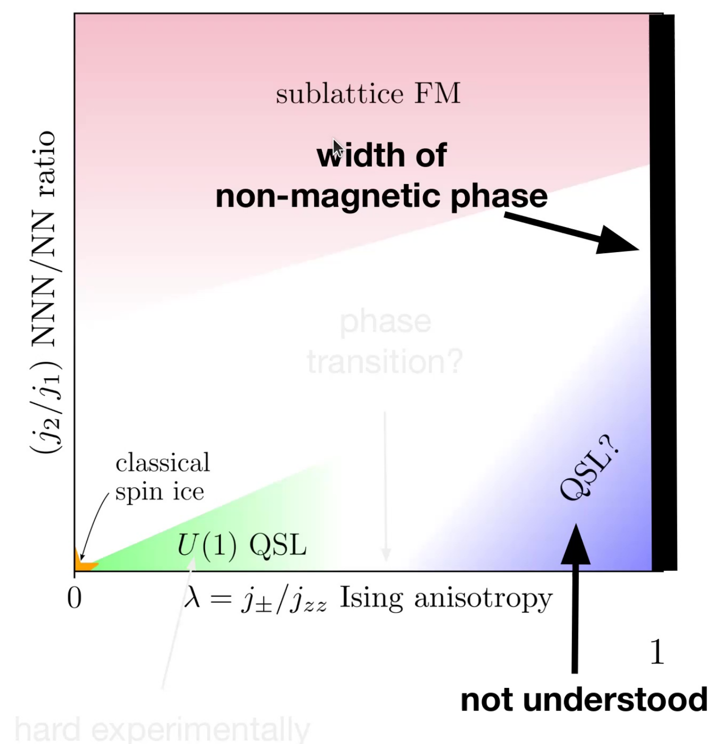
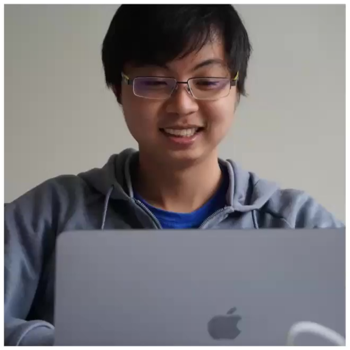


Titus Neupert (UZH)

Giuseppe Carleo (EPFL)

Mark H. Fischer (UZH)

Tom Westerhout (Radboud)



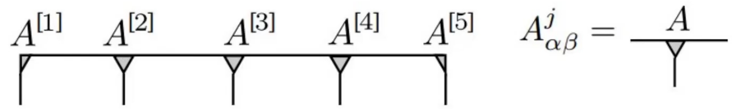
Kenny Choo (UZH → Hudson River Trading)

Apoorv Tiwari (UZH → KTH Stockholm)

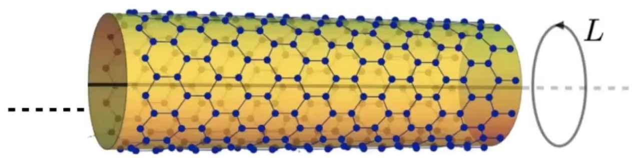
Numerics of frustrated magnets

- **1D**: ED (up to ~50 spins) or DMRG

$\psi_{j_1,j_2,j_3,j_4,j_5} \approx$



- **2D**: DMRG on **tube geometries**



Jiang et al., Nat. Phys. (2012), M. Fannes et al., 1992, Schuch et al., 2008

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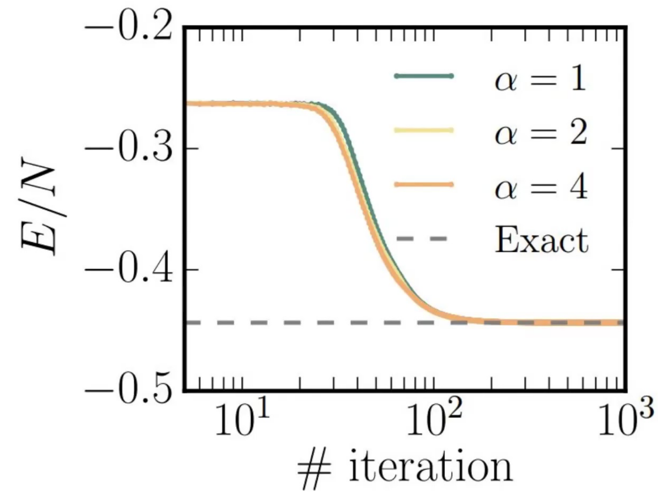
Variational Monte Carlo

- Variational principle

$$E_{\rm GS} \leqslant E_{\rm var.}(\boldsymbol{\theta}) = \langle \psi(\boldsymbol{\theta}) | \hat{H} | \psi(\boldsymbol{\theta}) \rangle$$

- **Quality** = smallness of energy
- Need ansätze that **capture** pyrochlore physics!



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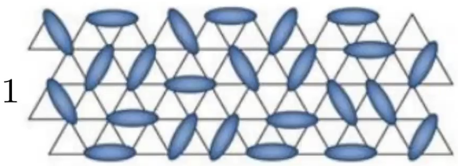
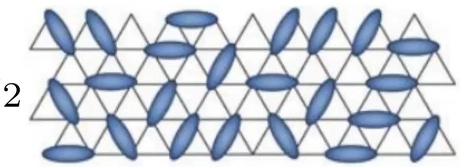
RVB-inspired Ansatz

- Choice of amplitudes — different QSLs!
- **Compress** the wave function

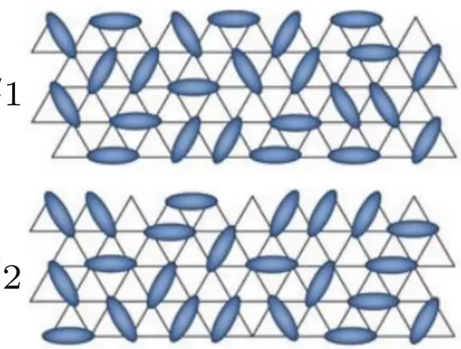
$|\Psi\rangle = \alpha_1$ 

$+\alpha_2$  $+ \ldots$

RVB-inspired Ansatz

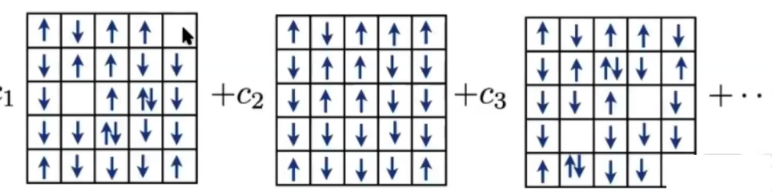
- Choice of amplitudes — different QSLs!
- **Compress** the wave function
- Occupy FS of a non-interacting **band "parton" model**

$$|\Psi\rangle = \alpha_1 \quad + \alpha_2 \quad + \ldots$$



$$|\Psi\rangle = \sum_{\boldsymbol{k} \in \mathrm{FS}} c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{\boldsymbol{k}\downarrow} |0\rangle$$

$$= c_1 \quad + c_2 \quad + c_3 \quad + \cdots$$



Variational ansätze (bias control)

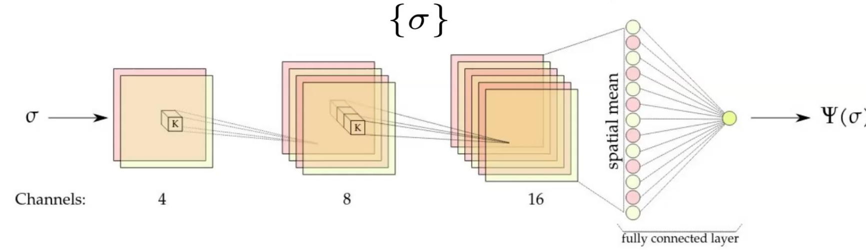
RVB
[*Misawa, Com. Phys. Comm. 2019*]

$$|\phi_{\rm pair}\rangle = \mathcal{P}_{\rm G}^{\infty} \exp\left(\sum_{i,j} f_{i,j}\hat{c}_{i,\uparrow}^{\dagger}\hat{c}_{j\downarrow}^{\dagger}\right)|0\rangle,$$

Neural quantum states
[*Carleo, Science 2017*]

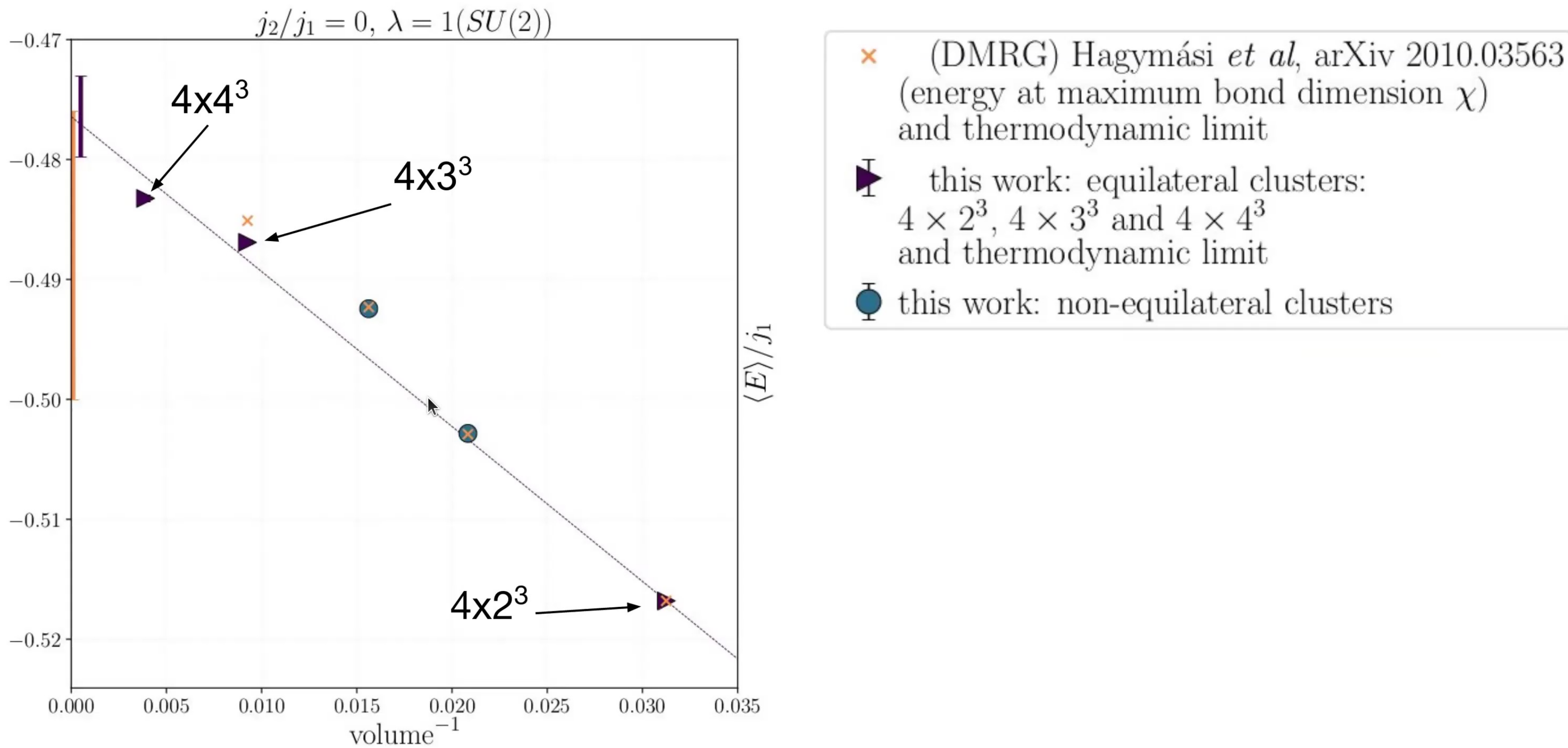
Ψ(σ) – neural network [σ⟶ Ψ(σ)]

$$|\psi_{\rm NN}\rangle = \sum_{\{\sigma\}} \Psi(\sigma)|\sigma\rangle$$



Spin, momentum, point group symmetry quantum number ξ projection: $|\psi_{\xi}\rangle = \sum_{n} \xi^{n}\hat{G}^{n}|\psi\rangle,$

Competitive energies!



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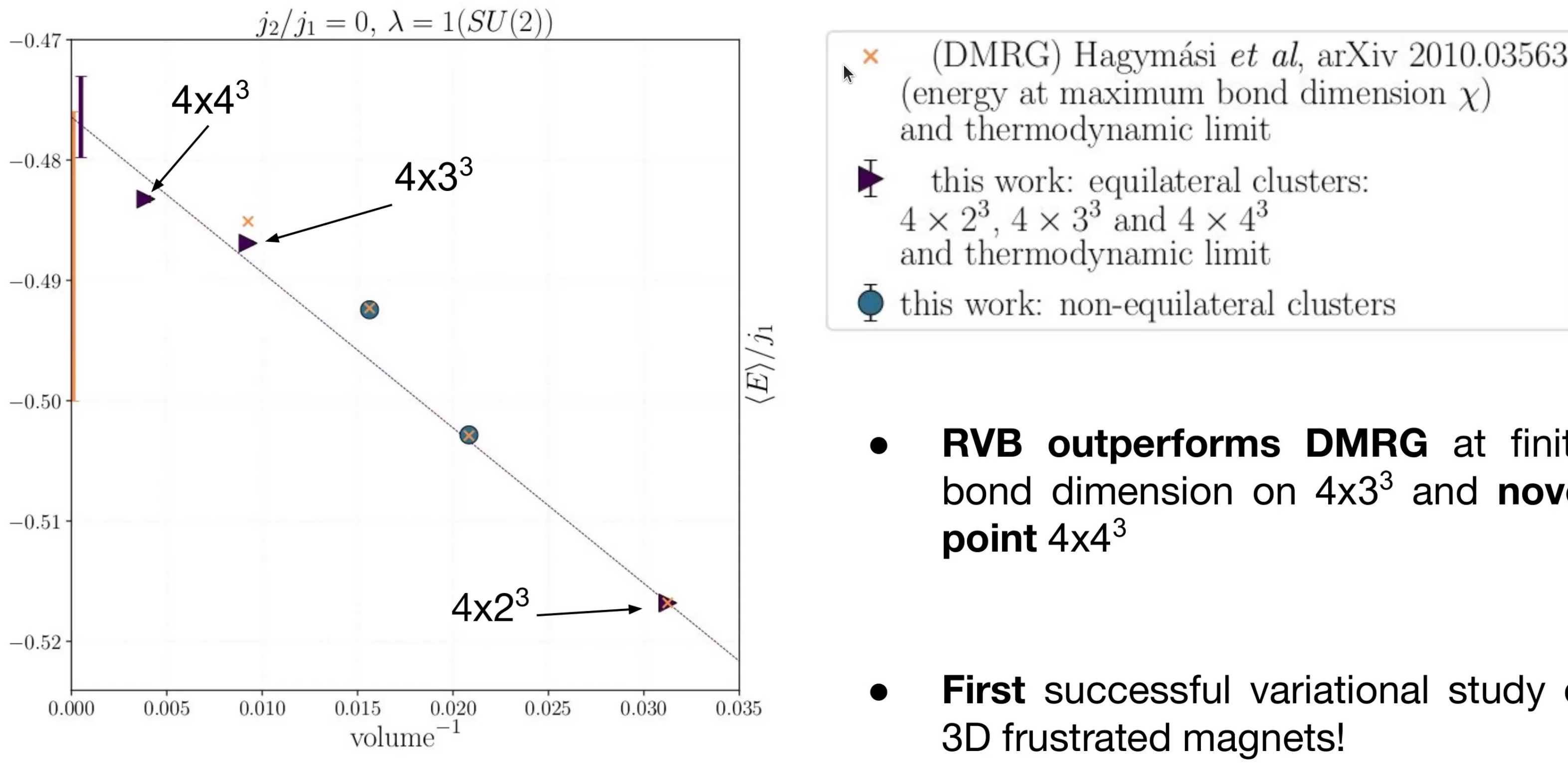


- **RVB outperforms DMRG** at finite bond dimension on 4x3^3 and **novel point** 4x4^3

- **First** successful variational study of 3D frustrated magnets!

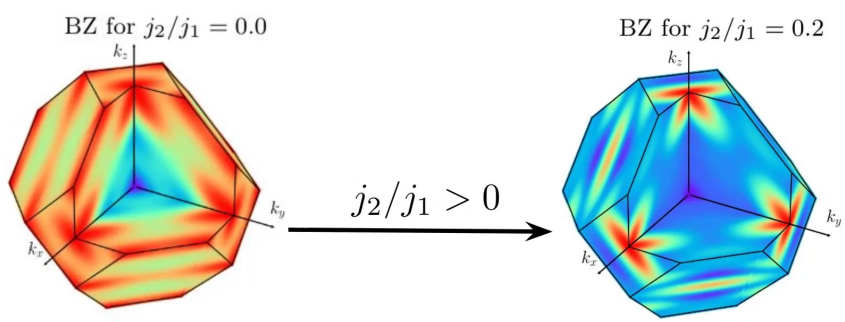
Magnetic order

- **k**-dependent magnetic wave operator

$$\hat{M}(\mathbf{k}) = \frac{1}{\Omega} \sum_i \hat{S}_i^z e^{i\mathbf{k}\mathbf{r}_i},$$

- Magnetic susceptibility

$$\chi_{M_{\mathbf{k}}} = \langle M^\dagger(\mathbf{k}) M(\mathbf{k}) \rangle$$



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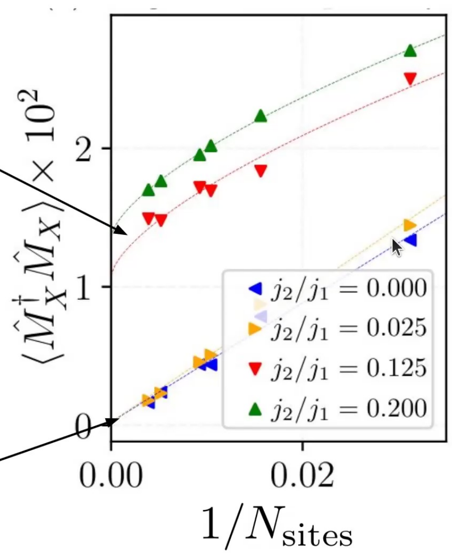
Thermodynamic Limit

non-zero in magnetic phase



zero in non-magnetic phase

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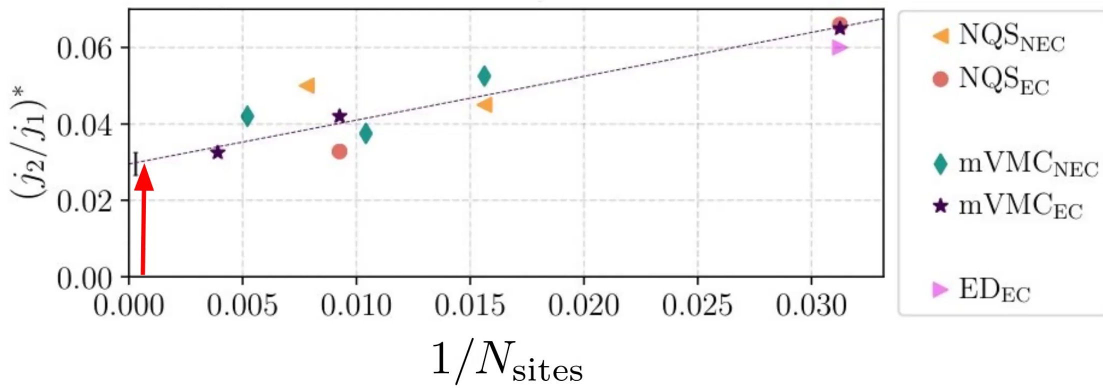
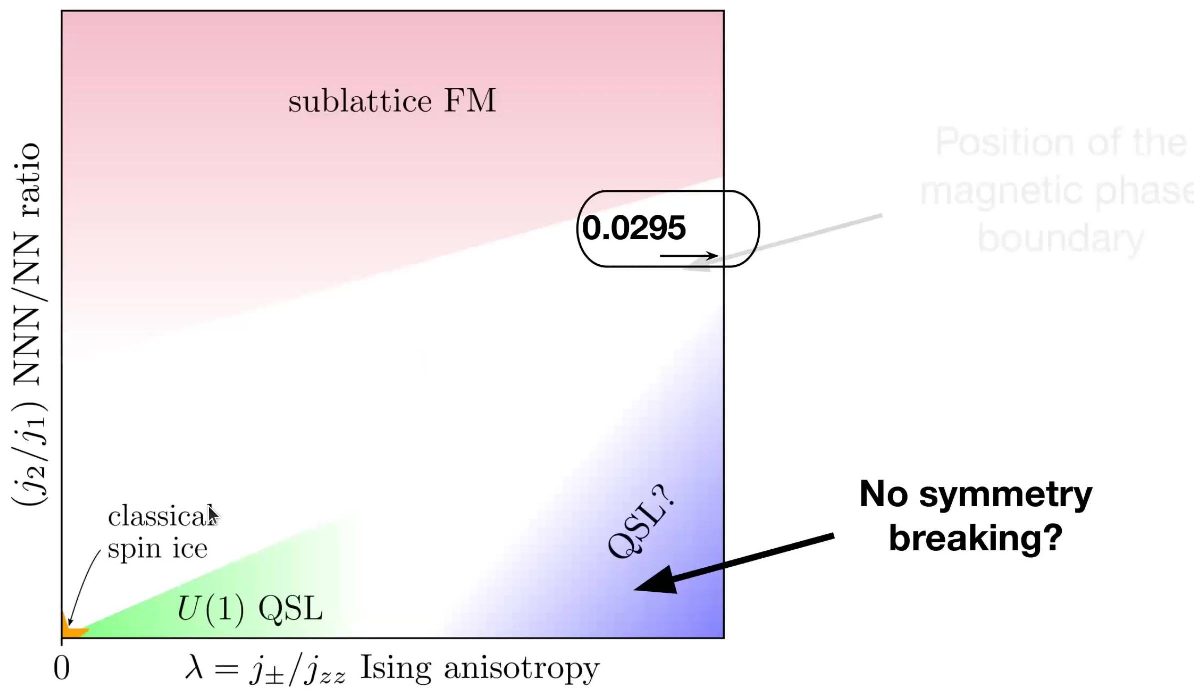
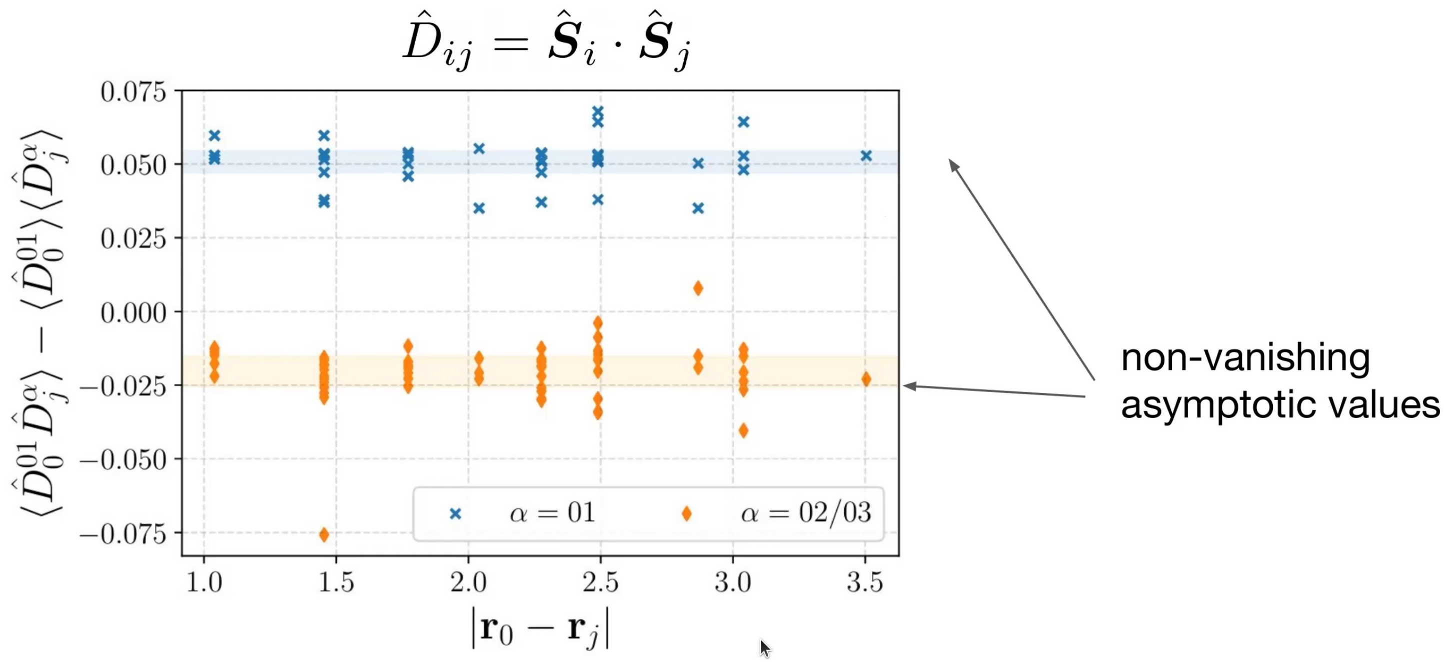
Non-magnetic phase width is finite!



- Non-magnetic phase **shrinks x7 times** w.r.t. PFRG
- Two VMC methods **agree**
- Phase width is **finite**


sublattice FM
0.0295
Position of the magnetic phase boundary
(j_2/j_1) NNN/NN ratio
classical spin ice
$U(1)$ QSL
QSL?
0
$\lambda = j_\pm/j_{zz}$ Ising anisotropy
No symmetry breaking?

Dimer-dimer correlations



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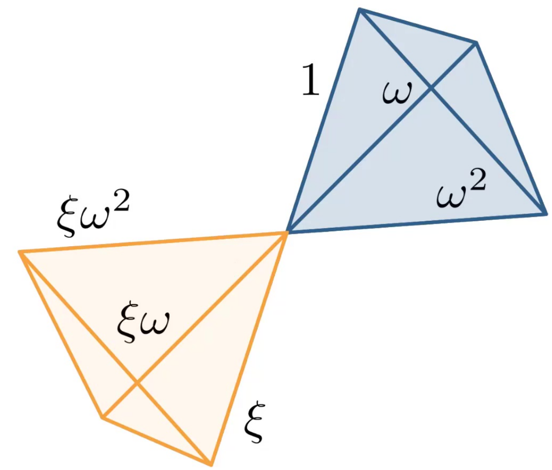
Dimer order parameter

- Dimer operators

$$\hat{\mathcal{O}}(\xi,\omega) = \frac{1}{3\Omega}\sum_{\langle i,j\rangle} q_{i,j}(\xi,\omega)\,\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j,$$

- Quantum numbers
  ξ = {-1, +1}
  ω = {1, exp(-2 π i / 3), exp(+2 π i / 3)}

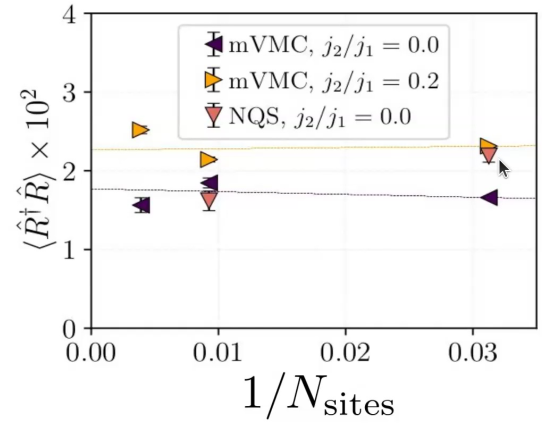
- Î = Ô(**ξ = -1**, ω = 1) ⟶ inversion
  R̂ = Ô(ξ = +1, **ω = exp(2 π i / 3)**) ⟶ rotation



Dimer order

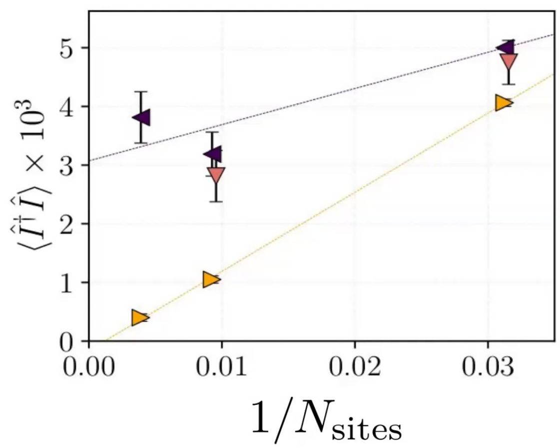
Rotation $\chi_R = \langle \hat{R}^\dagger \hat{R} \rangle$:

- k = 0: finite
- non-magnetic: finite



Inversion $\chi_{\hat{I}} = \langle \hat{I}^\dagger \hat{I} \rangle$:

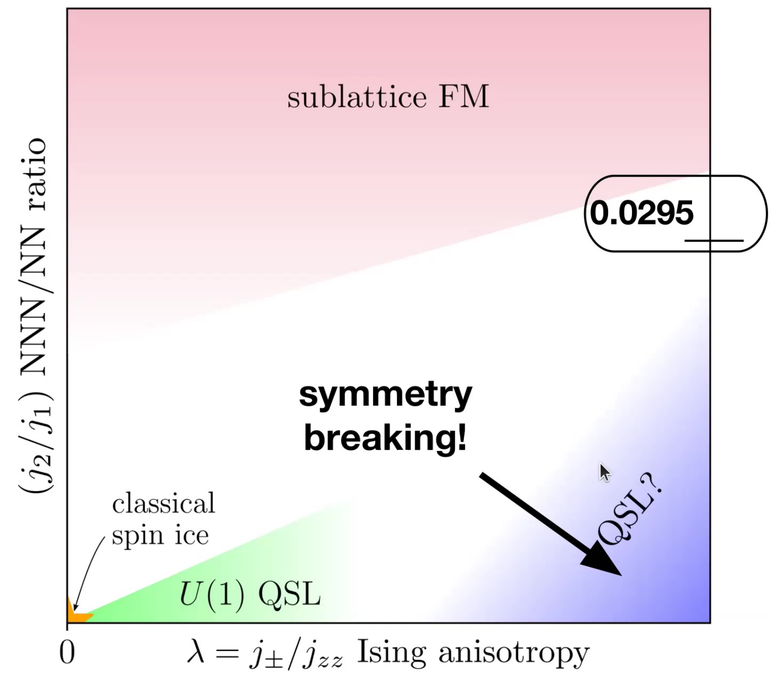
- k = 0: vanishes
- non-magnetic: finite



Classical study yields surprising results!

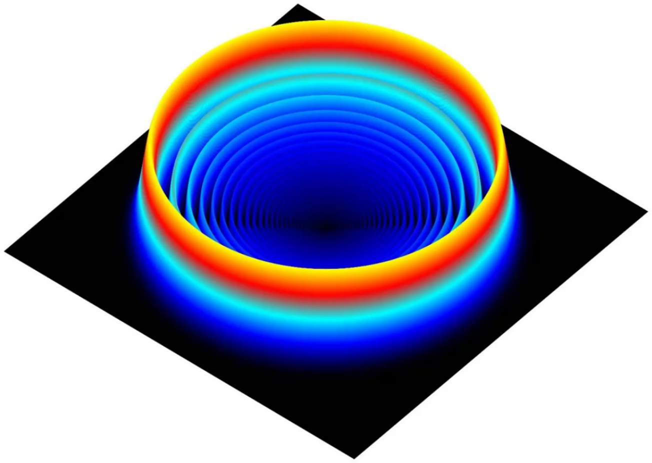
- Phase boundary shrinks to $\mathbf{j_2/j_1 = 0.0295(30)}$**!**
- **Symmetry-breaking** at $j_2/j_1 = 0 \rightarrow$ not a QSL?
- Variational Monte Carlo applied **first time** to a frustrated 3D magnet → competitive energies

*[**NA** et al, PRX 2021]*



Rydberg atoms

- Large **principal number** n
- Coherence times $\tau \sim n^3$
- Van der Waals $V_{\mathrm{vdW}}(r) \propto \frac{n^{11}}{r^6}$
- Dipole-dipole $V_{\mathrm{ddi}}(r) \propto \frac{n^4}{r^3}$



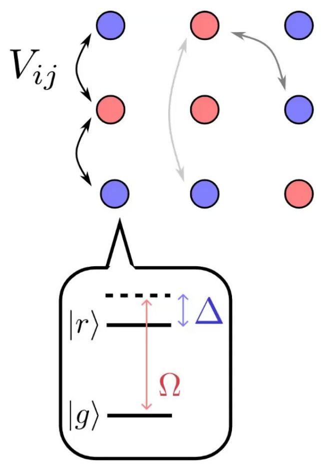
Jaksch et al., PRL (2000), M. Lukin et al., PRL (2001)

Programmable Rydberg Atom Simulator

- Sengupta-Sachdev (Ω – Rabi frequency, $\mathbf{\Delta}$ – laser detuning)

$$\hat{H} = \frac{\Omega}{2} \sum_{i \leqslant N} (|g_i\rangle\langle r_i| + \text{h.c.}) - \Delta \sum_{i \leqslant N} \hat{n}_i + \frac{1}{2} \sum_{i,j \leqslant N} V_{ij} \hat{n}_i \hat{n}_j,$$

$$\hat{n}_i|r_i\rangle = |r_i\rangle, \hat{n}_i|g_i\rangle = 0$$



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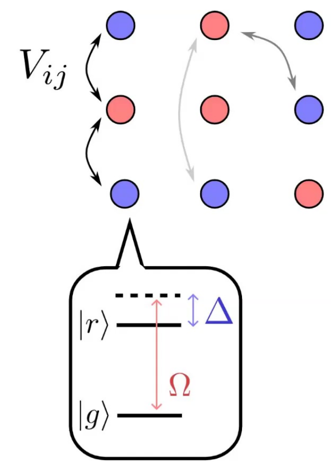
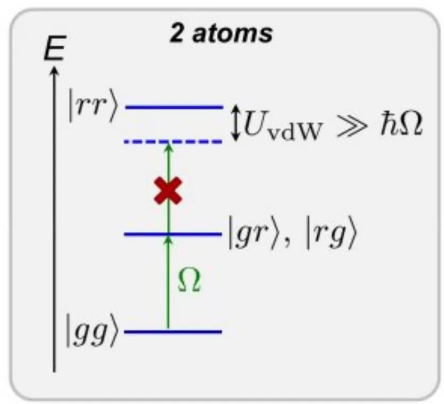


- **Rydberg blockade ⟶** no simultaneous excitement



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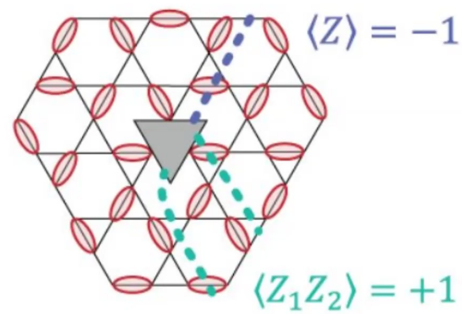
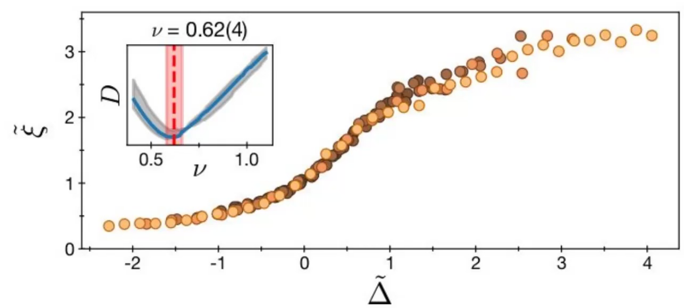
Recent highlights

- **Z_2 Kitaev QSL on the kagome lattice**
  [Semeghini et al., Science (2021)]



- **Critical exponent of the quantum Ising universality class in (2+1)**
  [Ebadi et al., Nature (2021)]

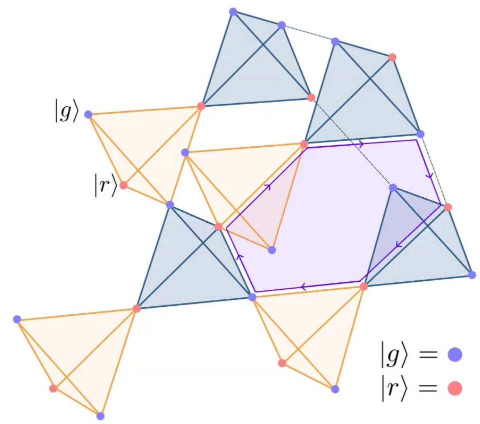


- **Quantum Approximate Optimization Algorithm**
  [Ebadi et al., Science (2022)]

U(1) QSL and Rydberg Atoms

- V(i,j) = {U for NN, 0 otherwise},
  $\mathbf{\Delta}$ = 3 U → **spin ice rule**

$$\hat{H}(\Omega = 0) = U \sum_{\text{tetr.}} \left(\sum_{i \in \text{tetr.}} \hat{n}_i - 2 \right)^2$$



NA et al., in progress

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Quantum Monte Carlo

- "Time" dimension to **decompose** $\Omega\, \sigma_x$
- (3+1)–dim. **classical** partition function
- Finite temperature – experimentally-relevant

$$\mathcal{Z} = \sum_{\{\alpha_{\rm cl}\}} \langle \alpha_{\rm cl} | e^{-\beta \hat{H}_{\rm cl.}} | \alpha_{\rm cl} \rangle, \text{ with}$$

$$\hat{H}_{\rm cl.} = \frac{1}{N_I} \sum_{a=0}^{N_I-1} \left(\sum_{i<j} V_{ij} n_{i,a} n_{j,a} - \Delta \sum_i n_{i,a} - \right.$$

$$\left. - \frac{N_I}{\beta} \log\coth\left(\frac{\beta\Omega}{2N_I}\right) \sum_i \sigma^z_{i,a} \sigma^z_{i,a+1}. \right)$$

Kalinowski et al., PRB (2022)

Quantum Monte Carlo

- "Time" dimension to **decompose** $\Omega\,\sigma_x$
- (3+1)–dim. **classical** partition function
- Finite temperature – experimentally-relevant
- NNN ordering requires large Ω – but higher-order flips?

$$\mathcal{Z} = \sum_{\{\alpha_{\rm cl}\}} \langle \alpha_{\rm cl} | e^{-\beta \hat{H}_{\rm cl.}} | \alpha_{\rm cl} \rangle, \text{ with}$$

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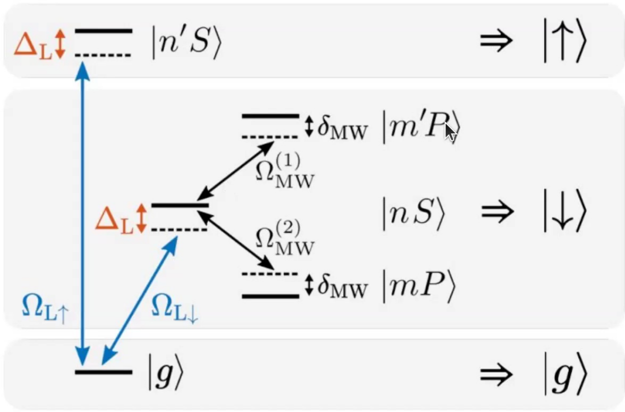
Kalinowski et al., PRB (2022)

Full λ axis accessible!

- **Admixing** Rydbergs with S and P parities
  [Jong Yeon Lee et al., arXiv:2207.08829]

$$\hat{H}_{\text{eff}} = \frac{C_6}{r^6} \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z + \frac{C_3}{r^3} \sum_{\langle i,j \rangle} \left(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y \right)$$



NA et al., in progress

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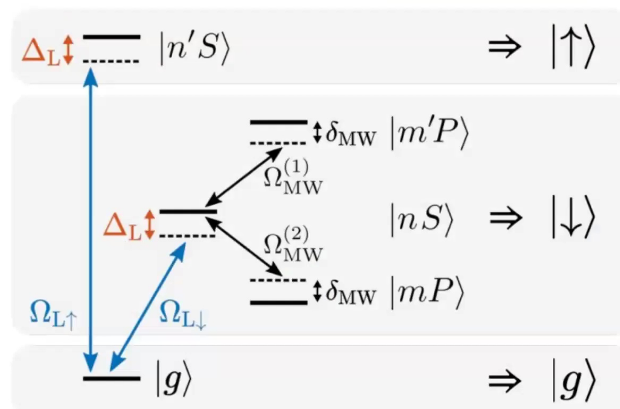
- Ising anisotropy **in a wide range**

$$\lambda = r^3 (C_3/C_6)$$

- **Whole λ–axis accessed!**



NA et al., in progress

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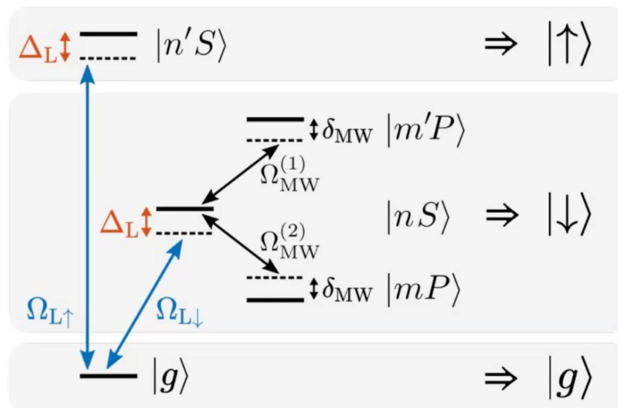
- Ising anisotropy **in a wide range**

$$\lambda = r^3 (C_3/C_6)$$

- **Whole λ–axis accessed!**

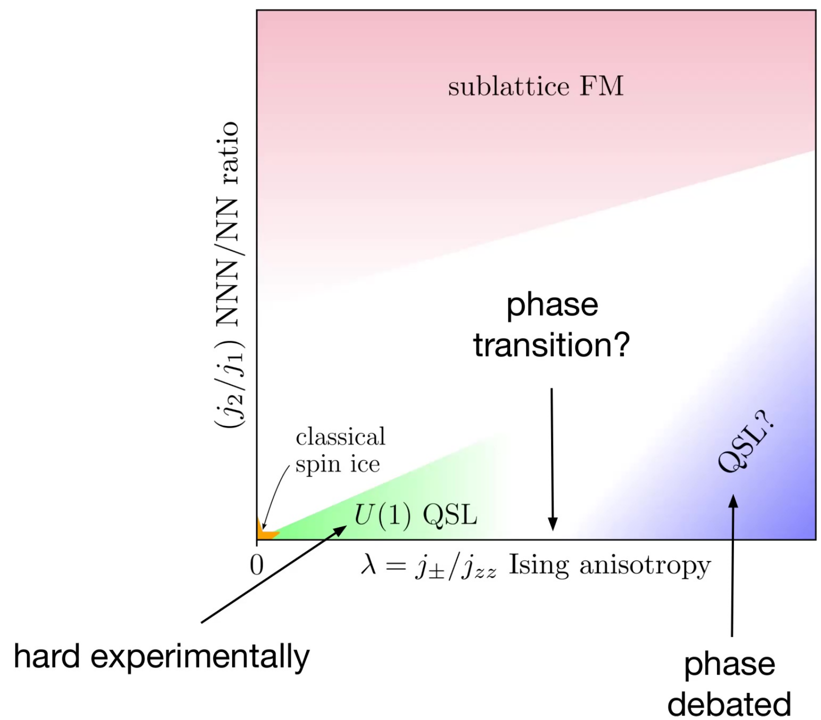
- Creating admixture having right anisotropy?



NA et al., in progress

Rydberg atoms can simulate pyrochlore physics!

- Two **complementary embeddings** to solve the λ–axis
- Finite-T QMC study for the experiment
- **Test on a real Rydberg device?**



NA et al., in progress