Triangular lattice antiferromagnets

Modelling ground states and excitations of strongly-correlated matter

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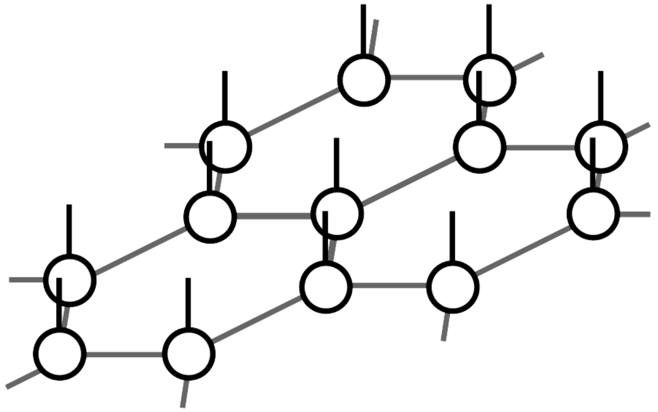
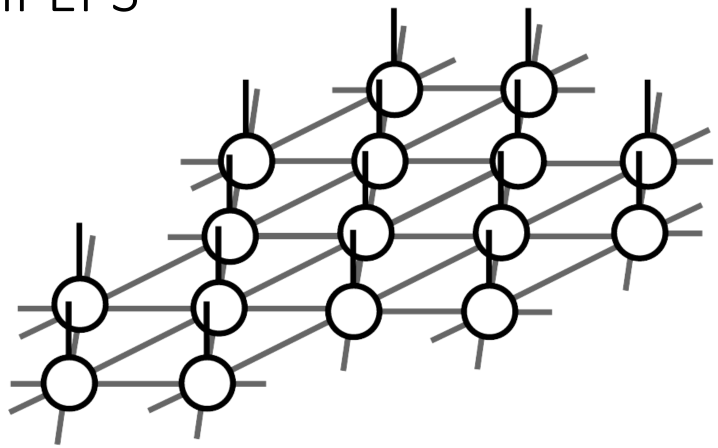
Outline

1. Motivations
2. Introduction to infinite tensor network states
3. Application
   - Incommensurate order with translationally invariant iPEPS
   - Excitations in XXZ model on triangular lattice





Optimizing **tensor contractions** for scientific applications

- quantum chemistry
- tensor networks
- QC simulations
- ML / NN and more

Goal: hardware/software support of your use cases by vendors:

NVIDIA AMD intel

Go to survey

https://forms.office.com/e/qeJFNWe4zX

Many-body electron problem – *ab initio*

$$\hat{H} = \sum_{I=1}^{N_a} \frac{\hat{P}_I}{2M_I} + \sum_{i=1}^{N_e} \frac{\hat{p}_I}{2m_e} - \sum_{I,i} \frac{Z_I e^2}{|\hat{r}_i - \hat{R}_I|} + \sum_{i>j} \frac{e^2}{|\hat{r}_i - \hat{r}_j|} + \sum_{I>J} \frac{Z_I Z_J e^2}{|\hat{R}_i - \hat{R}_j|}$$

We aim to understand the **phases** (ground states), **transitions** (universality), and **dynamics**

- Classically – state of the system given by $O(\boldsymbol{N})$ data
- Quantum mechanics – instead $\boldsymbol{O(exp(N))}$ is required

Many-body electron problem – *ab initio*

$$\hat{H} = \sum_{I=1}^{N_a} \frac{\hat{P}_I}{2M_I} + \sum_{i=1}^{N_e} \frac{\hat{p}_I}{2m_e} - \sum_{I,i} \frac{Z_I e^2}{|\hat{r}_i - \hat{R}_I|} + \sum_{i>j} \frac{e^2}{|\hat{r}_i - \hat{r}_j|} + \sum_{I>J} \frac{Z_I Z_J e^2}{|\hat{R}_i - \hat{R}_j|}$$

"The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved. ..."

— Paul A. M. Dirac 'Quantum Mechanics of Many-Electron Systems', Proceedings of the Royal Society (1929), A, 123, 714-733.

Many-body electron problem – *ab initio*

"(cont.) It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation."

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Many-body electron problem – *ab initio*

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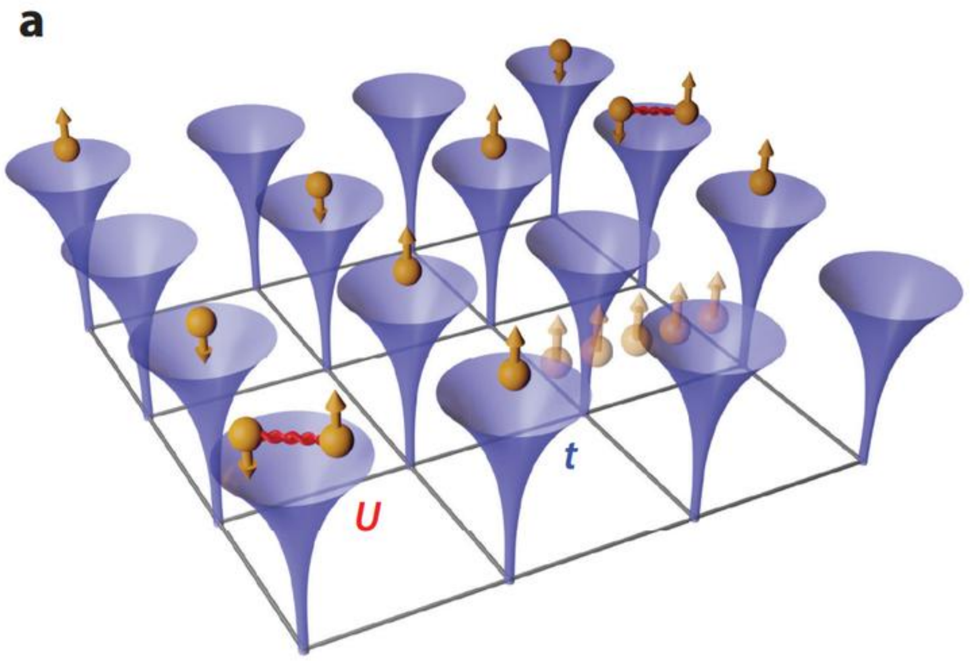
I. Fix nuclei: electrons move in an effective potential generated by static nuclei [Adiabatic approx.]

$$\hat{H}_{eff} = \sum_{i=1}^{N_e} \frac{\hat{p}_I}{2m_e} + \sum_{i>j} \frac{e^2}{|\hat{r}_i - \hat{r}_j|} + \sum_{i=1}^{N_e} V(\hat{r}_i)$$

II. Truncate: retain only **few orbitals per site** and **short-range** interactions

One example to rule them all: Cuprates



Annual Review of Cond. Mat. Phys. 2022

Effective lattice model:

single-band Hubbard model

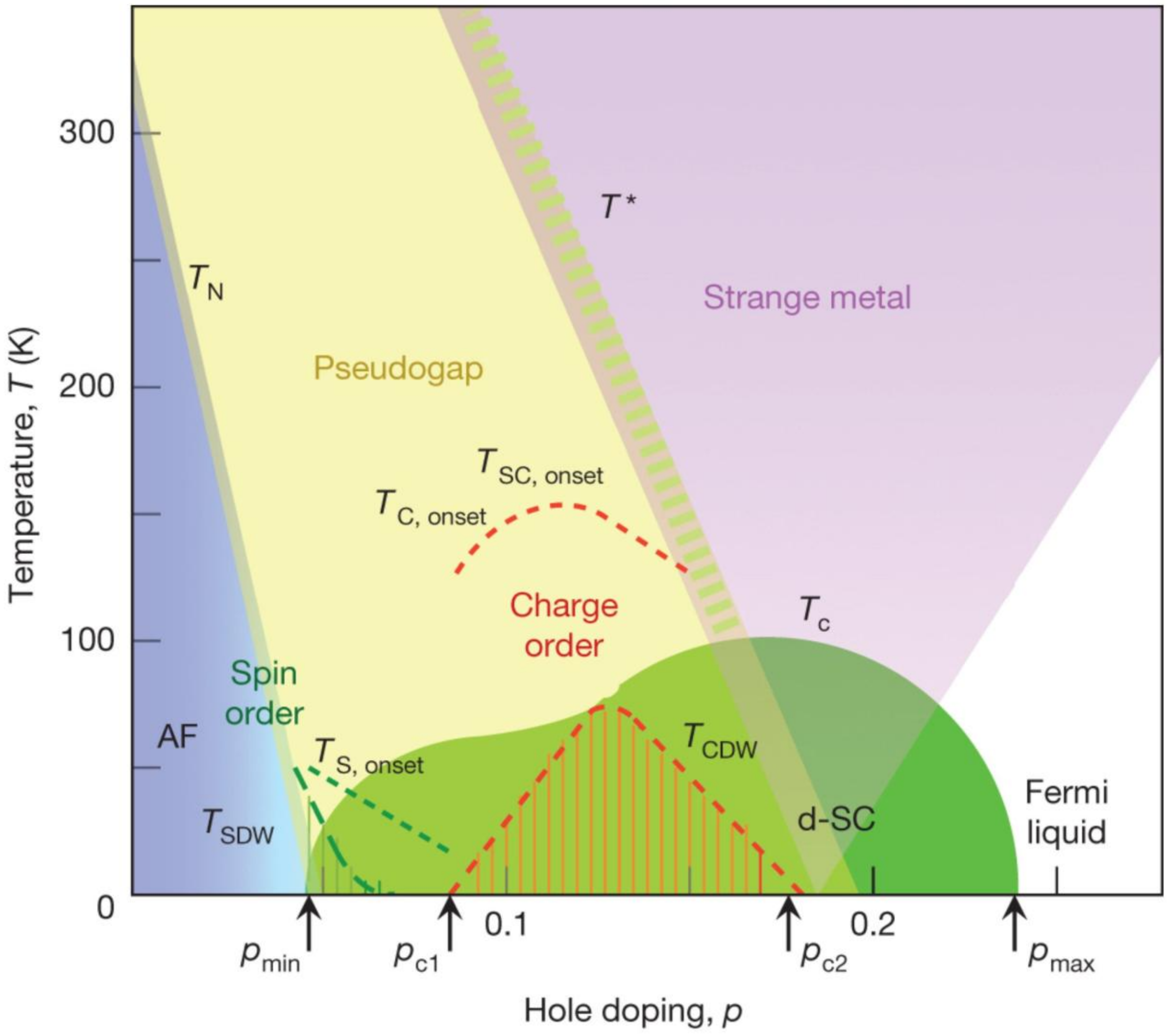
$$H = -t \sum_{\langle i,j \rangle,\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

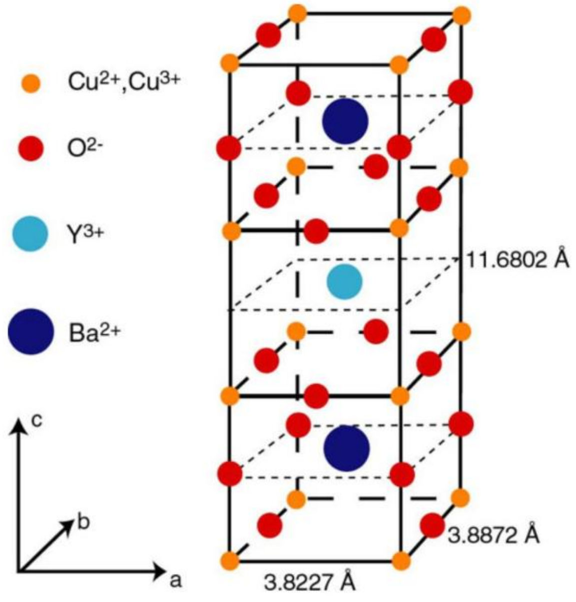
Or its **large-*U*** limit (and t' ...)

$$H = J \sum_{\langle i,j \rangle} S_i . S_j + J' \sum_{\langle\langle i,j \rangle\rangle} S_i . S_j + \dots$$

One example to rule them all: Cuprates

Keimer, Kivelson, Norman, Uchida, and Zaanen, *Nature* **518**, 179 (2015)





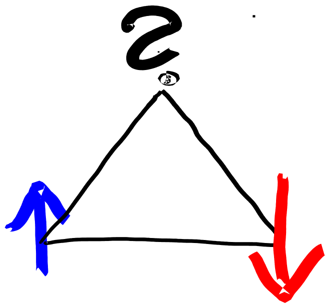
$YBa_2Cu_3O_{6+x}$

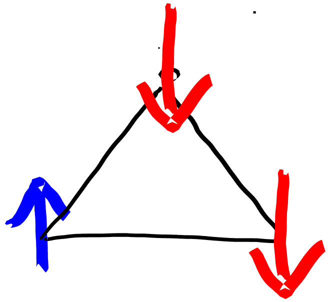
Triangular antiferromagnets

Ising antiferromagnet $J > 0$

$$H = J \sum_{\langle i,j \rangle} (S_i^z S_j^z)$$

- Classical example of **geometrical** frustration
- **Macroscopic degeneracy**: All tilings from





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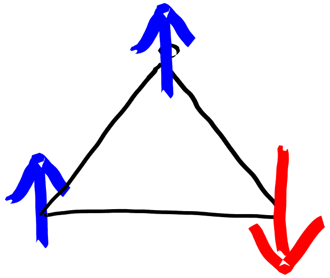


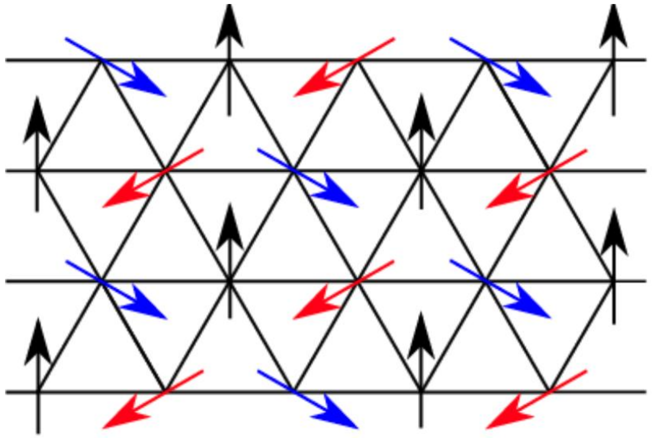
(and rotations)

Triangular antiferromagnets

Heisenberg spin-1/2 antiferromagnet $J > 0$

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

- Classically / Mean-field gives 120$^{\mathrm{o}}$ **order**



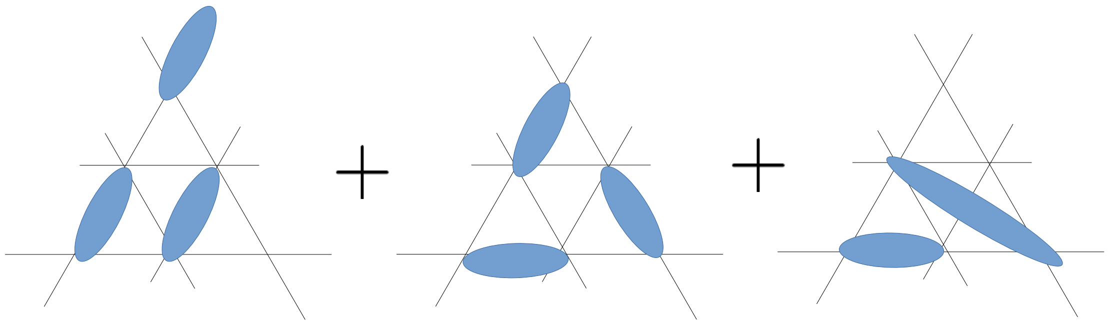
Triangular antiferromagnets

Heisenberg spin-1/2 antiferromagnet $J > 0$

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

- **Anderson**: Resonating Valence Bond (RVB) state

$$|\mathrm{RVB}\rangle = \sum_c \phi_c |c\rangle =$$



$$+ \dots$$

$$= |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$$

Triangular antiferromagnets

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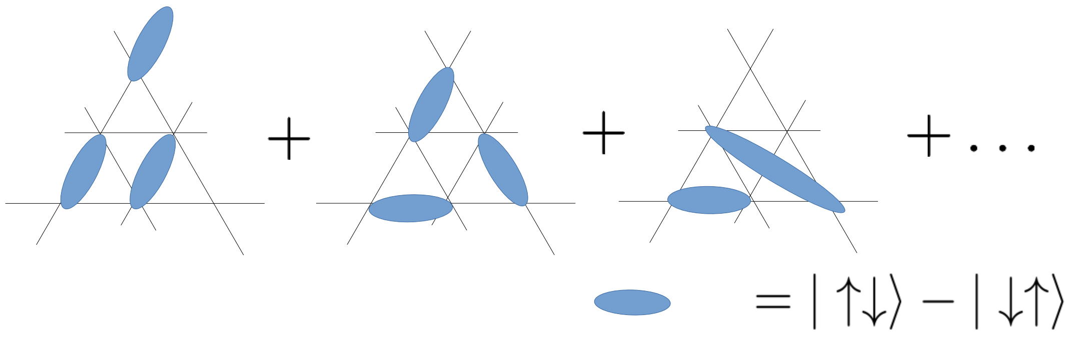
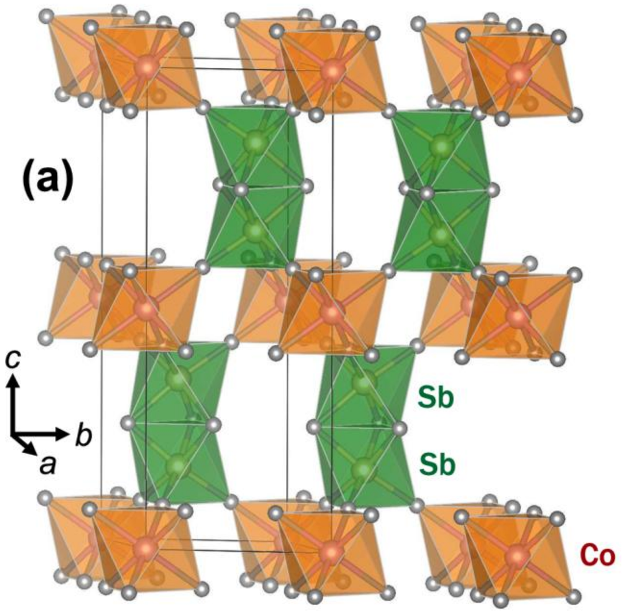


- **(Spin) Liquid: All symmetries are preserved**
- **Doped RVB – a mechanism of hole-doped high-Tc SC ?**

Triangular antiferromagnets: Gifts from Nature

Cobaltites: Co^{2+} in octahedral cage of Oxygens **"effective" spin-1/2**

$Ba_3CoSb_2O_9$



- **ideal TL** and mostly J_1 (XXZ)
- no Dzyaloshinskii–Moriya (DM)
- no Jahn-Teller
- easy plane (XY) or easy-axis (Ising)

Chernyshev, Pollica 2024;
Li, Gegenwart, and Tsirlin, J. Phys.: Condens. Matter 32, 224004 (2020)

Triangular antiferromagnets: Gifts from Nature

Cobaltites: Co^{2+} in octahedral cage of Oxygens **"effective" spin-1/2**

- **ideal TL** and mostly J_1 (XXZ)
- **120^o order**

$$H = J_1 \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z) + \cdots$$

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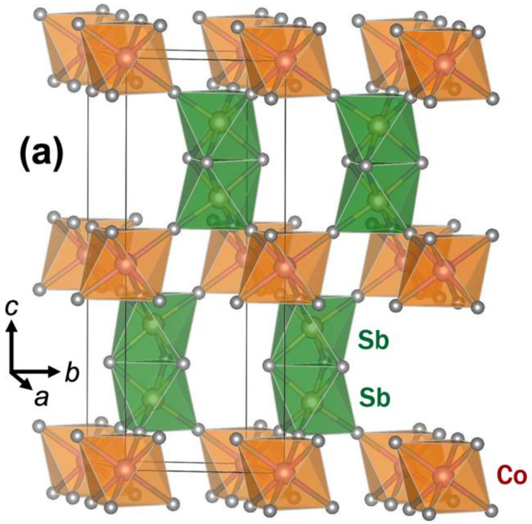

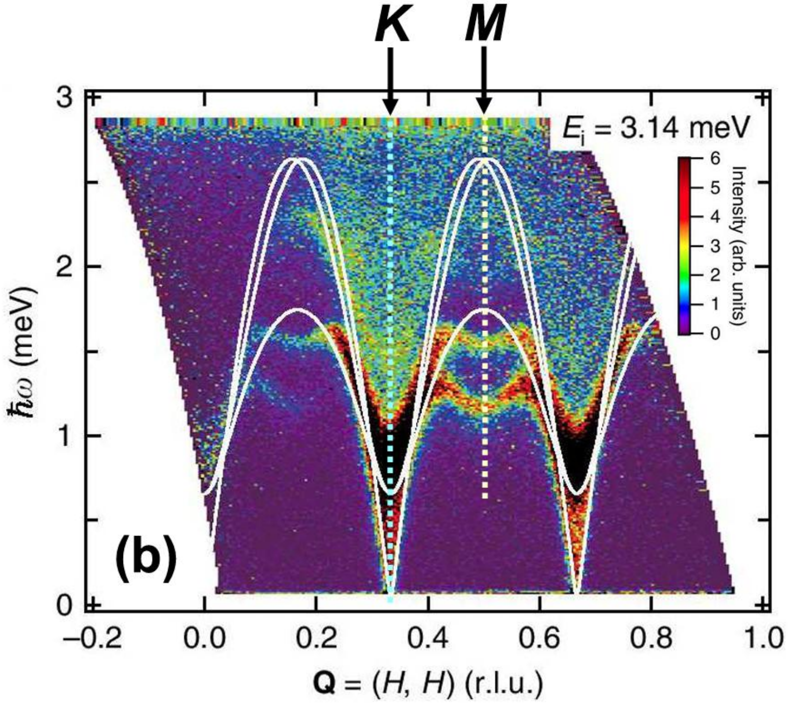

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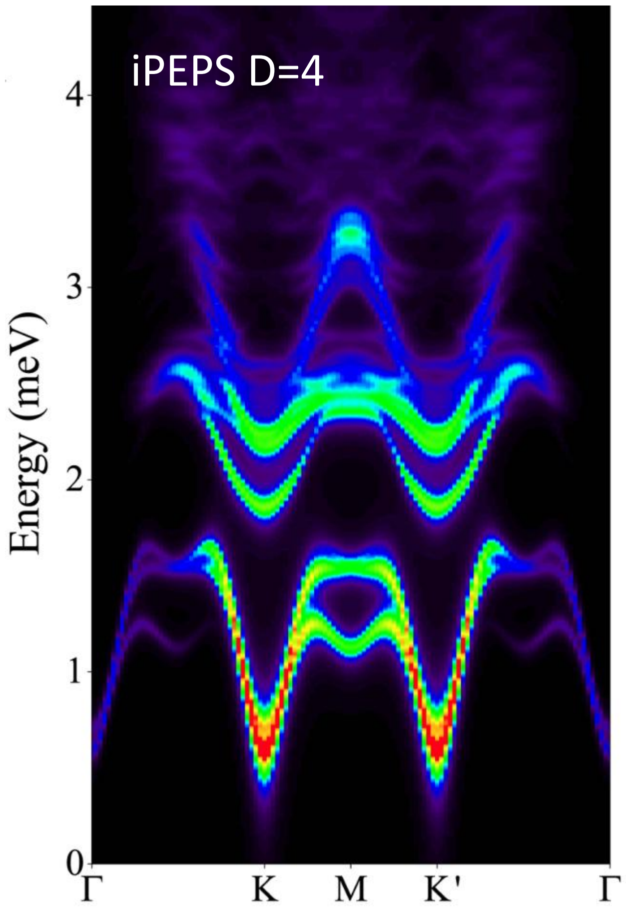

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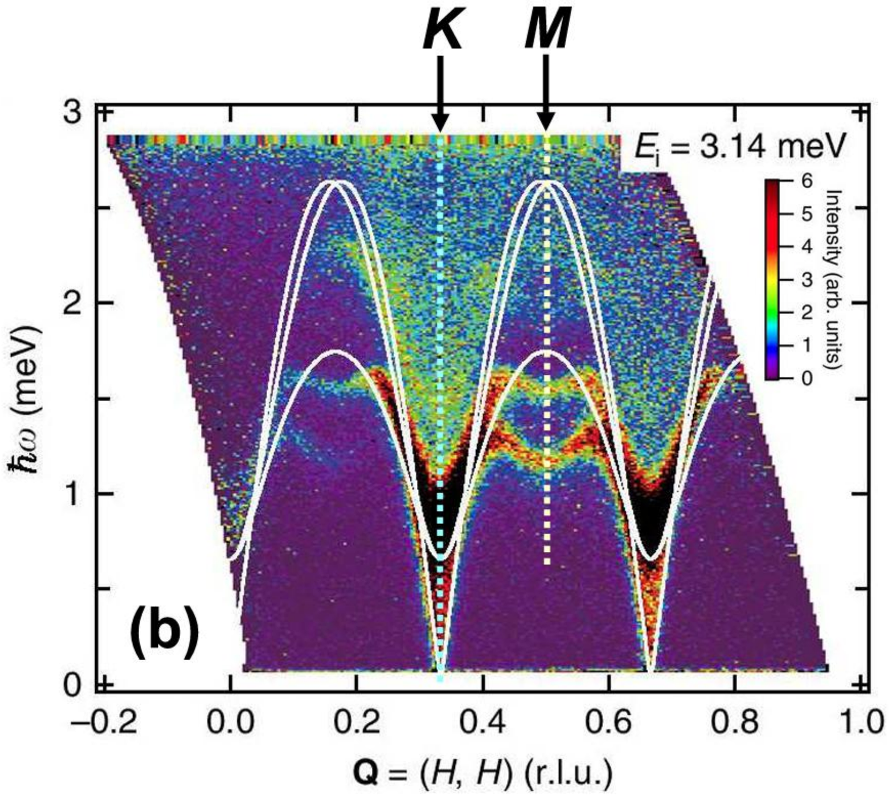
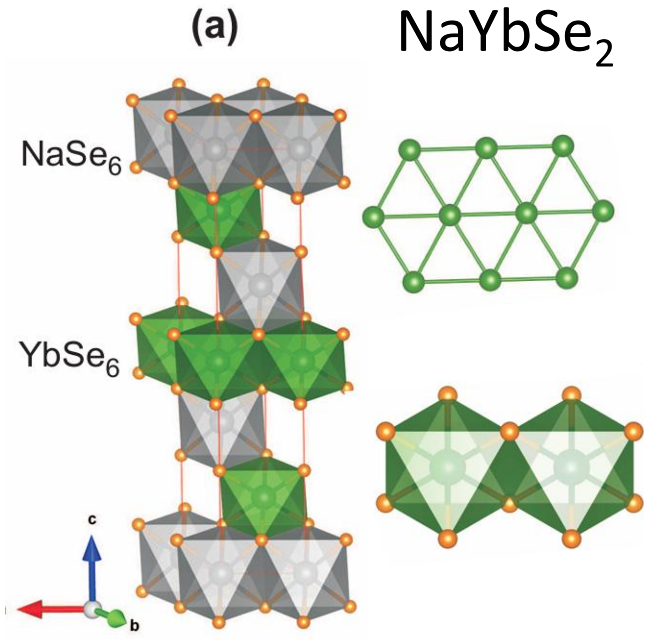


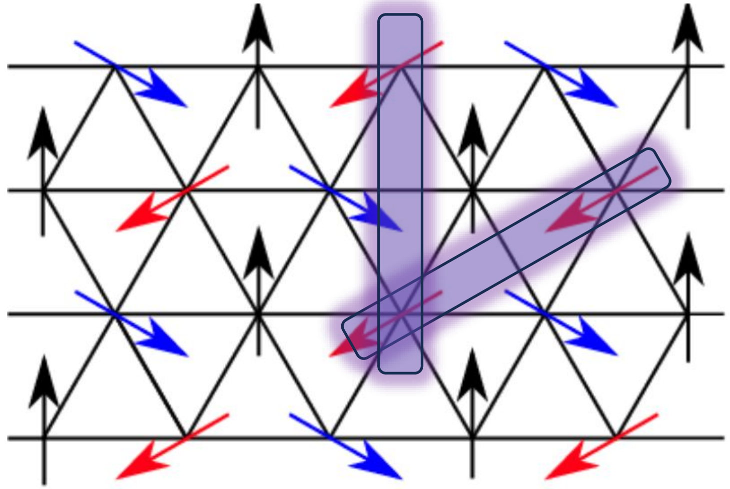
Chernyshev, Pollica 2024; Chi, Liu, Wan, Liao, and Xiang, PRL (2022)

Triangular antiferromagnets: Gifts from Nature

Rare-earth: i.e. Yb^{3+} in octahedral cage of Oxygens or Selenia give **"effective" spin-1/2**



- $J = 7/2$ + crystal-field splitting $\Rightarrow$ effective pseudo-spin $S = 1/2$
- **ideal TL** and also $\boldsymbol{J_2}$ - **Frustration!**

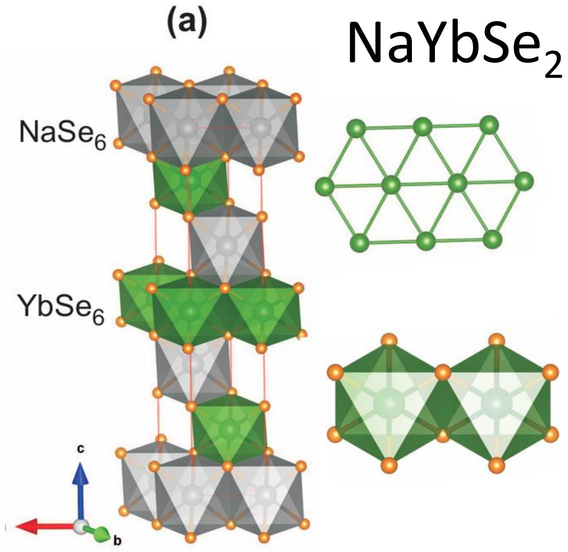


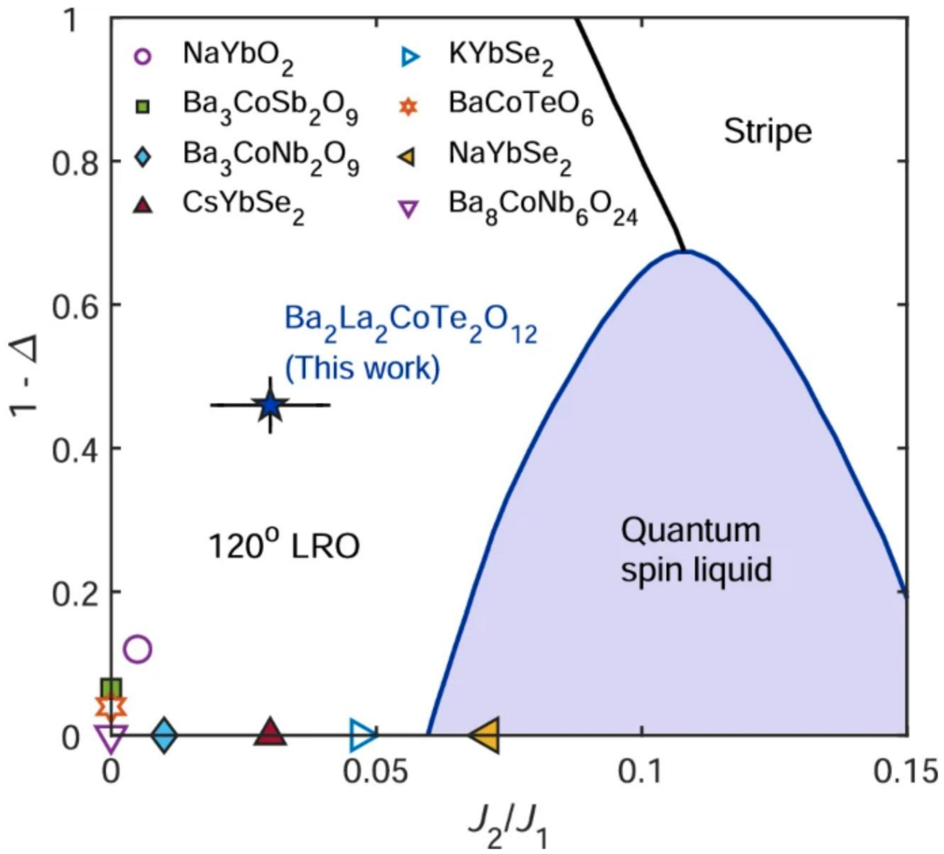
Ranjith et al. PRB 100, 224417 2019; Chernyshev, Pollica 2024;

Triangular antiferromagnets: Gifts from Nature

Rare-earth: i.e. Yb^{3+} in octahedral cage of Oxygens or Selenia give **"effective" spin-1/2**

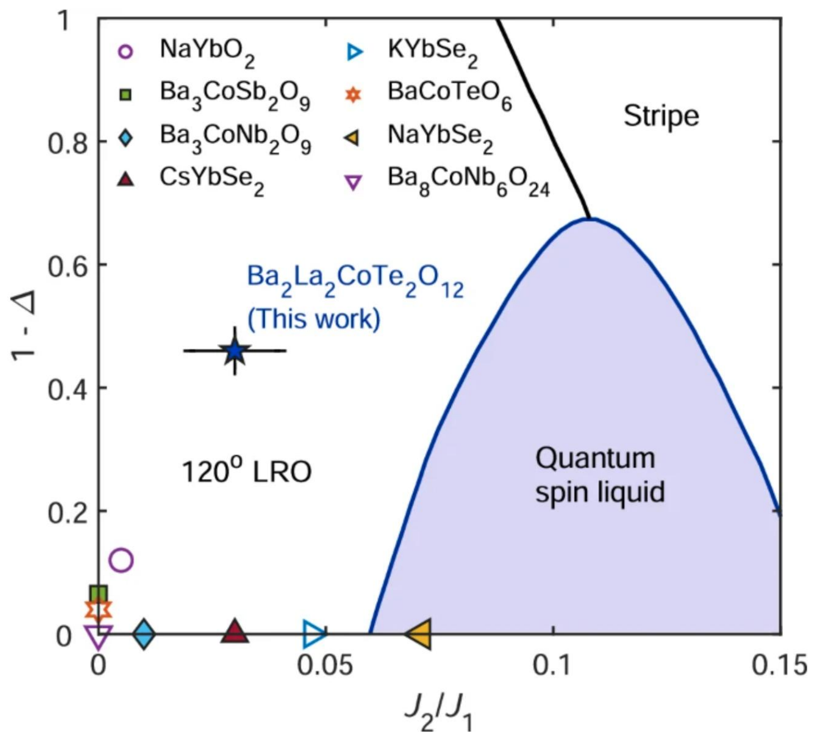
$$H = J_1 \sum_{\langle i,j \rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) + J_2 \sum_{\langle\langle i,j \rangle\rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) + \cdots$$

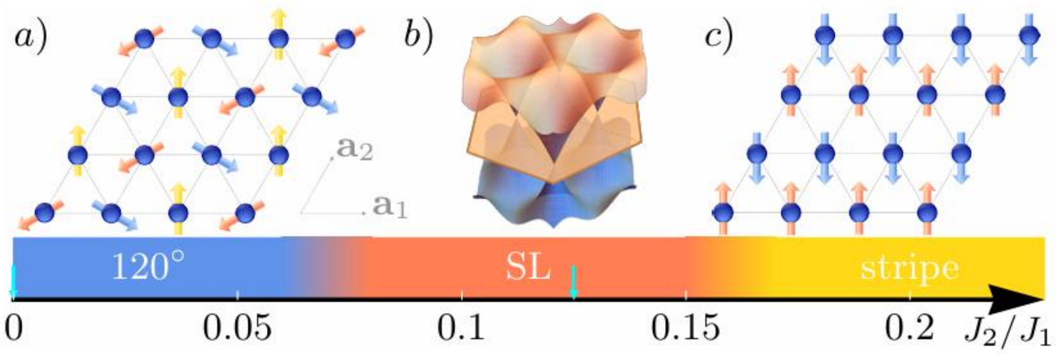




Park et al., Nat. Comm. 15, 7264 (2024); Ranjith et al. PRB 100, 224417 2019; Chernyshev, Pollica 2024;

Triangular antiferromagnets: Gifts from Nature





$$H = J_1 \sum_{\langle i,j \rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) + J_2 \sum_{\langle\langle i,j \rangle\rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) + \cdots$$

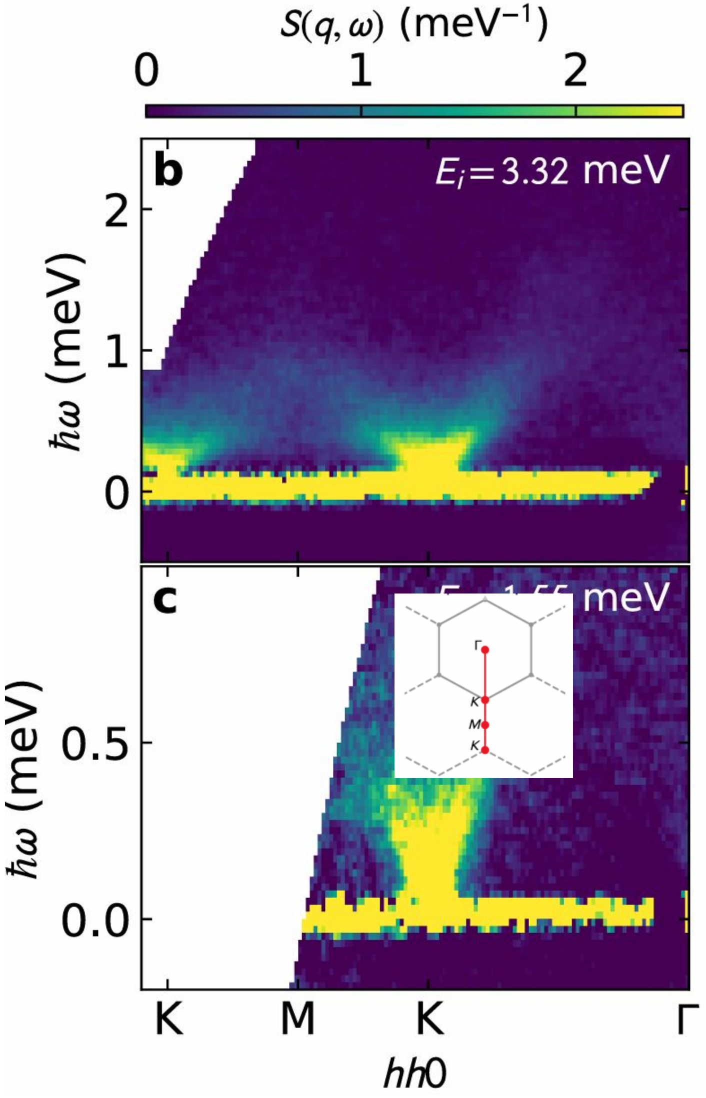
What is the **phase diagram** ?

- What is the **nature** of paramagnetic phase (QSL)?
  - Anderson's RVB ?
- **Dynamics** ?

Iqbal et al., PRB 93, 144411 (2016)

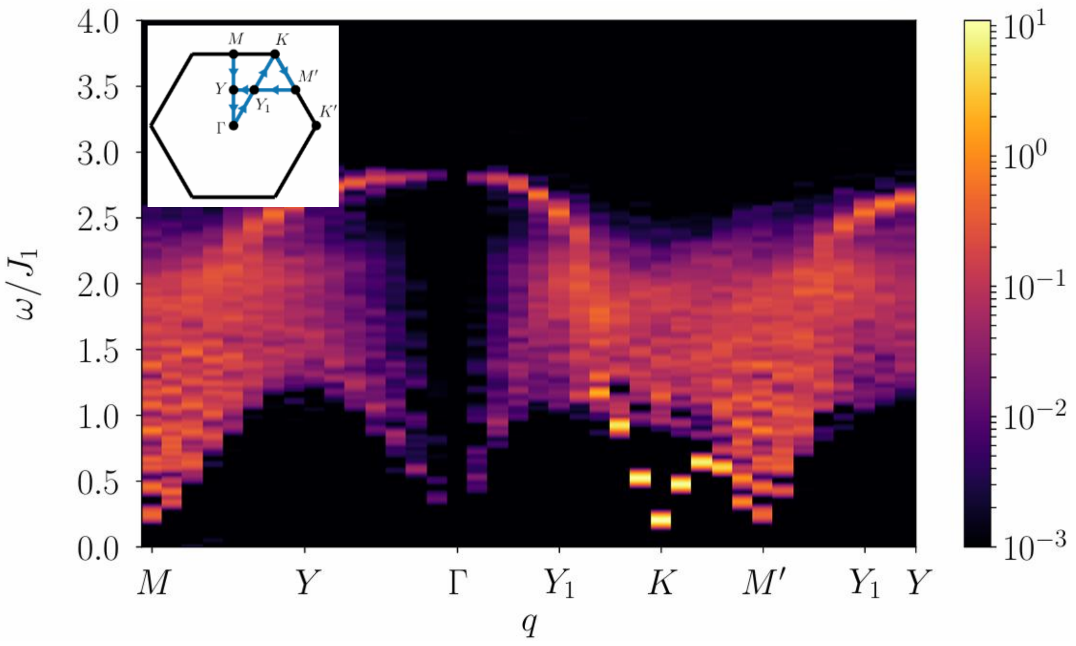
Triangular antiferromagnets: Gifts from Nature

NaYbSe_2 $\mathbf{J_2/J_1 \approx 0.07}$



$$H = J_1 \sum_{\langle i,j \rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) + J_2 \sum_{\langle\langle i,j \rangle\rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) + \cdots$$

$\boldsymbol{J_2/J_1 = 0.09}$ VMC of π-flux GPFW



Scheie et al. arXiv:2406.17773v1; Ferrari, Becca, PRX 9, 031026 (2019)

Variational method

1) **Parametrize**: parametrize many-body wavefunction $|\psi(\boldsymbol{p})\rangle$
2) **Optimize**: minimize the energy $\min_{\boldsymbol{p}} \langle\psi(\boldsymbol{p})|H|\psi(\boldsymbol{p})\rangle$
3) **Analyze**: read off physics from the optimal *ansatz* $|\psi(\boldsymbol{p_{opt}})\rangle$

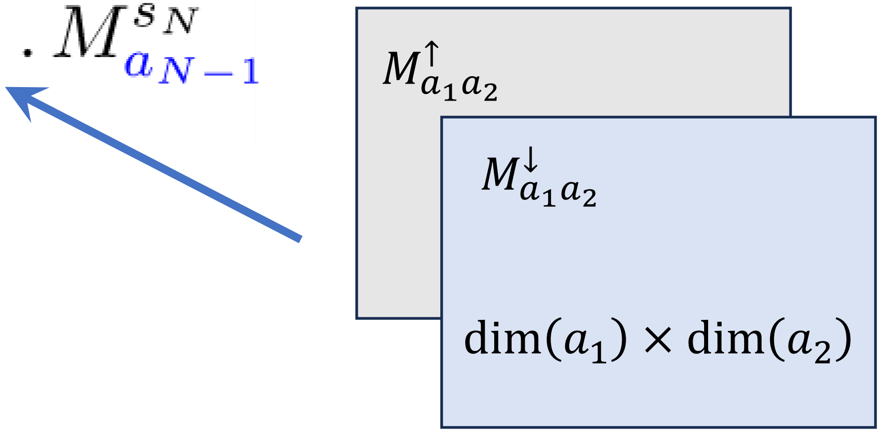
Matrix product states

Take simple spin-1/2 system with $\boldsymbol{N}$ spins. Wave function in spin-1/2 computational basis $s = \{\uparrow, \downarrow\}$

$$|\psi\rangle = \sum_{s_1 s_2 \ldots s_N} c_{s_1 s_2 \ldots s_N} |s_1 s_2 \ldots s_N\rangle$$

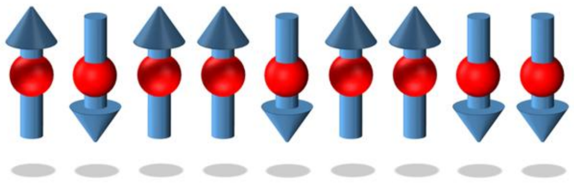
Express **any** given coefficient $c_{s_1 s_2 \ldots s_N}$ as a **product of matrices**

$$c_{s_1 s_2 \ldots s_N} = \sum_{a_1 a_2 \ldots a_{N-1}} \tilde{M}^{s_1}_{a_1} \tilde{M}^{s_2}_{a_1 a_2} \ldots \tilde{M}^{s_N}_{a_{N-1}}$$



Rank-3 tensor

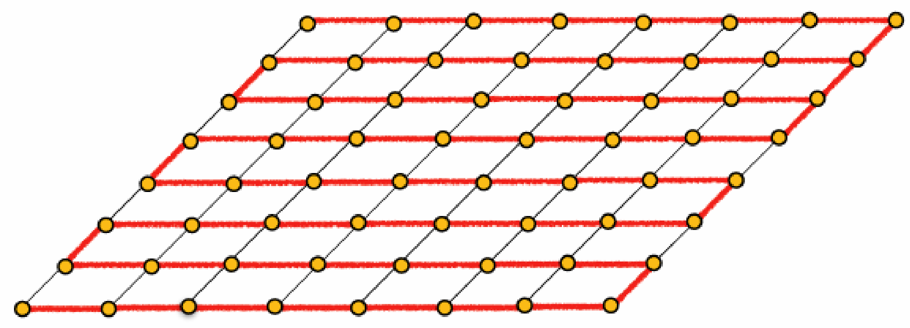
i.e. $c_{\uparrow\downarrow\downarrow\uparrow\uparrow} = \tilde{M}^{\uparrow}_{a_1} \tilde{M}^{\downarrow}_{a_1 a_2} \tilde{M}^{\downarrow}_{a_2 a_3} \tilde{M}^{\uparrow}_{a_3 a_4} \tilde{M}^{\uparrow}_{a_4}$



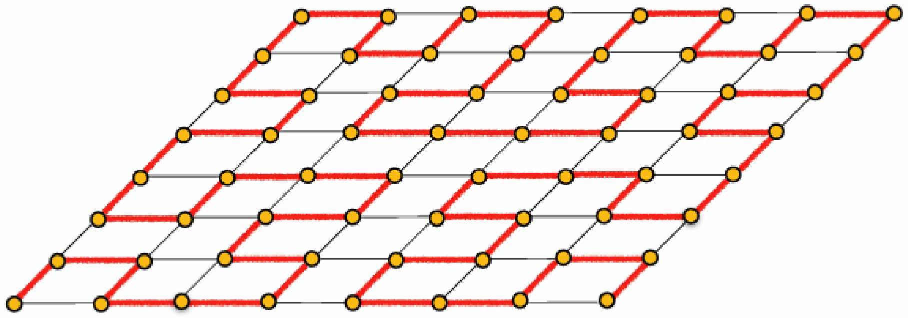
In two dimensions – Matrix product states

Let's keep doing what worked in 1D …

MPS



Hilbert curve



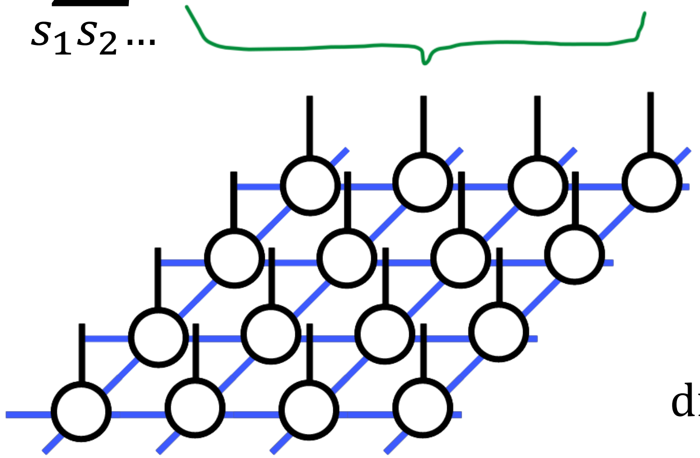
… except, the cost is exponential even for a gapped system !

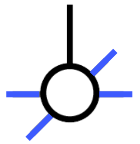
picture from Cataldi et al., Quantum 5, 556 (2021)

In two dimensions

iPEPS: infinite projected-entangled pair states **two-dimensional** tensor network
[F. Verstraete, M. M. Wolf, D. Perez-Garcia, J. I. Cirac, PRL, 2006]

$$|\psi(M)\rangle = \sum_{s_1 s_2 \dots} Tr_{aux}(M^{s_1} M^{s_2} \dots)|s_1 s_2 \dots\rangle$$



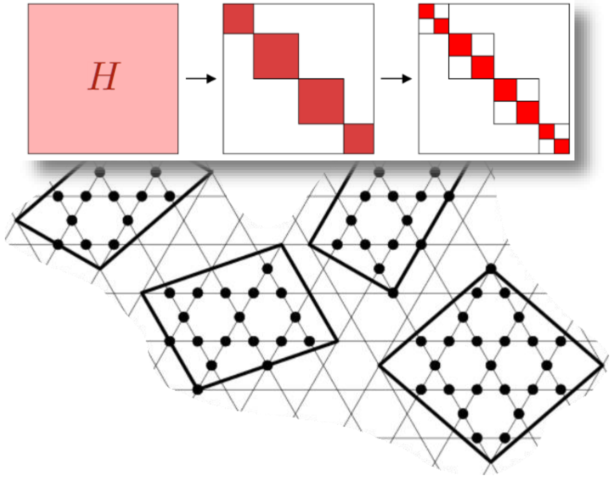


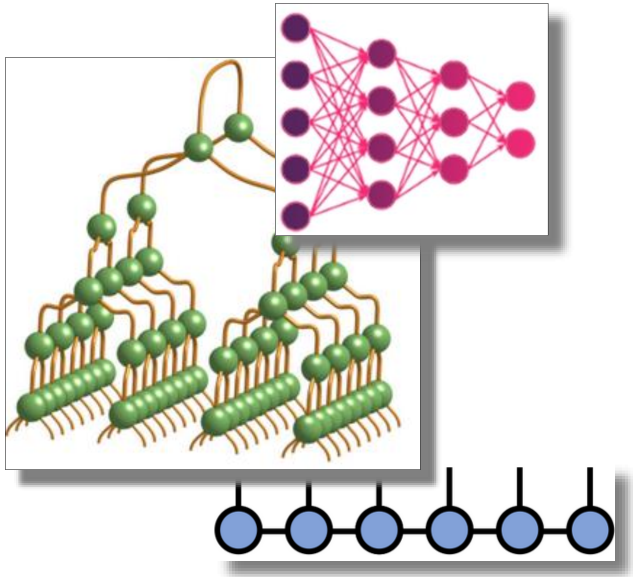
M^{s}_{uldr}

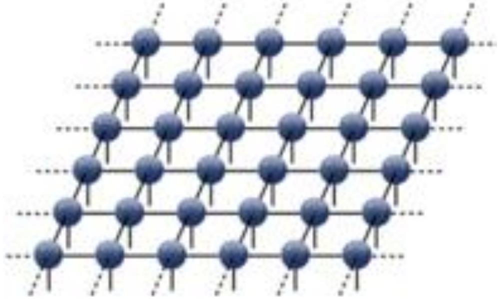
$\dim(u) = \dim(l) = \cdots = D$

Non-perturbative numerical methods

Exact diagonalization	Monte Carlo/Neural nets/ Finite tensor networks	Infinite Tensor networks







$O(20)$ $O(300)$ $O(\infty)^*$ N

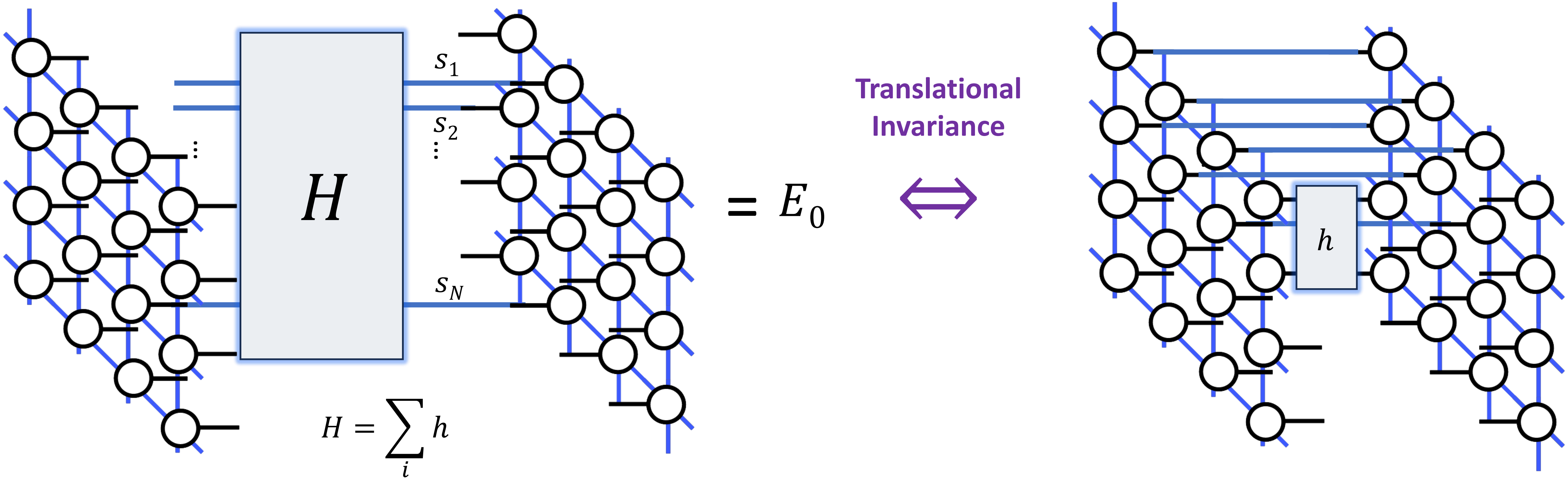
Full $\mathcal{H}$ $S \propto |\partial A|$ / $S \propto |A|$ $S \propto |\partial A|$

Entanglement entropy

Exact diagonalization studies, Sandvik; Seman et al., arXiv:1508.01523; Montangero, Rico, Silvi, Phil. Trans. R. Soc. A. (2014); TN.org, APS.org

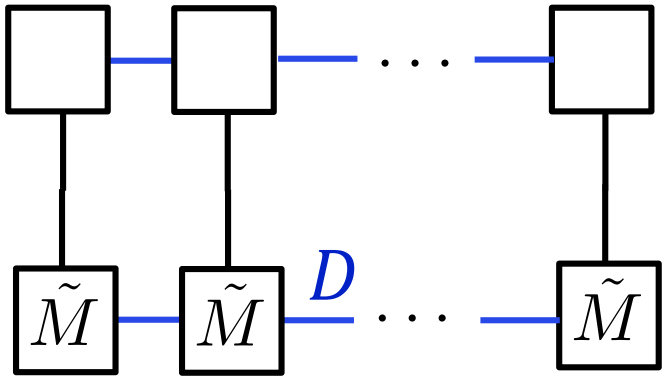
Infinite PEPS – Low-rank approximations

- Making sense of formally infinite networks:
  Density matrices [Marginals] through **environments**



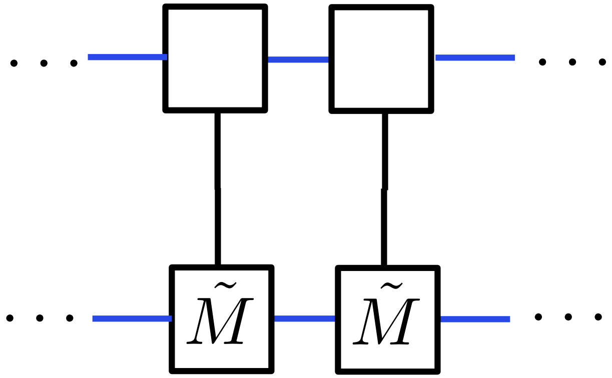
Reminder: (i)MPS

Observables are evaluated **exactly** at **polynomial cost**



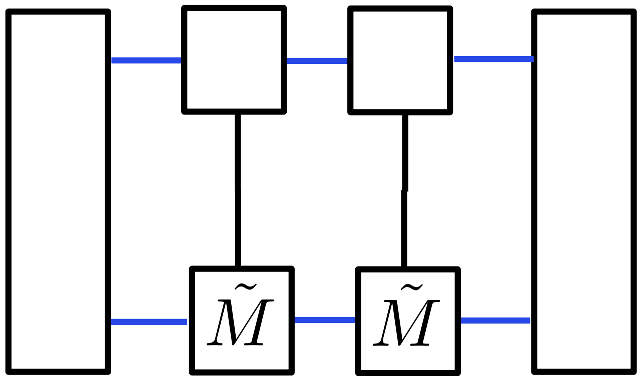
$O(D^3)$

For both **finite** and **infinite** MPS



$O(D^4)$

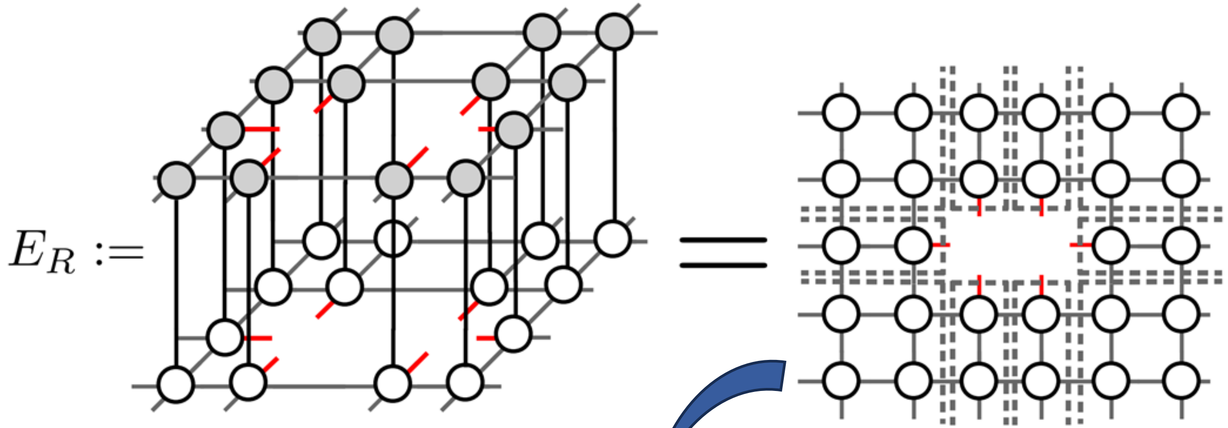
$\approx$



In two dimensions – Corner TM

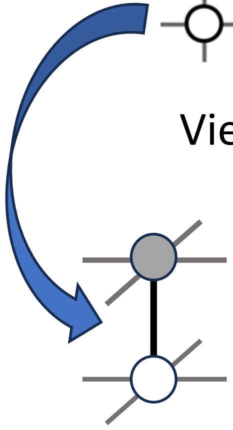
Observables are no longer easy to compute

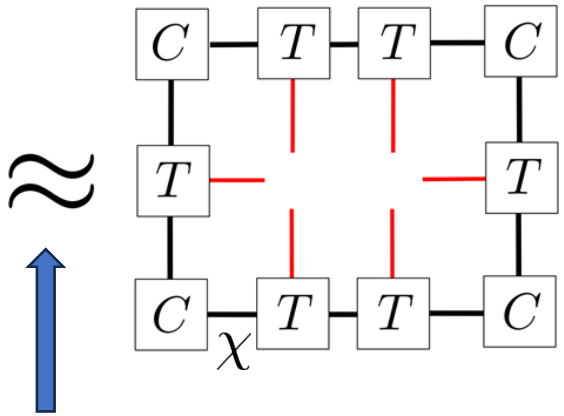
- **Effective environments**: presume existence of finite-sized (χ) tensor **C, T**



View from the "side"

View from the "top"





- CTMRG (Baxter, Nishino,Orus,Corboz,…)
- BoundaryMPS (Jordan, Verstraete, Vanderstraeten, Van Hecke, …)

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Observables are no longer easy to compute

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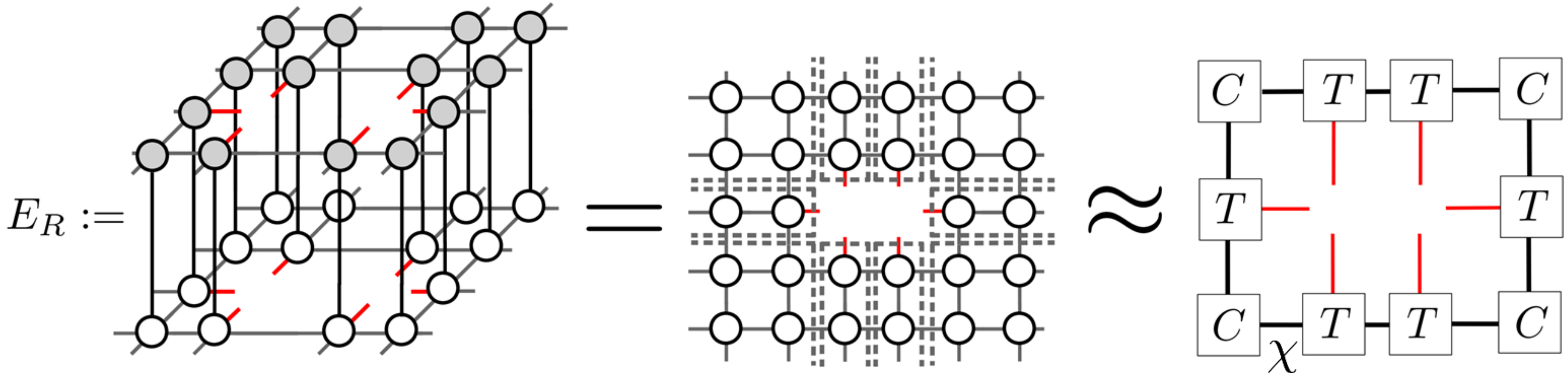
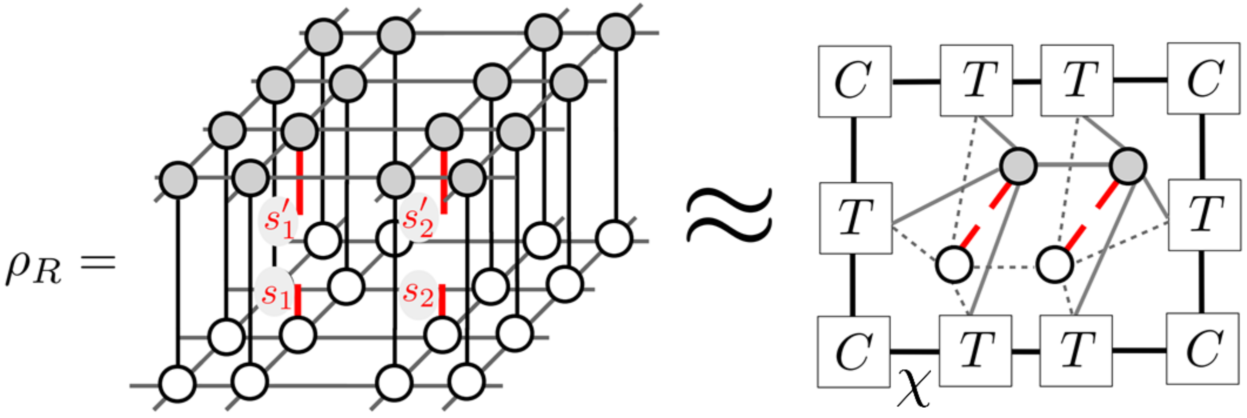


Fill in the on-site tensors…

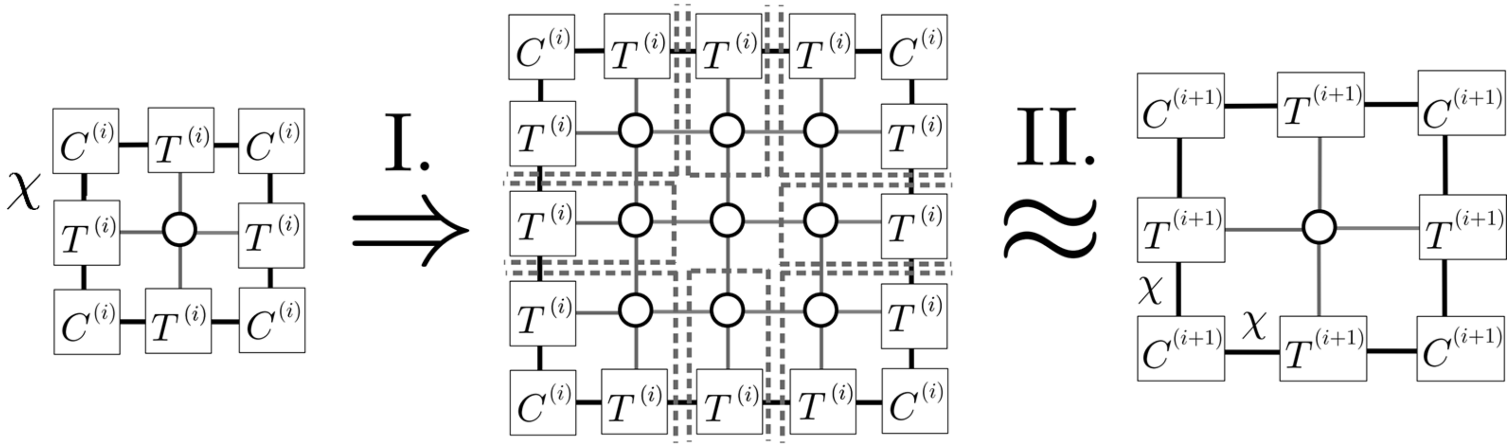


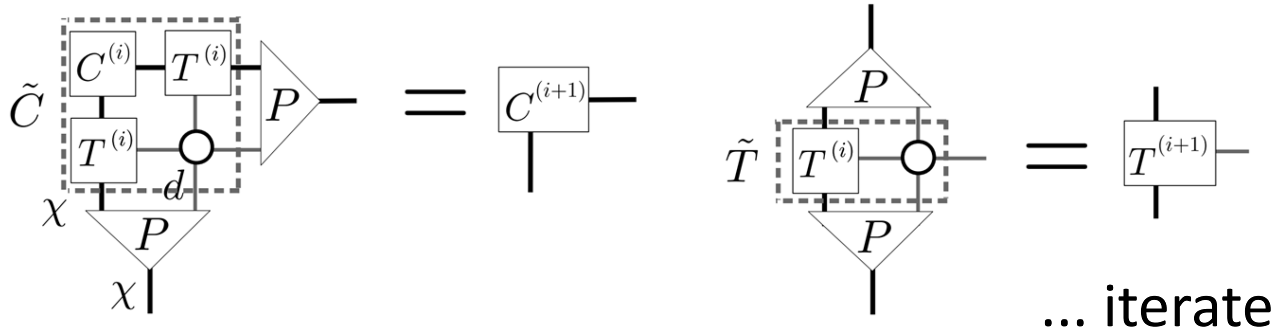
$$\langle \mathcal{O} \rangle_\chi \approx \mathrm{Tr}(\rho_R(\chi)\mathcal{O})$$

In two dimensions – Corner TM

Observables are no longer easy to compute

- **Effective environments**: presume existence of finite-sized (χ) tensor **C, T**
- Corner transfer matrix renormalization group (**CTMRG**). Complexity **O(χ^3D^6)**



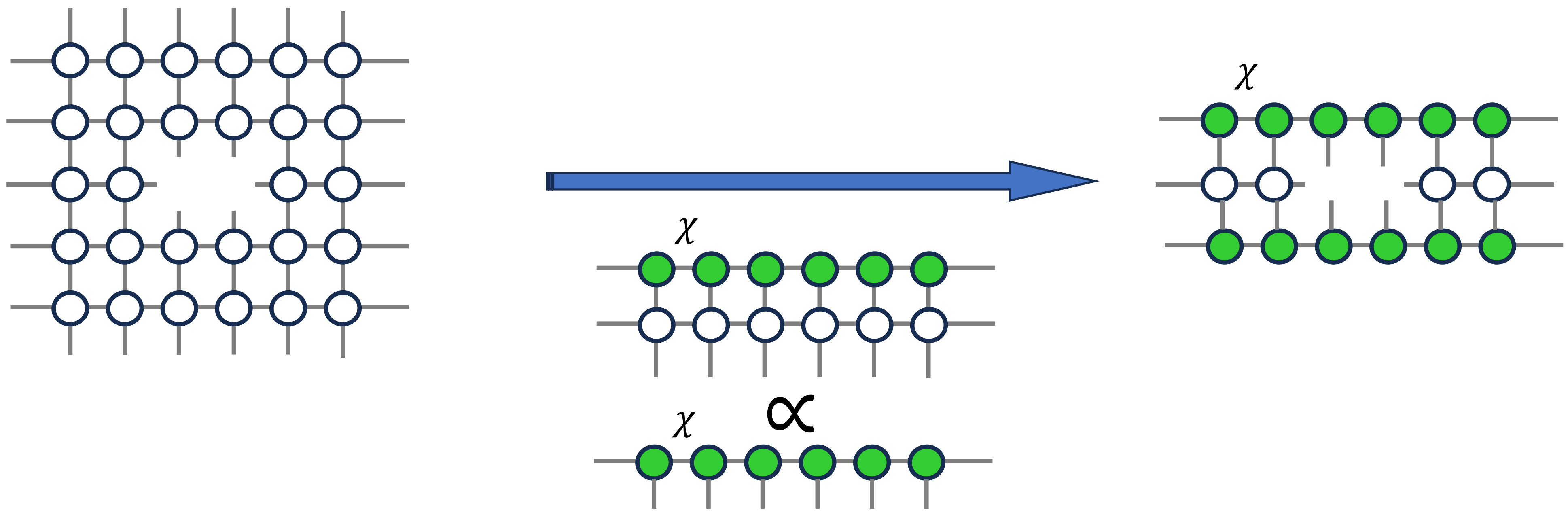


... iterate until **fixed point** C,T

In two dimensions – boundary MPS

Observables are no longer easy to compute

- **Effective environments**: presume existence of finite-sized (χ) tensor **C, T**
- Complexity **O(DMRG/TDVP)**

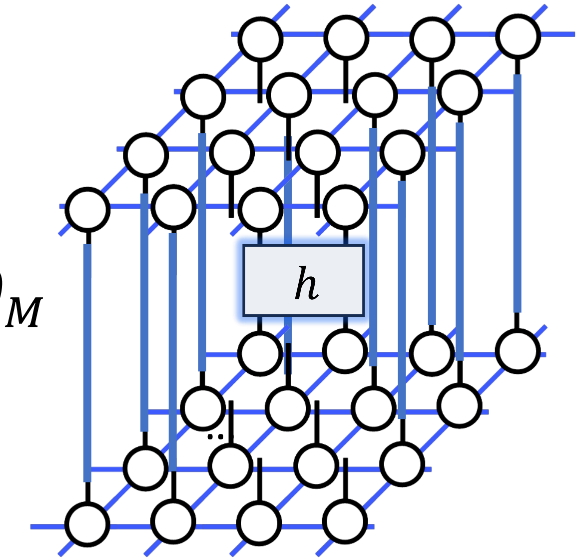


Optimizing iPEPS

Recently: Direct energy minimization

Two-dimensional networks: gradients with **backpropagation** (like ML) [Liao '19]

$$\text{grad} = \partial_M \langle iPEPS(M)|h|iPEPS(M)\rangle = \partial_M$$



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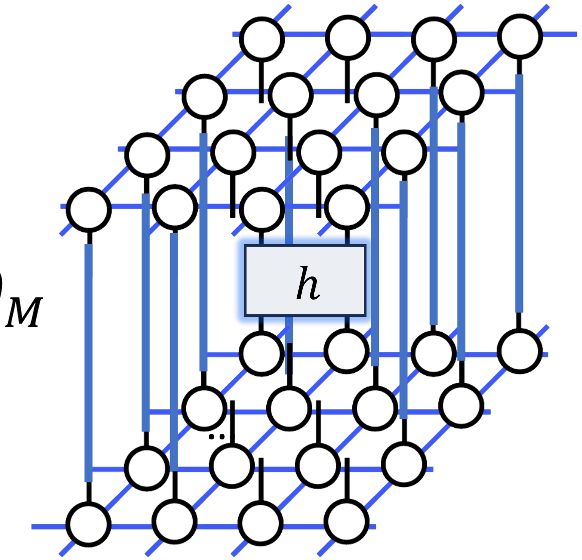
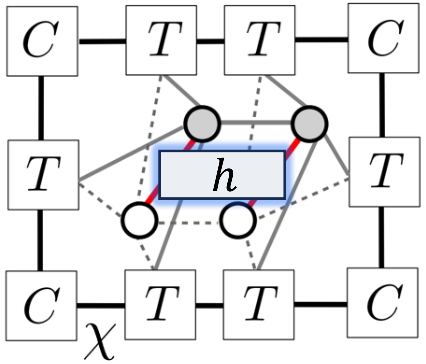
$\text{grad} = \partial_M \langle iPEPS(M)|h|iPEPS(M)\rangle = \partial_M$ 

$\approx \partial_M$ 

- Invented in the 1970’s. Now, a core technology behind training neural nets
- Works for any **computable** function (i.e. composed from simple functions)

Application – ground states

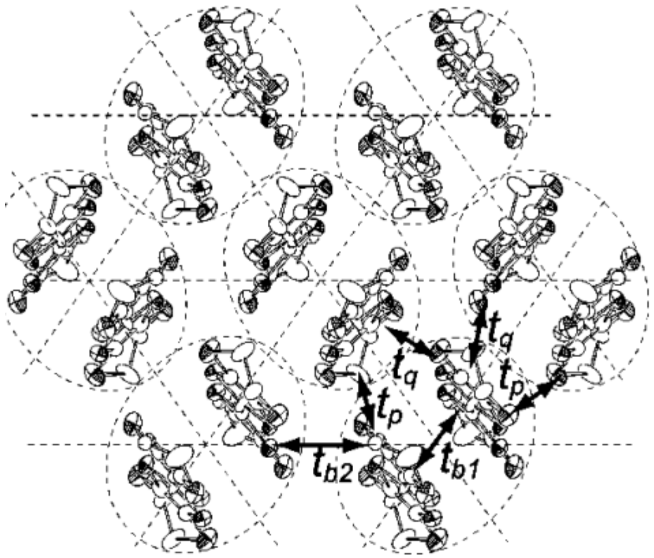
Incommensurate order with translationally invariant iPEPS

JH, Philippe Corboz,
PRL 133, 176502 (2024)

UNIVERSITY OF AMSTERDAM
Faculty of Science

Motivation

- Enabling **simulation** of (at least some) incommensurate orders
- Modelling of **triangular** lattice compounds (with **anisotropy**)



κ-$ET_2Cu_2CN_3$

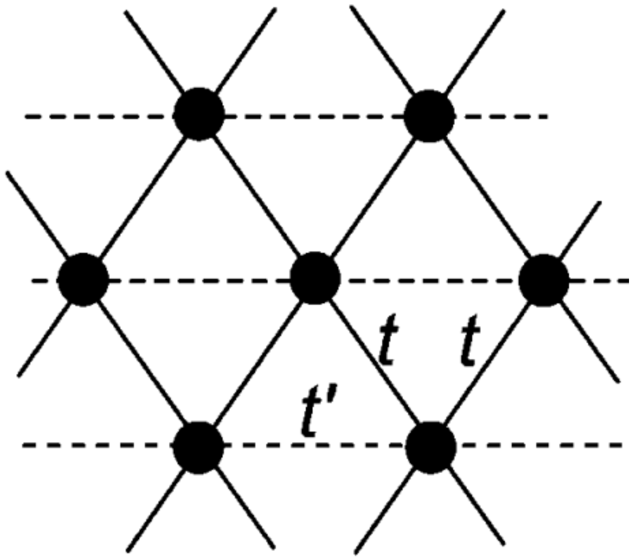
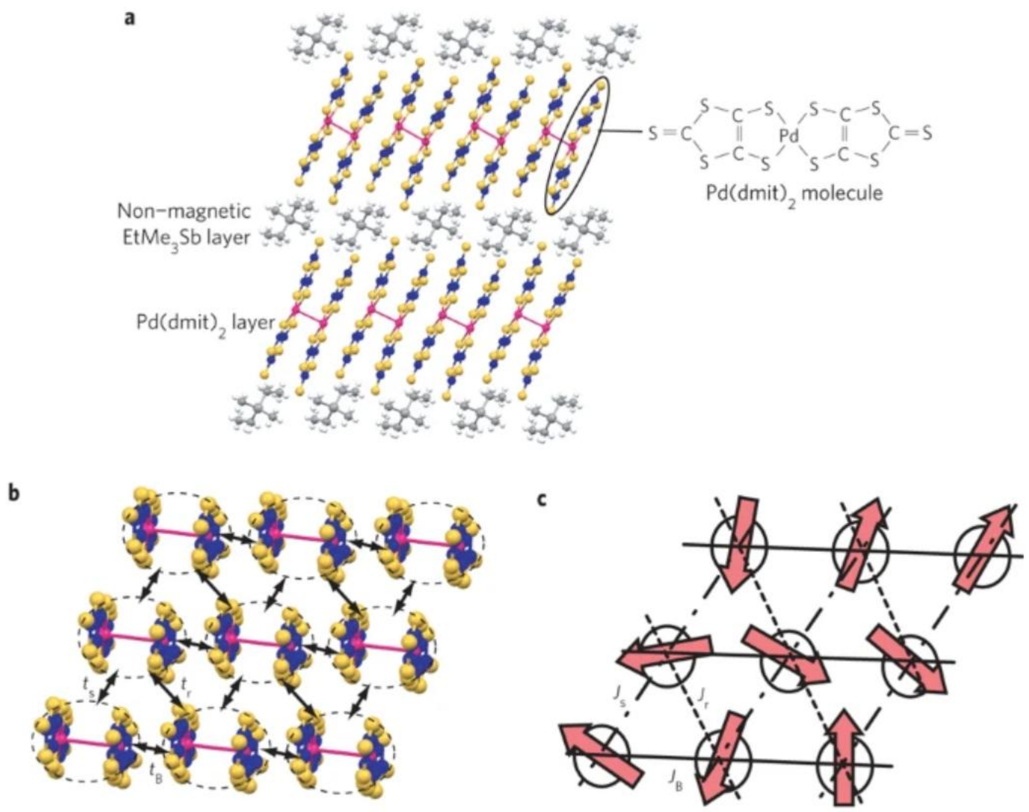


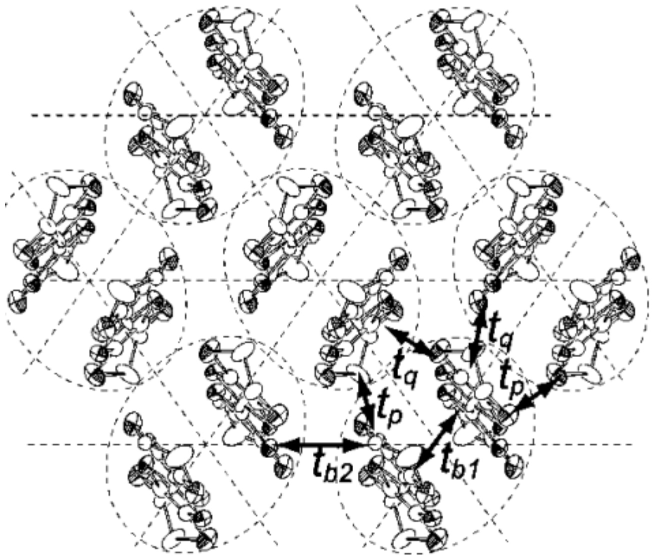
Figure 1: Crystal structure of $EtMe_3Sb[Pd(dmit)_2]_2$.



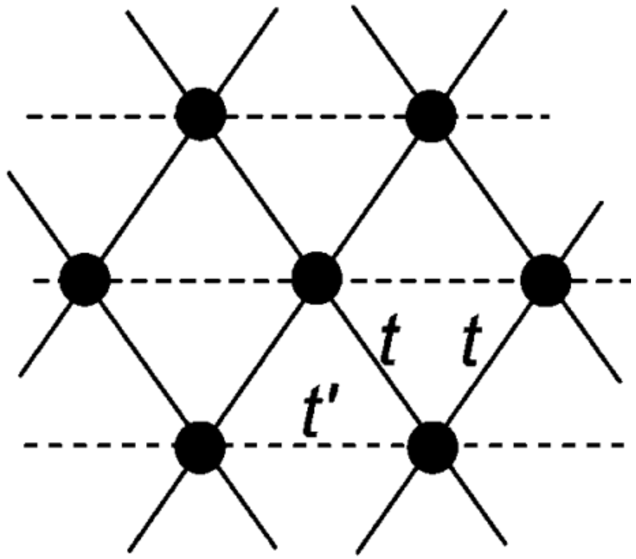
Y. Shimizu, K. Miyagawa, K. Kanoda, M. Maesato, and G. Saito, PRL 91 (2003)
T. Itou, A. Oyamada, S. Maegawa & R. Kato, Nat. Phys. 6 (2010)

Motivation

- Effective model: **TL spin-1/2 Heisenberg model**



κ-$ET_2Cu_2CN_3$

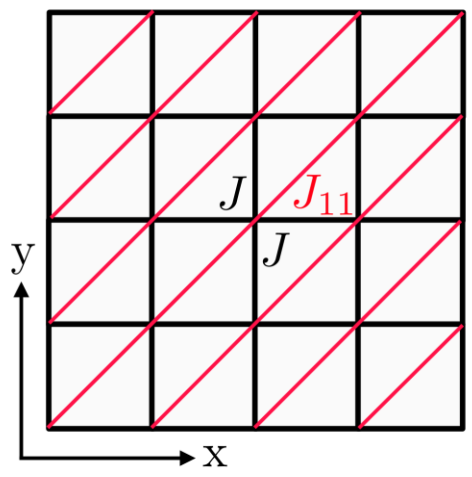


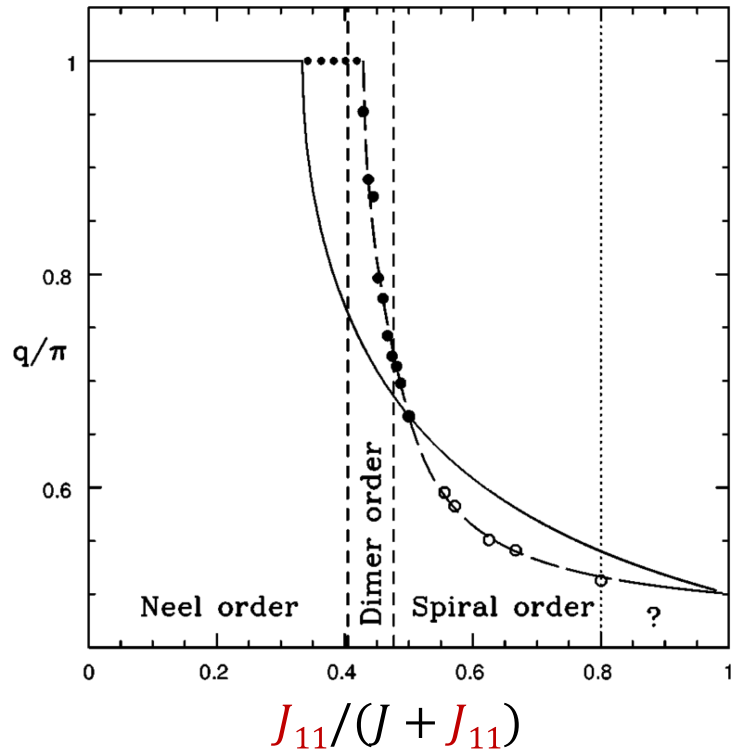
- Pairs of molecules form dimers as $t_{b1} \approx 2t_{b2}$
- Effective **spin-1/2**'s on triangular lattice
- Range of anisotropies t'/t

Y. Shimizu, K. Miyagawa, K. Kanoda, M. Maesato, and G. Saito, PRL 91 (2003)
T. Itou, A. Oyamada, S. Maegawa & R. Kato, Nat. Phys. 6 (2010)

Anisotropic TL Spin-1/2 Heisenberg model

$$H = \sum_{\mathbf{r}} J(\mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\hat{x}} + \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\hat{y}}) + J_{11}\mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\hat{x}+\hat{y}}$$

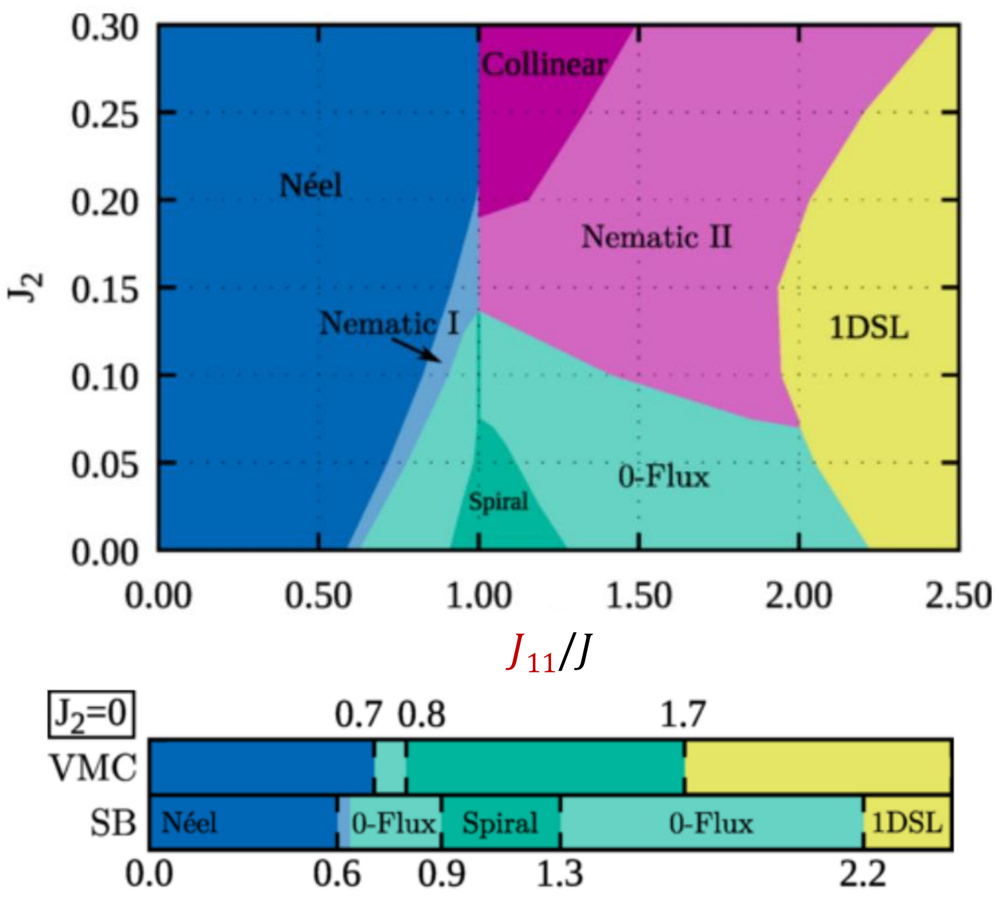


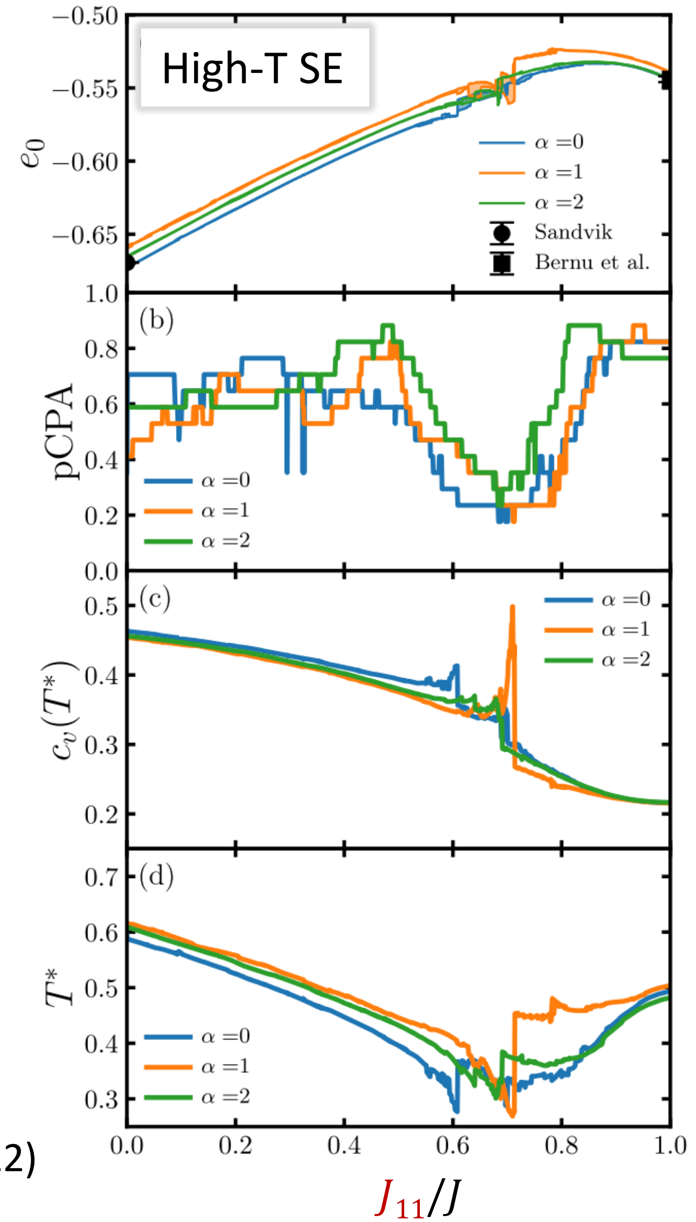


Zheng Weihong, Ross H. McKenzie, and Rajiv R. P. Singh, PRB **59**, (1999)

- Interpolates between **Néel** $q = (\pi, \pi)$ order at $J_{11} = 0$ and **120-degree** $q = (2\pi/3, 2\pi/3)$ order at $J_{11} = J$

Anisotropic TL Spin-1/2 Heisenberg model

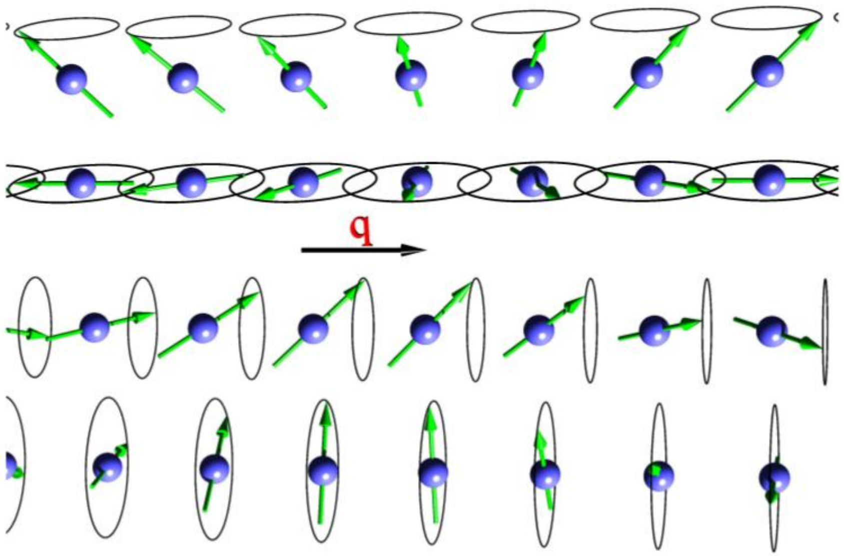




Elaheh Ghorbani, Luca F. Tocchio, and Federico Becca, PRB 93 (2016)
M. G. Gonzalez, E. A. Ghioldi, C. J. Gazza, L. O. Manuel, and A. E. Trumper, PRB 102, (2020)
Matías G. Gonzalez, Bernard Bernu, Laurent Pierre, Laura Messio, SciPost Phys. 12, 112 (2022)

Incommensurate order

Spin spirals with arbitrary momentum **q**

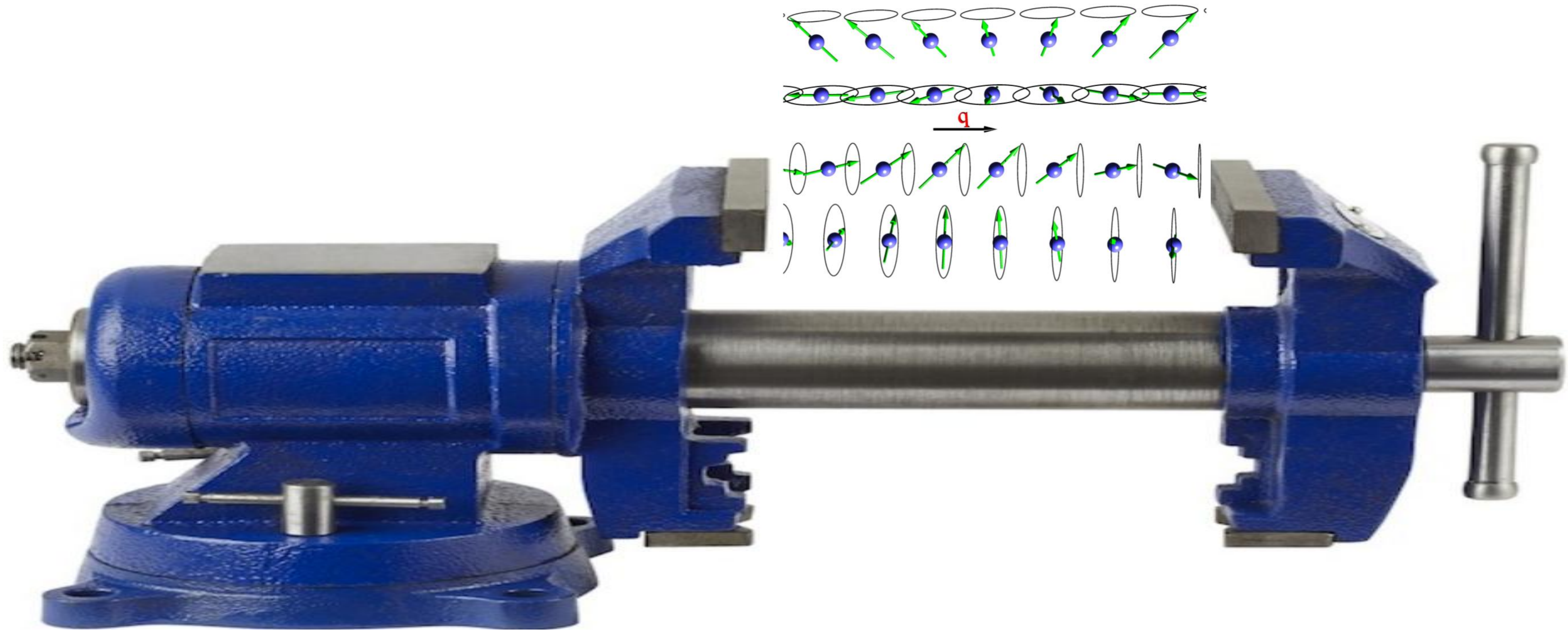


flapw.de

Incommensurate order

Spin spirals with arbitrary momentum **q**

- **Finite-size geometry (PBC) introduces spurious frustration**



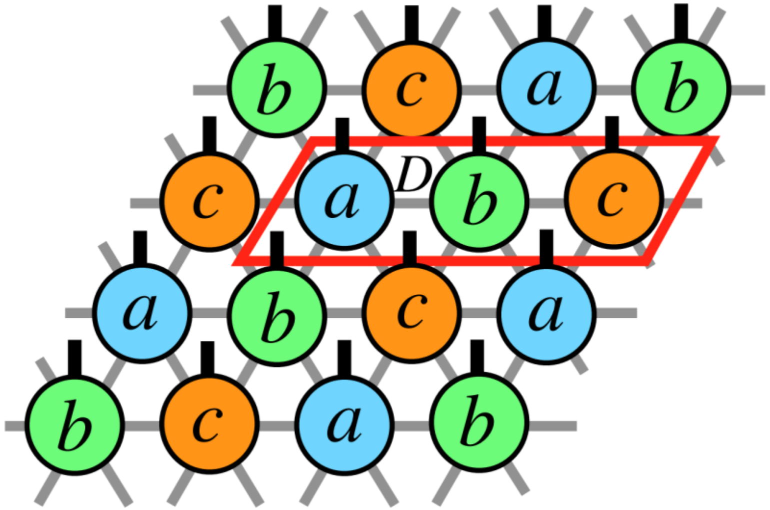
Incommensurate order

Spin spirals with arbitrary momentum **q**

- Finite-size geometry (PBC) introduces spurious frustration

Typical approach to spatial symmetry-breaking in iPEPS

- **Create unit cell with different tensors**



Incommensurate order with iPEPS

Spin spirals with arbitrary momentum **q**

- Finite-size geometry (PBC) introduces spurious frustration
- Typical iPEPS approach requires unit cells commensurate with q

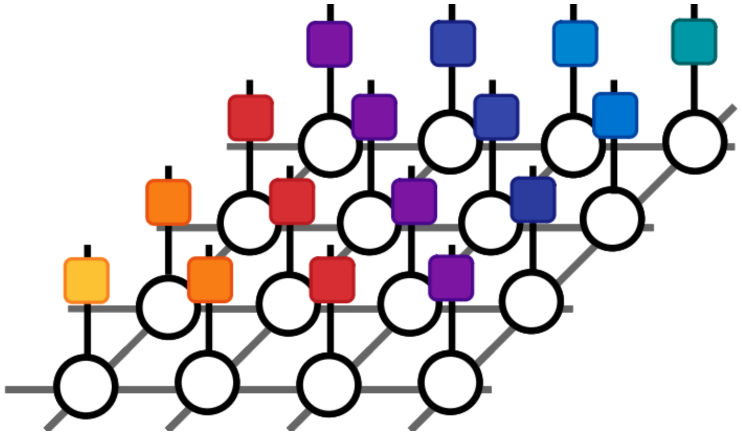
With iPEPS we can circumvent this obstacle

- **Use position-dependent unitary – spiral iPEPS**

$$|\psi(a, \boldsymbol{q})\rangle \; = \; U(\boldsymbol{q})|iPEPS(a)\rangle$$

$$U(\boldsymbol{q}) = \prod_{\boldsymbol{r}} u_{\boldsymbol{r}}\,(\boldsymbol{q}, \boldsymbol{r})$$

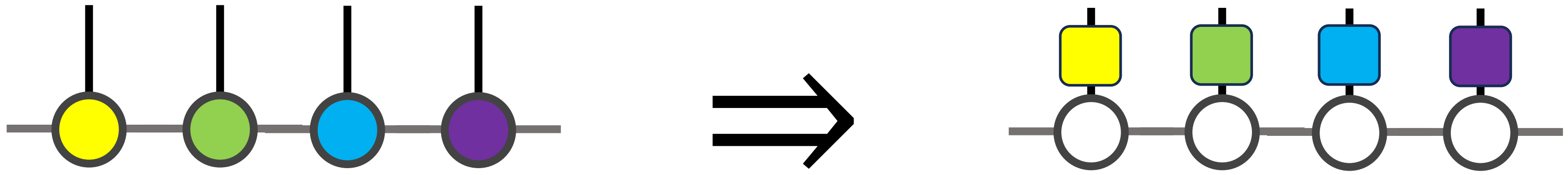
with $u_{\boldsymbol{r}}(\boldsymbol{q}, \boldsymbol{r}') = \exp[i\pi(\boldsymbol{q}.\boldsymbol{r}')S_{\boldsymbol{r}}^{y}]$



Incommensurate order with iPEPS

Spin spirals with arbitrary momentum **q**

- **Illustration on MPS - position-dependent unitary**
  H. Ueda and I. Maruyama, Phys. Rev. B 86, 064438 (2012)



$$|\psi(a,q)\rangle = U(q)|iMPS(a)\rangle$$

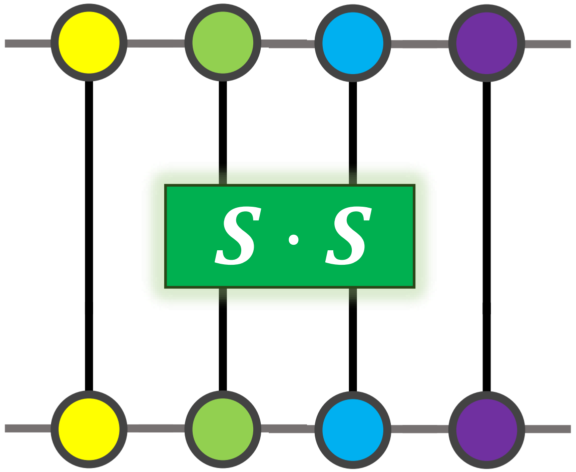
$$U(q) = \prod_r u_r\,(q,r) \text{ with } u_r(q,r') = \exp[i\pi(q.r')S_r^y]$$

Spiral iPEPS - Observables

Illustration on MPS:

To get **energy** we need **just** nearest-neighbour ρ_{NN}

$\langle S_r . S_{r+x} \rangle =$



Spiral iPEPS - Observables

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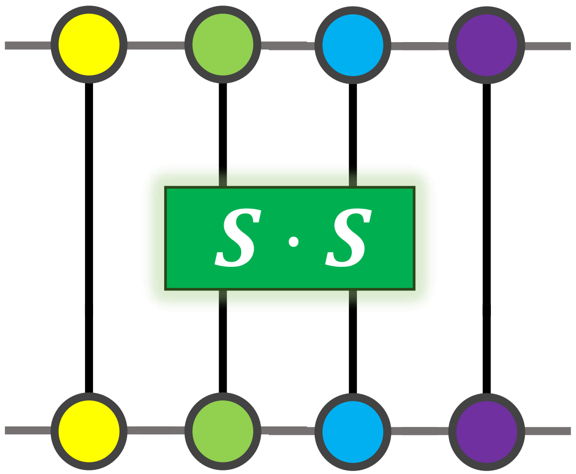
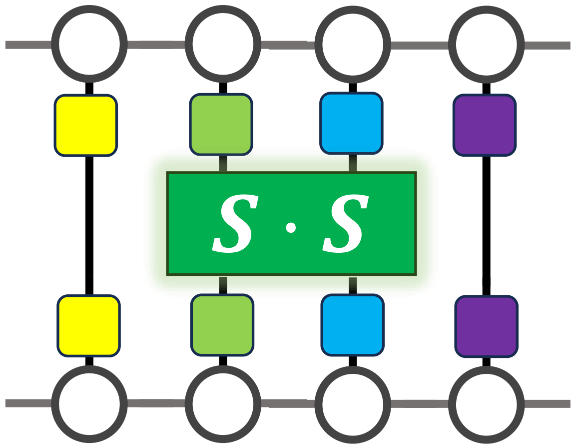


$\Rightarrow$



$$U^{\dagger}(q)\boldsymbol{S}_r \cdot \boldsymbol{S}_{r'}U(q) = \boldsymbol{S}_r \cdot \tilde{\boldsymbol{S}}_{r'}(q,\Delta)$$

where $\tilde{\boldsymbol{S}}^{\alpha}_{r'}(q,\Delta) = u^{\dagger}_{r'}(q,\Delta)\boldsymbol{S}^{\alpha}u_{r'}(q,\Delta)$ with $\Delta = r - r'$

Spiral iPEPS - Observables

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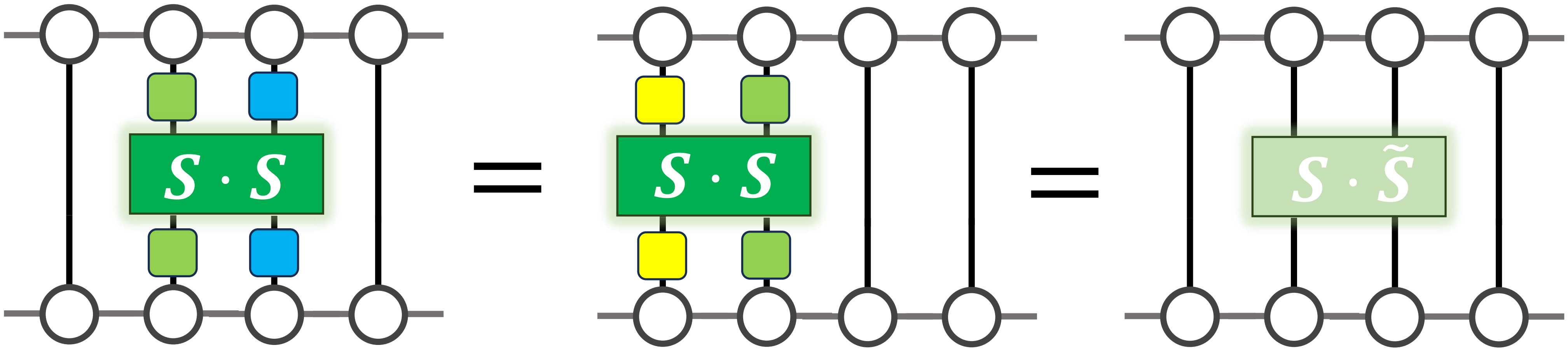
$\langle S_r . S_{r+x} \rangle =$ 

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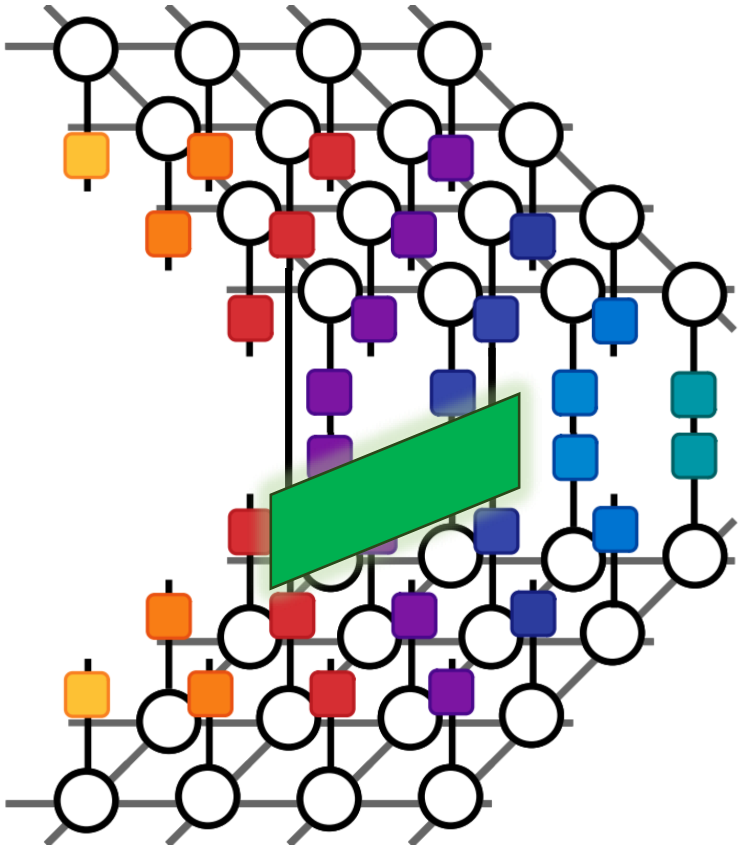
Spiral iPEPS - Observables

To get **energy** we need **just** nearest-neighbour ρ_{NN} and next-nearest neighbour ρ_{NNN} reduced density matrices

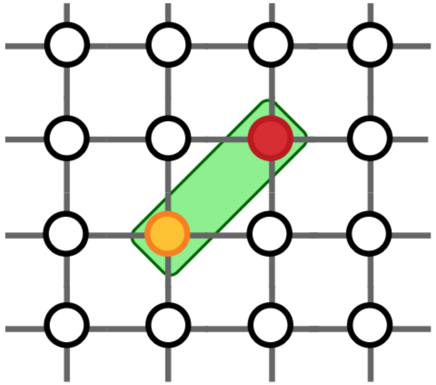
$\langle S_r . S_{r+x+y} \rangle =$



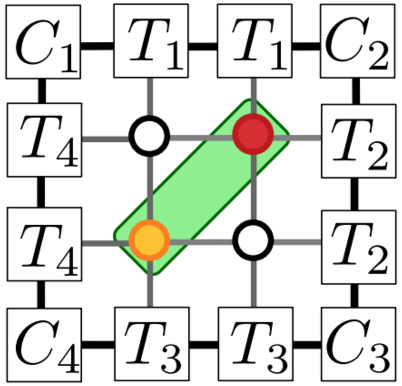
Optimizing spiral iPEPS

Gradients of on-site tensor and **momentum q** with backpropagation

$$grad = \partial_{a,\boldsymbol{q}}($$



$$\approx$$

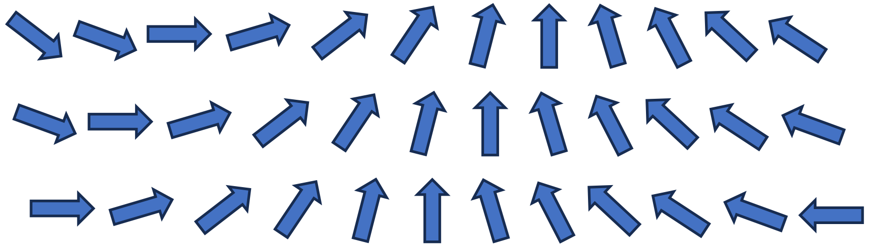


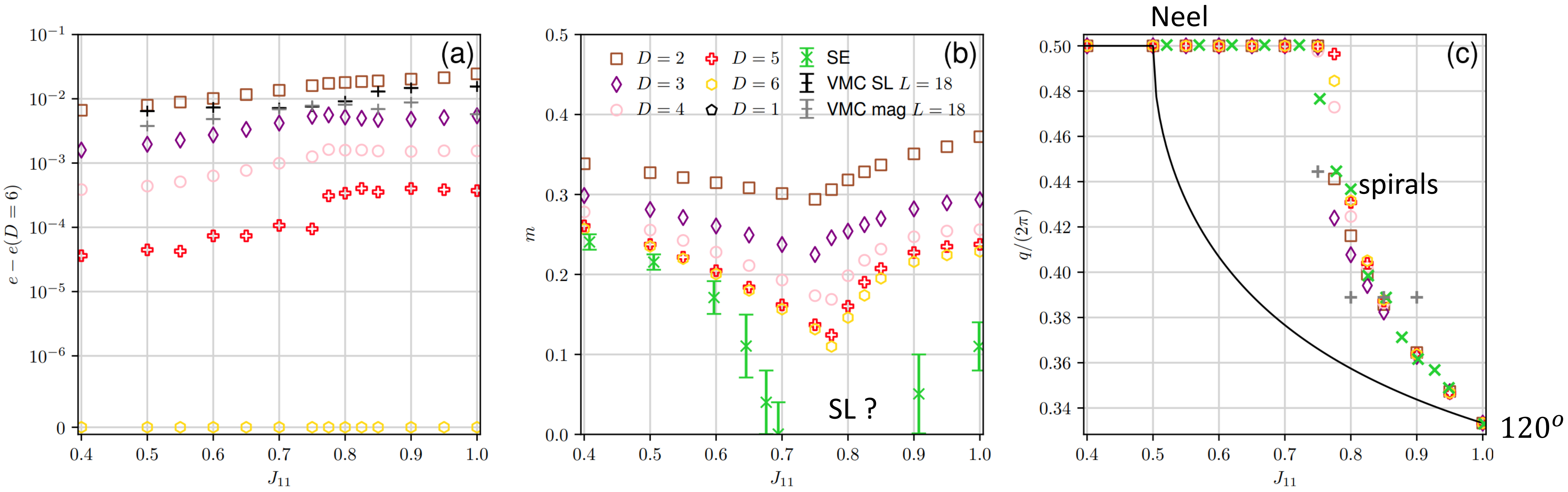
$$+ \ \ldots)$$

Optimizing spiral iPEPS

- We can carry out variational optimization – including the spiral's **q**

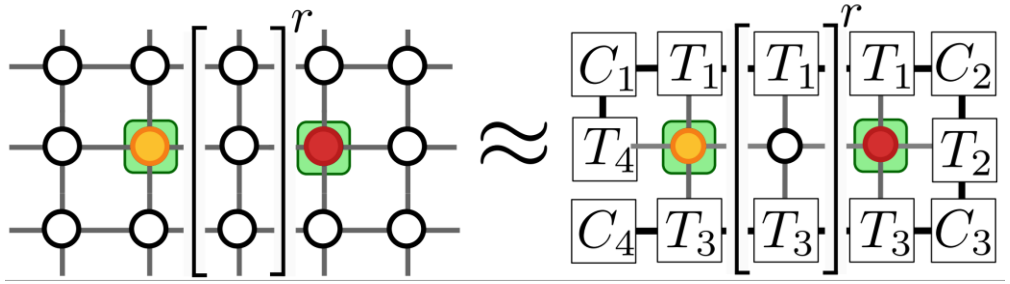
$$H = \sum_{\mathbf{r}} J(\mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\hat{x}} + \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\hat{y}}) + J_{11}\mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\hat{x}+\hat{y}}$$





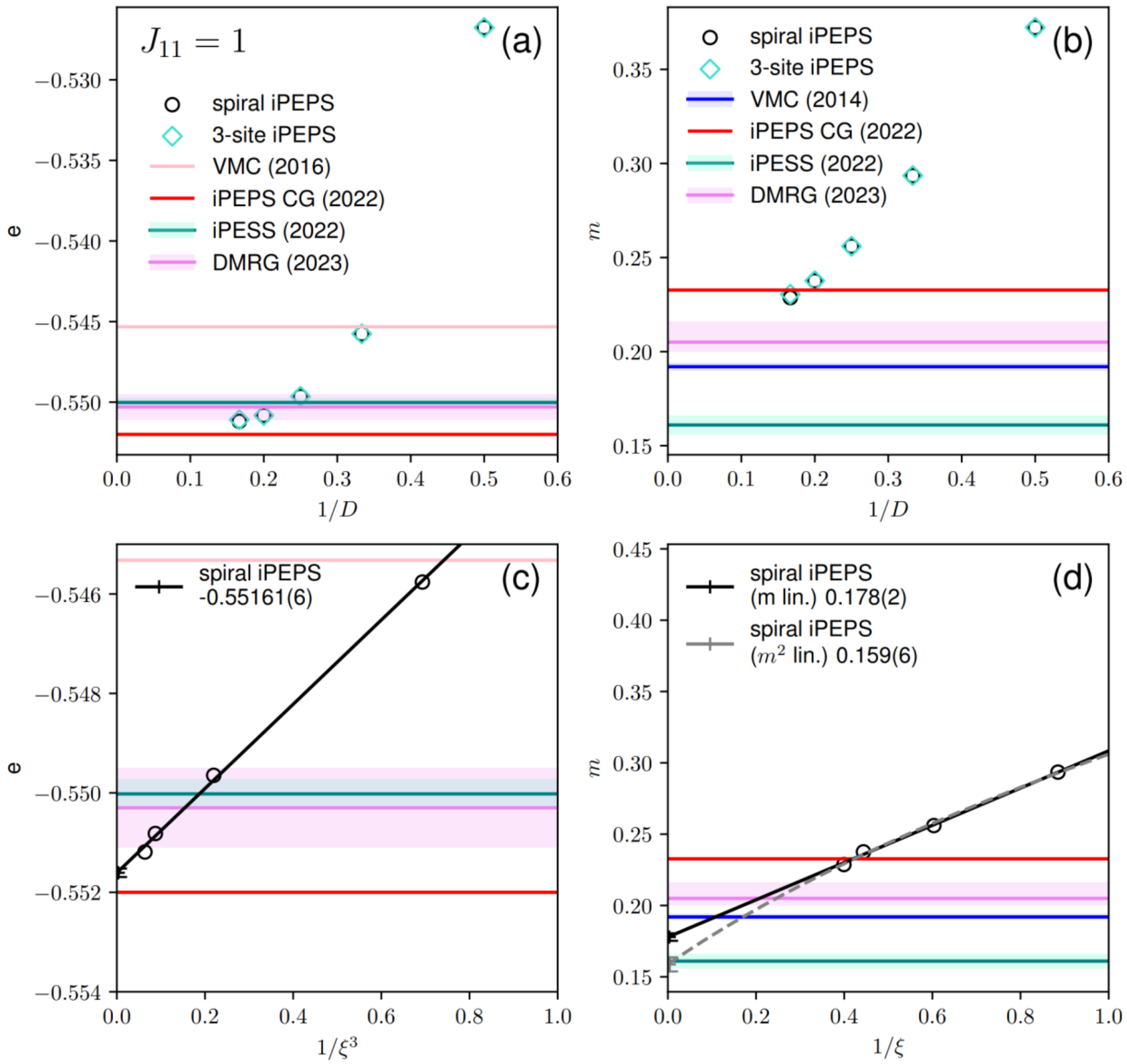
Correlation length scaling with spiral iPEPS

- **Isotropic triangular lattice $J = J_{11}$**
- Spectrum of transfer matrix T dictates decay of two-point corr. f.



$$T^r = |0\rangle\langle 0| + \sum_{i>0} |i\rangle \lambda_i^r \langle i|$$

Then $\xi = -1/\log(\lambda_1)$

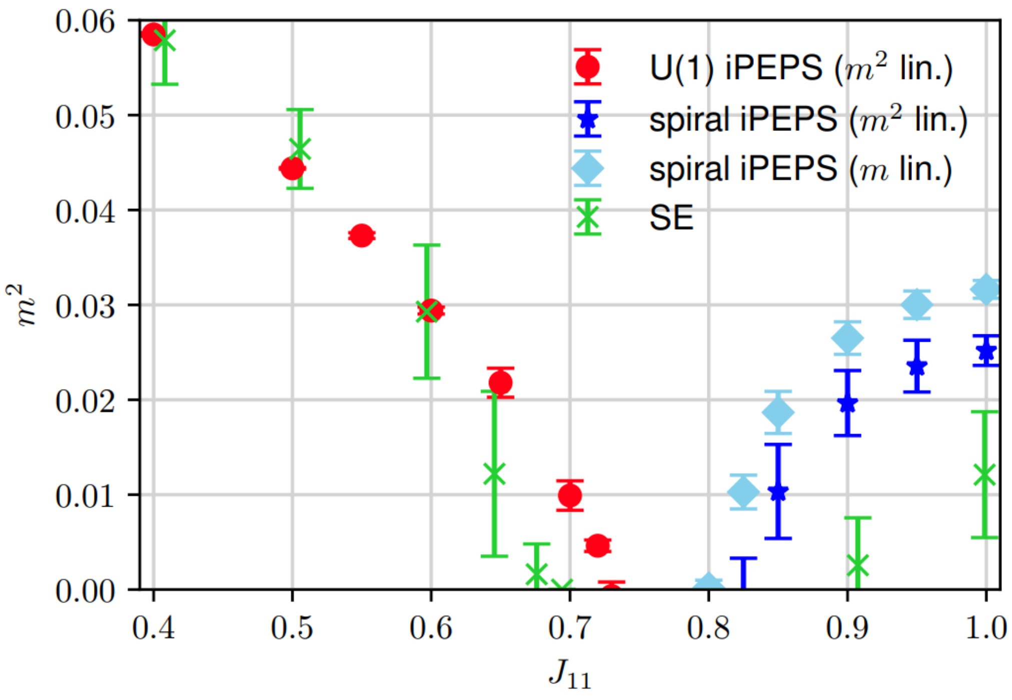


Correlation length scaling – phase diagram

- We can carry out variational optimization – including the spiral's **q**

$$H = \sum_{\mathbf{r}} J(\mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\hat{x}} + \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\hat{y}}) + J_{11} \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\hat{x}+\hat{y}}$$

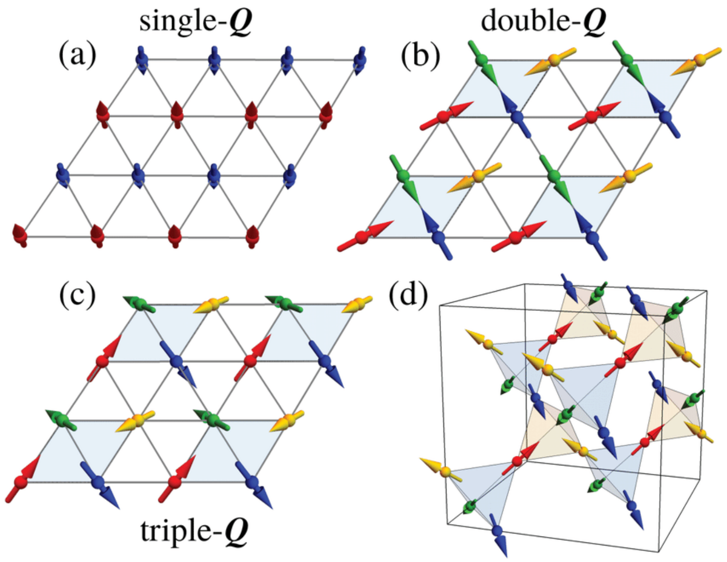
- With scaling theory, obtain extrapolation to $D \to \infty$
- Possible **spin-liquid** region

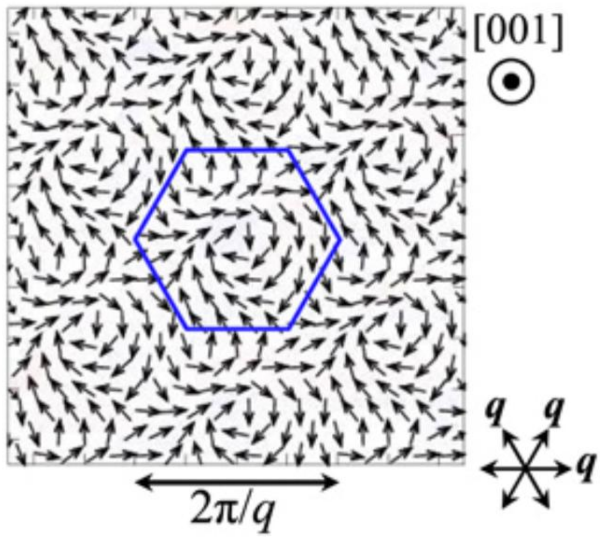


Rader and Lauchli; Corboz et al. PRX (2018)

Summary – Spiral iPEPS

- Allows for seamless exploration of phase diagrams, identifying single-**q** phases
- The computational cost **does not depend** on q
- Question: Can we leverage position-dependent unitaries for other magnetic textures ?





Takagi et al., Science Advances, Vol 4, Issue 11 (2018)

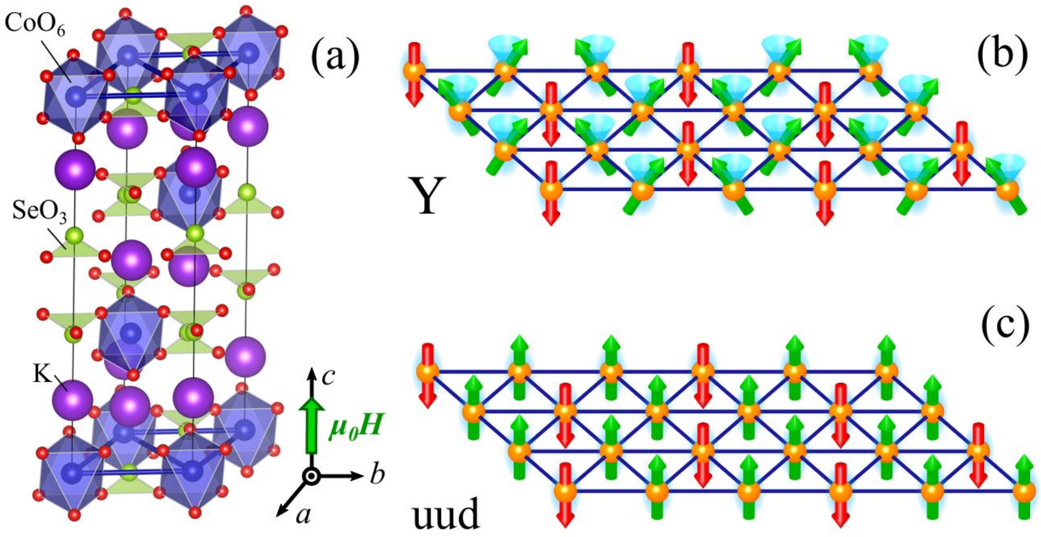
Application – excited states

Dynamical structure factor of $K_2Co(SeO_3)_2$

Yi Xu, JH, Boris Ponsioen,
Andriy H. Nevidomskyy
Phys. Rev. B 111, L060402 (2025)

RICE
UNIVERSITY OF AMSTERDAM
Faculty of Science

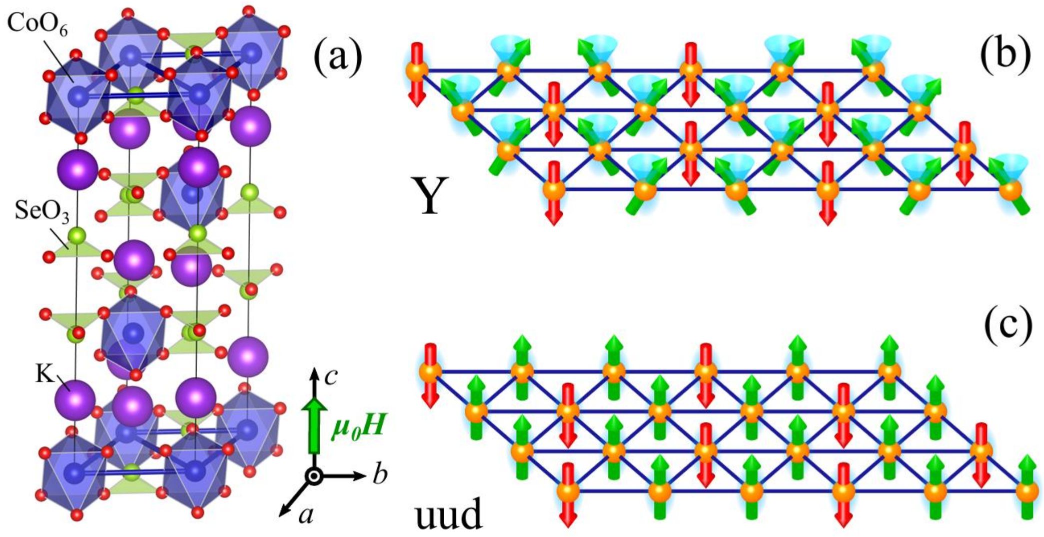
XXZ Antiferromagnet on triangular lattice



Zhu et al., Phys. Rev. Lett. 133, 186704 (2024)

- Large Δ, hence close to Ising limit

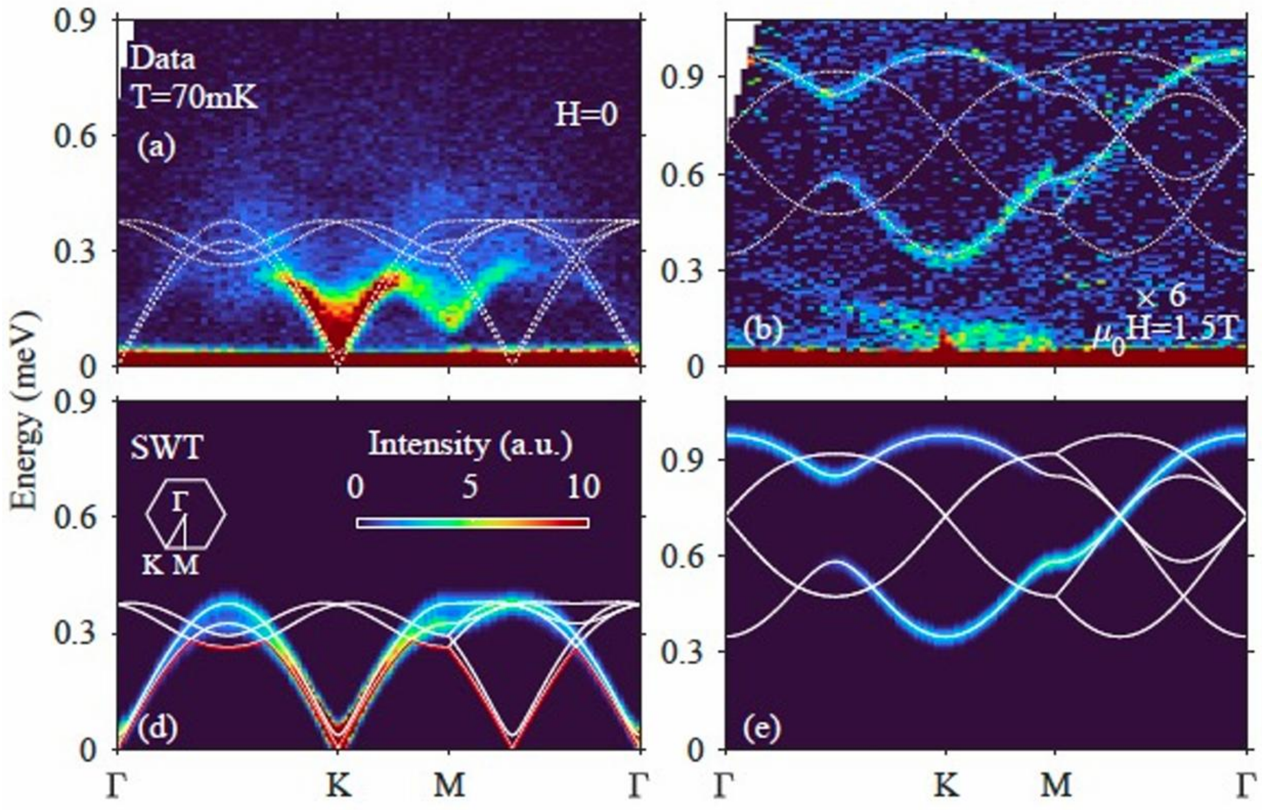
XXZ Antiferromagnet on triangular lattice



Zhu et al., Phys. Rev. Lett. 133, 186704 (2024)

- Large Δ, hence close to Ising limit

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \left(S_i^x S_j^x + S_i^y S_j^y + \Delta\, S_i^z S_j^z \right), \quad + ???$$



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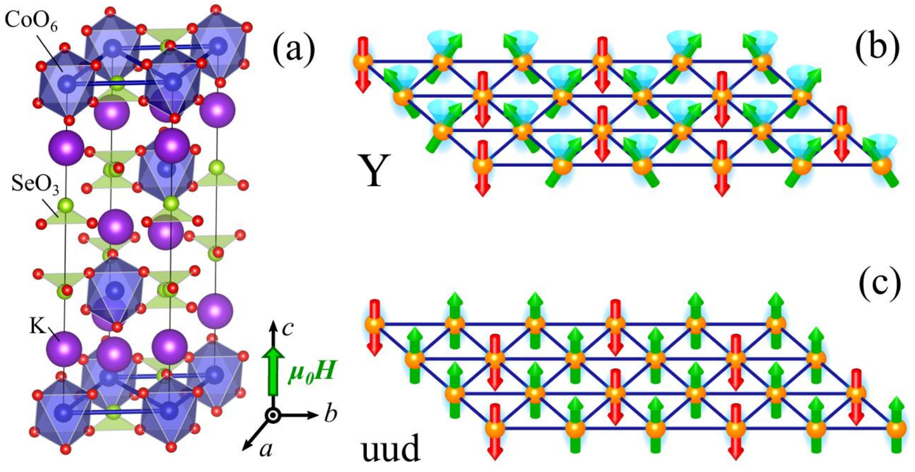


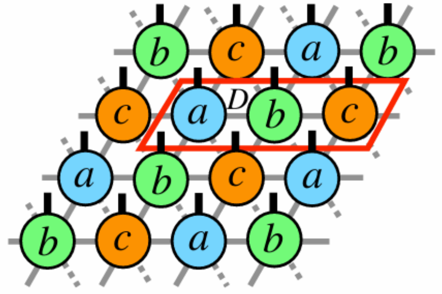
Zhu et al., Phys. Rev. Lett. 133, 186704 (2024)

$$\hat{H} = \sum_{\langle ij \rangle} \left[J_{zz} S_i^z S_j^z + J_{xy} \left(S_i^x S_j^x + S_i^y S_j^y \right) \right] - g\mu_B B_z \sum_i S_i^z$$

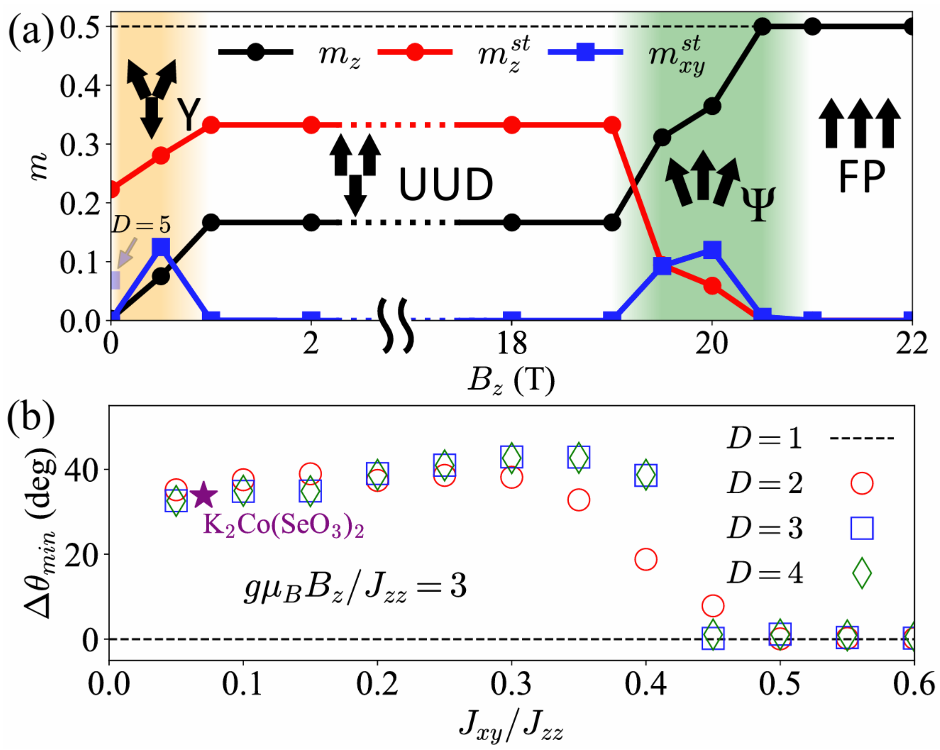
$J_{zz} = 2.98\text{meV}, J_{xy} = 0.21\text{meV}$

Estimates from fitting INS data arXiv:2402.15869

iPEPS parametrization:

$$|\Psi(A = [a, b, c])\rangle = \sum_{\{s\}}$$  $$|\{s\}\rangle$$

XXZ Antiferromagnet on triangular lattice



$$m_{xy}^{st} = |1/3 \sum_{n\in u.c.} e^{\frac{2in\pi}{3}} [\langle S_n^x\rangle \hat{x} + \langle S_n^y\rangle \hat{y}|)$$

$$m_z^{st} = |1/3 \sum_{n\in u.c.} e^{\frac{2in\pi}{3}} \langle S_n^z\rangle|$$

$$\hat{H} = \sum_{\langle ij\rangle} \left[J_{zz} S_i^z S_j^z + J_{xy}\left(S_i^x S_j^x + S_i^y S_j^y\right)\right] - g\mu_B B_z \sum_i S_i^z$$

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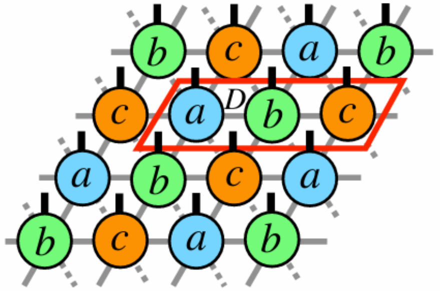
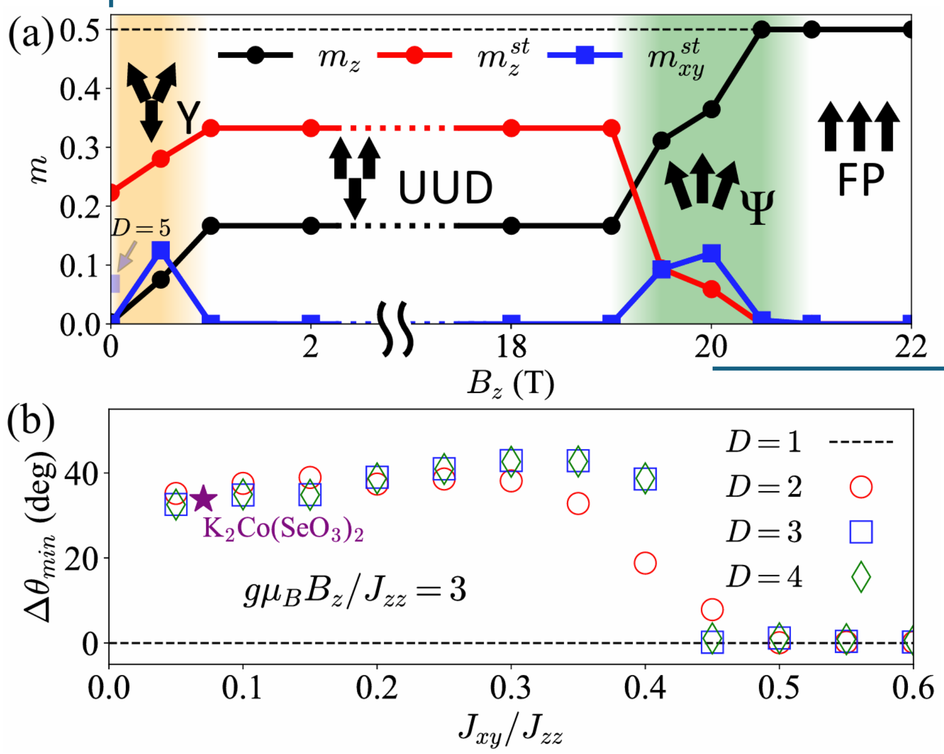
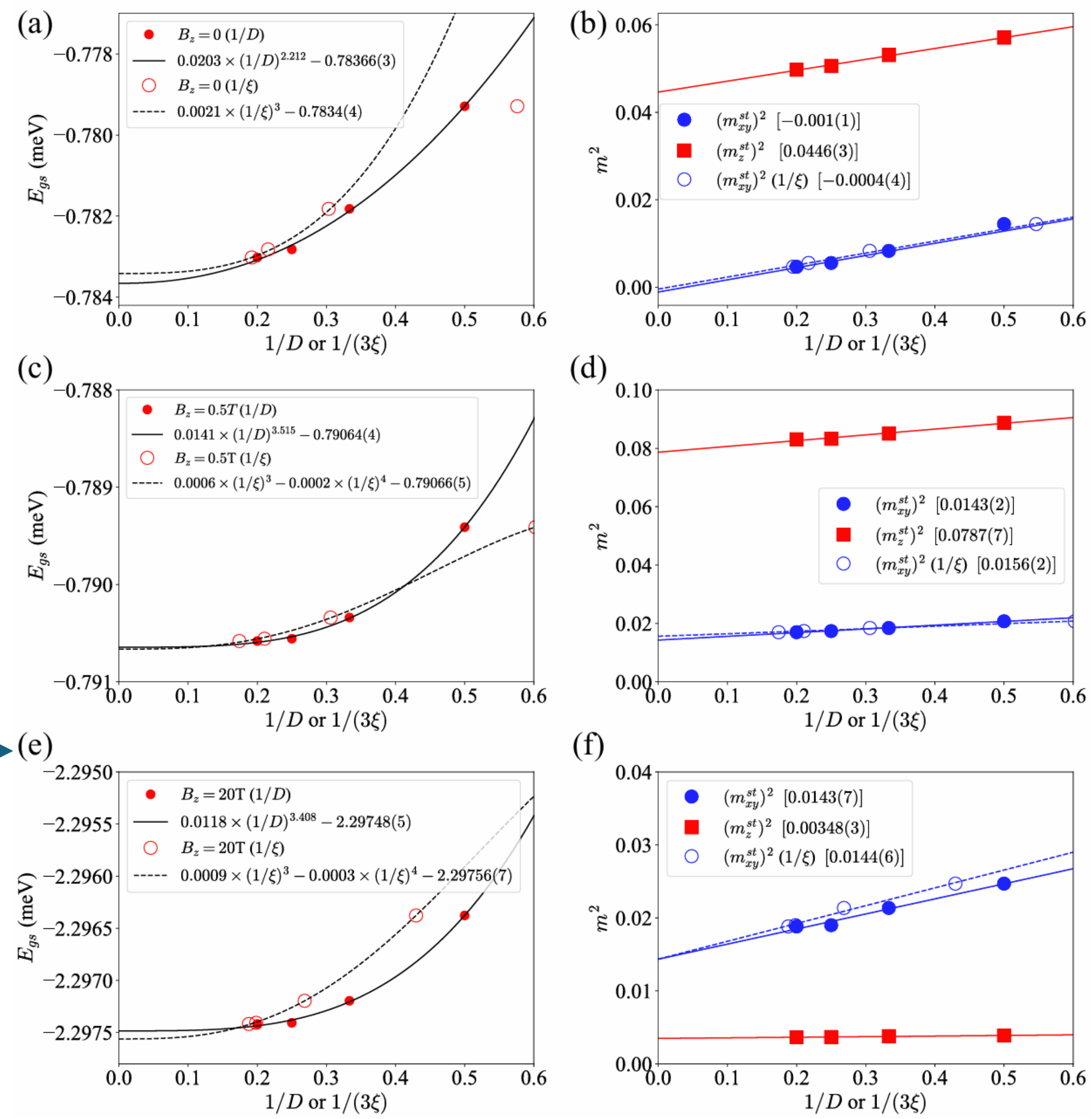
$$|\Psi(A=[a,b,c])\rangle = \sum_{\{s\}}$$  $$|\{s\}\rangle$$

XXZ Antiferromagnet on triangular lattice





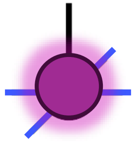
$$m^{st}_{xy} = \left|1/3 \sum_{n\in u.c.} e^{\frac{2in\pi}{3}} [\langle S^x_n\rangle \hat{x} + \langle S^y_n\rangle \hat{y}]\right|$$

$$m^{st}_{z} = \left|1/3 \sum_{n\in u.c.} e^{\frac{2in\pi}{3}} \langle S^z_n\rangle\right|$$

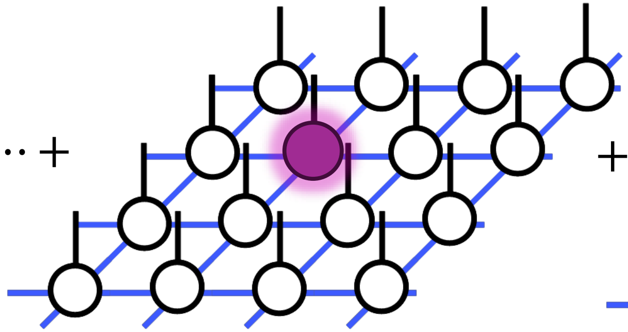
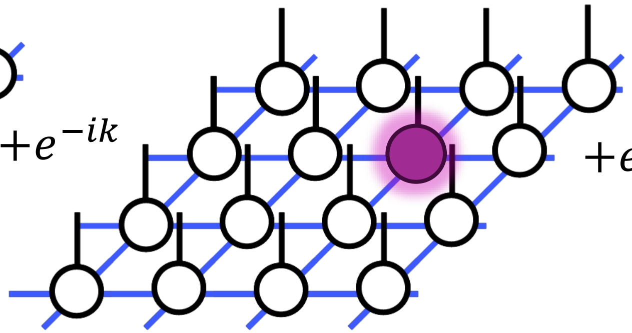
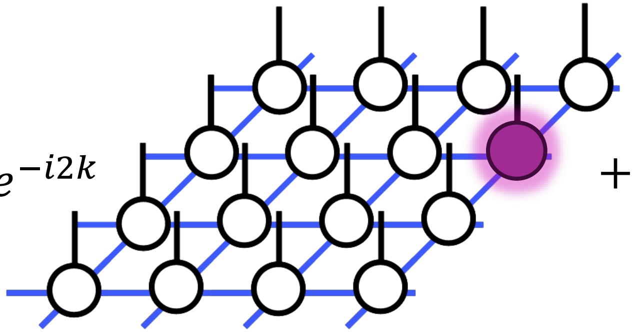
Tangent space

Spanned by plane-wave superposition of local defects *B*

$$|\Phi_k(B; M)\rangle = \sum_r e^{-i\boldsymbol{k}.\boldsymbol{r}} |\Psi_r(B; M)\rangle$$

B^s_{uldr} 

$\dim(u) = \dim(l) = \cdots = D$

$= \cdots +$  $+ e^{-ik}$  $+ e^{-i2k}$  $+ \cdots$

$|\Psi_r(B; M)\rangle$ $\quad$ $|\Psi_{r+1}(B; M)\rangle$ $\quad$ $|\Psi_{r+2}(B; M)\rangle$

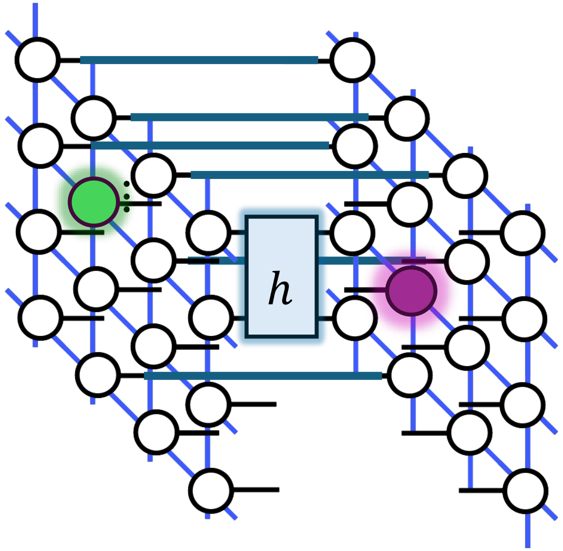
L. Vanderstraeten; B. Ponsioen, P. Corboz; Tu et al.

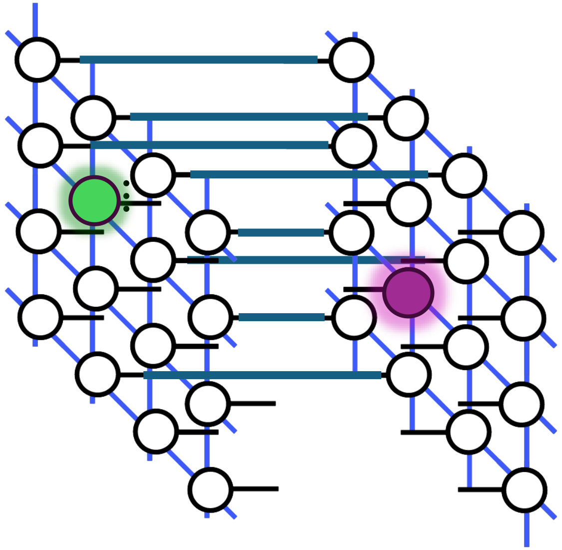
Tangent space

Project full Hamiltonian onto **tangent space** and solve

$\hat{H} P_{\boldsymbol{q}} |\psi\rangle = E_{\boldsymbol{q}} P_{\boldsymbol{q}} |\psi\rangle$ where $P_{\boldsymbol{q}} = \sum \left|\Phi_{\boldsymbol{q}}(B; M)\right\rangle \langle \Phi_{\boldsymbol{q}}(B; M)|$

→Generalized eigenvalue problem $\sum_{\beta} (\mathbb{H}^e_{\mathbf{k}})_{\alpha\beta} u^{(\gamma)}_{\beta} = \sum_{\beta} E_{\gamma} (\mathbb{F}^e_{\mathbf{k}})_{\alpha\beta} u^{(\gamma)}_{\beta}$





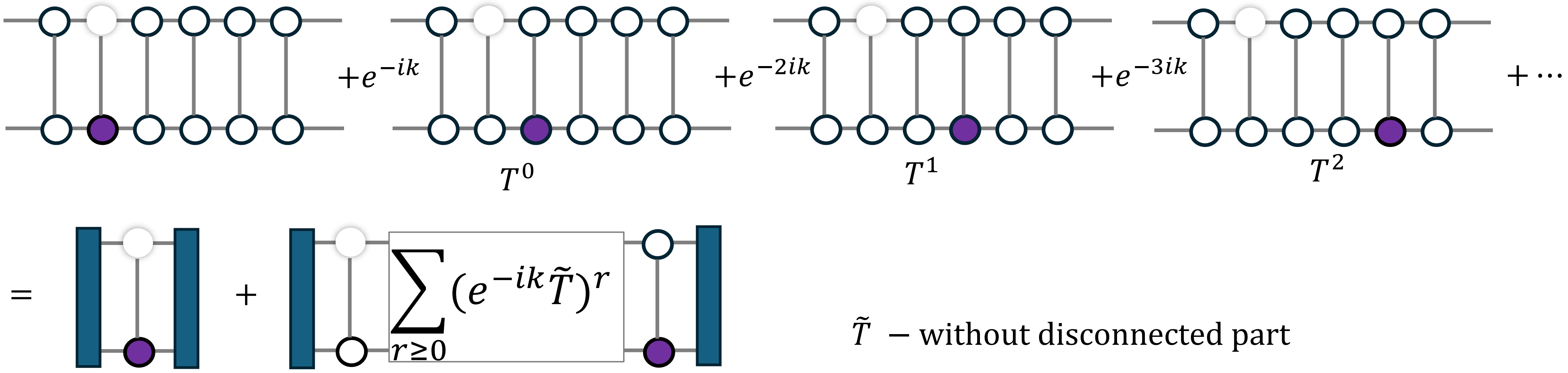
$(\mathbb{H}^e_{\mathbf{k}})_{\alpha\beta} \equiv E^e_{\mathbf{k}}(B_\alpha, B_\beta) = \frac{1}{N_s} \langle \Phi_{\mathbf{k}}(B_\alpha) | (\hat{H} - E_{gs}) | \Phi_{\mathbf{k}}(B_\beta) \rangle$

$F^e_{\mathbf{k}}(B_\alpha, B_\beta) = \frac{1}{N_s} \langle \Phi_{\mathbf{k}}(B_\alpha) | \Phi_{\mathbf{k}}(B_\beta) \rangle$

2- and 3-point summations: glimpse from 1D

$$F^e_{\mathbf{k}}(B_\alpha, B_\beta) = \frac{1}{N_s}\langle \Phi_{\mathbf{k}}(B_\alpha) | \Phi_{\mathbf{k}}(B_\beta)\rangle = \langle \Phi_{r=0}\,(.)|\Phi_k(B_\beta)\rangle$$

Translational invariance



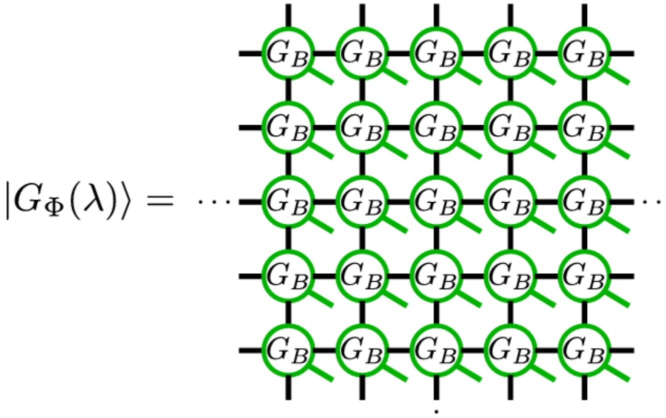
$\tilde{T}$ – without disconnected part

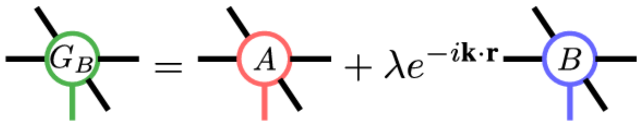
2- and 3-point summations: iPEPS

PRX QUANTUM **5**, 010335 (2024)

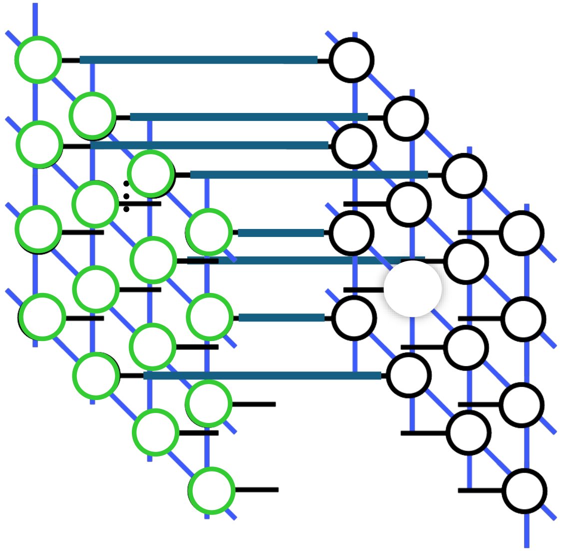
Generating Function for Projected Entangled-Pair States

Wei-Lin Tu,[1,*] Laurens Vanderstraeten,[2,†] Norbert Schuch,[3,4,‡] Hyun-Yong Lee,[5,6,7,§]
Naoki Kawashima,[8,9,¶] and Ji-Yao Chen[10,‖]





$$\partial_B \Big|_{\lambda=1, B=0}$$



$$F^e_{\mathbf{k}}(B_\alpha, B_\beta) = \frac{1}{N_s}\langle \Phi_{\mathbf{k}}(B_\alpha)|\Phi_{\mathbf{k}}(B_\beta)\rangle = \langle \Phi_{r=0}\,(.)|\Phi_k(B_\beta)\rangle$$

Dynamical structure factor - UUD

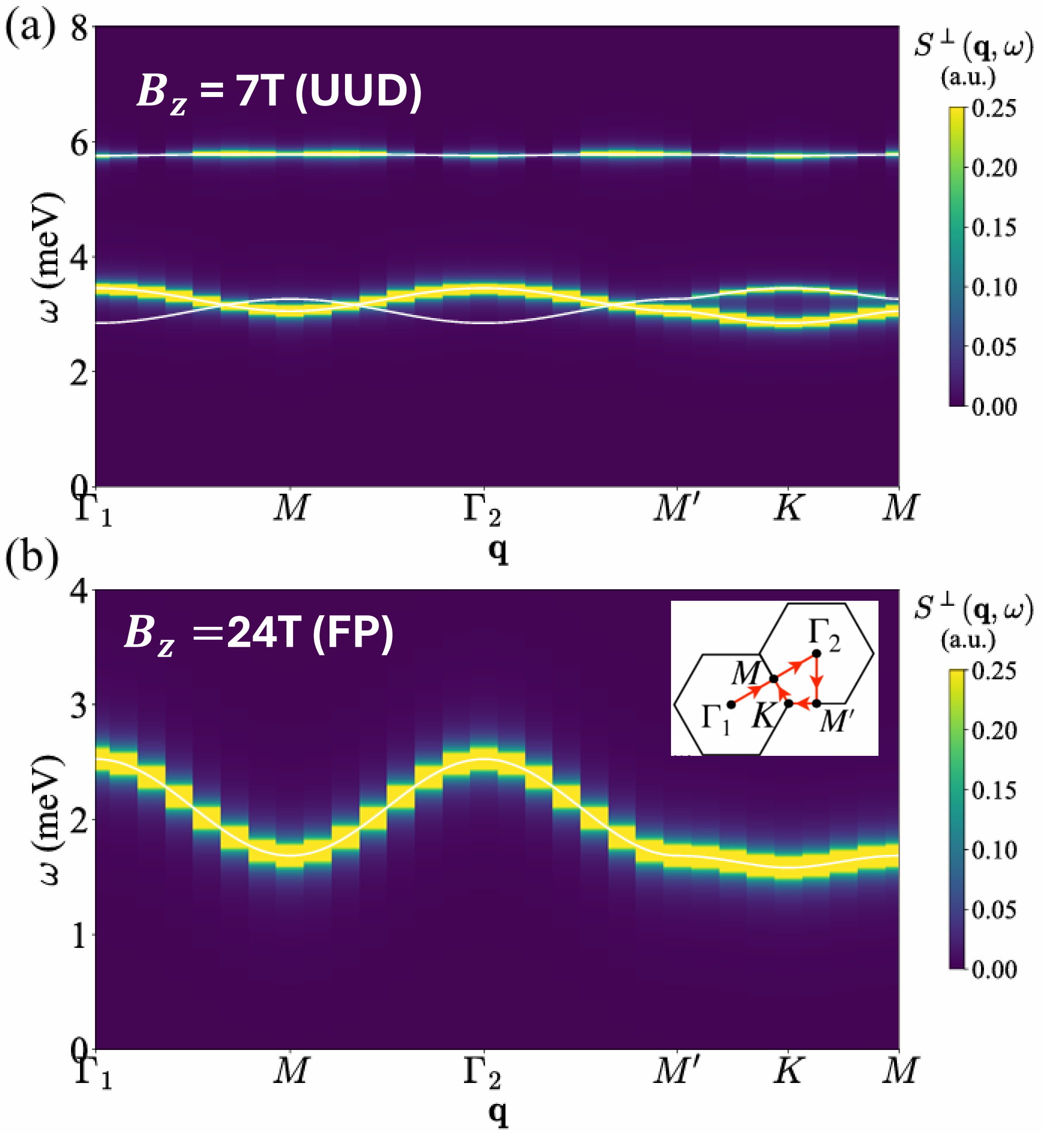
$$S^{\sigma\sigma}(\mathbf{q},\omega) \equiv \langle\Psi(A)|\hat{s}^{\sigma}_{-\mathbf{q}}\hat{s}^{\sigma}_{\mathbf{q}}\,\delta(\omega-\hat{H}+E_0)|\Psi(A)\rangle$$

For iPEPS excitation ansatz

$$S^{\sigma\sigma}(\mathbf{q},\omega) = \sum_{\alpha} p^{\sigma}_{\alpha}(\mathbf{q})\delta(\omega-\tilde{E}_{\mathbf{q}\alpha}+E_0)$$

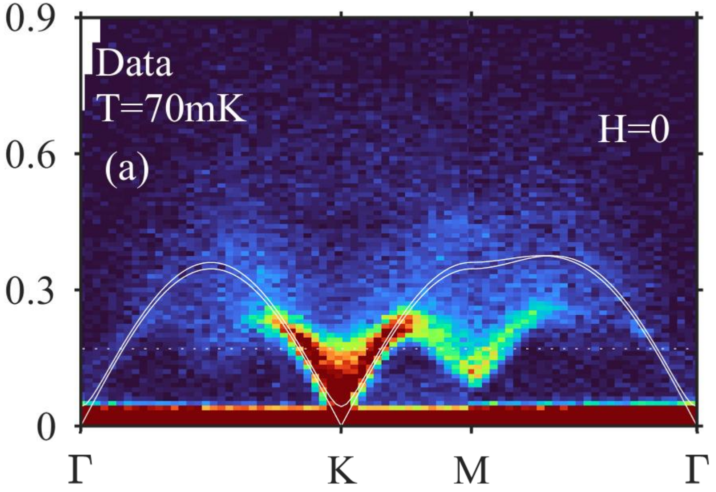
$$p^{\sigma}_{\alpha}(\mathbf{q}) = |\langle\Phi_{\mathbf{q}}(\tilde{B}_{\alpha})|\hat{s}^{\sigma}_{\mathbf{q}}|\Psi(A)\rangle|^2$$

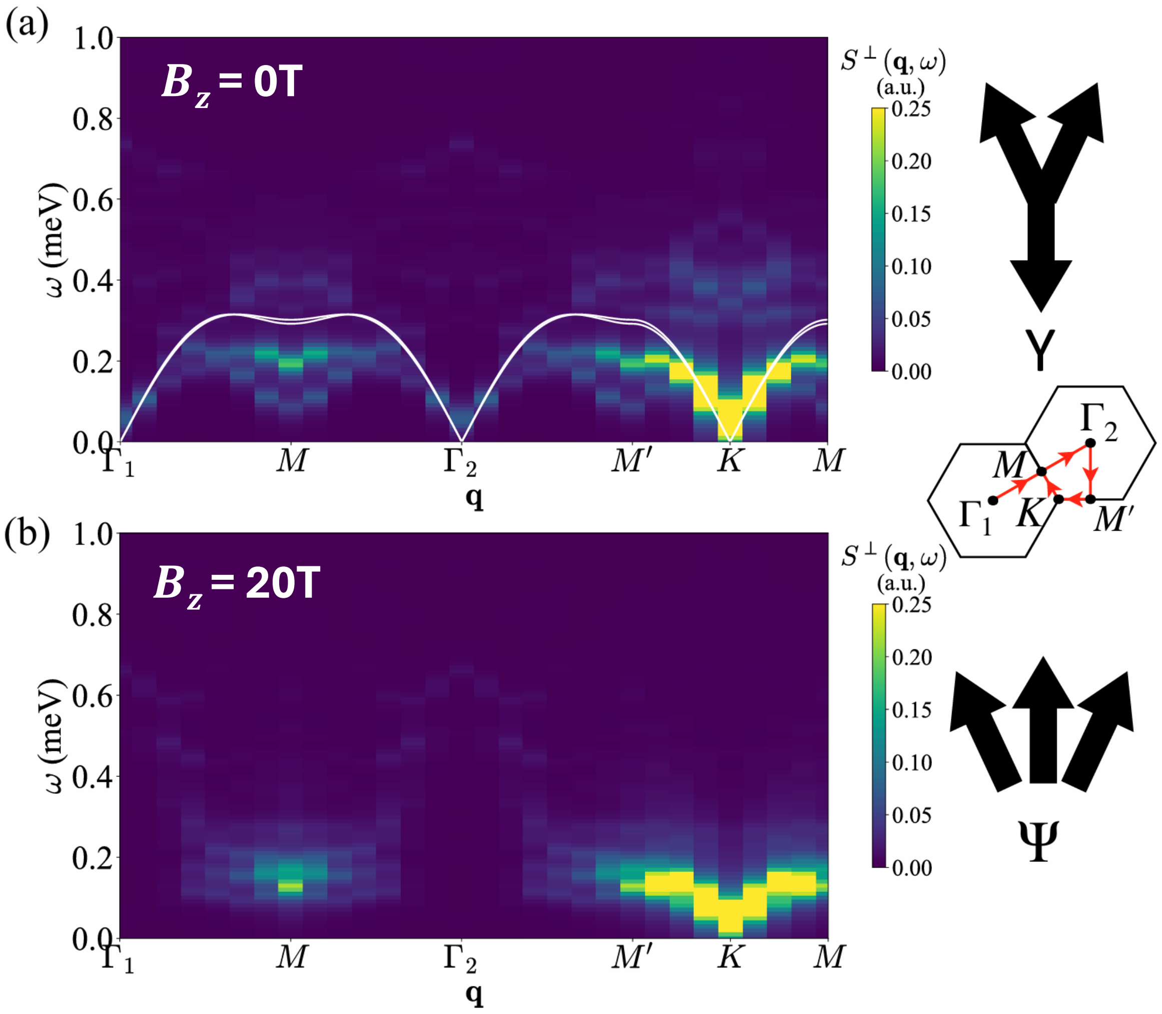
- In case of product states, equivalent to single-mode approximation



Dynamical structure factor - SuperSolid

$$S^{\sigma\sigma}(\mathbf{q},\omega) \equiv \langle \Psi(A)|\hat{s}^{\sigma}_{-\mathbf{q}}\hat{s}^{\sigma}_{\mathbf{q}}\,\delta(\omega - \hat{H} + E_0)|\Psi(A)\rangle$$





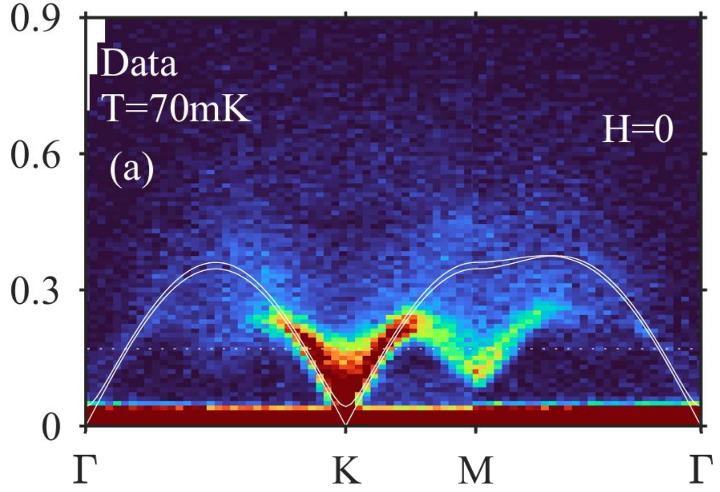
For iPEPS excitation ansatz

$$S^{\sigma\sigma}(\mathbf{q},\omega) = \sum_{\alpha} p^{\sigma}_{\alpha}(\mathbf{q})\delta(\omega - \tilde{E}_{\mathbf{q}\alpha} + E_0)$$

$$p^{\sigma}_{\alpha}(\mathbf{q}) = |\langle \Phi_{\mathbf{q}}(\tilde{B}_{\alpha})|\hat{s}^{\sigma}_{\mathbf{q}}|\Psi(A)\rangle|^2$$

Dynamical structure factor – roton mode

$$S^{\sigma\sigma}(\mathbf{q},\omega) \equiv \langle \Psi(A)|\hat{s}^{\sigma}_{-\mathbf{q}}\hat{s}^{\sigma}_{\mathbf{q}}\,\delta(\omega - \hat{H} + E_0)|\Psi(A)\rangle$$



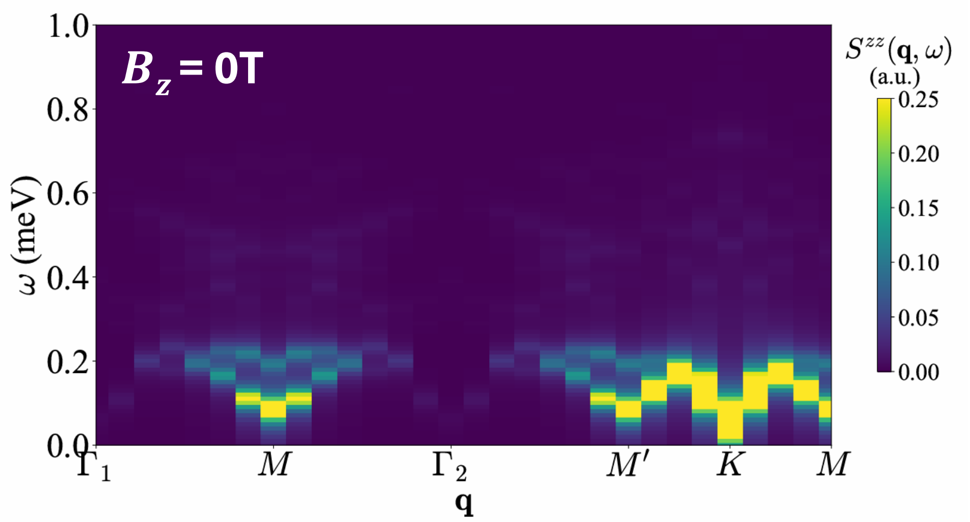


FIG. S2. Out-of-plane component of the dynamical spin structure factor, $S^{zz}(\boldsymbol{q},\omega)$, for the Y phase at $B_z = 0$, produced by $D = 3$ PEPS simulations with $n_b = 50$ states kept. The Lorentzian broadening factor is chosen to be $\eta = 0.02$ meV.

For iPEPS excitation ansatz

$$S^{\sigma\sigma}(\mathbf{q},\omega) = \sum_{\alpha} p^{\sigma}_{\alpha}(\mathbf{q})\delta(\omega - \tilde{E}_{\mathbf{q}\alpha} + E_0)$$

$$p^{\sigma}_{\alpha}(\mathbf{q}) = |\langle \Phi_{\mathbf{q}}(\tilde{B}_{\alpha})|\hat{s}^{\sigma}_{\mathbf{q}}|\Psi(A)\rangle|^2$$

Summary - KCSO

- Simulate **zero temperature** phase diagram of KCSO's effective model
  - New high-field super-solid phase ?

- Simulate **low-energy dynamics** (at zero temperature)
  - Captures low-energy dispersion beyond (non-linear) spin-waves

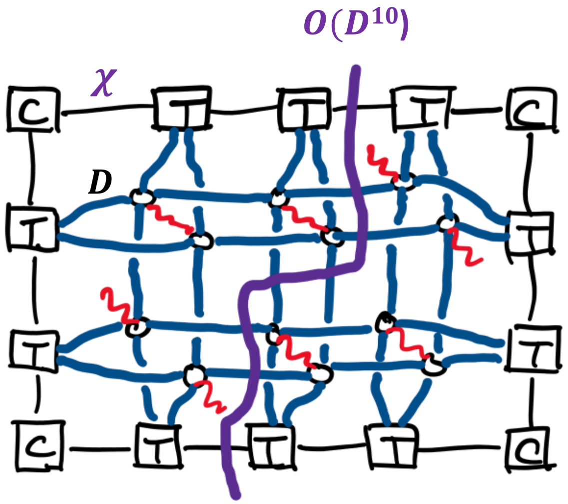
- Can we resolve the **zero-field** situation ? Scaling indicates vanishing superfluid order.

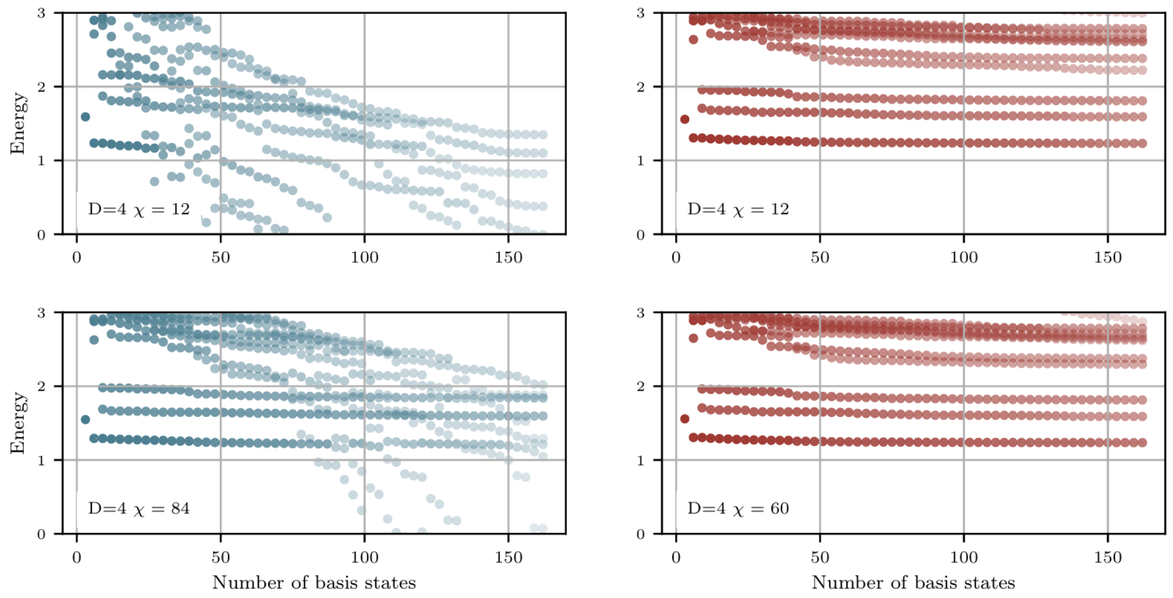
Challenges (not just) on triangular lattice

- Gradient minimization of energy from approximate environments unless protected by explicit point-group symmetry of the lattice

- Stability of excited states

- Sharp scaling of evaluation of NNN interaction (J_2)





Ponsioen, JH, Corboz

Mature software

github.com/jurajHasik/peps-torch

github.com/yastn/yastn

YASTN power PEPS simulations in D-wave's recent

"Computational supremacy in quantum simulation"
by King et al (D-wave and collaborators) Science (2025)



with Marek M. Rams, Gabriela Wójtowicz, and Aritra Sinha

JAGIELLONIAN UNIVERSITY IN KRAKÓW

And other

- **1D:** ITensor**,** TenPy**,** many more …
- 2D: **Quantumghent**, variPEPS, ADpeps, and not many more

Thank you !

Many thanks to collaborators:
Boris Ponsioen,
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Andriy Nevidomskyi (Rice)
Aritra Sinha,
Gabriela Wójtowicz,
Marek Rams (Krakow)