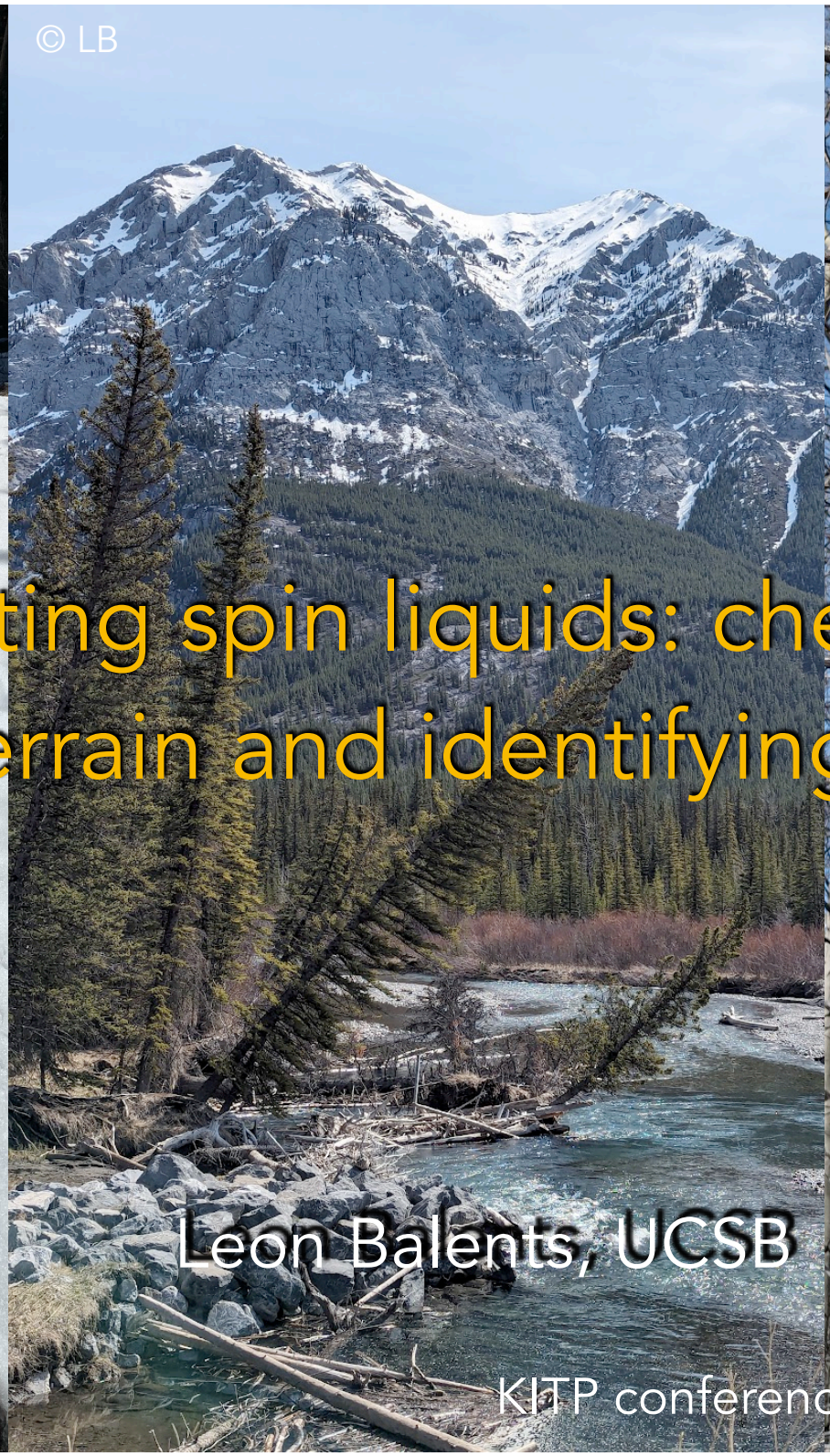


Hunting spin liquids: checking out the terrain and identifying the tracks

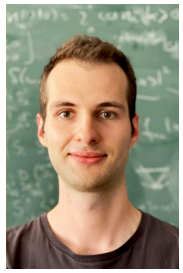
Leon Balents, UCSB

KITP conference "Gapless24", May 2024

Collaborators

Zhenhao Song
UCSB

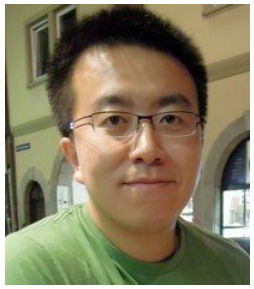
Zhu-Xi Luo
Harvard
→ Georgia Tech



Urban Seifert
U. Köln

Hongchen Jiang
SLAC

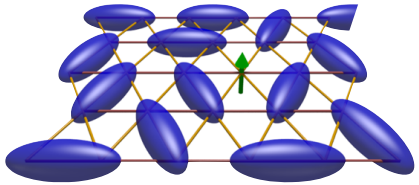
Oleg Starykh
U. Utah



Zi-Yang Meng
HKU

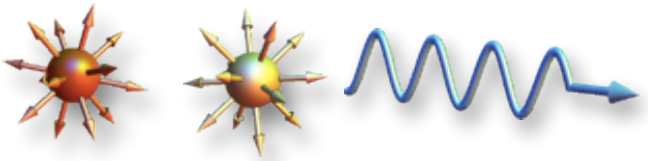
Quantum spin liquids

- Topological QSLs



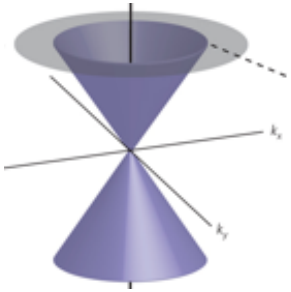
TQFT

- U(1) QSL



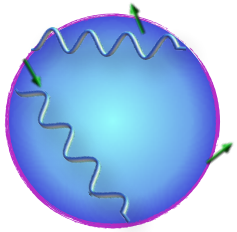
4d Maxwell

- Dirac QSLs

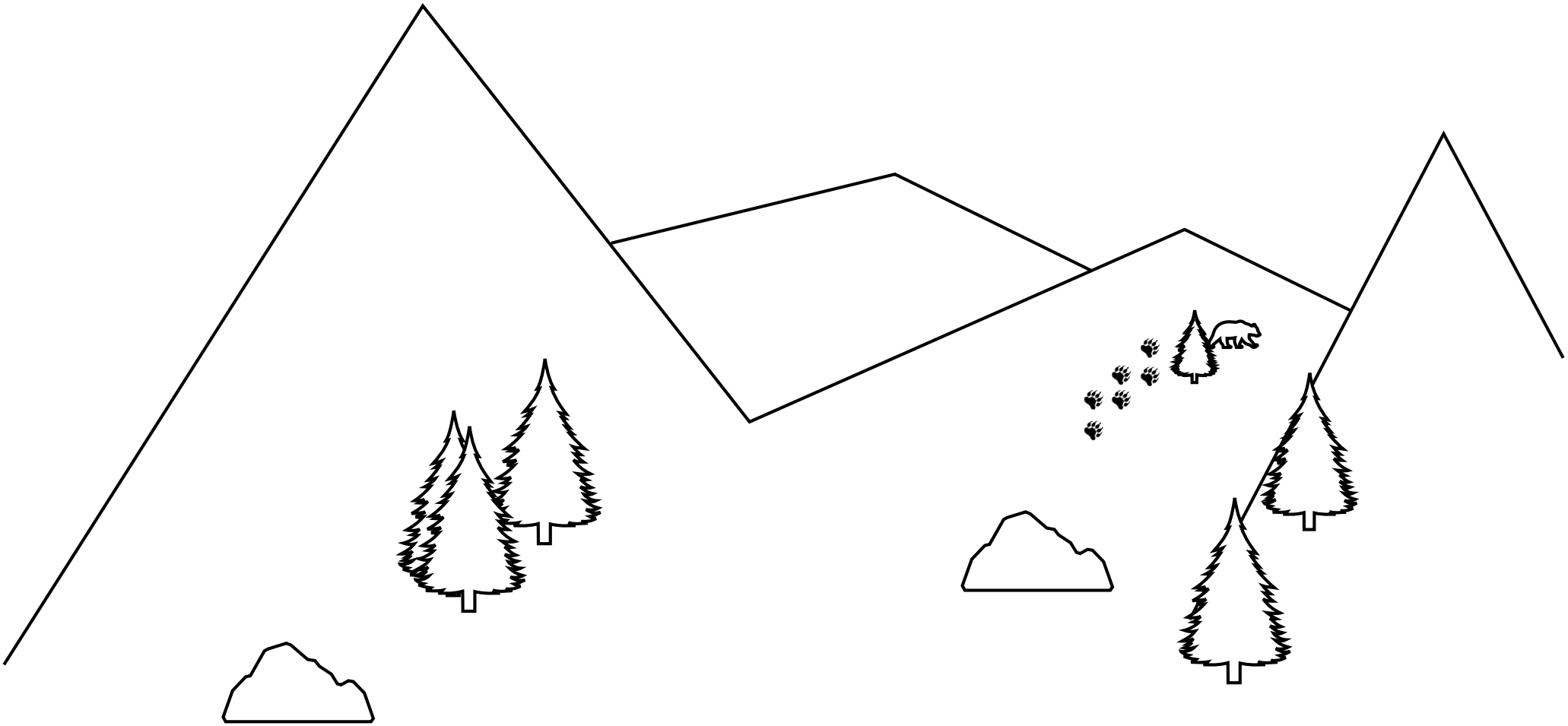


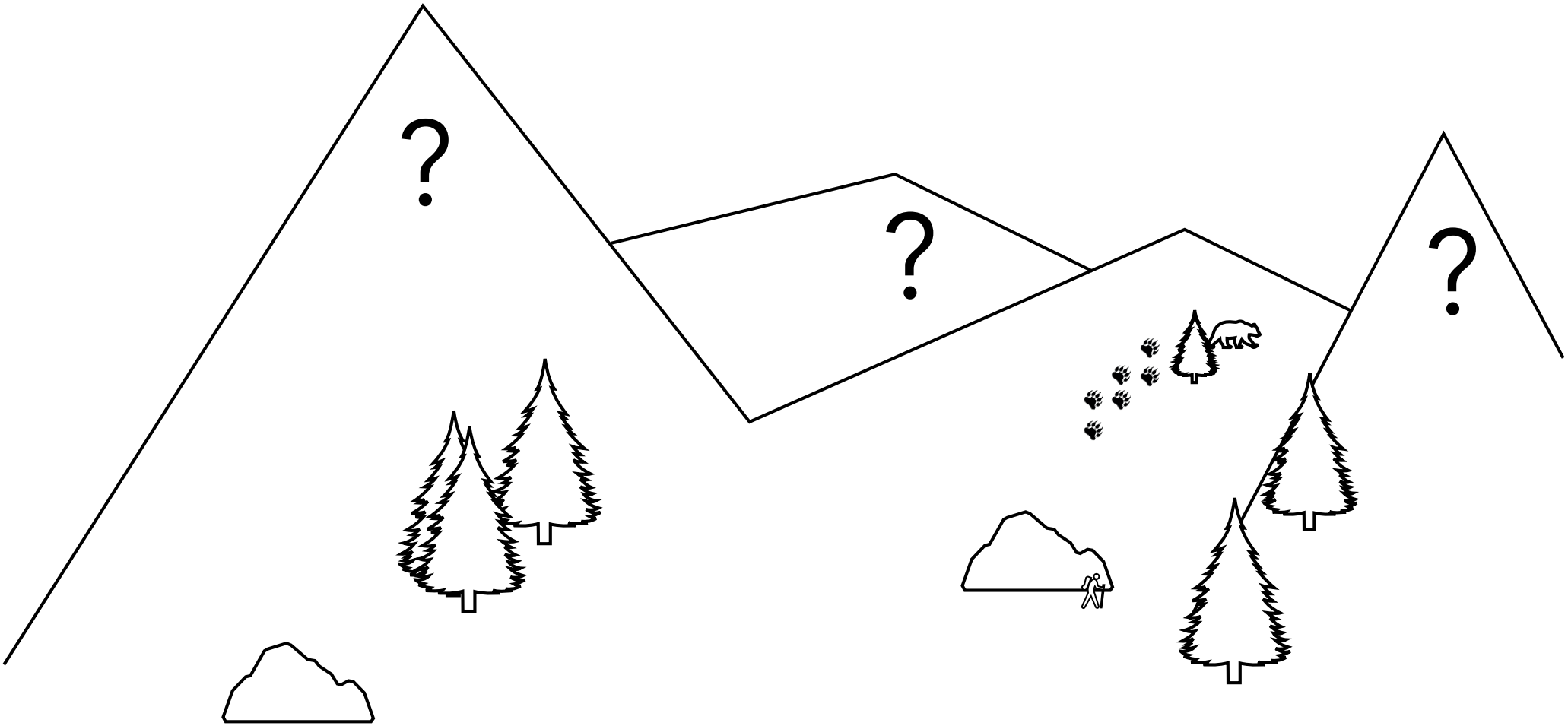
QED3

- Spinon Fermi surface



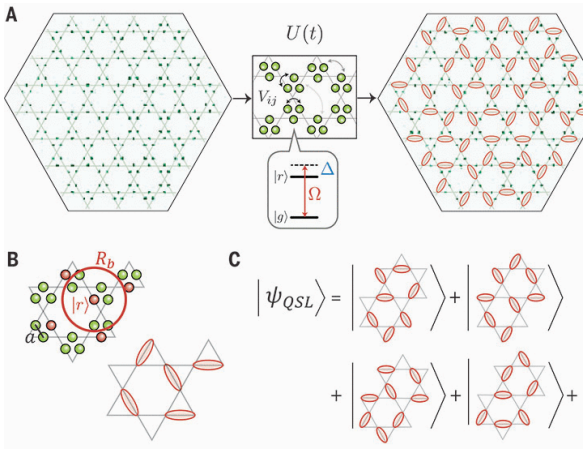
QED3 with
$\mu \neq 0$





Spin liquid terrain

Quantum simulator

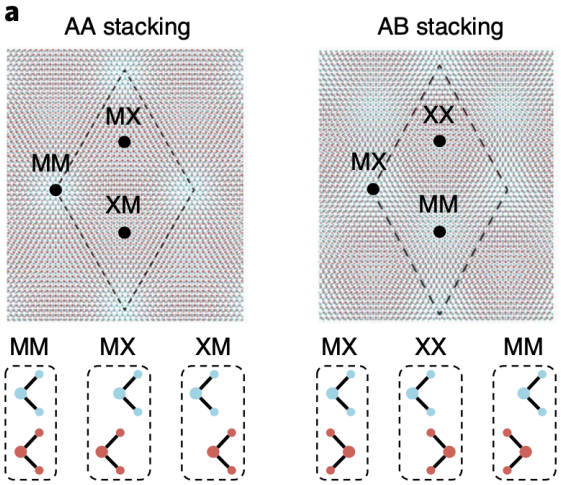


219 qubits

Very high degree of control

athermal

2d materials



10^6 qubits

Some control

meV scales

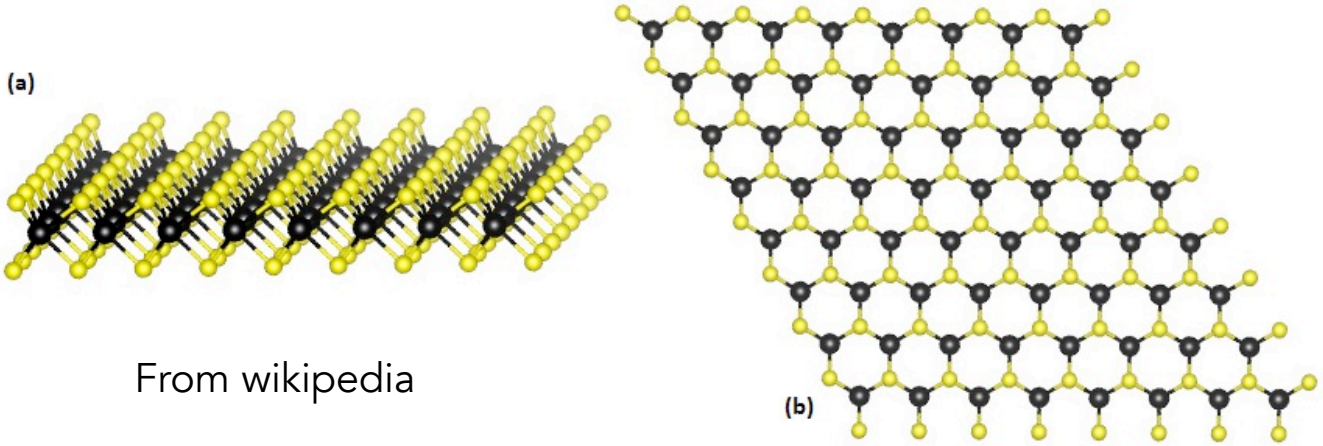
Crystals

10^{22} qubits

Caveat emptor

eV scales

TMD



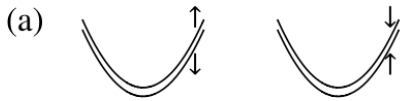
From wikipedia

MX_2

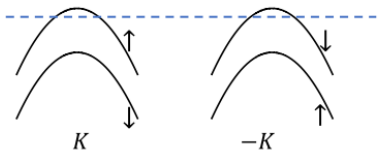
M=transition metal,
W, Mo, Nb etc.

X=chalcogenide
S,Se,Te

Typical band structure of TMD

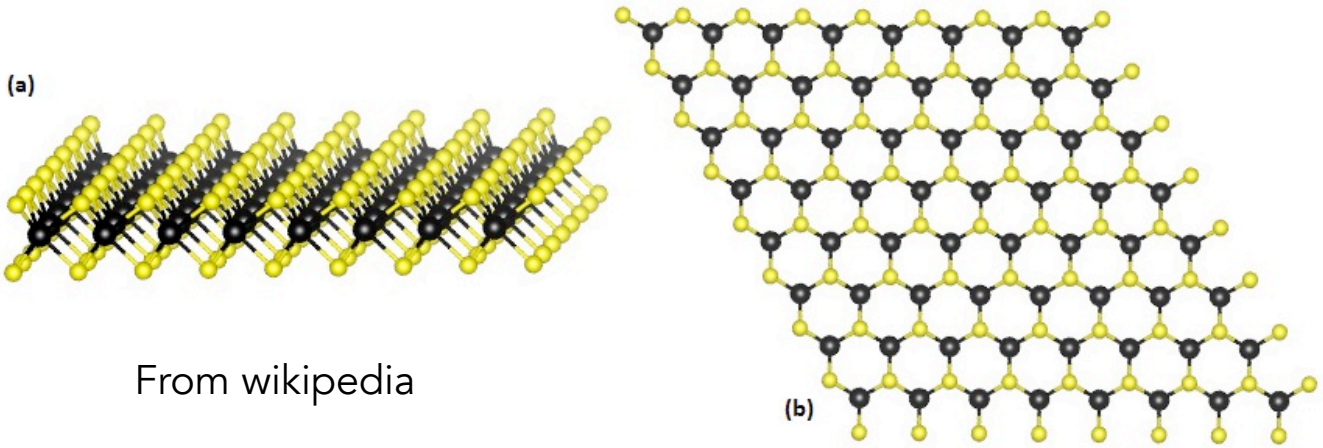


F. Wu *et al*, 2018



- Quadratic dispersion: non-relativistic Schrödinger equation
- Spin-valley locking

TMD



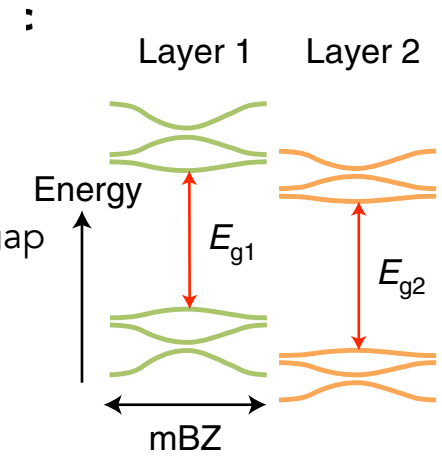
From wikipedia

MX_2

M=transition metal,
W, Mo, Nb etc.

X=chalcogenide
S,Se,Te

Typical band structure of bilayer



Large semiconducting gap

moiré bands localized around
band edge momenta

	graphene	TMD
Typical energy scales	$W \approx 10$–100 meV $U \approx 20$–40 meV	$W \approx 1$–100 meV $U \approx 100$–200 meV

K.-F. Mak, J. Shan, 2022

Hubbard simulator

PHYSICAL REVIEW LETTERS **121,** 026402 (2018)

Hubbard Model Physics in Transition Metal Dichalcogenide Moiré Bands

Fengcheng Wu,[1] Timothy Lovorn,[2] Emanuel Tutuc,[3] and A. H. MacDonald[2]

PHYSICAL REVIEW B **102**, 201104(R) (2020)

Quantum phase diagram of a Moiré-Hubbard model

Haining Pan, Fengcheng Wu, and Sankar Das Sarma

Article

Simulation of Hubbard model physics in WSe_2/WS_2 moiré superlattices

https://doi.org/10.1038/s41586-020-2085-3
Received: 18 August 2019

Yanhao Tang[1], Lizhong Li[1], Tingxin Li[1], Yang Xu[1], Song Liu[2], Katayun Barmak[3], Kenji Watanabe[4], Takashi Taniguchi[4], Allan H. MacDonald[5], Jie Shan[1,6,7]✉ & Kin Fai Mak[1,6,7]✉

PHYSICAL REVIEW B **104**, 075150 (2021)

Editors' Suggestion

Hartree-Fock study of the moiré Hubbard model for twisted bilayer transition metal dichalcogenides

Jiawei Zang,[1] Jie Wang,[2] Jennifer Cano,[2,3] and Andrew J. Millis[1,2]

moiré (extended) Hubbard model

$$H = \sum_s \sum_{i,j} t_s(\boldsymbol{R}_i - \boldsymbol{R}_j) c^\dagger_{i,s} c_{j,s} + \frac{1}{2} \sum_{s,s'} \sum_{i,j} U(\boldsymbol{R}_i - \boldsymbol{R}_j) c^\dagger_{i,s} c^\dagger_{j,s'} c_{j,s'} c_{i,s},$$

complex hopping Longer-range interactions

Caution: does not apply if active band is topologically non-trivial

The Hubbard model is hard

D. Arovas *et al*, ARCMP, 2022

~60 years!

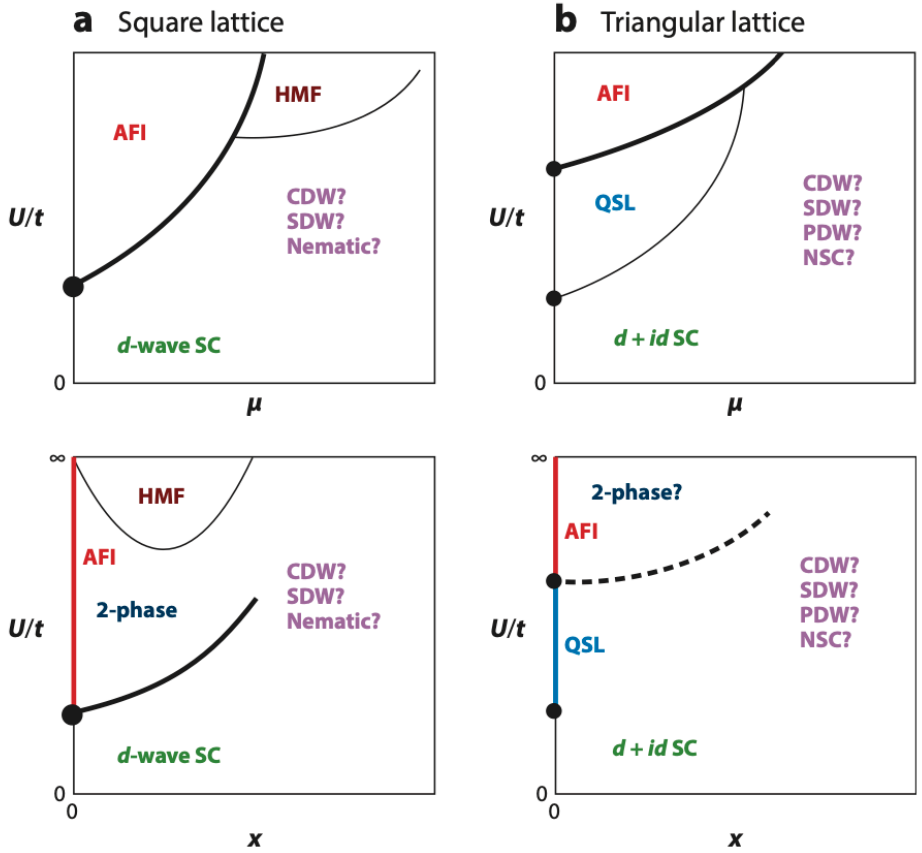


Figure 5

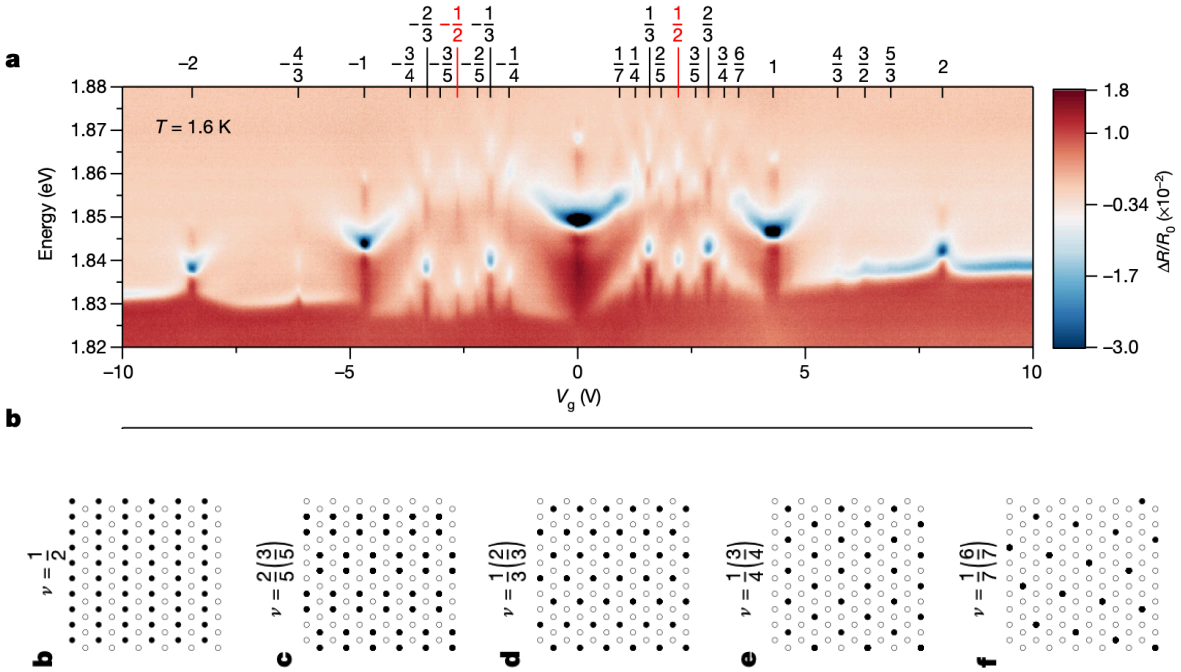
Speculative ground state phase diagrams of the Hubbard model as a function of U and chemical potential, μ

c.f.

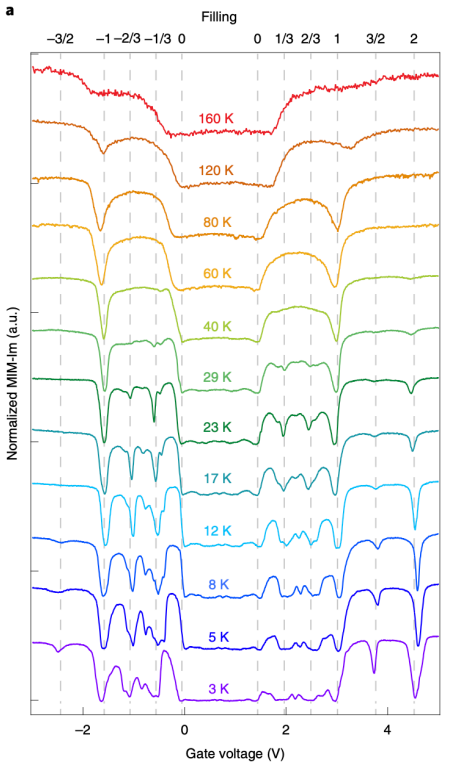
Simons Collaboration on the Many Electron Problem

Moiré Hubbard simulator

WS_2/WSe_2 bilayers



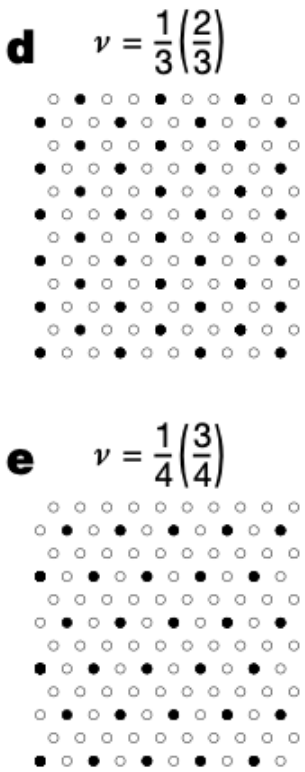
Y. Xu *et al*, 2020



X. Huang *et al*, 2021

Fractional filling insulators: charge order

Emergent lattices



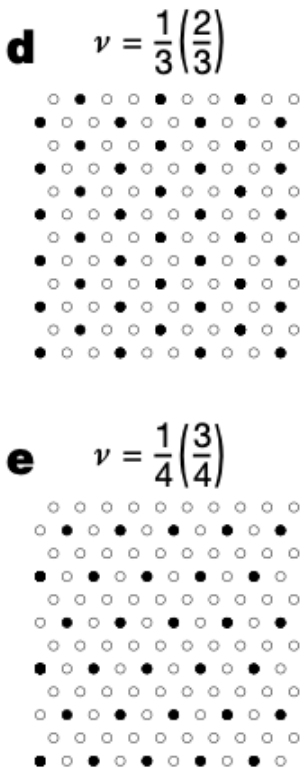
Triangular/honeycomb

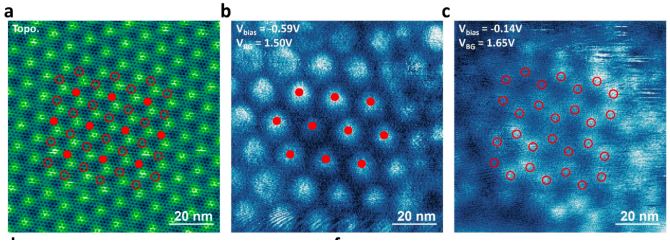
Triangular/kagomé

The Wigner crystallization is essentially classical

What are the spins doing?

Emergent lattices





H. Li *et al*, 2022

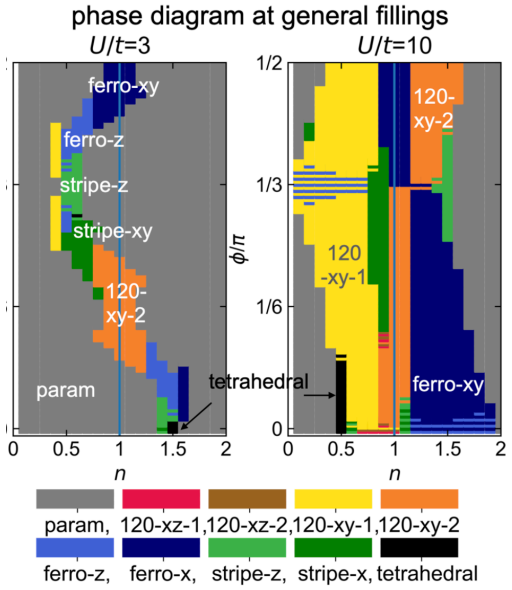
Electron and hole excitations in twisted WS_2 imaged via graphene capping layer

Triangular/kagomé

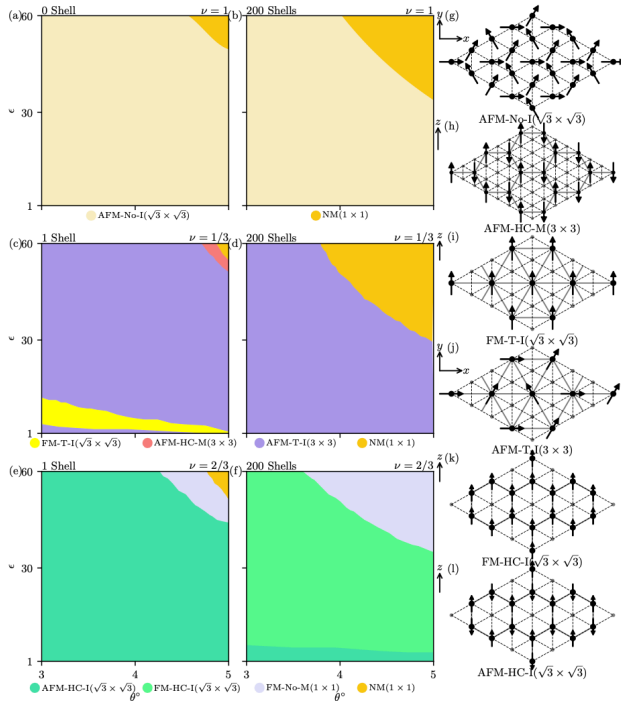
The Wigner crystallization is essentially classical

What are the spins doing?

Hartree-Fock studies



J. Zang *et al*, 2021



H. Pan + S. Das Sarma, 2022

+ many more

These studies are incapable of finding spin liquids

(Much fewer studies with other techniques, not global)

Slave rotor

$$c_{i\alpha} = f_{i\alpha} b_i$$

$$f_i^\dagger f_i = n_i$$ gauge constraint

$$b_i = e^{i\varphi_i}$$

$$[n_i, \varphi_j] = i\delta_{ij}$$

S. Florens + A. Georges, 2004

Slave rotor

$$c_{i\alpha} = f_{i\alpha} b_i \qquad f_i^\dagger f_i = n_i$$ gauge constraint

$$b_i = e^{i\varphi_i}$$

$$[n_i, \varphi_j] = i\delta_{ij}$$ S. Florens + A. Georges, 2004

Due to the constraint, density-density interactions can be cast entirely into the boson sector

$$H = \sum_{ij;\alpha} t_{ij,\alpha} f_{i\alpha}^\dagger f_{j\alpha} b_i^\dagger b_j + \frac{1}{2}\sum_{i,j} U_{ij} n_i n_j$$

$$\downarrow$$

$$H_{mf} = \sum_{ij;\alpha} t_{ij,\alpha}^{\text{eff}} f_i^\dagger f_j + K_{ij} b_i^\dagger b_j + \frac{1}{2}\sum_{i,j} U_{ij} n_i n_j$$

Slave rotor

$$c_{i\alpha} = f_{i\alpha} b_i \qquad f_i^\dagger f_i = n_i$$ gauge constraint

$$b_i = e^{i\varphi_i}$$

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Due to the constraint, density-density interactions can be cast entirely into the boson sector

MF conditions $$t^{\text{eff}}_{ij,\alpha} = t_{ij,\alpha}\langle b_i^\dagger b_j\rangle \quad K_{ij} = \sum_\alpha t_{ij,\alpha}\langle f^\dagger_{i,\alpha} f_{j,\alpha}\rangle$$

$$H_{mf} = \sum_{ij;\alpha} t^{\text{eff}}_{ij,\alpha} f_i^\dagger f_j + K_{ij} b_i^\dagger b_j + \frac{1}{2}\sum_{i,j} U_{ij} n_i n_j$$

Slave rotor

$$c_{i\alpha} = f_{i\alpha} b_i \qquad f_i^\dagger f_i = n_i$$ gauge constraint

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Physics:
Phases become
U(1) gauge fields

c.f. Senthil 2008

Secondary MF

MF conditions $t^{\rm eff}_{ij,\alpha} = t_{ij,\alpha}\langle b^\dagger_i b_j\rangle \quad K_{ij} = \sum_\alpha t_{ij,\alpha}\langle f^\dagger_{i,\alpha} f_{j,\alpha}\rangle$

$$H_{mf} = \sum_{ij;\alpha} t^{\rm eff}_{ij,\alpha} f^\dagger_i f_j + K_{ij} b^\dagger_i b_j + \frac{1}{2}\sum_{i,j} U_{ij} n_i n_j$$

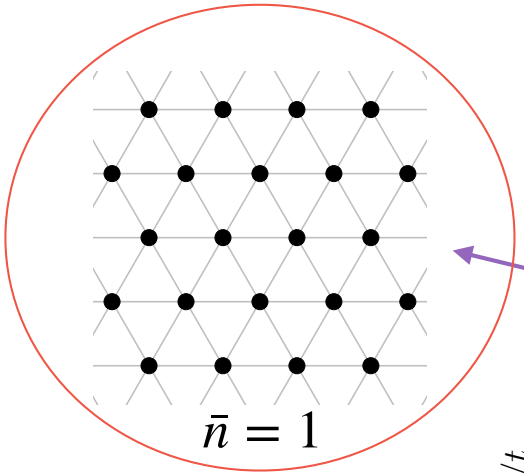
Boson rotor model still non-trivial: a canonical model for Bose Mott and Bose crystal transitions

For a tractable calculation we carry out a secondary MF for the boson problem, and work to quadratic order in the fluctuations around it. This is sufficient to obtain all necessary expectation values, and becomes exact in the large U limit.

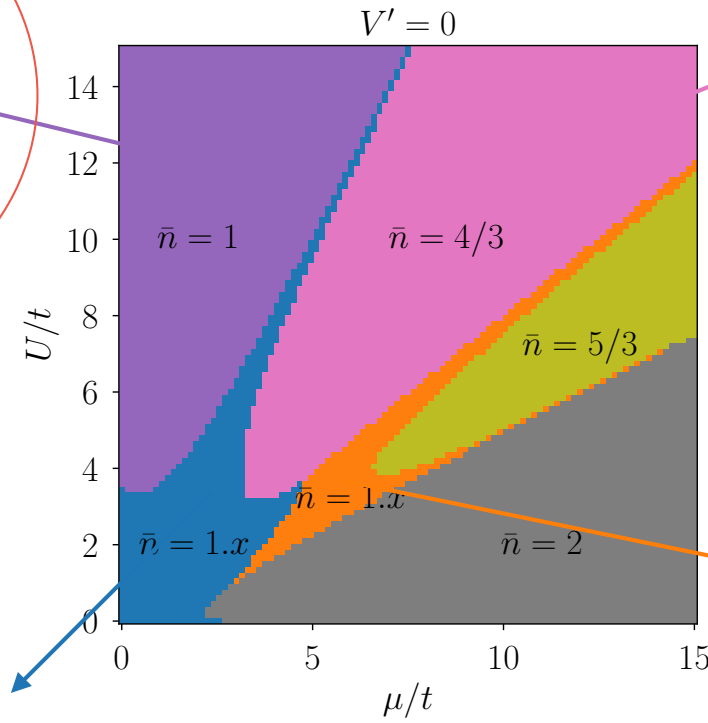
Mean Field results

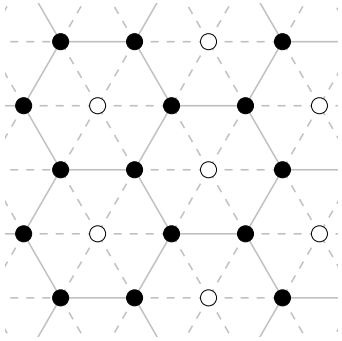
On-site repulsion: U nearest neighbor repulsion: $V = U/4$

next nearest neighbor repulsion: $V' = 0$



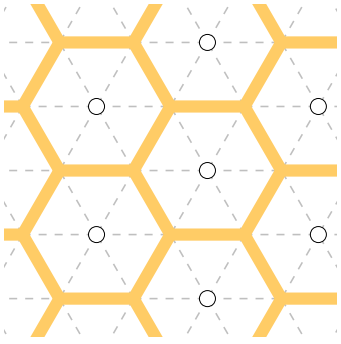
$\bar{n} = 1$





$\bar{n} = 4/3$

$\bar{n} = 1.x$



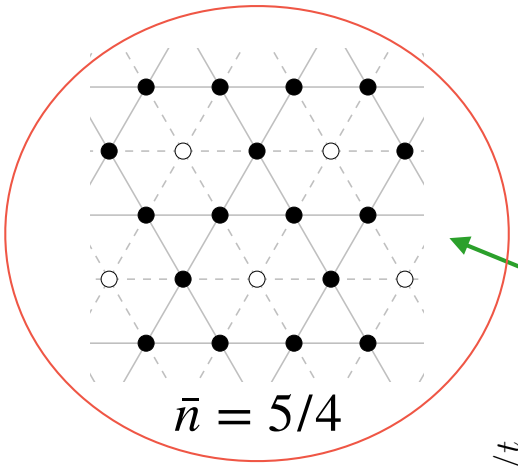
$\bar{n} = 1.x$

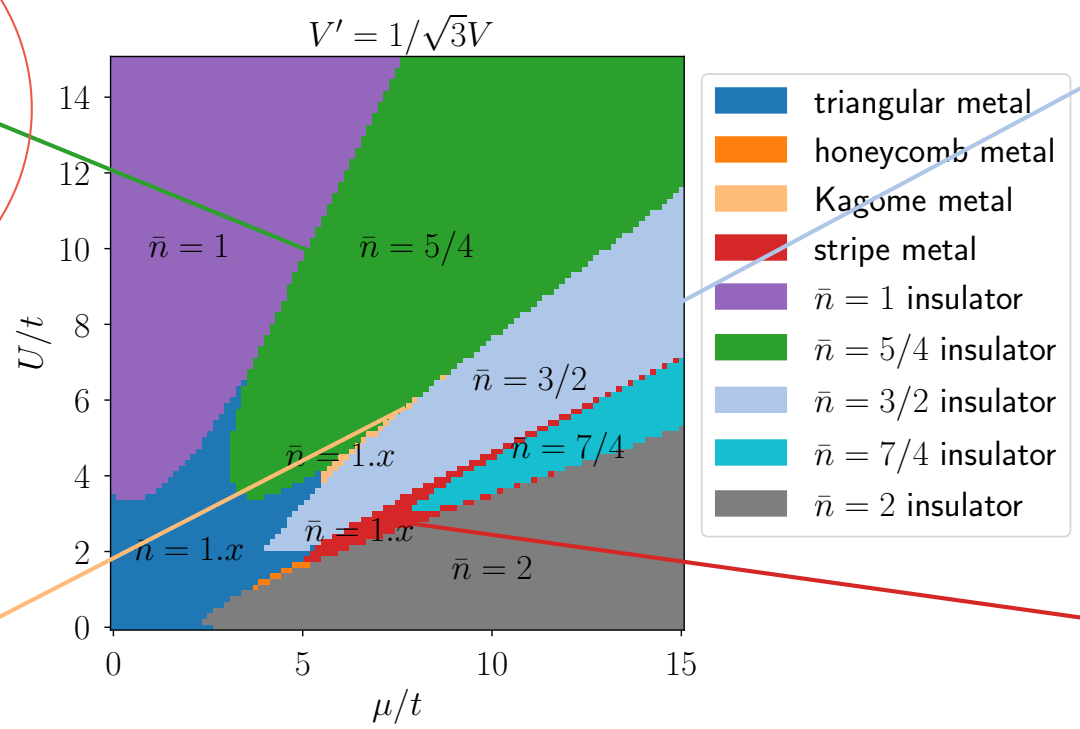
3-site and 4-site unit cell ansatz

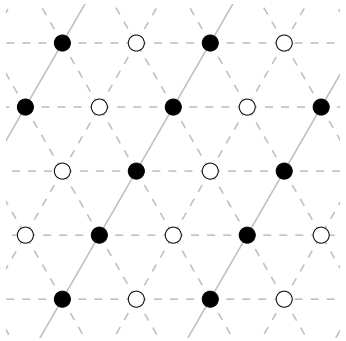
Mean Field results

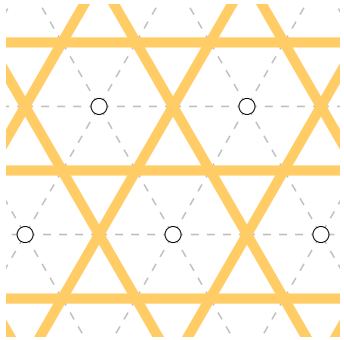
On-site repulsion: U nearest neighbor repulsion: $V = U/4$

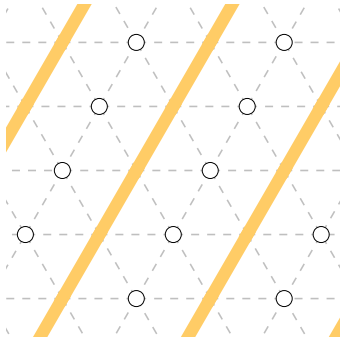
next nearest neighbor repulsion: $V' = 1/\sqrt{3}V$





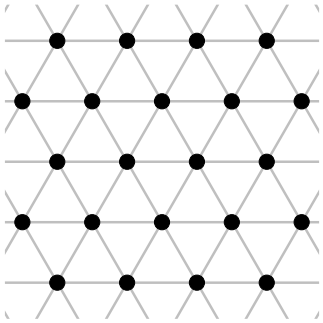




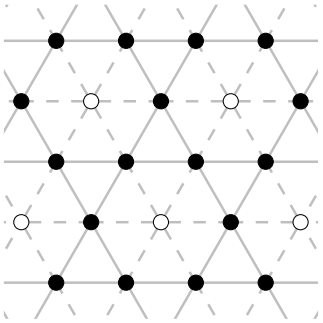


3-site and 4-site unit cell ansatz

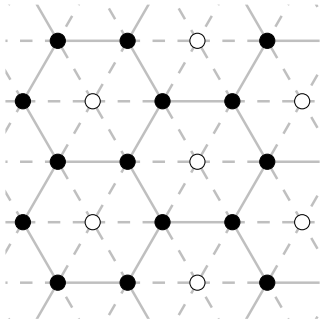
All the phases



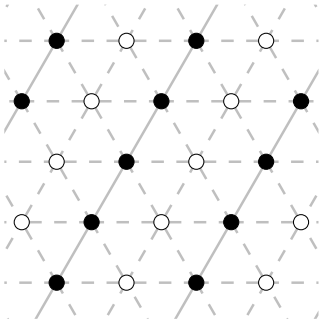
(c) $\bar{n} = 1$



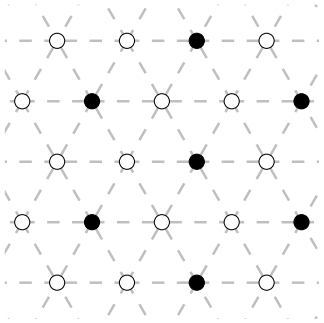
(d) $\bar{n} = 5/4$



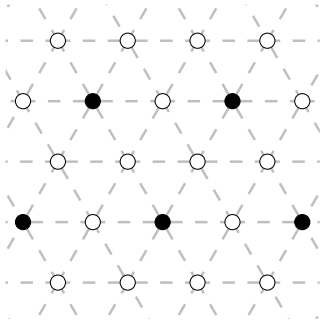
(e) $\bar{n} = 4/3$



(f) $\bar{n} = 3/2$

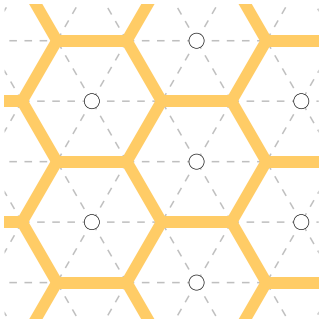


(g) $\bar{n} = 5/3$

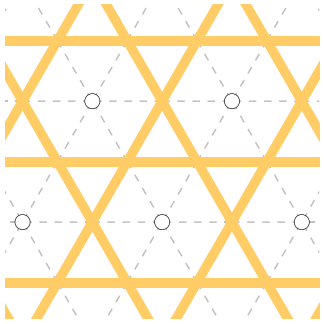


(h) $\bar{n} = 7/4$

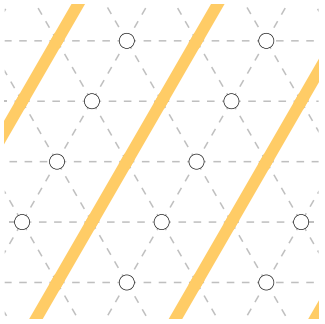
(i) triangular metal



(j) honeycomb metal



(k) kagome metal

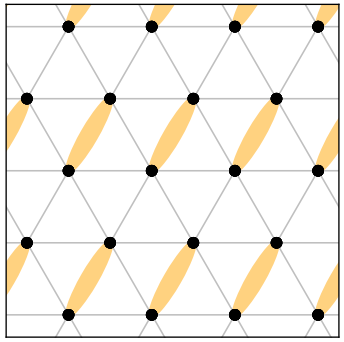


(l) stripe metal

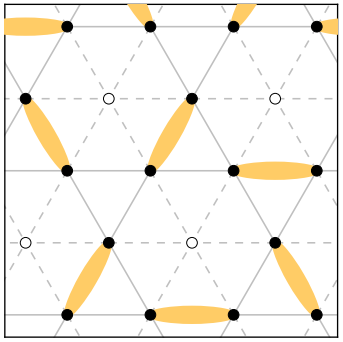
?? Can we find spin liquids in any of these states?

VBS states

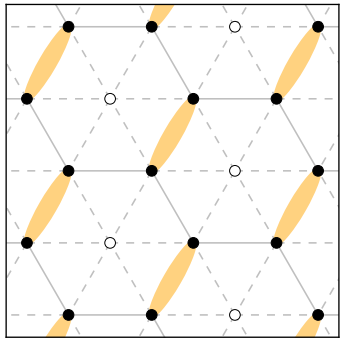
At mean field level, dimer (VBS) states always have the lowest energy



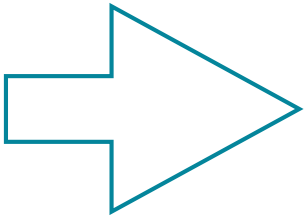
$n = 1$

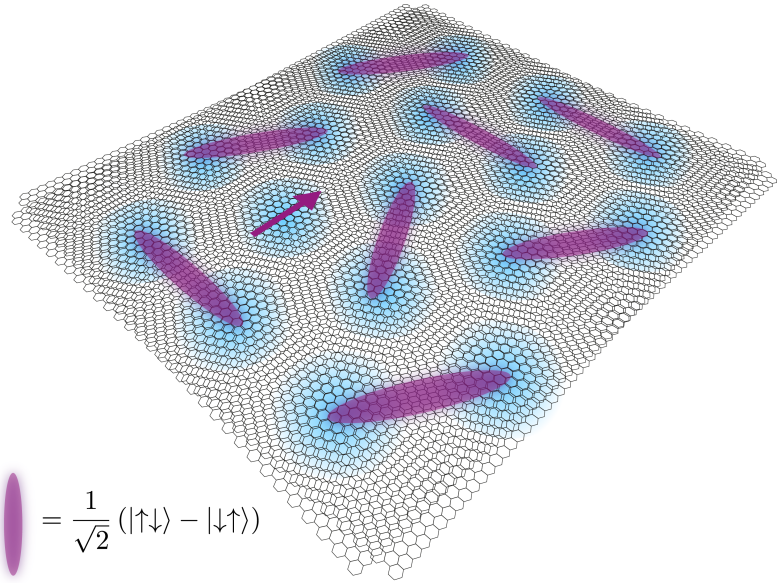


$n = 5/4$



$n = 4/3$



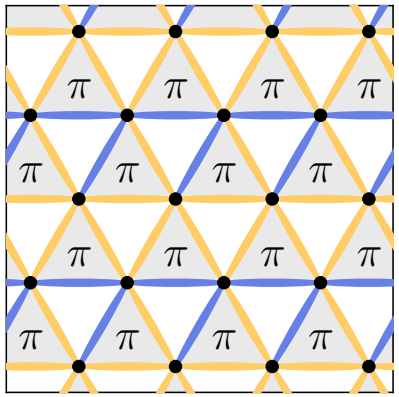


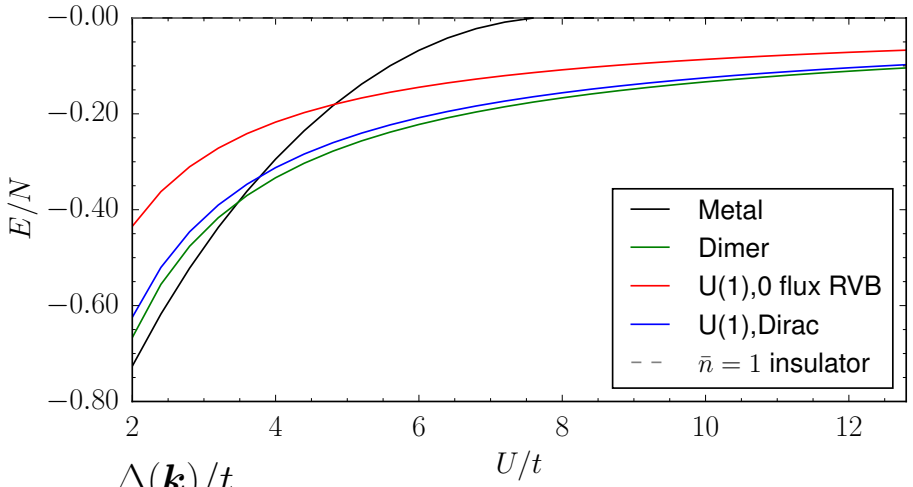
BUT...

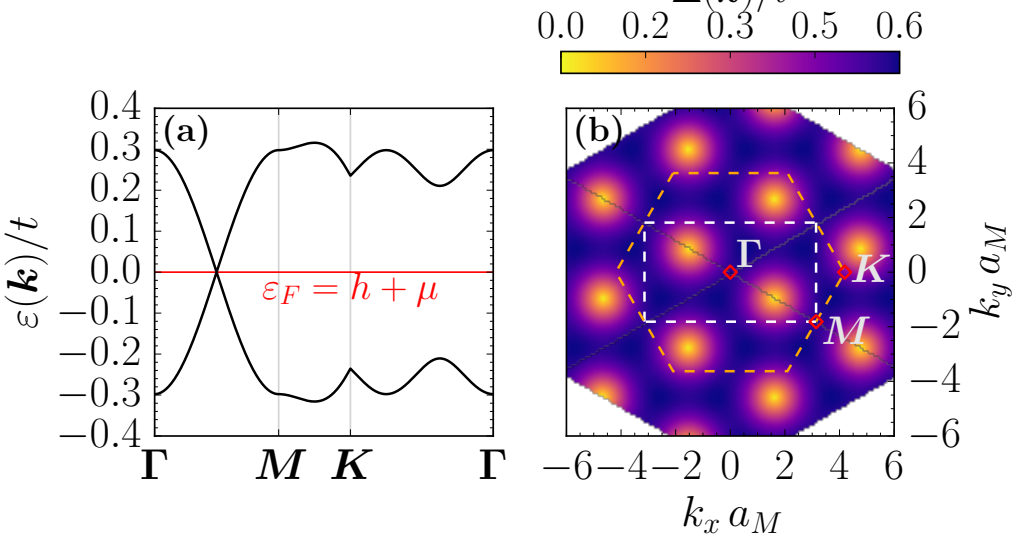
Triangular

Dirac spin liquid states are quite energetically competitive,

and are likely to be favored after Gutzwiller projection back to physical space







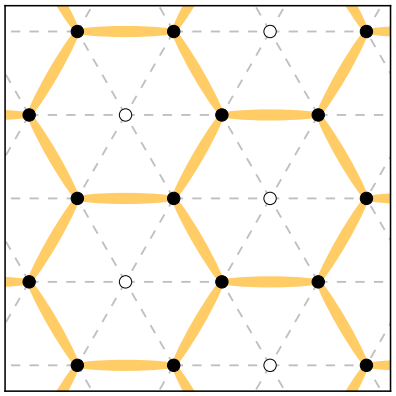
Low energy theory: N=4 QED in 2+1 dim

$$\langle S^\alpha(\mathbf{x}) S^\alpha(\mathbf{y})\rangle \sim \frac{-e^{i\mathbf{K}\cdot(\mathbf{x}-\mathbf{y})}}{|\mathbf{x}-\mathbf{y}|^{2\Delta_\Phi}} + \text{h.c.} + \ldots$$

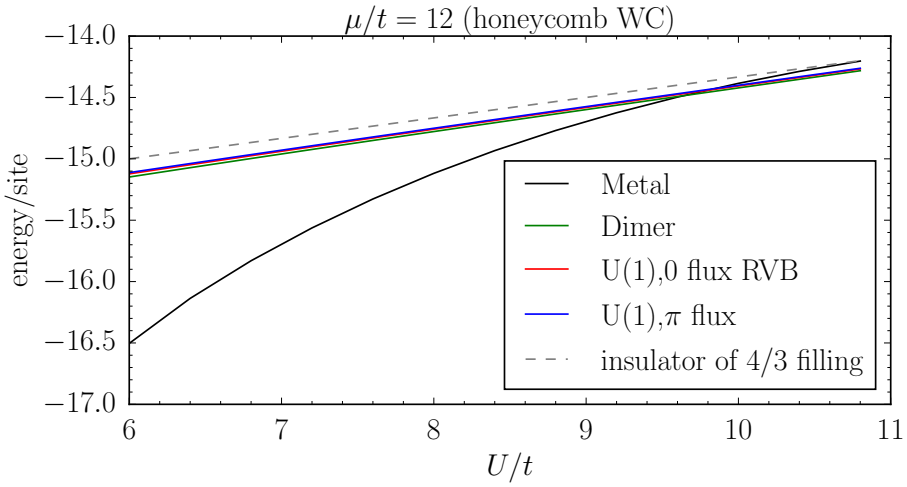
$$\Delta_\Phi \approx 1.02$$

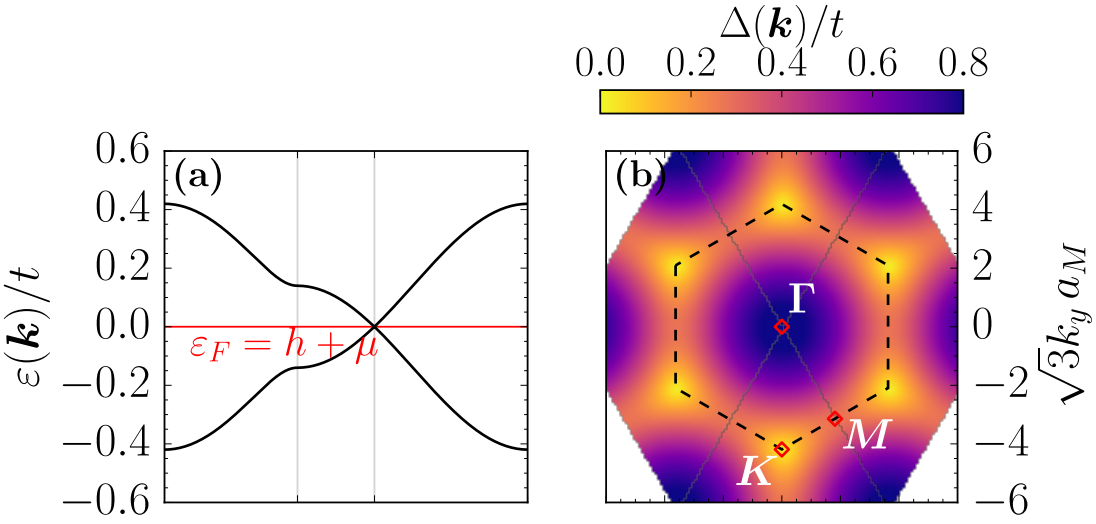
Albayrak *et al.*, arXiv 2021

Honeycomb



Resonance valence bond



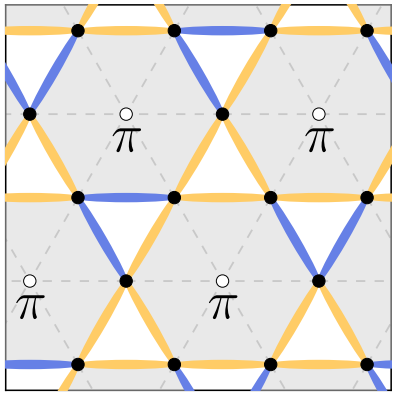


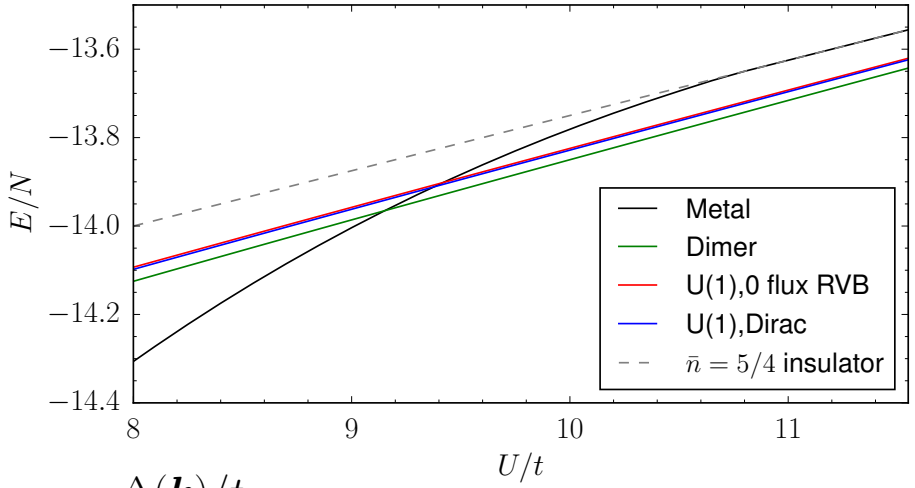
U(1) Dirac spin liquid

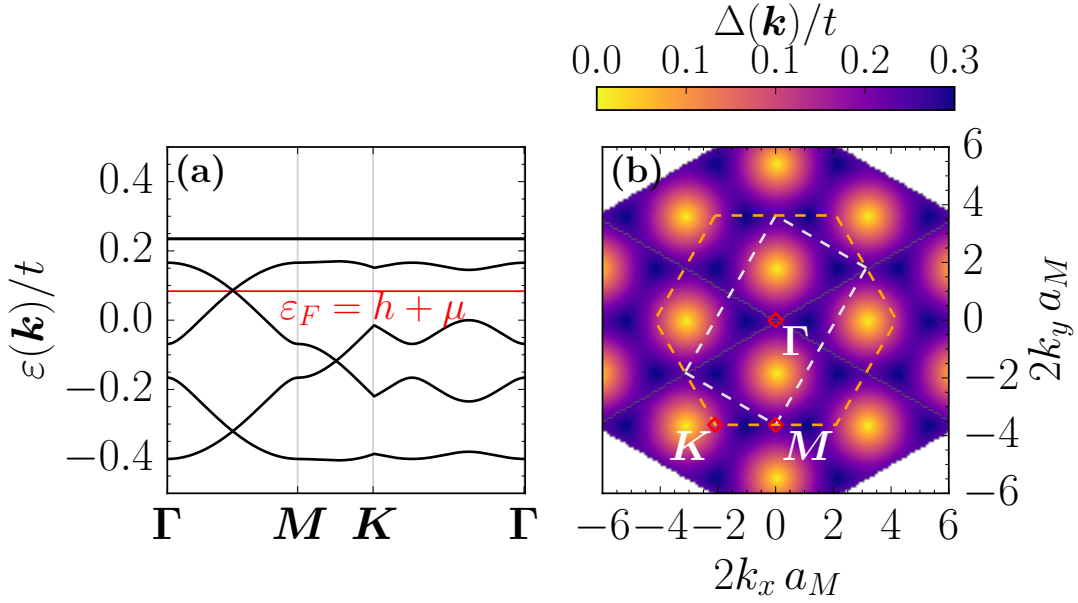
Unstable to monopole proliferation

X.-Y. Song *et al., Nature Commun* 2019

Kagome







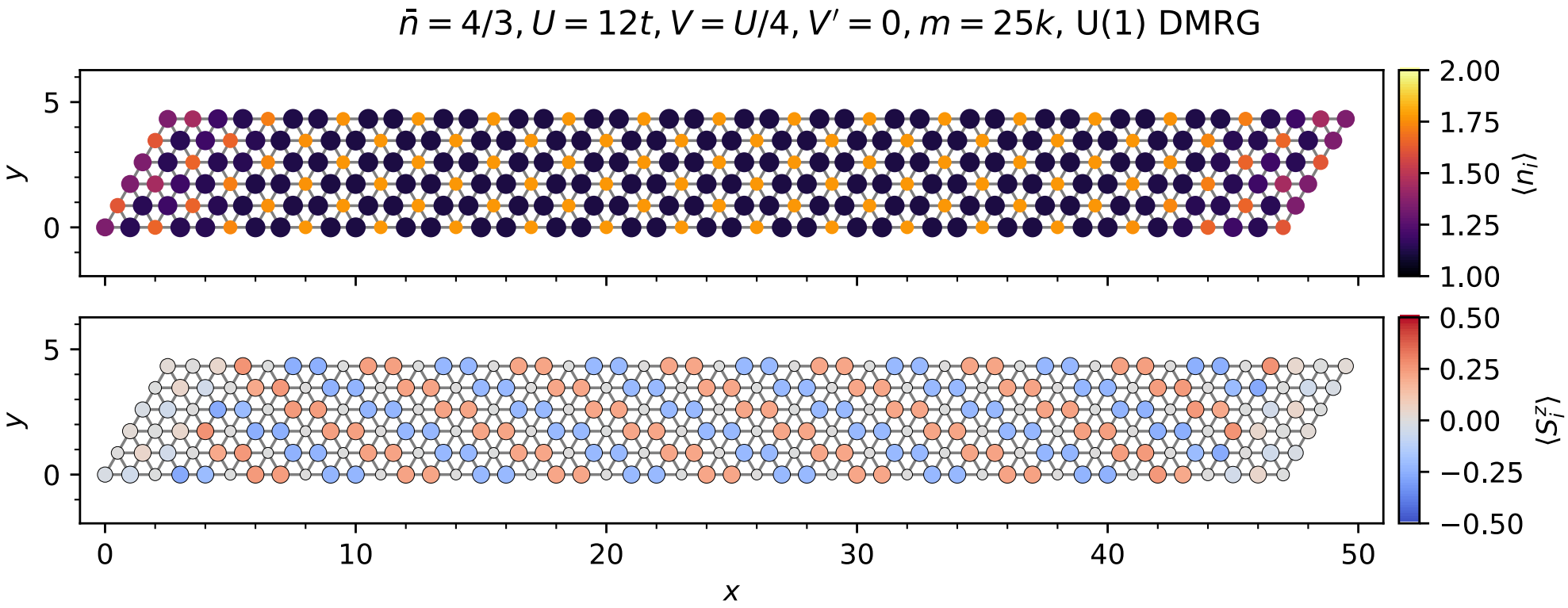
U(1) Dirac spin liquid

Emergent SU(4) symmetry

Beyond MF

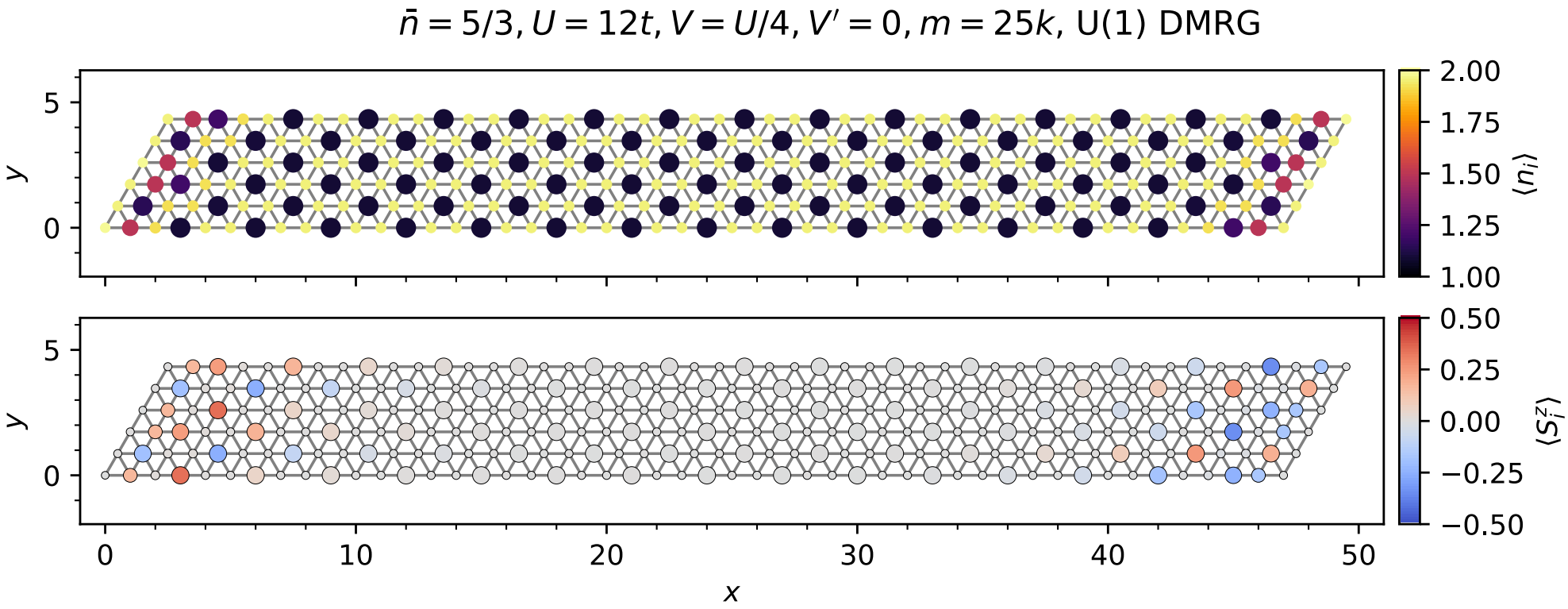
- Small energy differences in MF results: we need to be more precise!
- Turn to Density Matrix Renormalization Group
- Recent advances make it possible to directly study substantially large Hubbard (not Heisenberg or t-J) models, despite larger Hilbert space
- We are completely reliant upon the expertise of Hongchen Jiang (SLAC)!

Honeycomb CDW



Not a spin liquid. Zig-zag spin order.

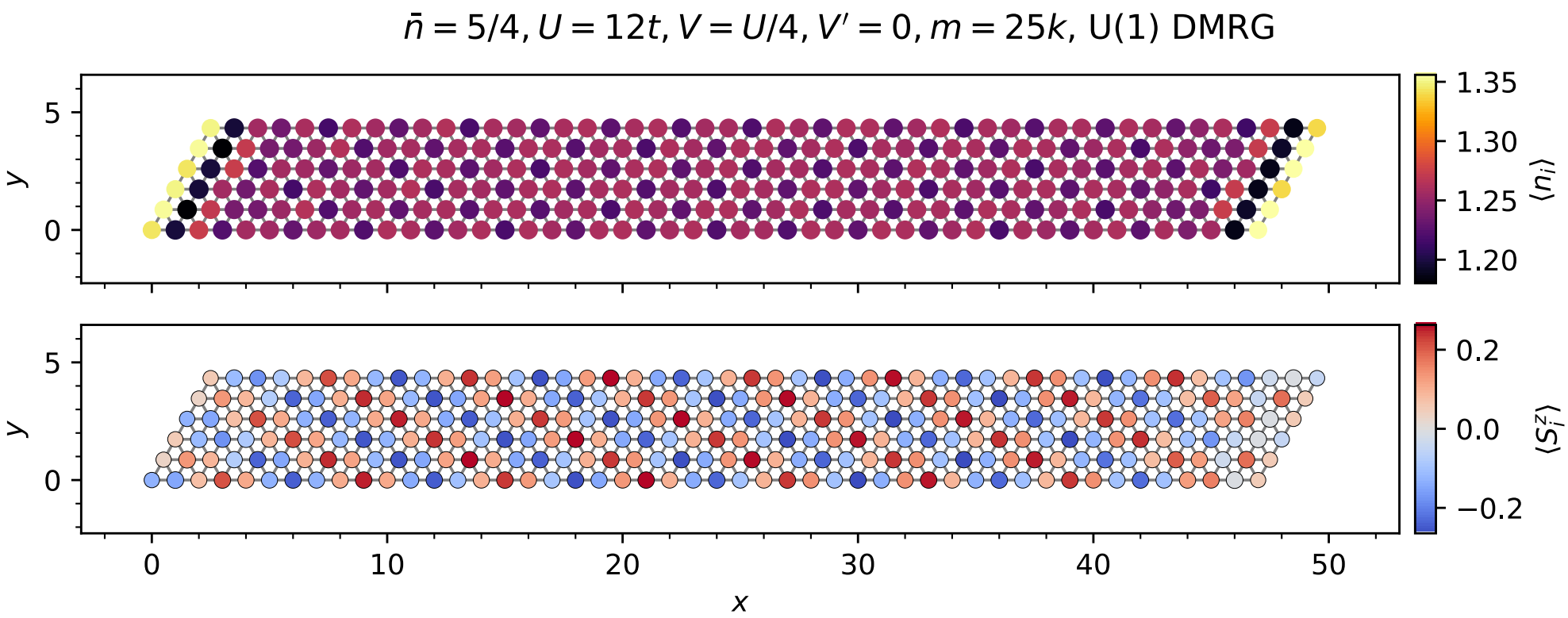
Inverse honeycomb CDW



Might be a spin liquid.

No visible moments in bulk.

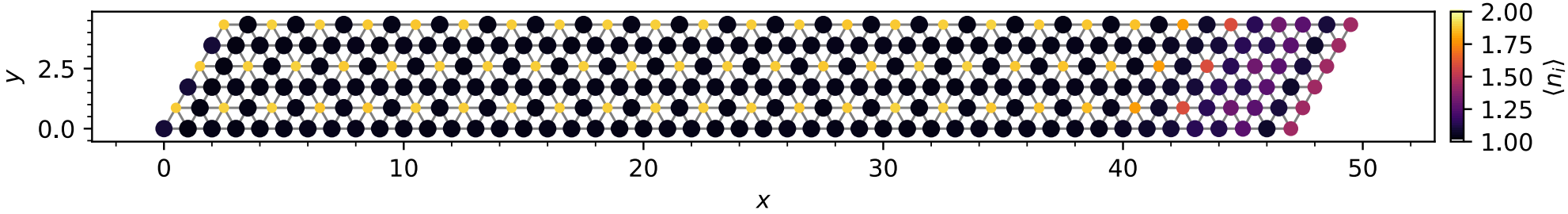
Weak n=5/4 CDW

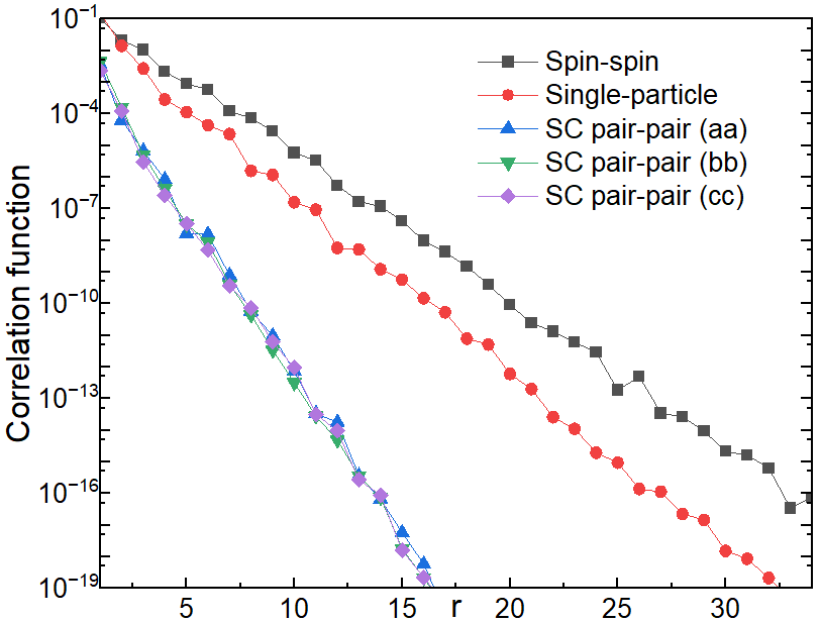


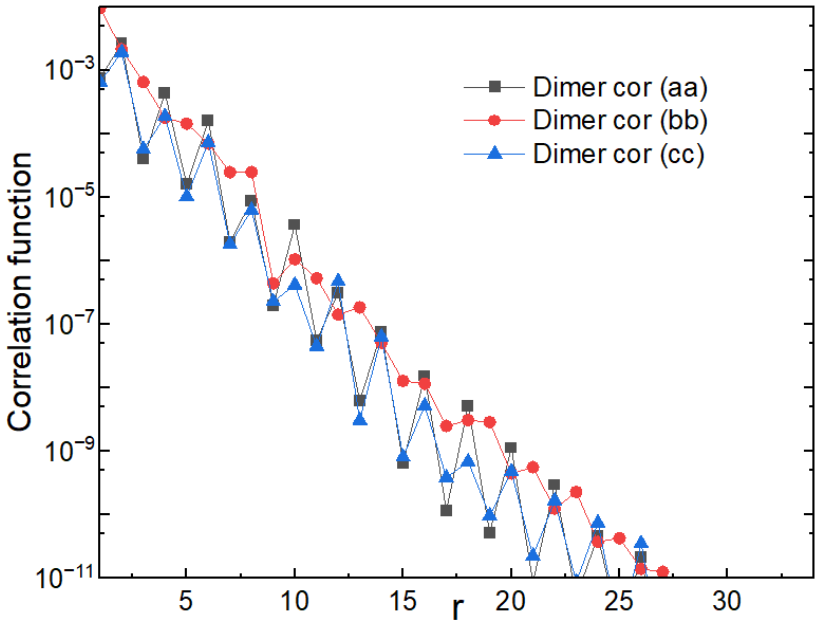
Without NNN interaction, we see small charge order, consistent with a collinear SDW and induced secondary CDW order.

Kagome CDW

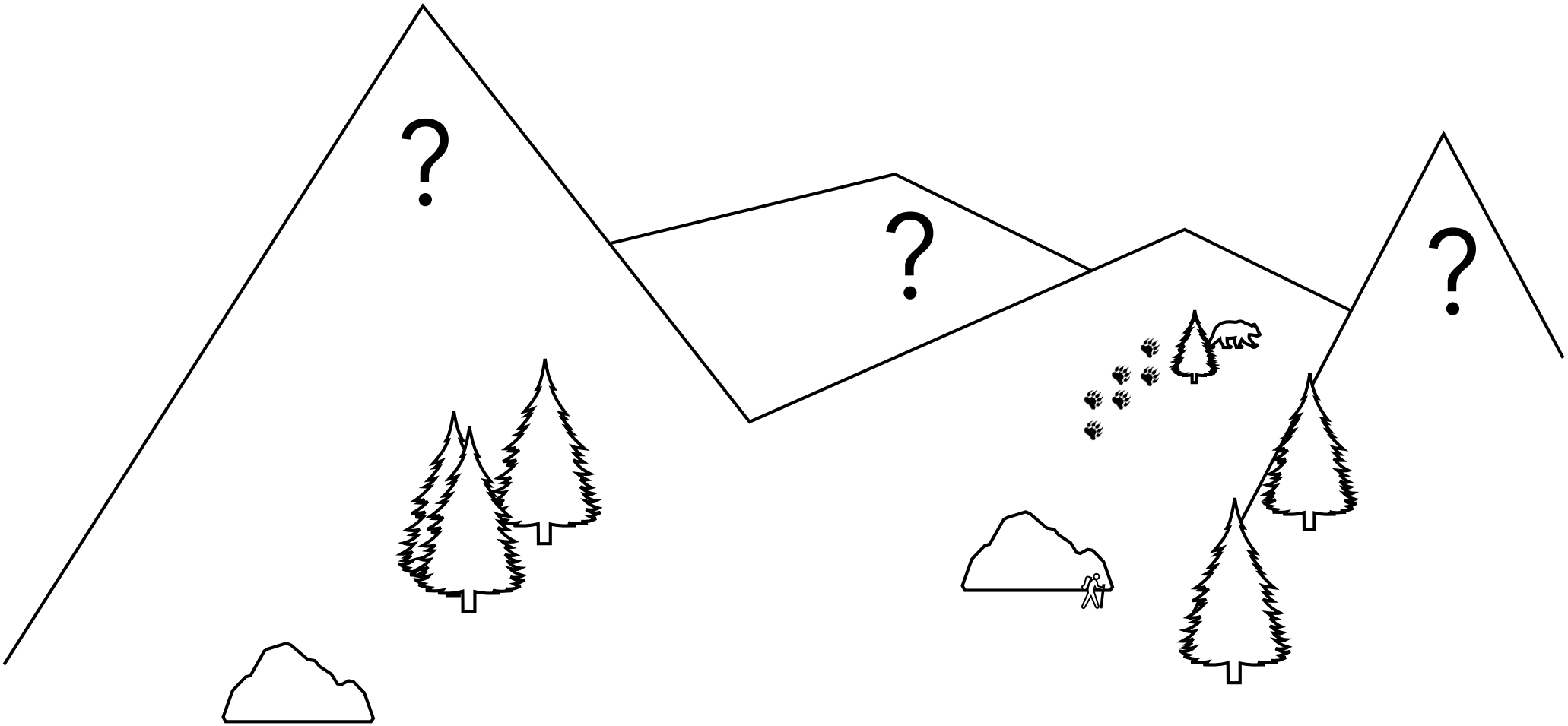
$\bar{n} = 5/4, U = 12t, V = U/4, V' = V/\sqrt{3}, m = 8k$, SU(2) DMRG

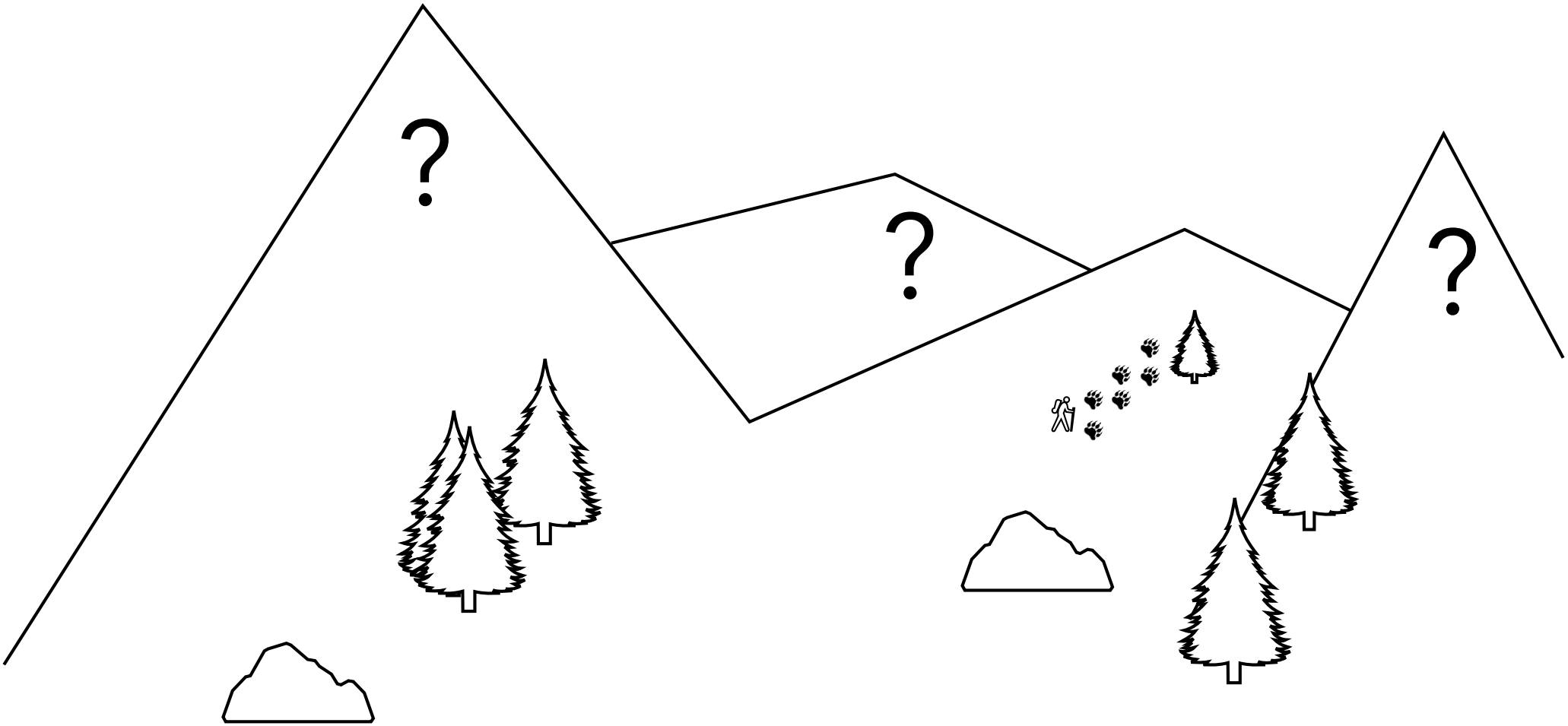




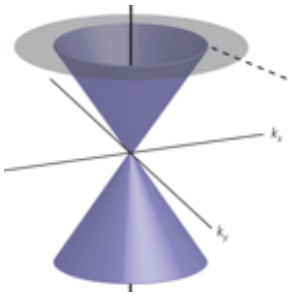


Consistent with a spin liquid. Not clear what type.



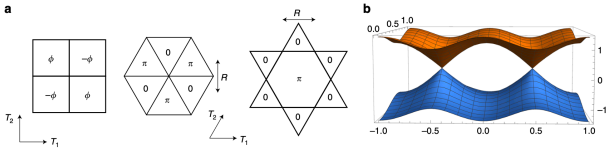


Dirac QSL

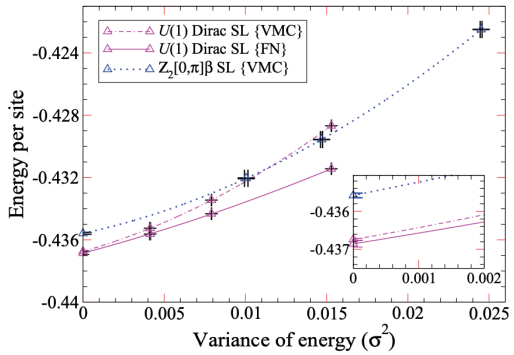


- A realization of QED_3 in a spin system
- Very often found to be energetically best amongst trial wave functions.

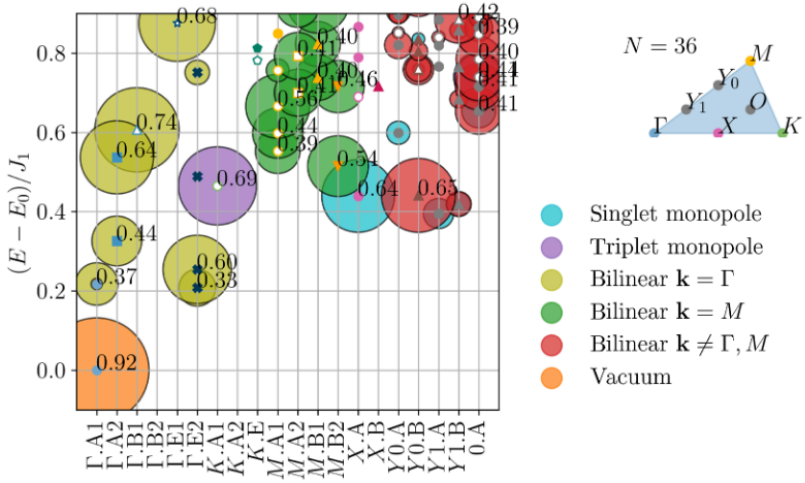
$$\mathscr{L} = \bar{\psi}\gamma^{\mu}(\partial_{\mu} - ia_{\mu})\psi + \cdots$$



X.-Y. Song *et al*, 2019

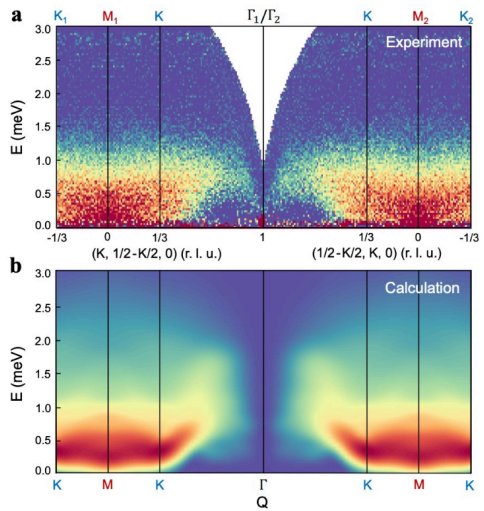


Y. Iqbal *et al*, 2013



A. Wietek *et al*, 2024

$YbZn_2GaO_5$



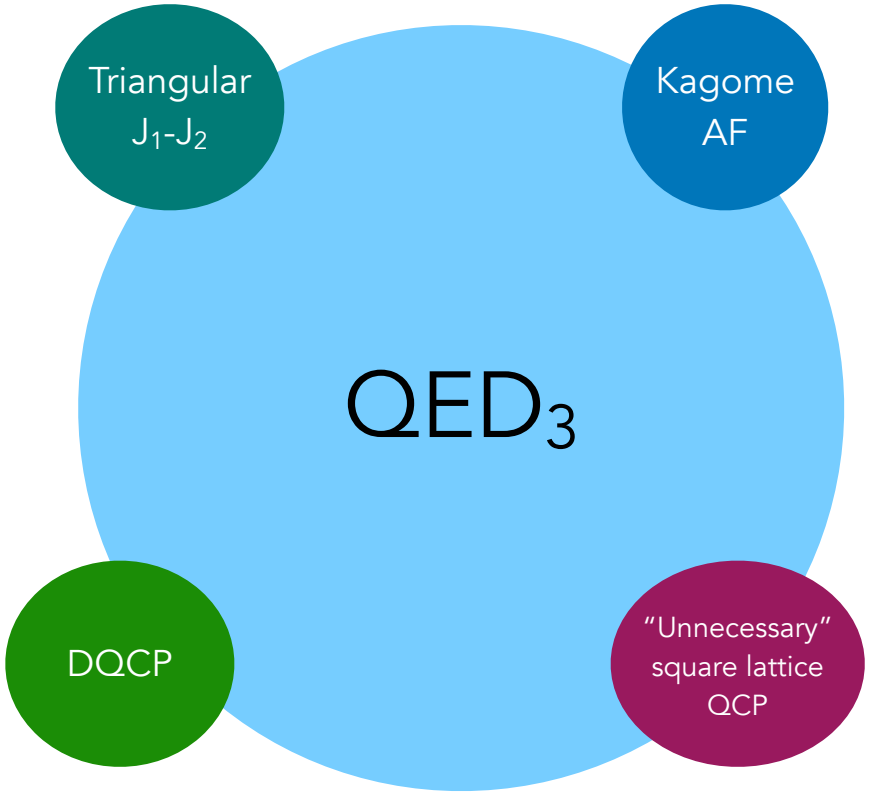
Xu *et al*, 2024

Spins and QED_3

Each system has its own:

- Microscopic (exact) symmetries
- Operator dictionary
- Perturbations to CFT

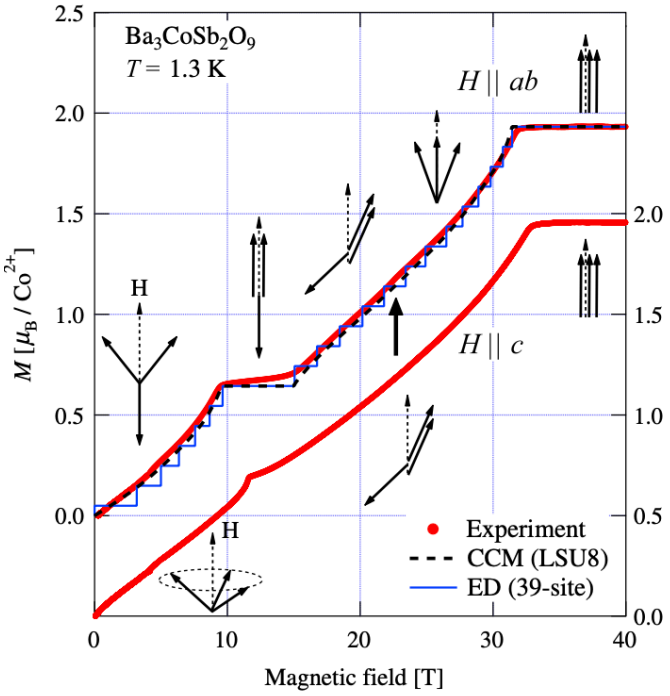
X.-Y. Song *et al*, 2019



We seek some qualitative and quantitative signatures

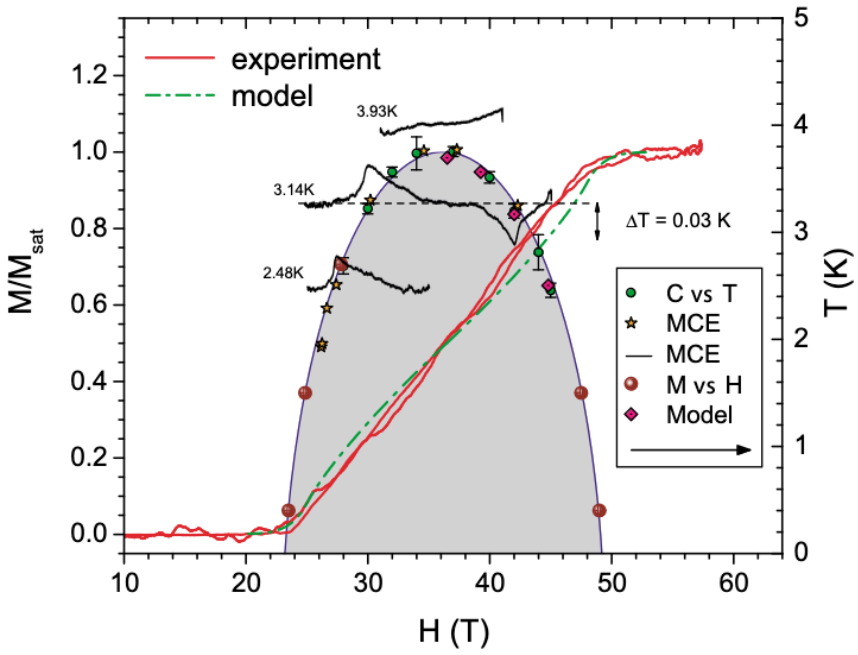
Applied field

- Essential tuning knob available in experiment



T. Suzuki *et al*, 2013

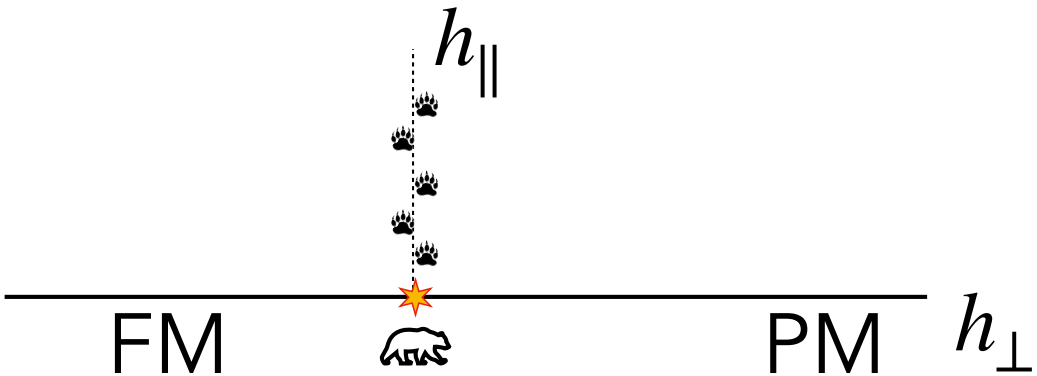
$BaCuSi_2O_6$

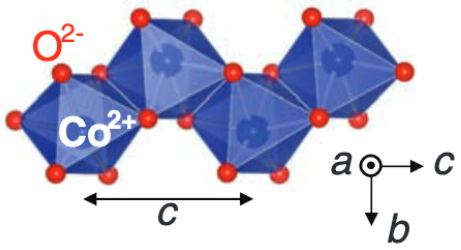


M. Jaime *et al*, 2006

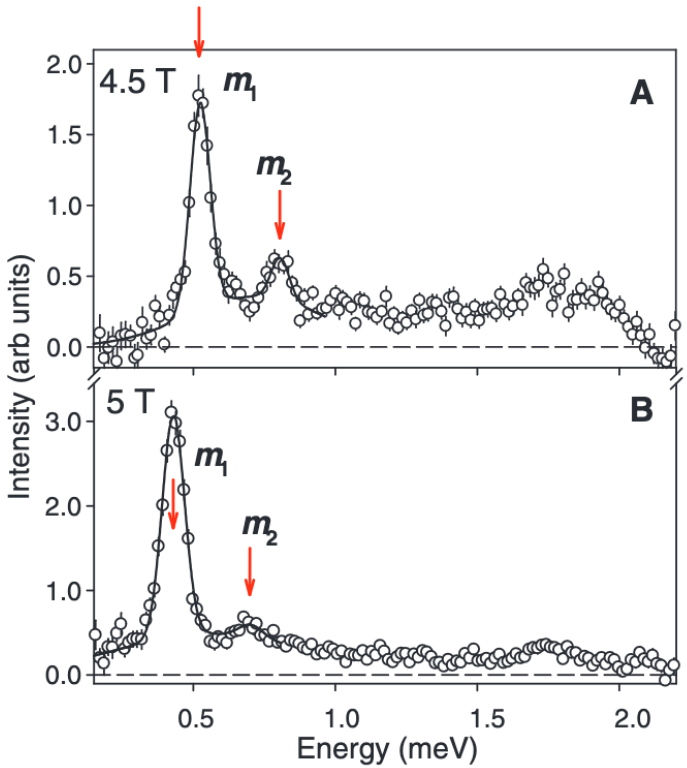
- Field couples via Zeeman term $-HS^z$
- Non-zero dM/dH usually indicates symmetry breaking

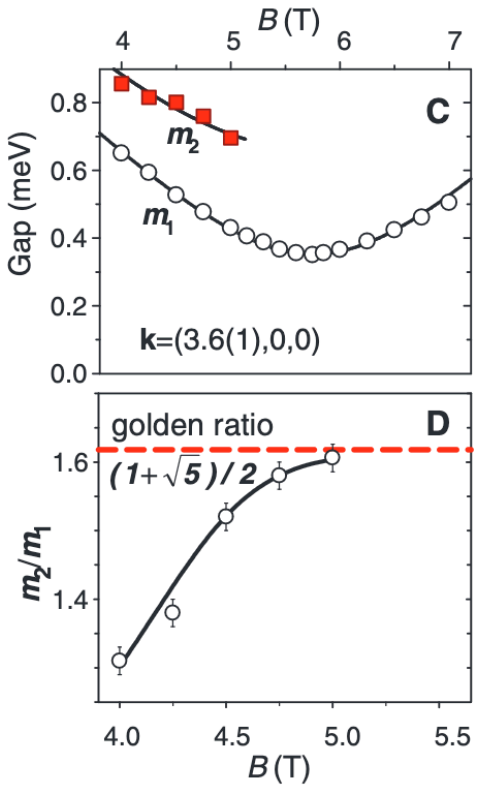
Proof of principle





R. Coldea *et al*, 2010

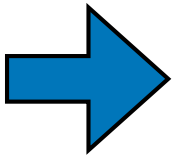




Applied field

$$H = H_{\mathrm{QED3}} - h\psi^{\dagger}\sigma^{z}\psi$$

- Field couples to conserved SU(2) charge $M = S^{z}$
- $SU(2)_{spin}$ is a subgroup of SU(N) symmetry of QED3
- Conformal QED3 also has emergent $U(1)_{flux}$ conservation symmetry



States labeled by M and Φ

$$E = E_0(M, \Phi) - hM$$

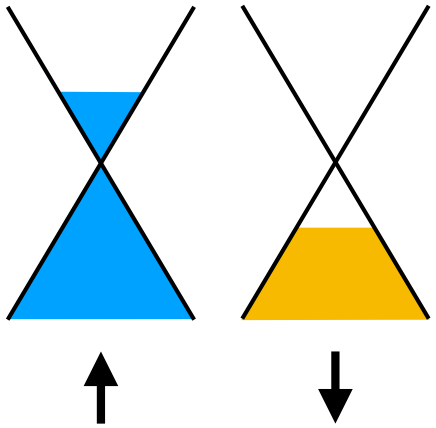
Applied field

$$E = E_0(M, \Phi) - hM$$

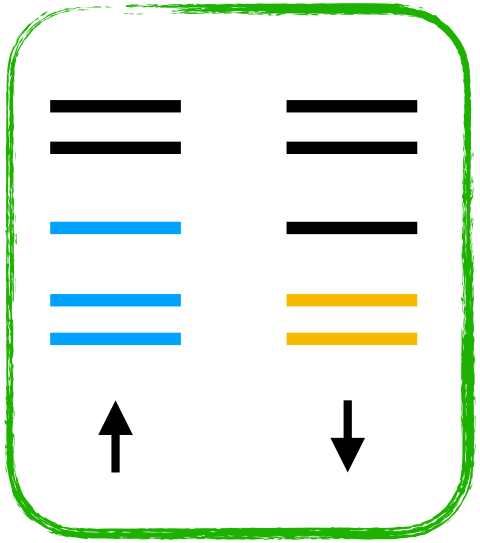
- Key question: what value of Φ minimizes E?

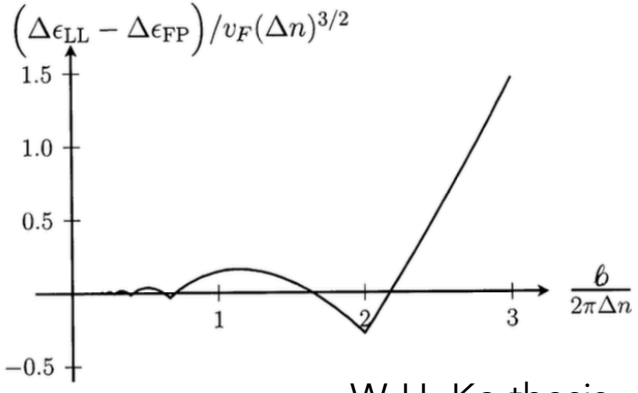
[Y. Ran *et al*, 2009]: $\Phi = \pm 2\phi_0$

n.b. sign breaks TRS



vs

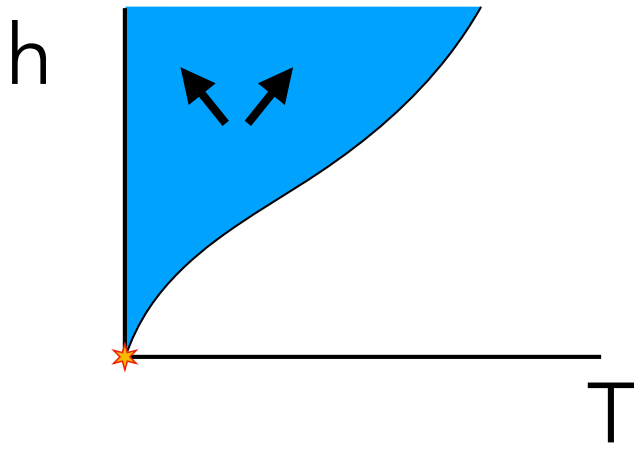




W-H. Ko thesis

LL state

- Ran *et al:* LL state *is* a magnetically ordered state!
  - It breaks TRS
  - It has a fermion gap, so monopole-monopole correlations are long-ranged
  - Response to probe gauge field A^{μ}_{spin} shows that $U(1)_{\text{spin}}$ symmetry is spontaneously broken



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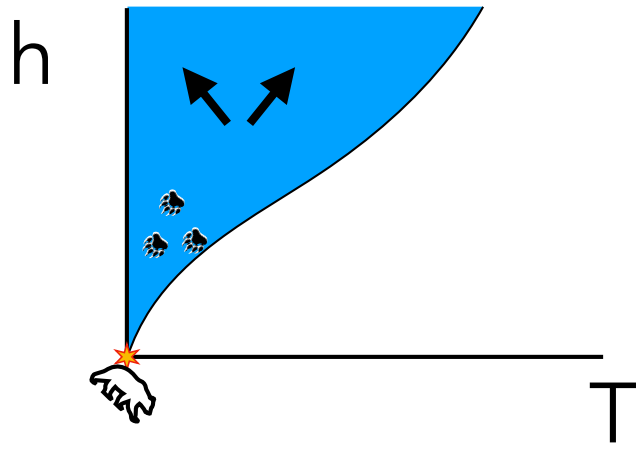
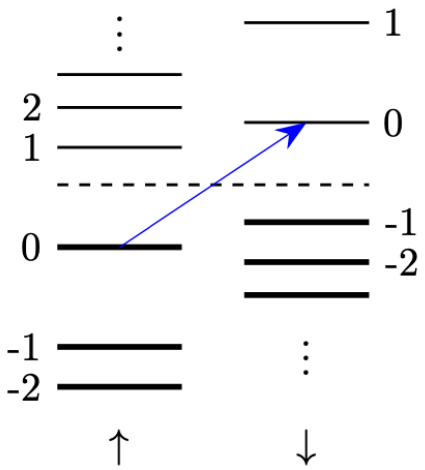


Can we still see signs of QED3 in the ordered phase?

Spectroscopy

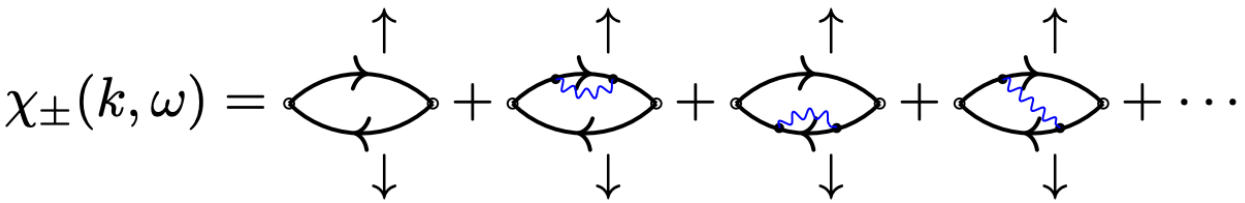
- Ran *et al* analysis of ordered phase is entirely based on energies $\ll \hbar\omega_c$
- QED3 theory should be valid for any small energy, including multiples of $\hbar\omega_c$
- Project: seek signs of QED3 structure on these scales in observables.

Dynamical spin correlations



LL transitions:

"magneto-excitons"



"Excitonic" corrections will give dispersion, broadening

A fully worked example

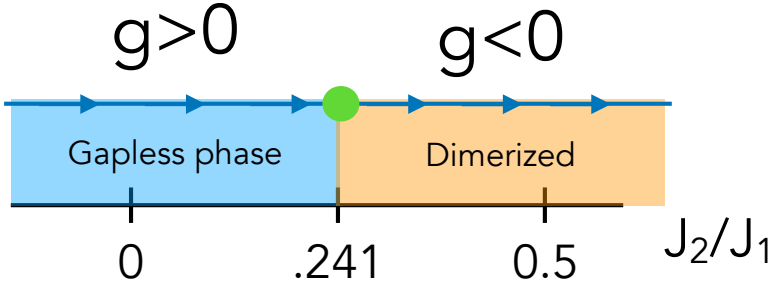
A. Keselman *et al* (2020)

$$H = \sum_i \left[J_1 \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \vec{S}_i \cdot \vec{S}_{i+2} - B S_i^z \right]$$

- Bosonization and refermionization:

$$H_0 = v \int dx \left(\psi_R^\dagger (-i\partial_x) \psi_R + \psi_L^\dagger (i\partial_x) \psi_L \right)$$

$$V = -g \int dx \, \vec{J}_R \cdot \vec{J}_L = -g \int dx \, \left[J_R^z J_L^z + \tfrac{1}{2} J_R^+ J_L^- + \tfrac{1}{2} J_R^- J_L^+ \right]$$



$$\vec{S}_i \sim \vec{J}_R(x_i) + \vec{J}_L(x_i) + (-1)^i \vec{N}(x_i)$$

$$\vec{J}_{R/L} = \tfrac{1}{2} \psi_{R/L}^\dagger \vec{\sigma} \, \psi_{R/L}$$

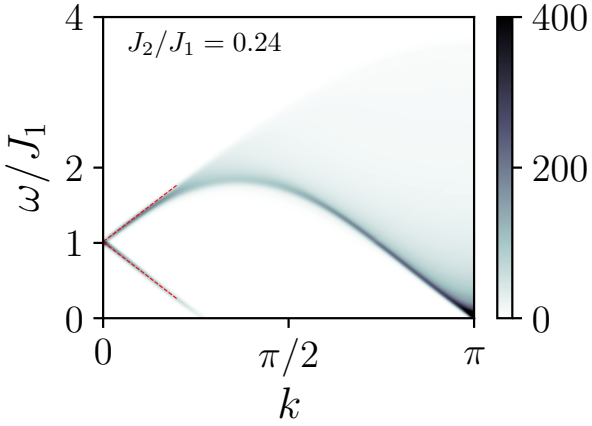
Small k spin correlations ~ fermion bilinear

A fully worked example

MPS methods: DMRG+TEBD

Near QCP

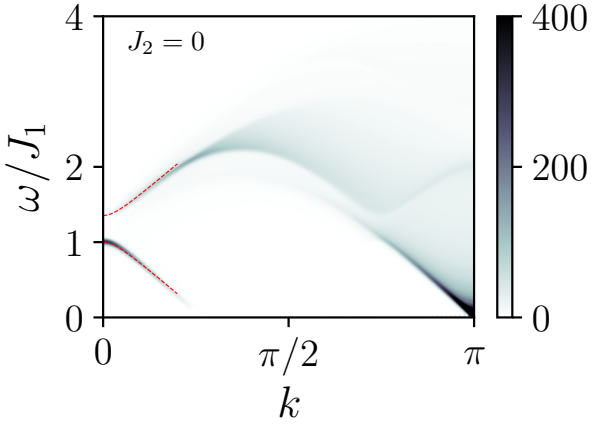
$g \approx 0$



well-approximated by free fermion spin correlations (at small k)

NN chain

B/J_1=1



Excitonic corrections evident due to interaction g (at small k)

A fully worked example

MPS methods: DMRG+TEBD

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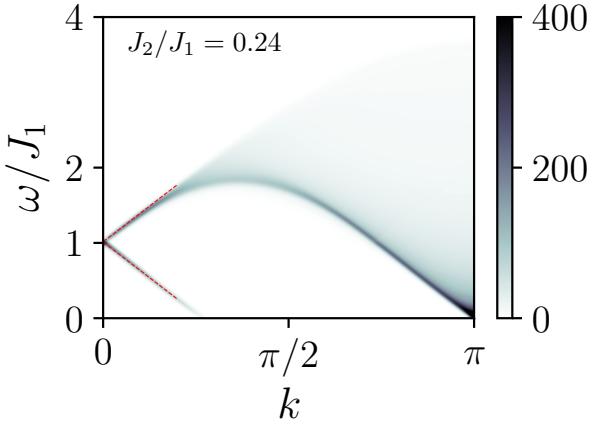

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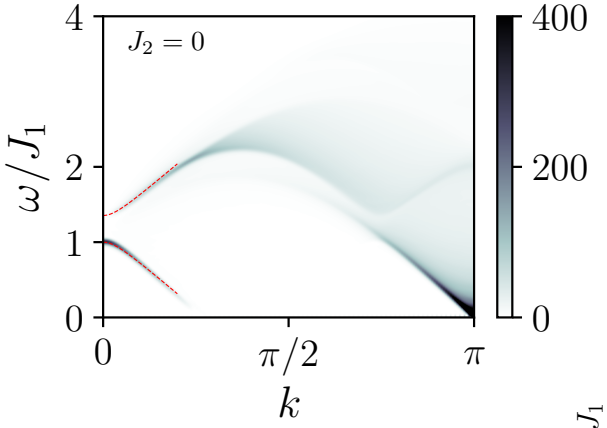
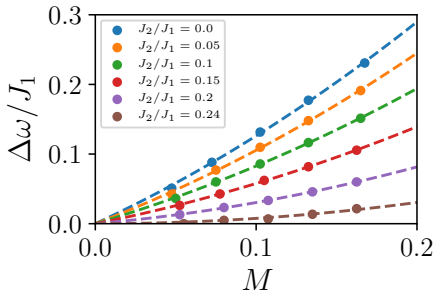
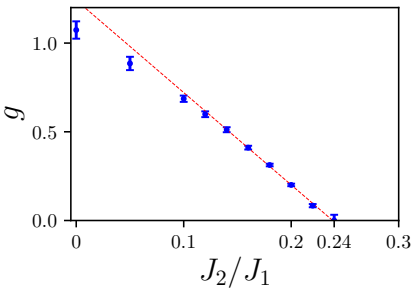


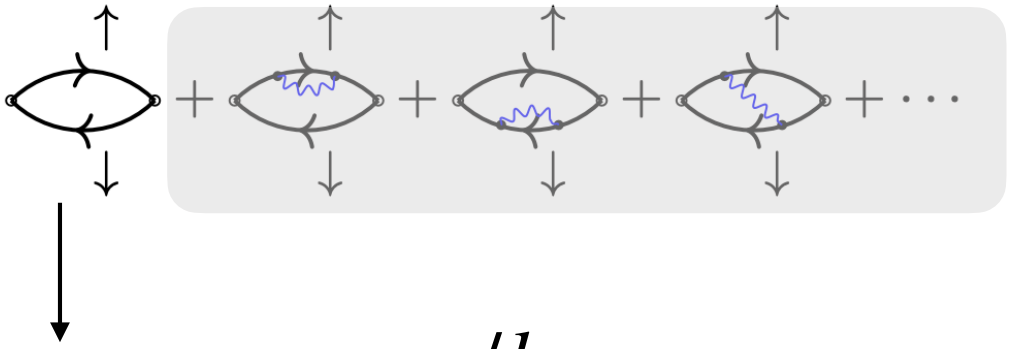
Excitonic corrections evident due to interaction g (at small k)





The QED3 case

$$\chi_{\pm}(k,\omega) =$$

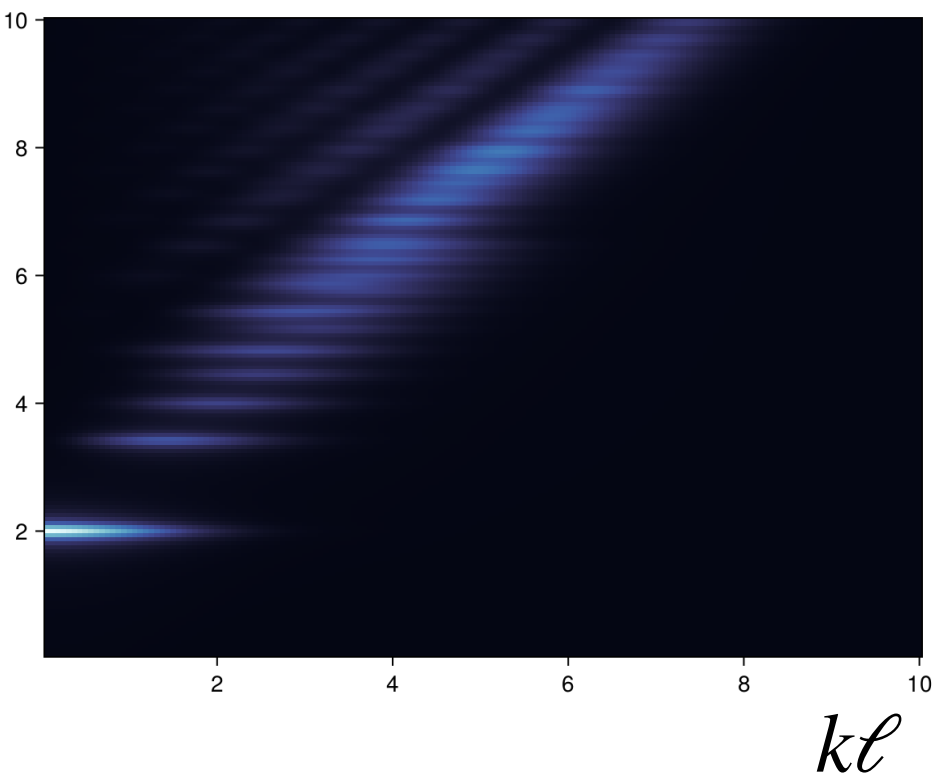


$$\mathrm{Im}[\Pi^{+-}(\nu+\mathrm{i}\eta,\boldsymbol{k})] \sim \pi \times \frac{\mathrm{e}^{-|\boldsymbol{k}|^2\ell^2/2}}{2\pi\ell^2}\left[\delta_\eta(\nu-2h)+\sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{\ell^2|\boldsymbol{k}|^2}{2}\right)^n\delta_\eta(\nu-2h-E_n)\right.$$

$$+\frac{1}{4}\sum_{n=1,m=1}^{\infty}(-1)^{n+m}\left[\delta_\eta(\nu-(E_m+E_n+2h))-\delta_\eta(\nu-(-E_m-E_n+2h))\right]\times\left\{\mathcal{L}_{0,0}^{n,m}(\ell^2|\boldsymbol{k}|^2/2)+\mathcal{L}_{1,1}^{n,m}(\ell^2|\boldsymbol{k}|^2/2)\right.$$

$$\left.\left.-2\frac{E_n}{E_m}\mathcal{L}_{0,1}^{n,m}(\ell^2\boldsymbol{k}^2/2)\right\}\right]$$

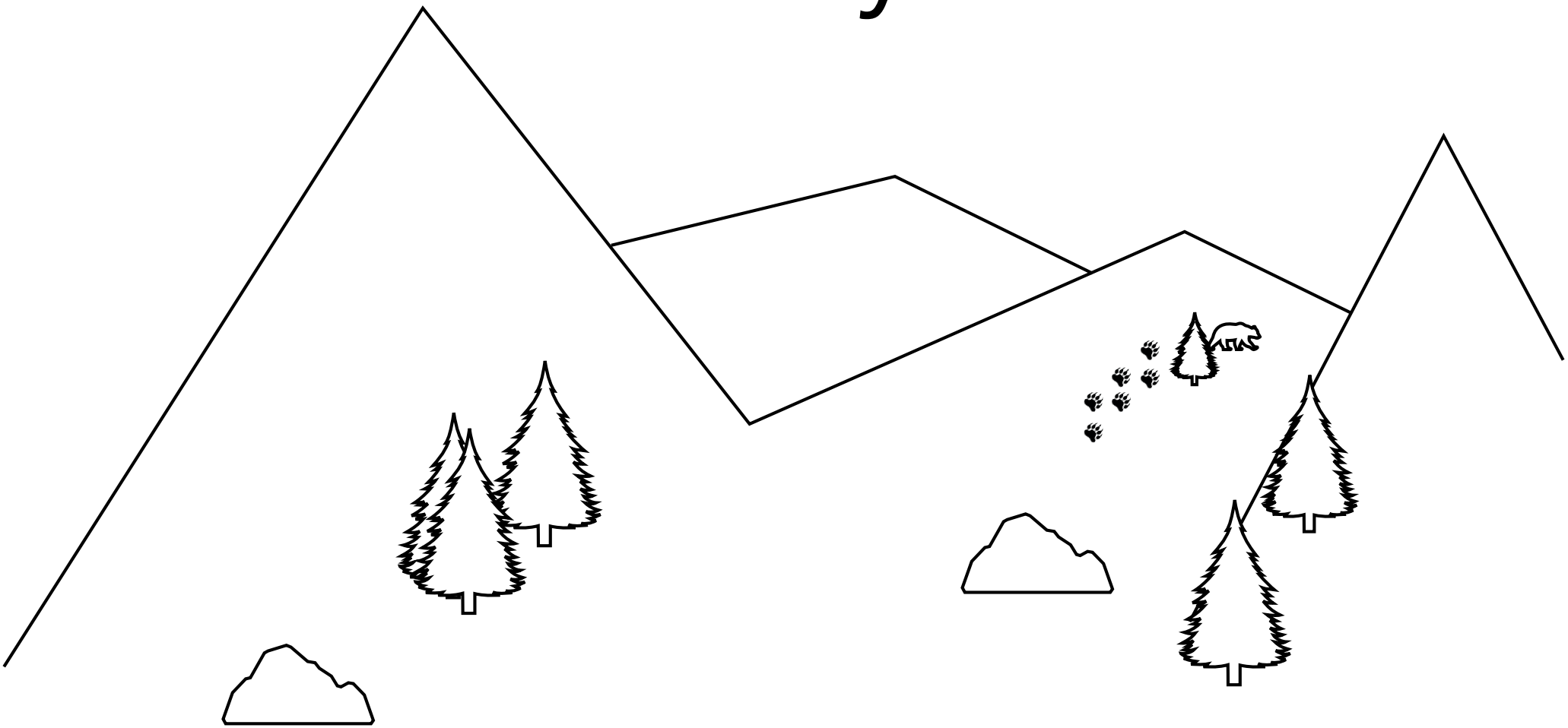
Will be interesting to see how this structure is affected by excitonic corrections



Issues

- Full treatment of gauge fluctuations: lattice gauge simulation? (No sign problem!)
- Some spin correlations are represented by monopole operators: how to calculate these contributions?
- Role of perturbations to the CFT Hamiltonian

Thank you



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