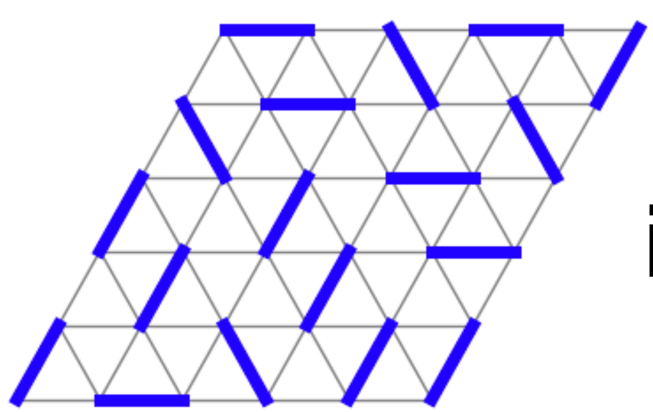
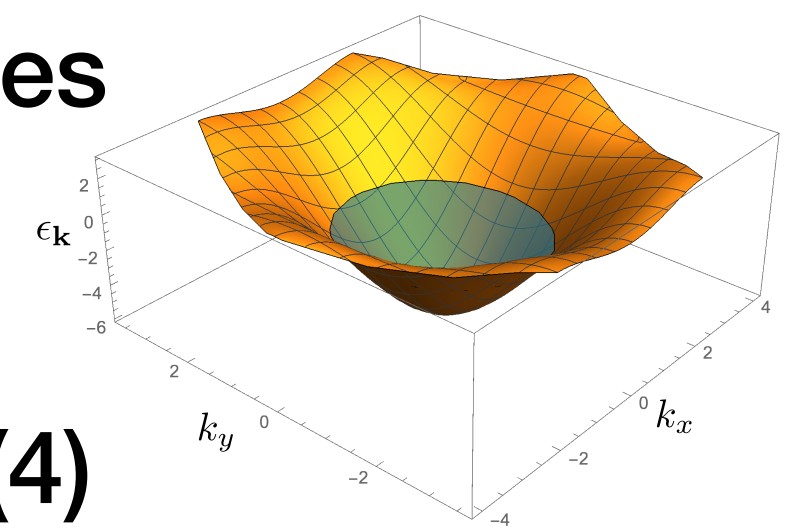
Kavli Institute for Theoretical Physics
University of California, Santa Barbara

GORDON AND BETTY MOORE FOUNDATION

Valence-bond and gapless liquid states in triangular lattice SU(4) antiferromagnets



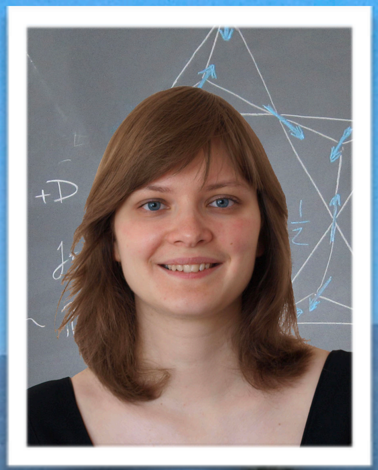


Anna Keselman, KITP

Correlated Systems with Multicomponent Local Hilbert Spaces, November 24, 2020

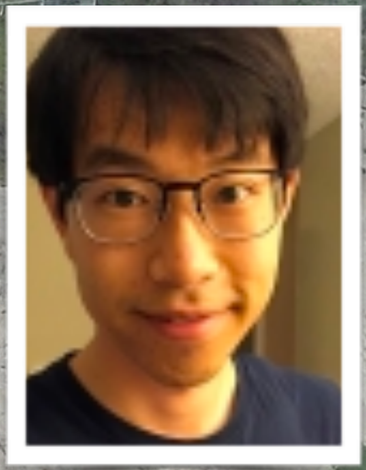
Collaborators

Leon Balents,
KITP

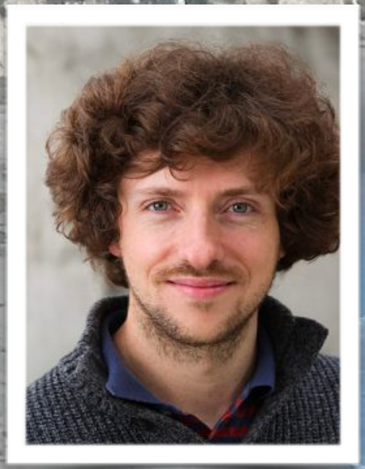


Lucile Savary,
Lyon

Cenke Xu,
UCSB



Chao-Ming Jian,
Cornell



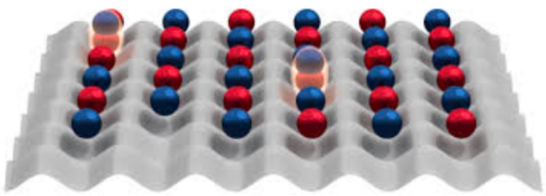
Bela Bauer,
MS Station Q

Systems with (approximate) SU(4) symmetry

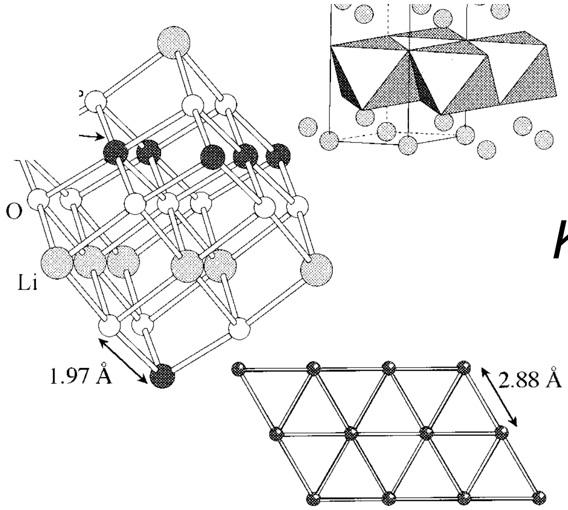
Cold atoms

(Alkaline-earth Fermi gases)

Gorshkov et al., Nat. Phys. 2010

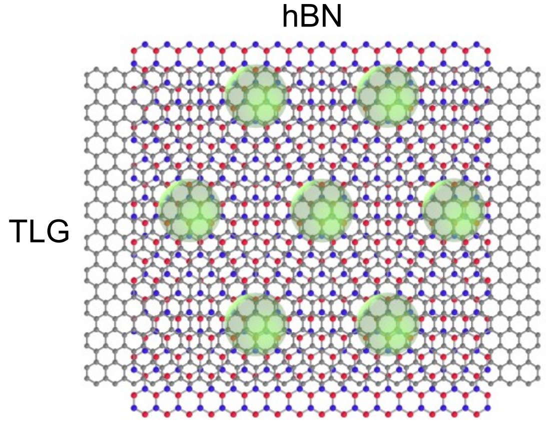


Transition metal compounds



Kugel, Khomskii, 1973

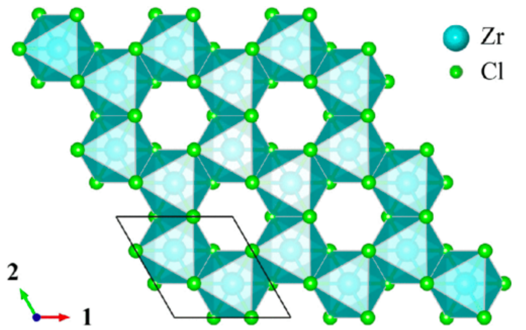
Moiré superlattices



Chen et al., Nat. Phys. 2019

and many more…

$\alpha - \mathrm{ZrCl_3}$



Yamada et al., PRL 2018

SU(4) “spin” systems

Hubbard model

$$H = -t \sum_{\langle i,j\rangle, a=1,..,4} c^{\dagger}_{i,a} c_{j,a} + U \sum_i (n_i - \bar{n})^2$$

$$n_i = \sum_{a=1,..,4} n_{i,a}$$

SU(4) fermions

$c_{i,a=1,2,3,4}$

“flavor” = (spin, valley/orbit)

$1 = (\uparrow, K) \quad 3 = (\uparrow, K')$

$2 = (\downarrow, K) \quad 4 = (\downarrow, K')$

$U \gg t$

$\bar{n} \in \mathbb{Z}$

Different representations of SU(4)

SU(4) Antiferromagnetic “Heisenberg” model

$$H = J \sum_{\langle i,j\rangle} \sum_{a,b=1}^{4} T^{ab}_i T^{ba}_j$$

$$J \sim \frac{t^2}{U} > 0$$

$$T^{ab}_i = c^{\dagger}_{i,a} c_{i,b}$$

SU(4) “spin” operators

SU(4) antiferromagnet

$$H = J \sum_{\langle i,j \rangle} \sum_{a,b=1}^{4} T_i^{ab} T_j^{ba}$$

$$T_i^{ab} = c_{i,a}^\dagger c_{i,b}$$

SU(4) "spin" operators

$$T_i^{aa} = c_{i,a}^\dagger c_{i,a} = n_{i,a}$$

SU(2) Heisenberg:

$$H = 2J \sum_{\langle i,j \rangle} \Big[S_i^+ S_j^- + S_i^- S_j^+ + \underbrace{n_{i,\uparrow} n_{j,\uparrow} + n_{i,\downarrow} n_{j,\downarrow}}_{= \frac{1}{2} S_i^z S_j^z + const.} \Big] = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + const.$$

$$S_i^+ = c_{i,\uparrow}^\dagger c_{i,\downarrow}$$

An equivalent form:

$$H = J \sum_{\langle ij \rangle, \alpha, \beta} \left(S_i^\alpha S_j^\alpha + V_i^\beta V_j^\beta + 4 (S^\alpha V^\beta)_i (S^\alpha V^\beta)_j \right)$$

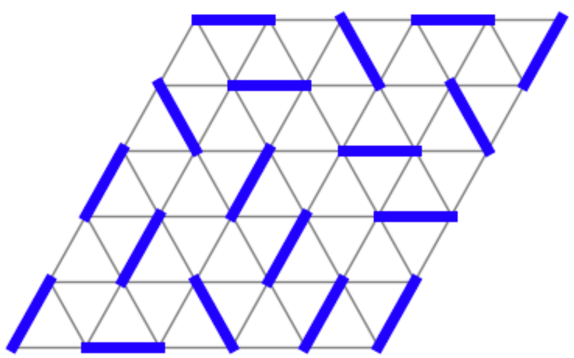
SU(4) symmetric point of the SU(2)xSU(2) Kugel-Khomskii model

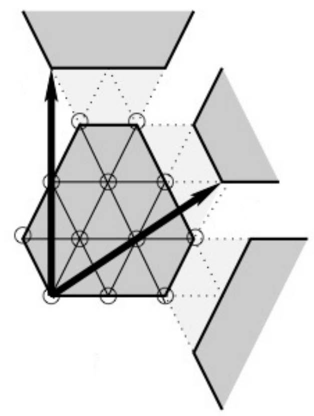
$$\tilde{S}_i = \left\{ c_{i,s,v}^\dagger \sigma_{s,s'}^\alpha \delta_{v,v'} c_{i,s',v'}, \quad c_{i,s,v}^\dagger \delta_{s,s'} \tau_{v,v'}^\beta c_{i,s',v}, \quad c_{i,s,v}^\dagger \sigma_{s,s'}^\alpha \tau_{v,v'}^\beta c_{i,s',v'} \right\}$$

3 + 3 + 9 = 15 operators

Outline - SU(4) “spins” on the triangular lattice

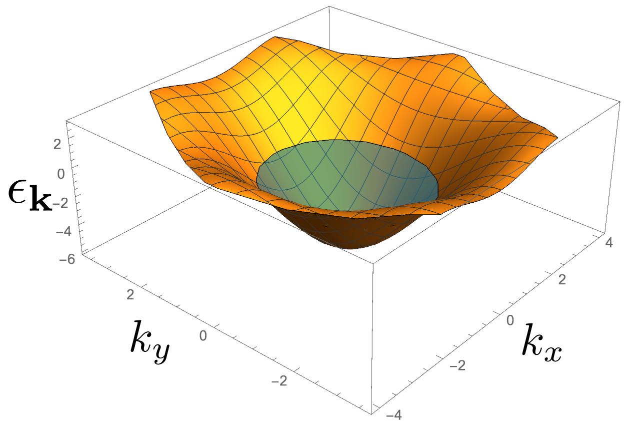
- **Half filling - dimer description and valence bond states**

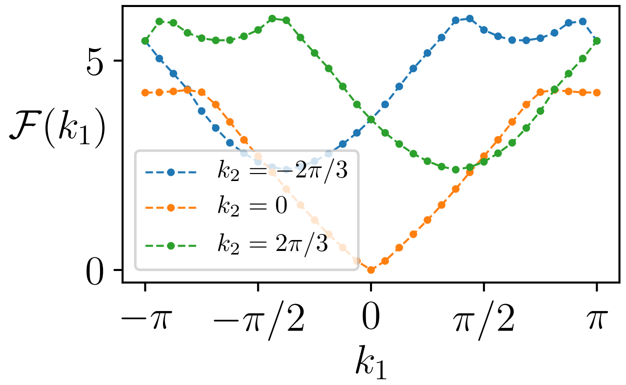




AK, Lucile Savary, Leon Balents, SciPost 2019

- **Quarter filling - evidence for a gapless quantum liquid**





AK, Bela Bauer, Cenke Xu, Chao-Ming Jian, PRL 2020

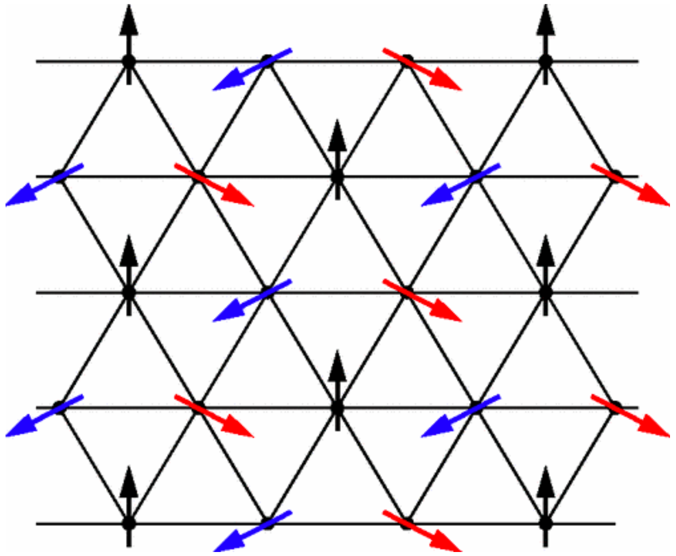
SU(4) "spins" at half filling

2 particles per site $|ab\rangle_i = c^\dagger_{i,a} c^\dagger_{i,b} |0\rangle_i$

6 possible states per site $\{|12\rangle, |13\rangle, |14\rangle, |23\rangle, |24\rangle, |34\rangle\}$

Classical (mean-field) limit

$$|\Psi\rangle = \prod_i |\psi\rangle_i$$

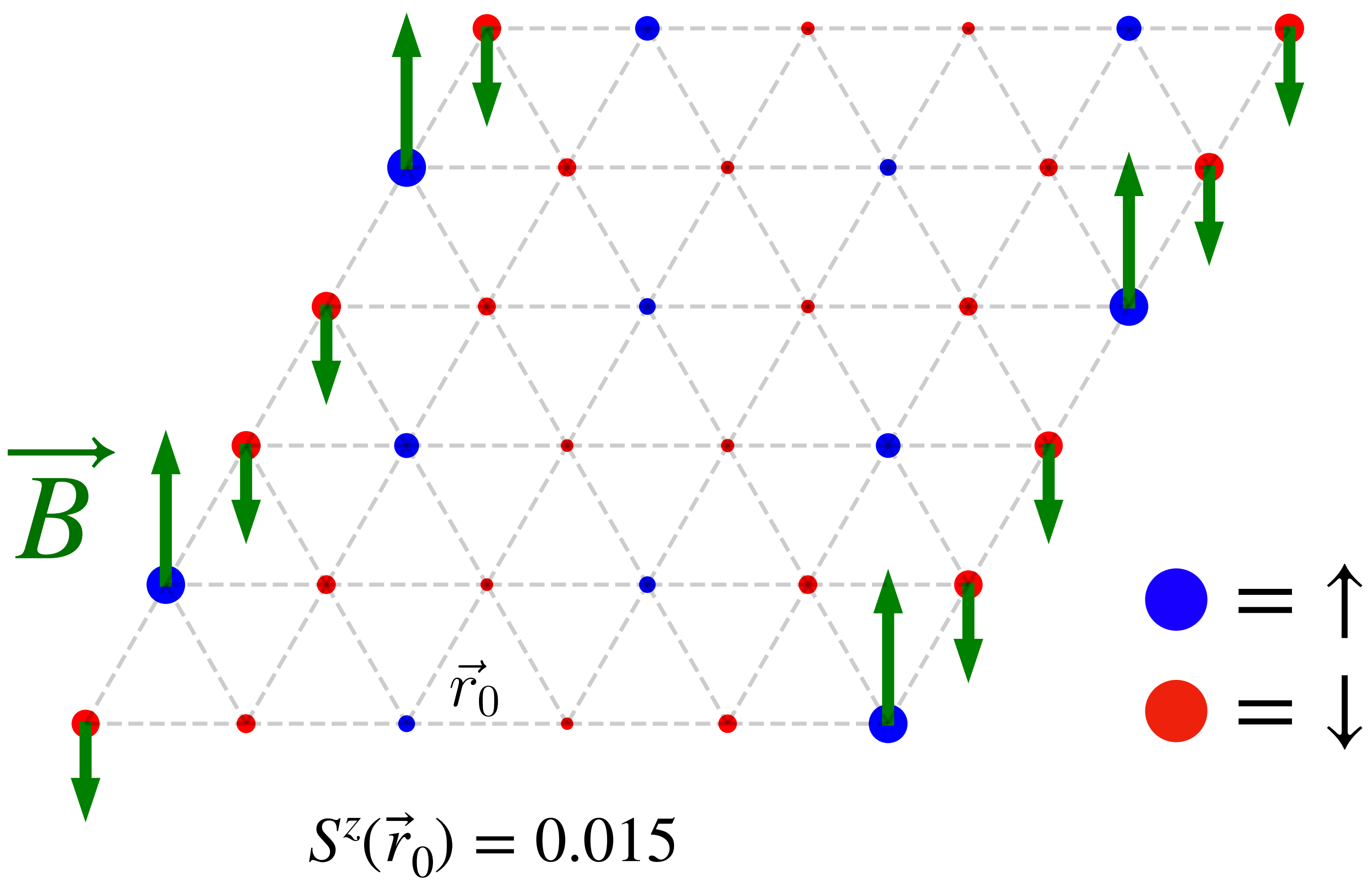


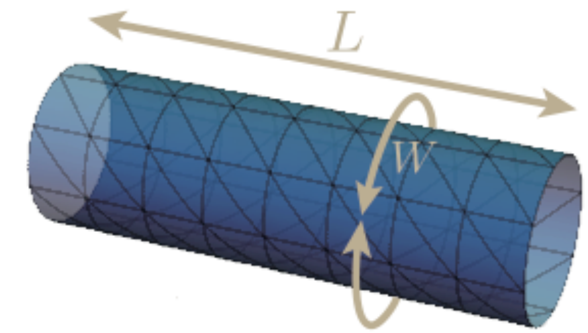
120° order!

(up to SU(4) rotations)

Probing long range order in the SU(4) model

Cylinder with pinning fields at the boundaries

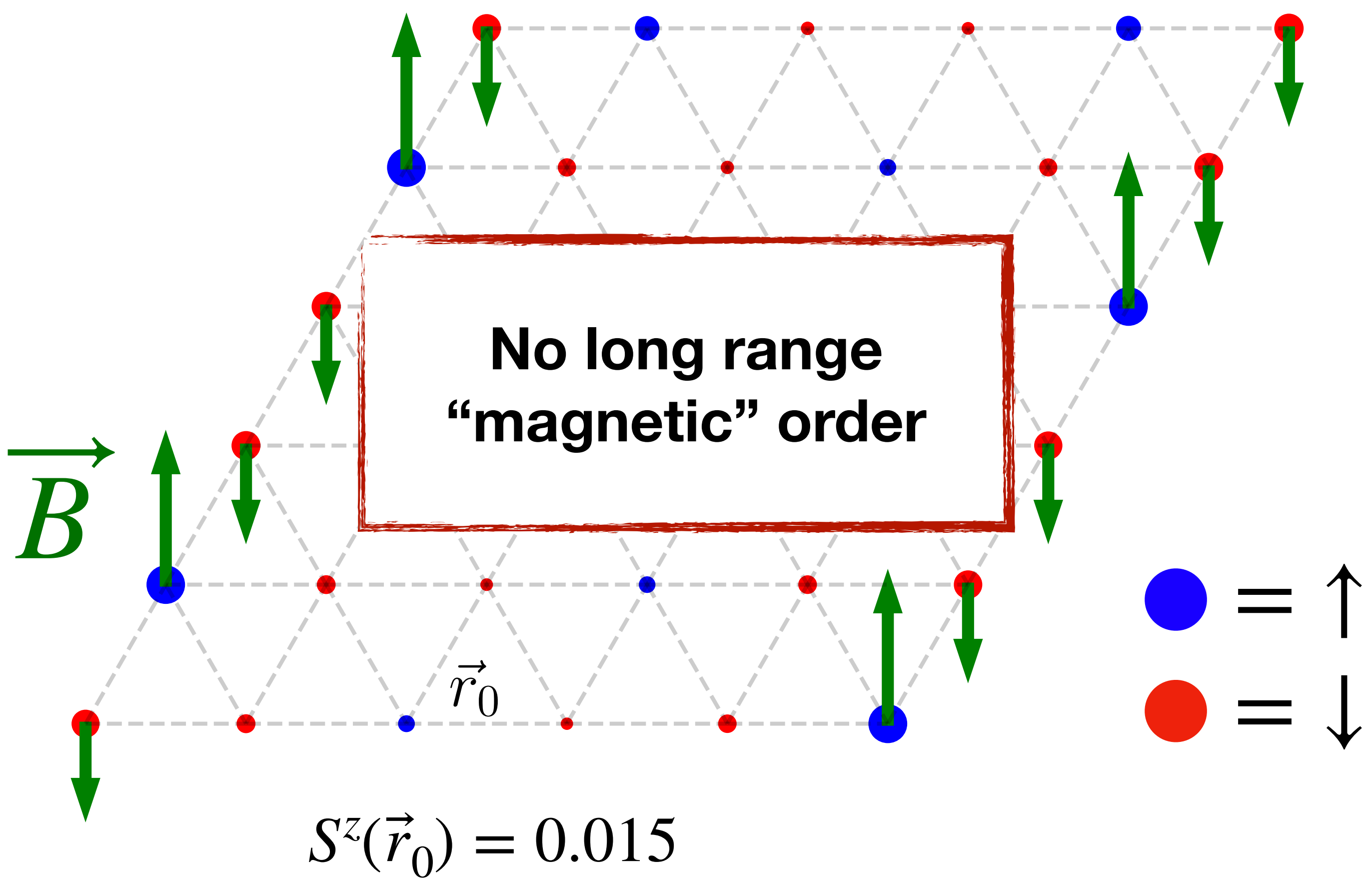


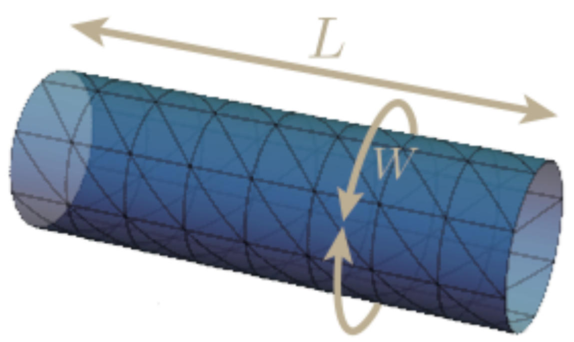


Expectation value of the spin along the field direction

Probing long range order in the SU(4) model

Cylinder with pinning fields at the boundaries





Expectation value of the spin along the field direction

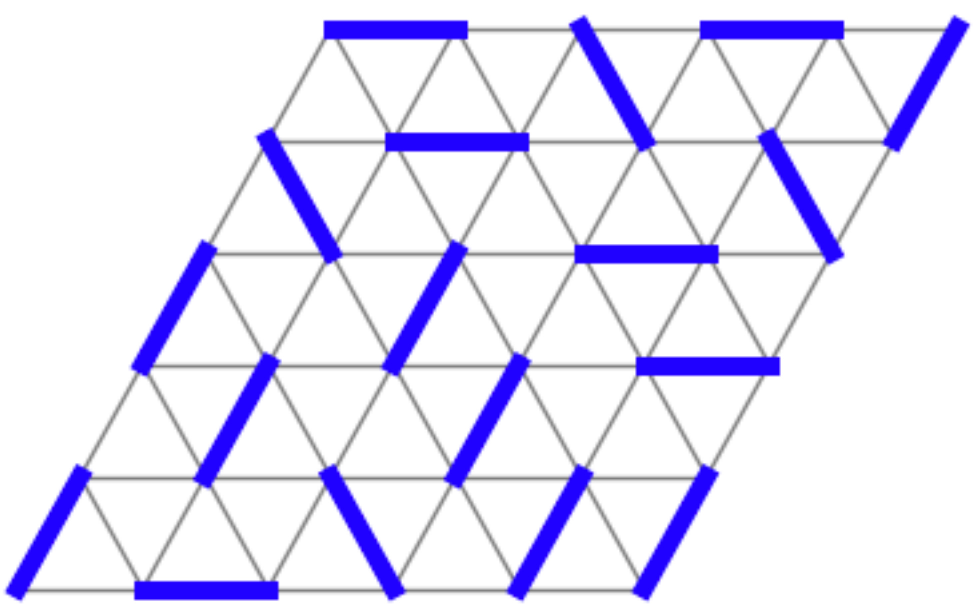
In agreement with a recent PF-FRG study by Kiese et al. PRR 2020

SU(4) spins at half-filling

2 particles per site $|ab\rangle_i = c^\dagger_{i,a} c^\dagger_{i,b} |0\rangle_i$

SU(4) singlet

$$|s\rangle_{ij} = \frac{1}{2\sqrt{6}} \sum_{a,b,c,d=1,..,4} \epsilon_{abcd} |ab\rangle_i |cd\rangle_j$$



Singlet coverings are candidates for the ground state on a lattice!

From SU(4) spins to dimers

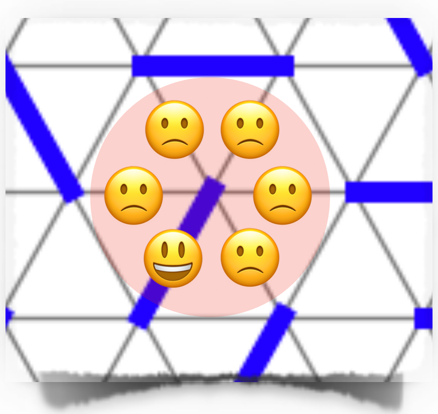
Can the nearest-neighbor singlet coverings capture the low energy physics of the SU(4) spin model?

- Large N limit -

  For SU(N) at half-filling ground state description in terms of dimer coverings is exact

Rokhsar 1990

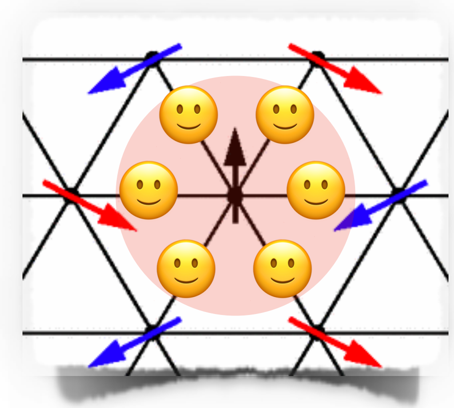
- Classical order vs dimer covering -



For SU(2), spin-1/2: $E^{\mathrm{SU(2)}}_{\mathrm{dimer}} = E^{\mathrm{SU(2)}}_{120^\circ}$

For SU(4):

$$\frac{E^{\mathrm{SU(4)}}_{\mathrm{dimer}}}{N_{bonds}} = -\frac{5}{6}J \quad < \quad -\frac{1}{2}J = \frac{E^{\mathrm{SU(4)}}_{120^\circ}}{N_{bonds}}$$



Dimer coverings have significantly lower energy!

Quantum dimer models

Projecting the spin Hamiltonian onto the
nearest-neighbor singlet-coverings subspace

singlet covering

$$|\psi\rangle = \sum_C \psi_C |C\rangle$$

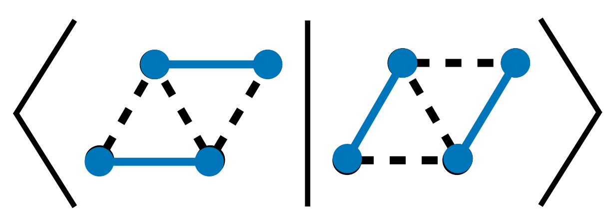
Effective Hamiltonian for
orthogonal dimers

$$H_{\text{dimer}} = S^{-1/2} H_{\text{proj}} S^{-1/2}$$

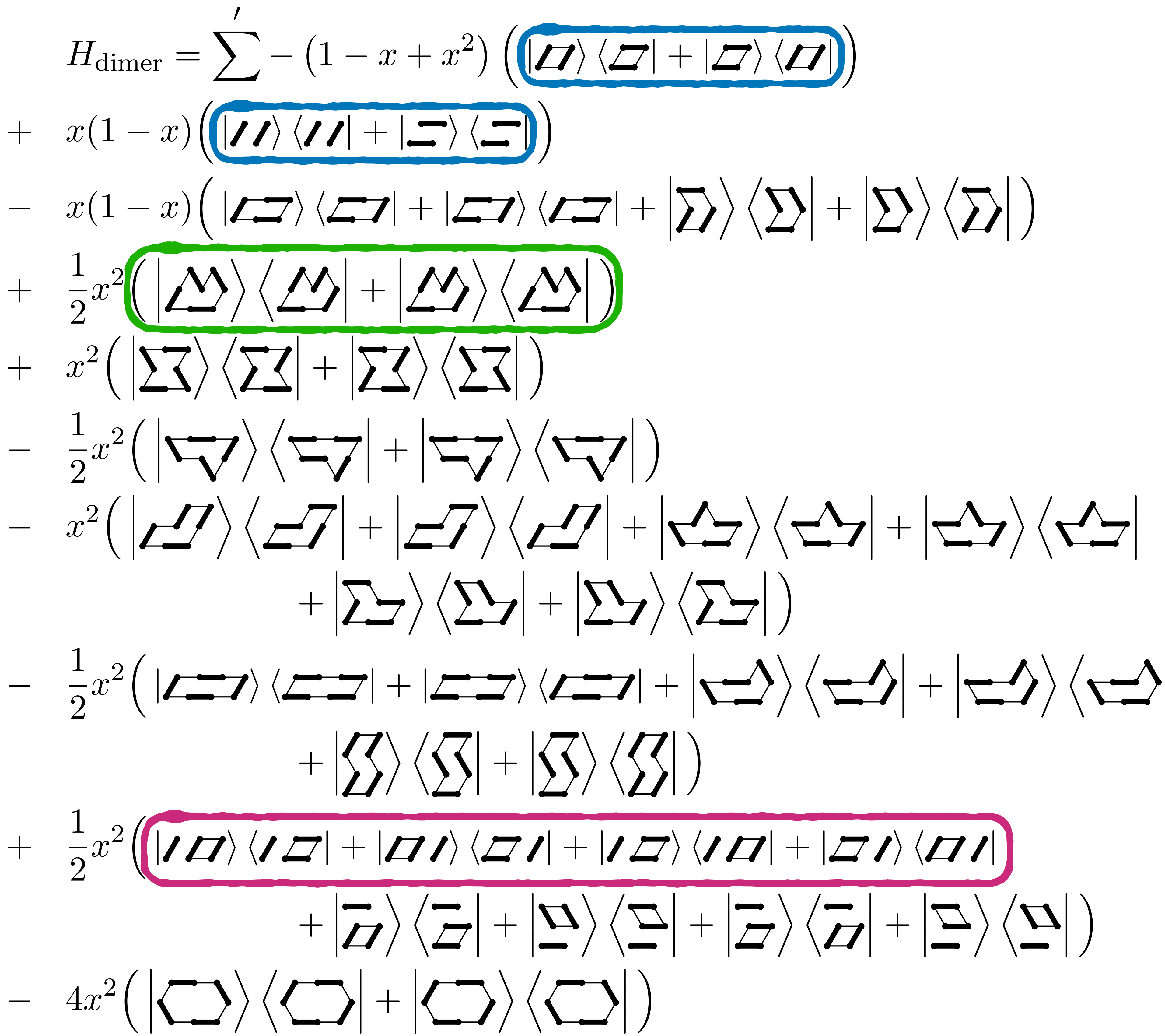
$$E(\psi) = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \rightarrow H_{\text{proj}}\psi = E_0 S \psi \rightarrow H_{\text{dimer}}\psi = E_0 \psi,$$

$$H_{\text{proj},C'C} = \langle C' | H | C \rangle, \; S_{C'C} = \langle C' | C \rangle$$

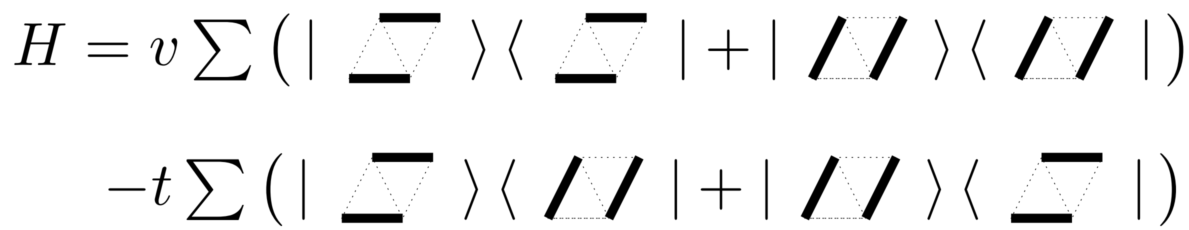
*singlet coverings are not orthogonal!

$x =$  $= \frac{1}{6}$

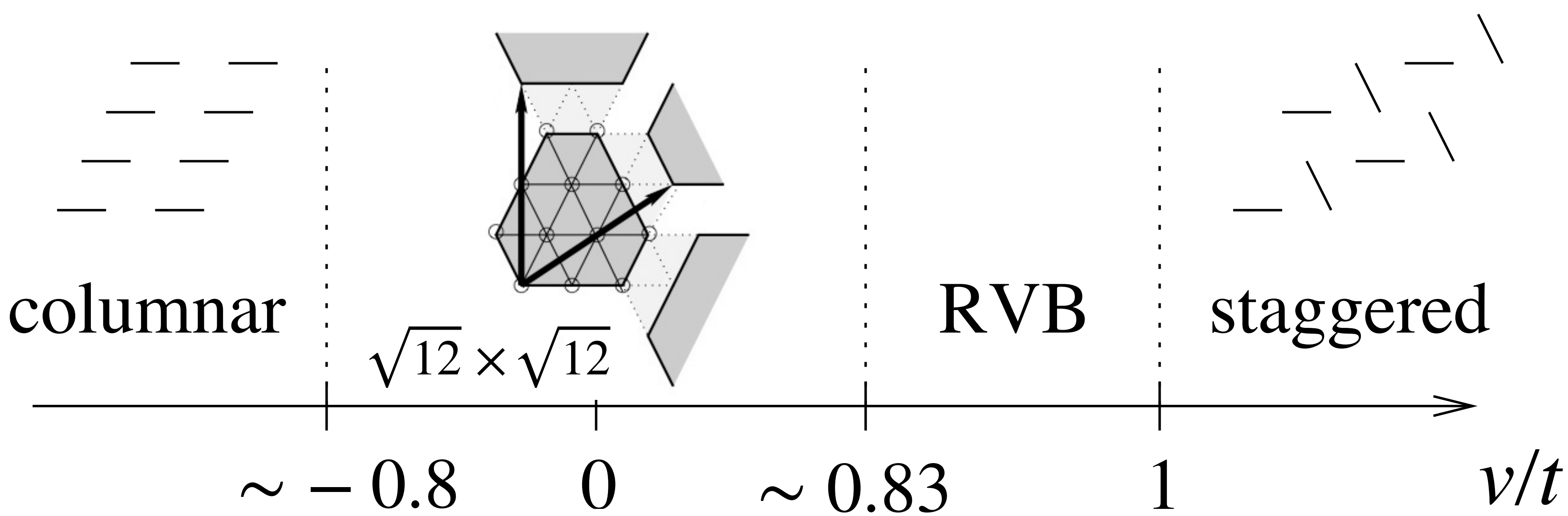
Rokhsar, Kivelson 1988


$H_{\text{dimer}} = \sum{}' -(1 - x + x^2)$
$+ \; x(1-x)$
$- \; x(1-x)$
$+ \; \frac{1}{2}x^2$
$+ \; x^2$
$- \; \frac{1}{2}x^2$
$- \; x^2$
$- \; \frac{1}{2}x^2$
$+ \; \frac{1}{2}x^2$
$- \; 4x^2$

Quantum dimer model



Phase diagram on the triangular lattice:

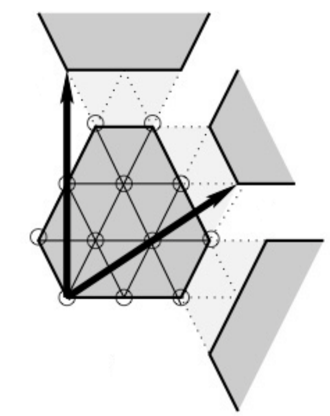


Moessner, Sondhi 2001, Ralko et al. 2005

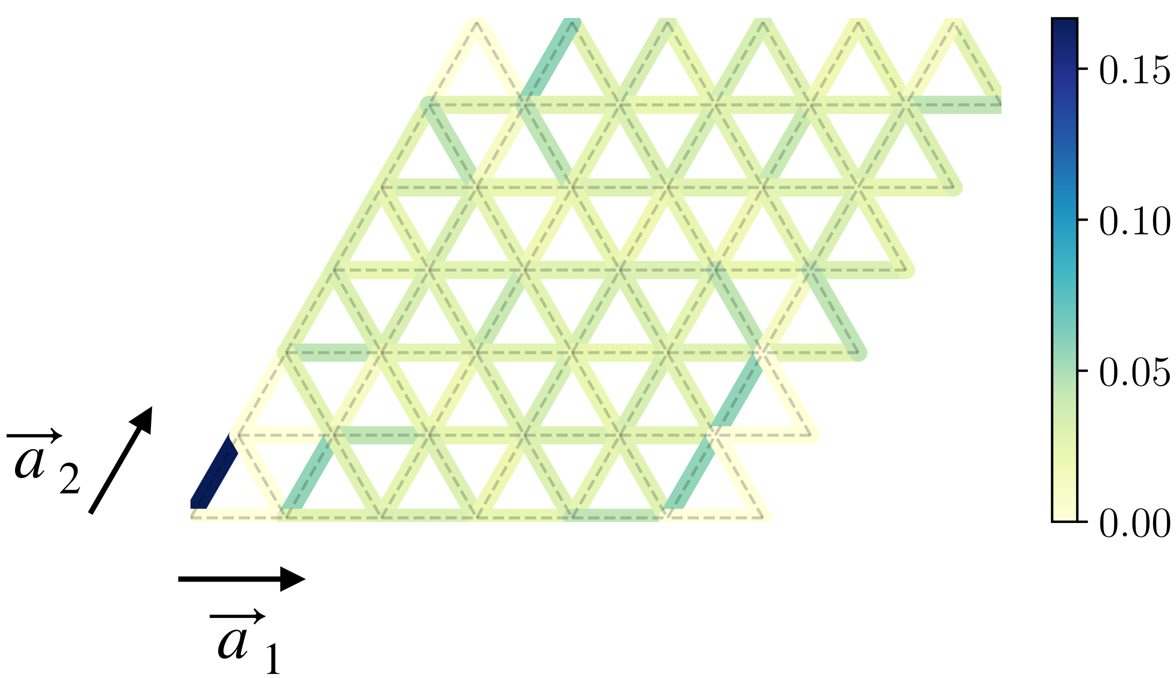
Back to the full dimer model - Exact Diagonalization

6x6 lattice with periodic boundary conditions

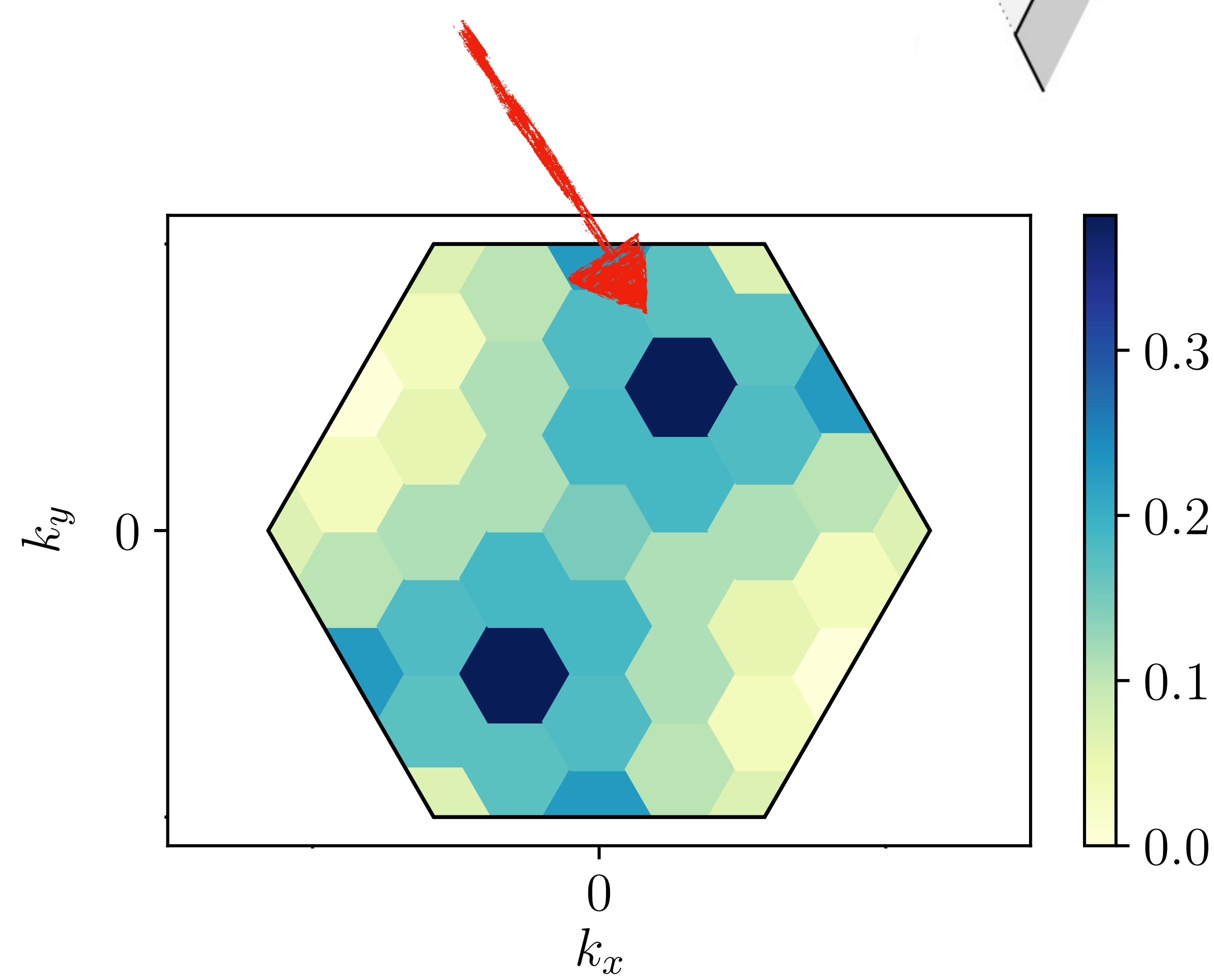
Ground state breaks translational invariance forming a 12-site unit cell!



Bond-bond correlations in the ground state:

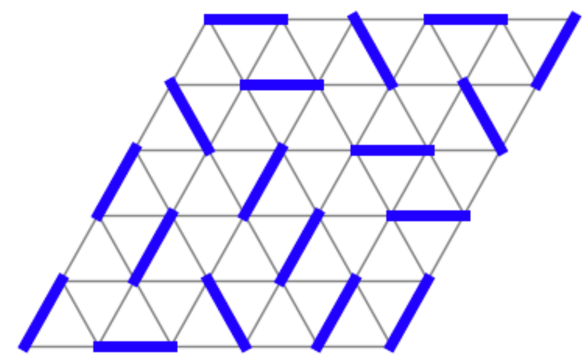


FT

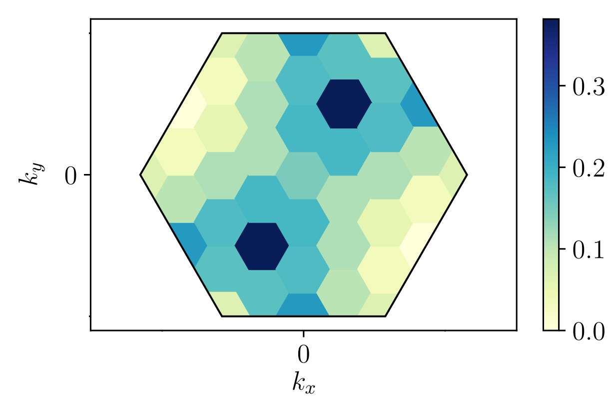


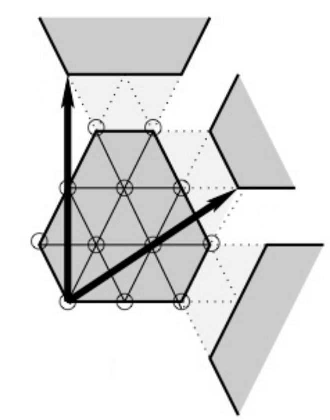
Half-filling - summary so far

Low energy properties of the Mott phase at half filling can be captured by an effective dimer model



The ground state of the effective dimer model is a valence bond solid state with a 12-site unit cell





Breaking SU(4) symmetry

Hund's coupling

$$H = J \sum_{\langle i,j \rangle} T_i^{ab} T_j^{ba} - J_H \sum_i |\vec{S}_i|^2$$

At large J_H , electrons on each site pair up into a spin-triplet

$$|1\rangle = |K \uparrow\rangle$$
$$|2\rangle = |K \downarrow\rangle$$
$$|3\rangle = |K' \uparrow\rangle$$
$$|4\rangle = |K' \downarrow\rangle$$

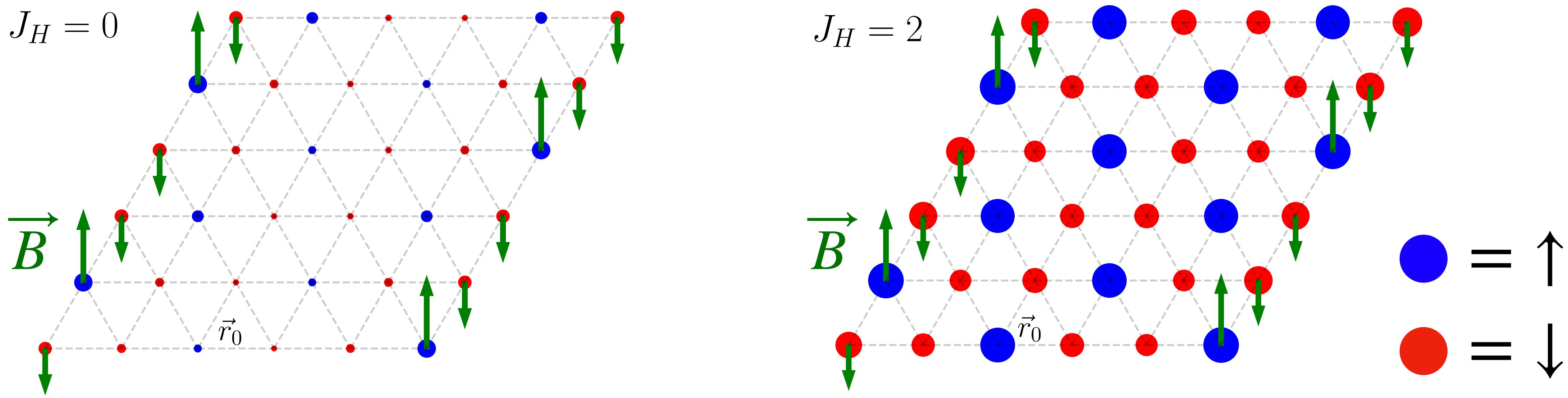
→

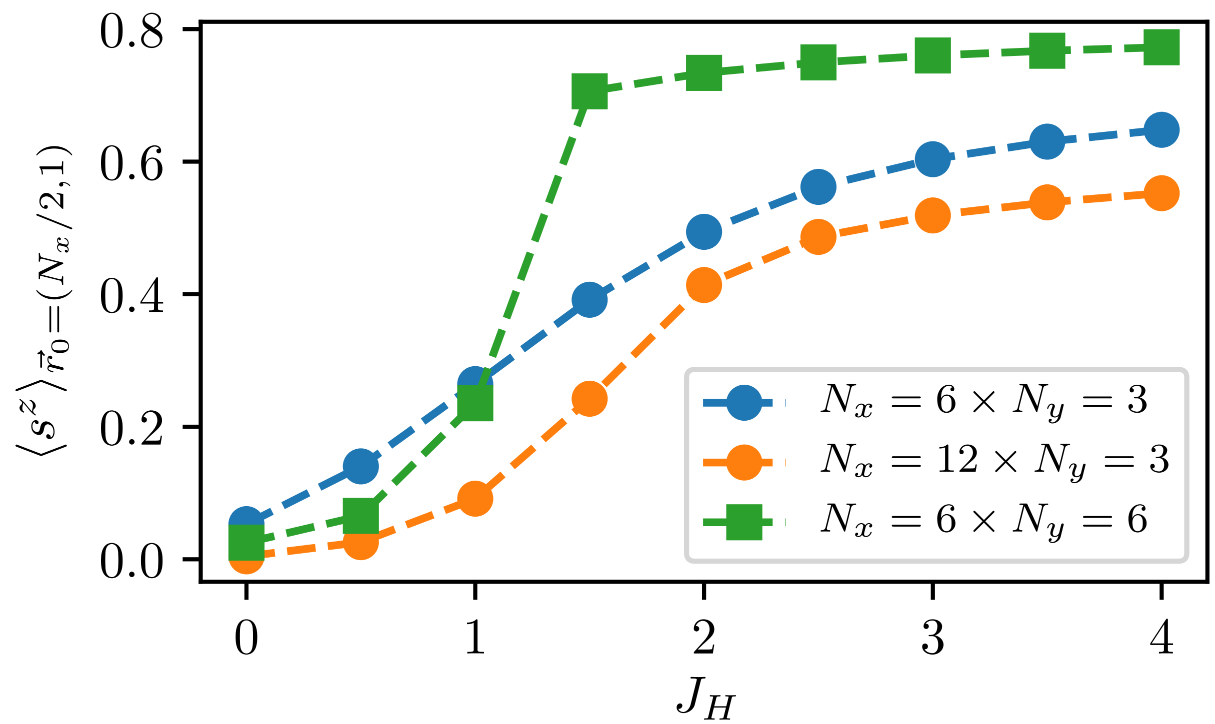
$$|13\rangle = |S = 1, m_z = +1\rangle$$
$$\frac{1}{\sqrt{2}}\left(|14\rangle + |23\rangle\right) = |S = 1, m_z = 0\rangle$$
$$|24\rangle = |S = 1, m_z = -1\rangle$$

$J_H \gg J$ $\quad$ $H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$ $\quad$ **Spin-1 Heisenberg model!**

120° magnetic order at large J_H

S_z expectation value obtained using DMRG

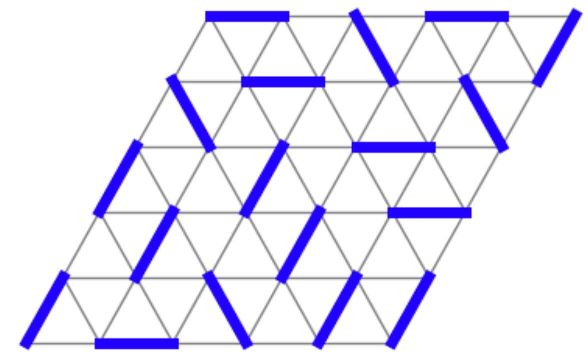




Phase transition from valence bond to magnetic order?

Half-filling - summary

Low energy properties of the Mott phase at half filling can be captured by an effective dimer model



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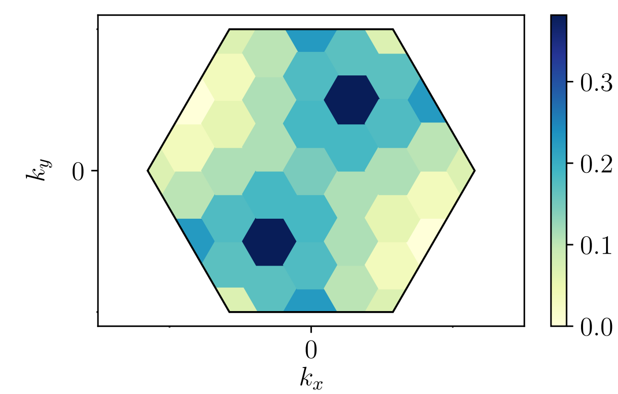
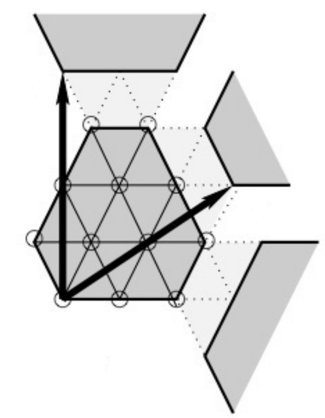
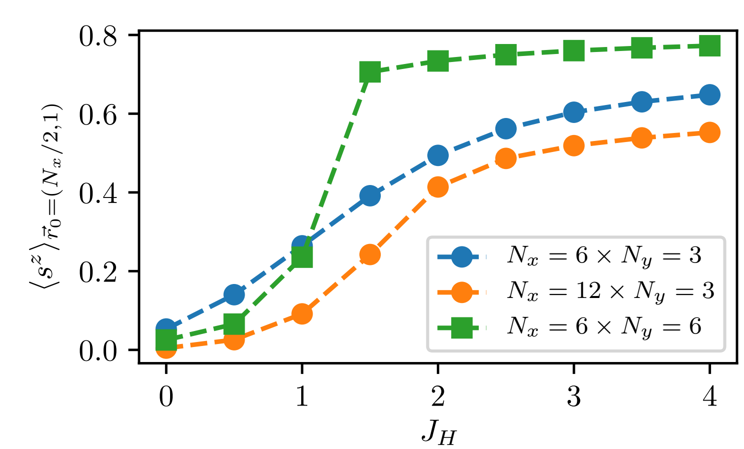


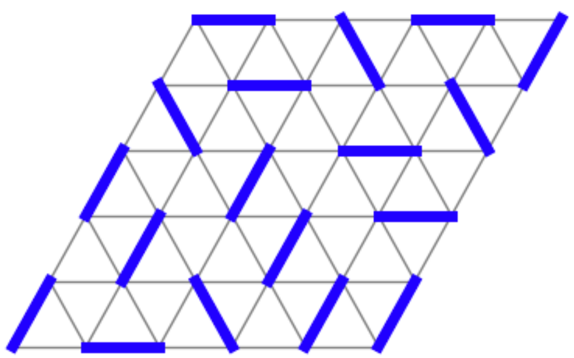


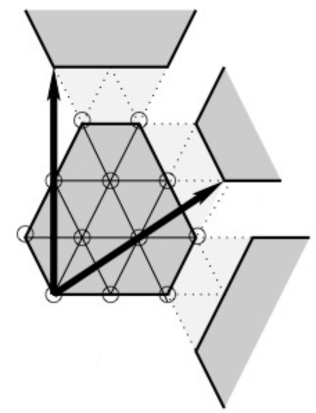
Breaking SU(4) symmetry by a Hund's coupling term drives the system into a magnetically ordered state



Outline - SU(4) “spins” on the triangular lattice

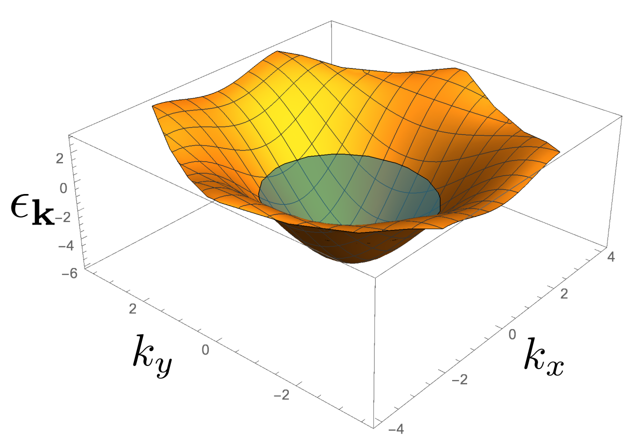
- **Half filling - dimer description and valence bond states**

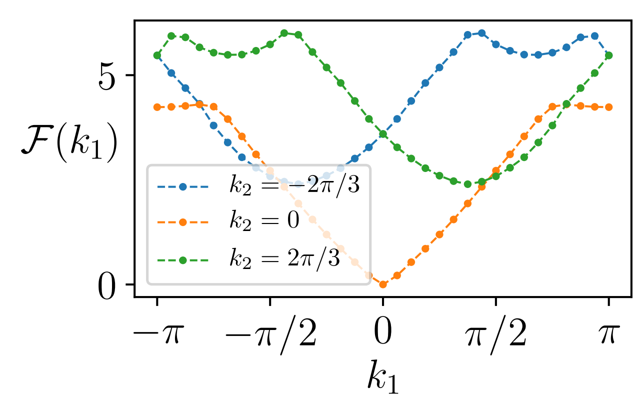




AK, Lucile Savary, Leon Balents, SciPost 2019

- **Quarter filling - evidence for a gapless quantum liquid**

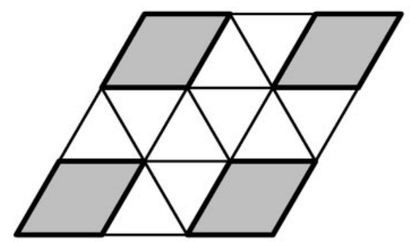




AK, Bela Bauer, Cenke Xu, Chao-Ming Jian, PRL 2020

SU(4) Heisenberg antiferromagnets at quarter-filling

Triangular lattice



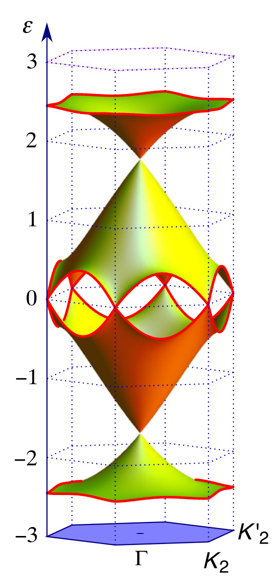
4 spins on a plaquette can form a singlet ⇒ expect plaquette order?

Li et al., PRL 1998

Variational study with singlet plaquettes as a starting points suggests spin-orbital liquid

Penc et al., PRB 2003

Honeycomb lattice



evidence for an algebraic (Dirac) spin-orbital liquid

Corboz et al., PRX 2012

Parton construction

$$S_i^\alpha = \frac{1}{2} f_{i,a}^\dagger \sigma^\alpha f_{i,a}, \qquad V_i^\beta = \frac{1}{2} f_{i,a}^\dagger \tau^\beta f_{i,a}, \qquad (S^\alpha V^\beta)_i = \frac{1}{4} f_{i,a}^\dagger \sigma^\alpha \tau^\beta f_{i,a}$$

Abrikosov fermions $\quad \{f_{i,a}, f_{j,b}^\dagger\} = \delta_{i,j}\delta_{a,b}$

with the constraint $\quad n_i = \sum_{a=1}^{4} f_{i,a}^\dagger f_{i,a} = 1$

Gutzwiller projection:

Numerically project out all states with occupancy $n_i \neq 1$

Parton mean field

$$H = J \sum_{\langle ij \rangle} \left(2\mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{2} \right) \left(2\mathbf{V}_i \cdot \mathbf{V}_j + \frac{1}{2} \right)$$

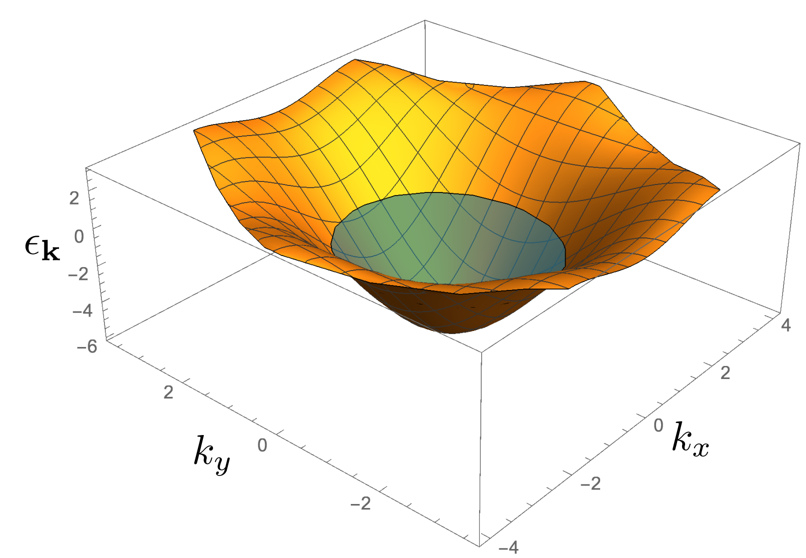
$$S_i^{\alpha} = \frac{1}{2} f_i^{\dagger} \sigma^{\alpha} f_i,\ V_i^{\beta} = \frac{1}{2} f_i^{\dagger} \tau^{\beta} f_i,\ (S^{\alpha} V^{\beta})_i = \frac{1}{4} f_i^{\dagger} \sigma^{\alpha} \tau^{\beta} f_i$$

$$H = -J \sum_{\langle i,j \rangle} \chi_{ij}^{\dagger} \chi_{ij} + const. \qquad \chi_{ij} = \sum_a f_{i,a}^{\dagger} f_{j,a}$$

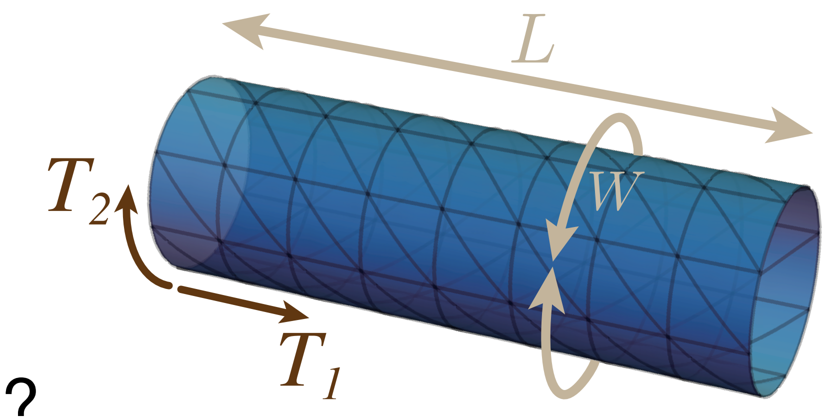
$$\langle \chi_{ij} \rangle = \chi_0,\ t = J\chi_0$$

$$H_{\mathrm{MF}} = -t \sum_{\langle i,j \rangle, a=1,..,4} f_{i,a}^{\dagger} f_{j,a} \qquad \nu = \frac{1}{4}$$

$\left| \Psi_{\mathrm{MF}} \right\rangle$ - Slater determinant state



Finite-circumference cylinders



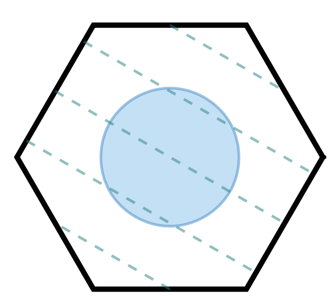
Periodic boundary conditions for the ***spins***

What are the boundary conditions for the ***partons***?

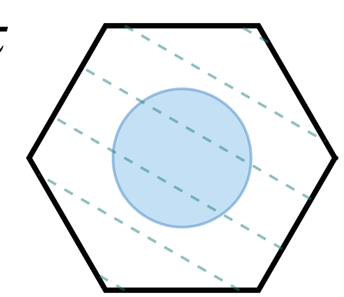
From symmetry constraints: $\Phi = 0$ or $\Phi = \pi$

Different cuts through the Fermi surface for finite circumference!

$\Phi = 0$



$\Phi = \pi$



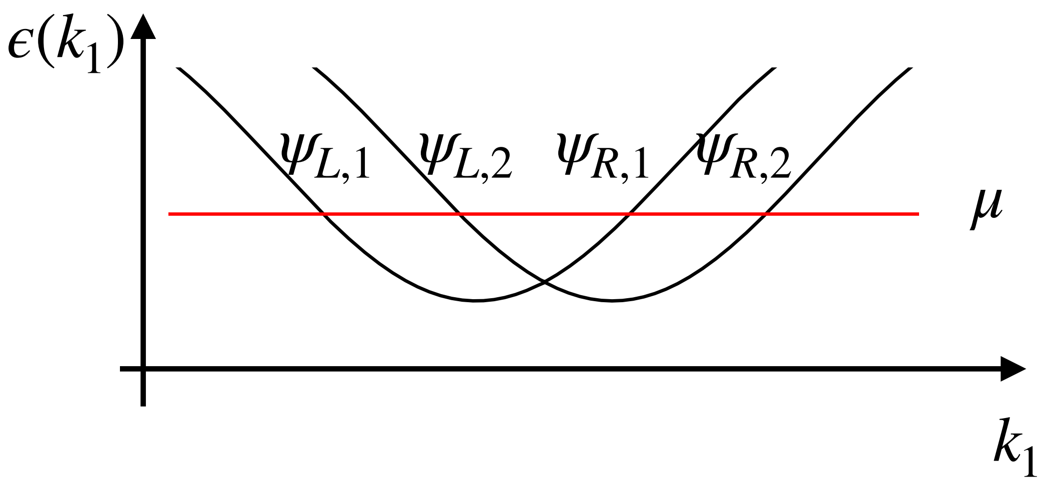
Finite-circumference cylinders

Low energy theory

$$\mathscr{L} = \sum_m \sum_{a=1}^{4} \left[\psi^\dagger_{L,m,a}(i\partial_t - iv_m\partial_x)\psi_{L,m,a} + \psi^\dagger_{R,m,a}(i\partial_t + iv_m\partial_x)\psi_{R,m,a}\right]$$

1D bands

Coupling to the gauge field $\partial_{\mu=x,t} \to \partial_\mu - a_\mu$



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↗ 1D bands

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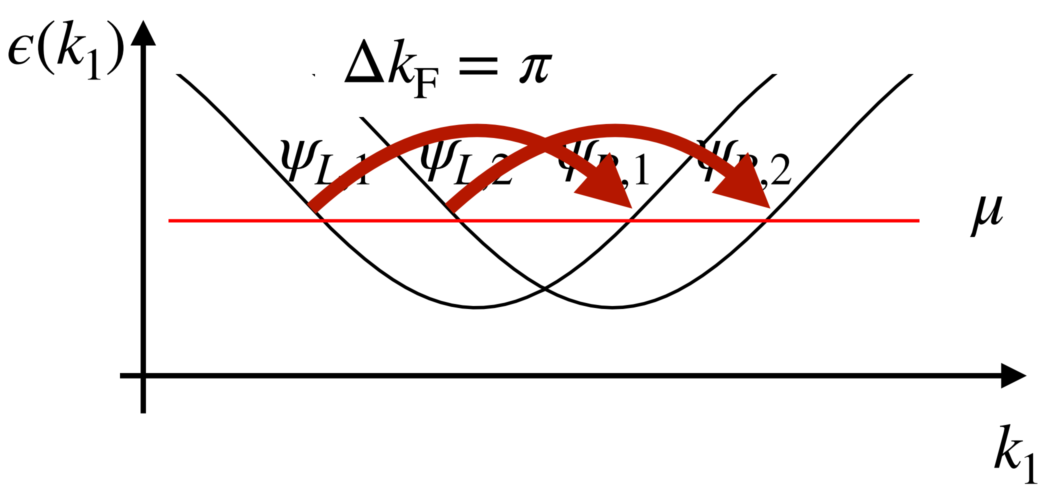
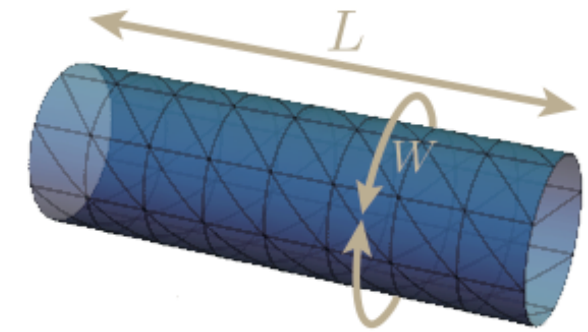


Umklapp scattering is a relevant perturbation for W=2 and W=4

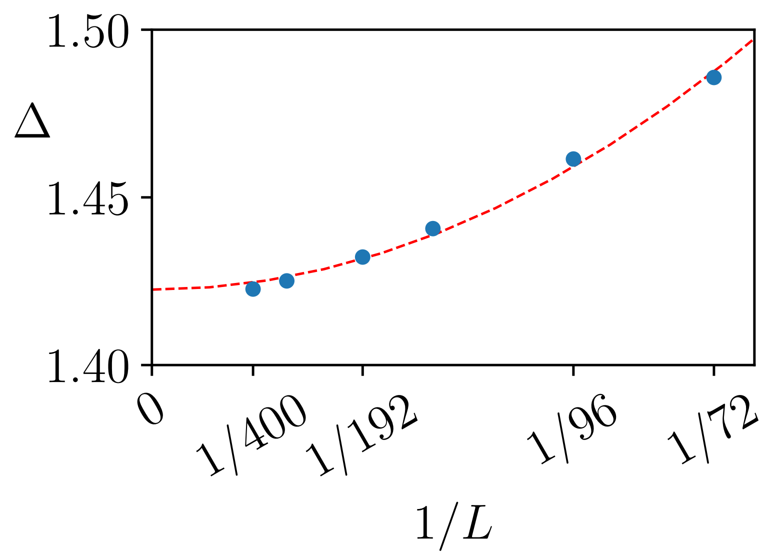
→ **will break translation invariance and open a gap!**

DMRG results

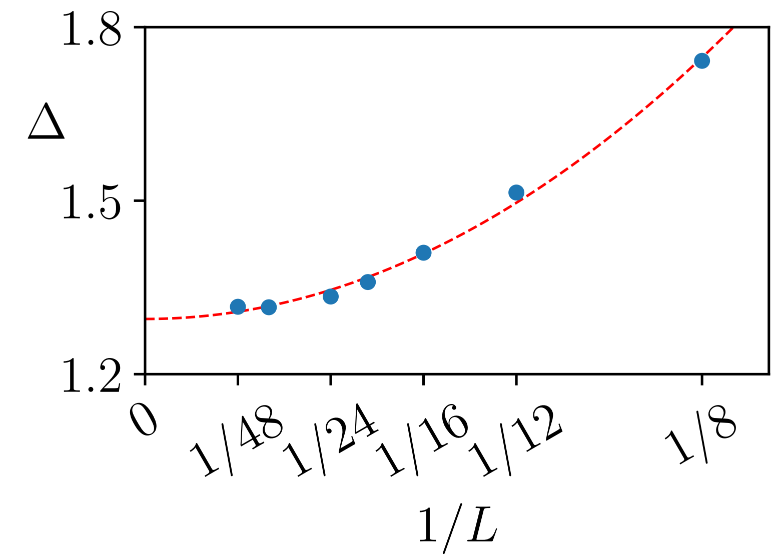


Spin gap

$W = 2$



$W = 4$

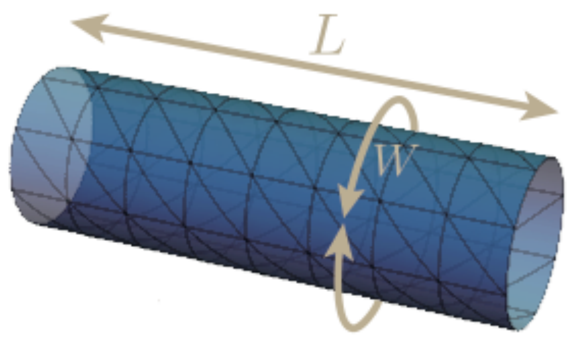


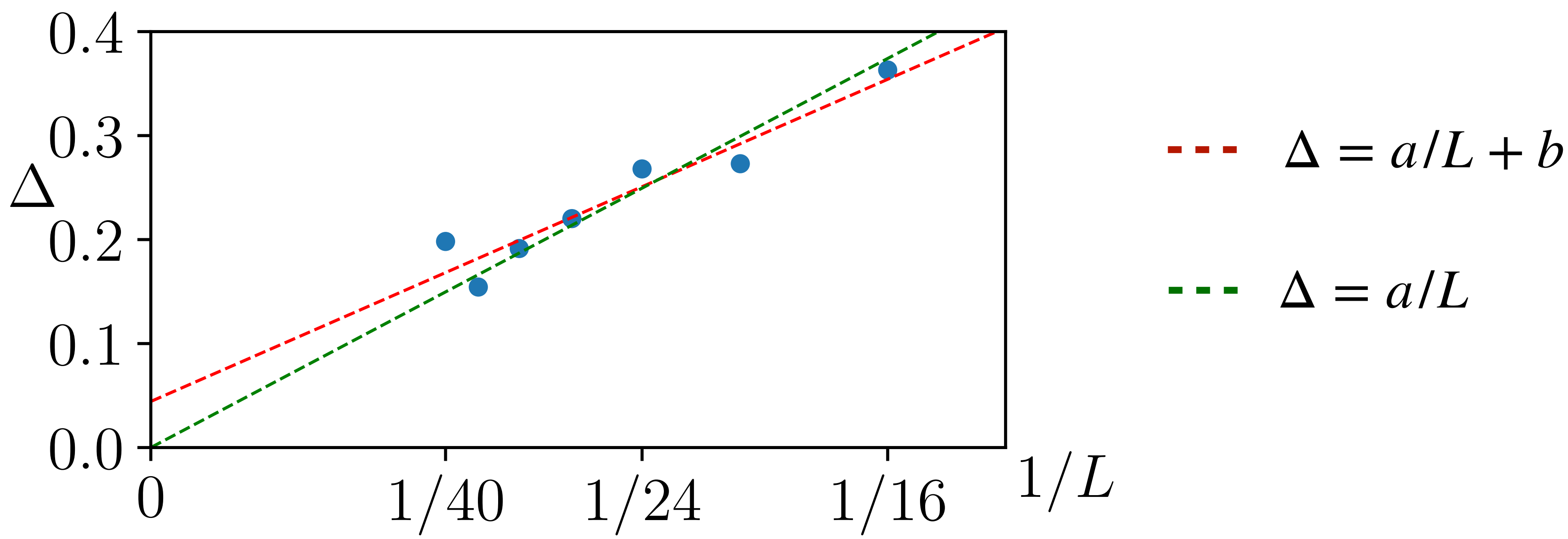
Bond expectation values $\langle \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_j \rangle$

Gapped phases with a two-site unit cell - consistent with the field theory

DMRG results

Spin gap $W = 3$

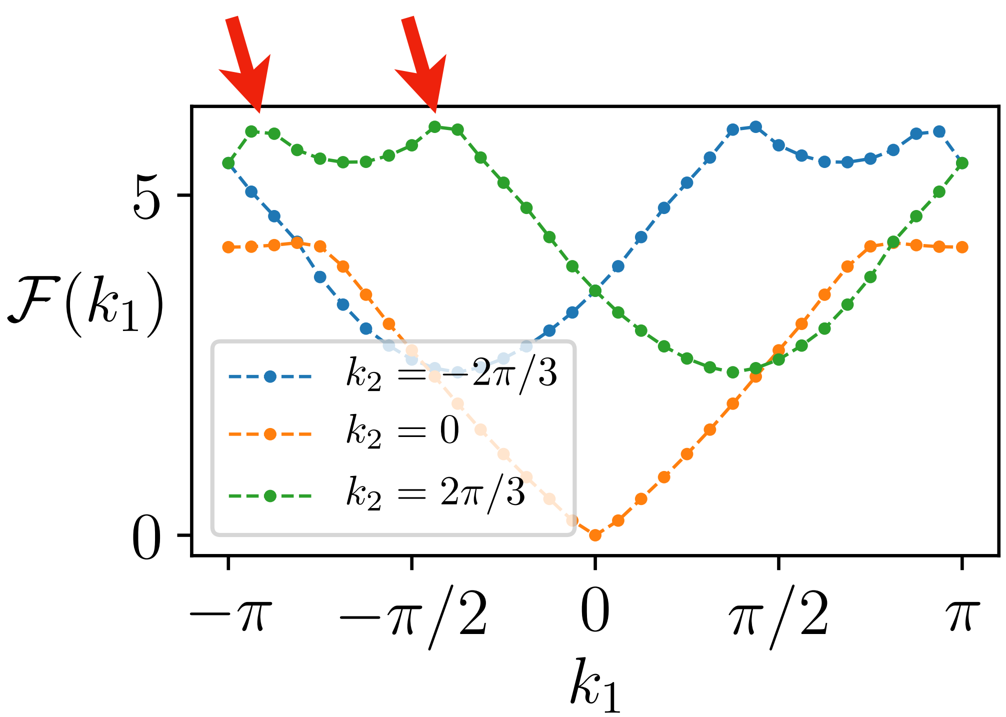


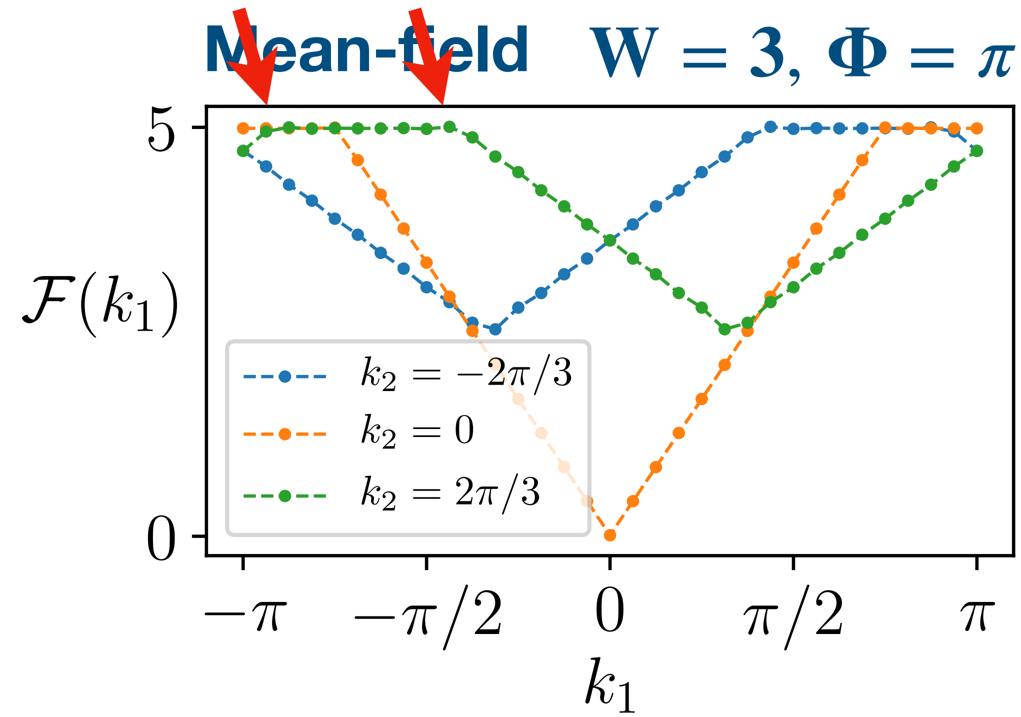


Consistent with a gapless state

DMRG results $W = 3$

Structure factor $\mathscr{F}(\overrightarrow{k}) = \sum_i e^{i\overrightarrow{k}\cdot(\vec{r}_i - \vec{r}_{i_0})} \sum_\alpha \langle \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_{i_0} \rangle$





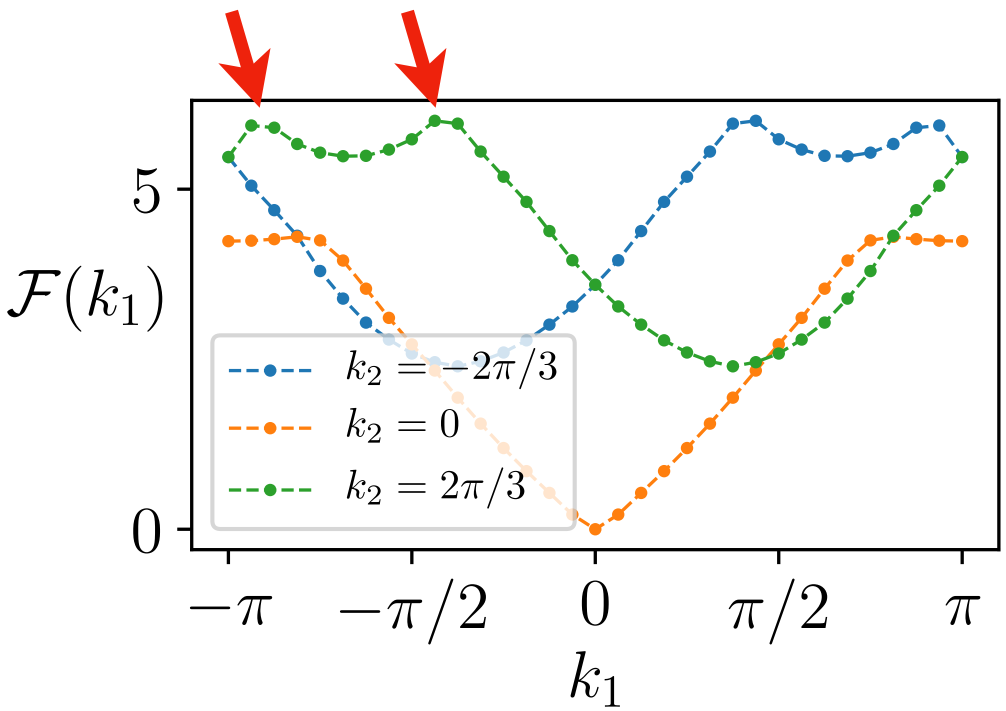
Cusps in the structure factor appear at the same values, corresponding to "$2k_F$"s !

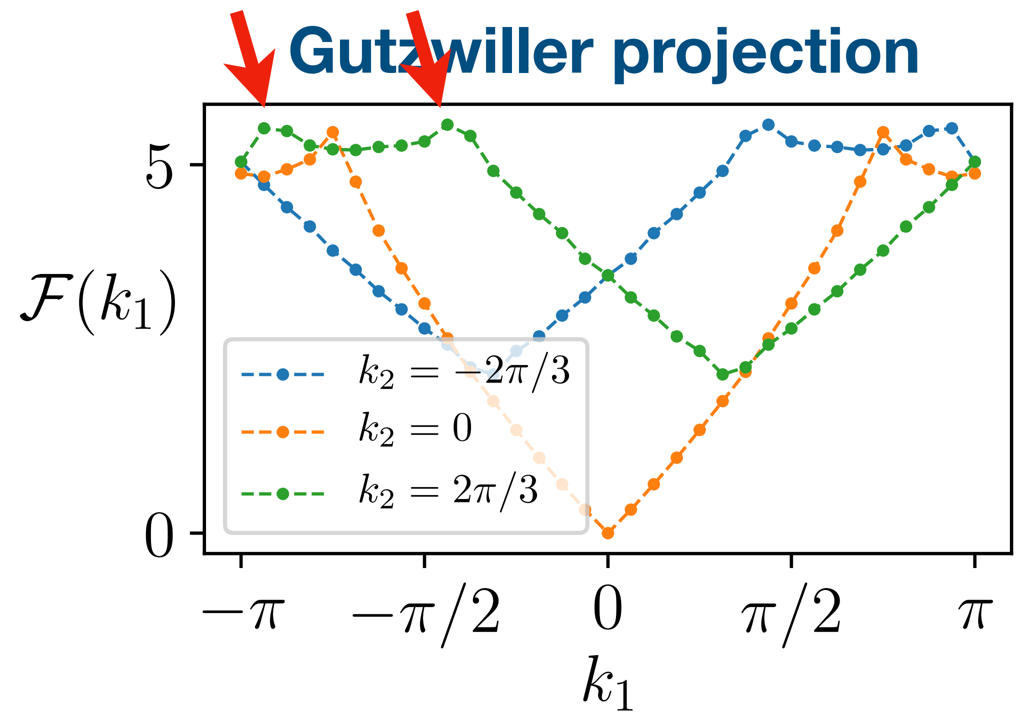
See e.g. *Sheng, Motrunich, Fisher, PRB 2009*

DMRG results

$W = 3$

Structure factor $$\mathscr{F}(\vec{k}) = \sum_i e^{i\vec{k}\cdot(\vec{r}_i - \vec{r}_{i_0})} \sum_\alpha \langle \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_{i_0} \rangle$$





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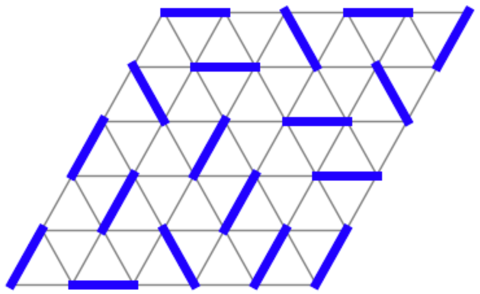
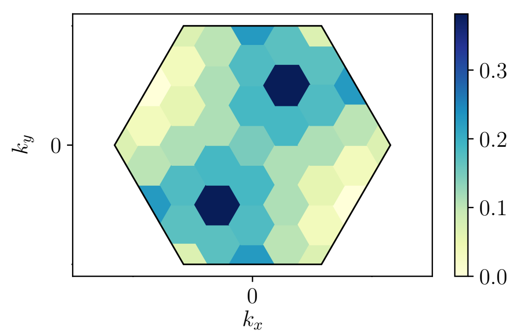
Summary

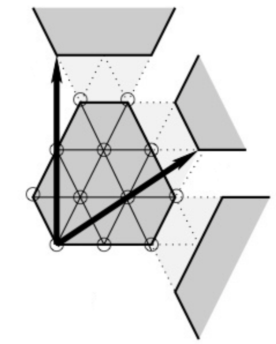
- **Half filling**

Low energy properties of the Mott phase at half filling can be captured by an effective dimer model

The ground state of the effective dimer model is a valence bond solid state with a 12-site unit cell



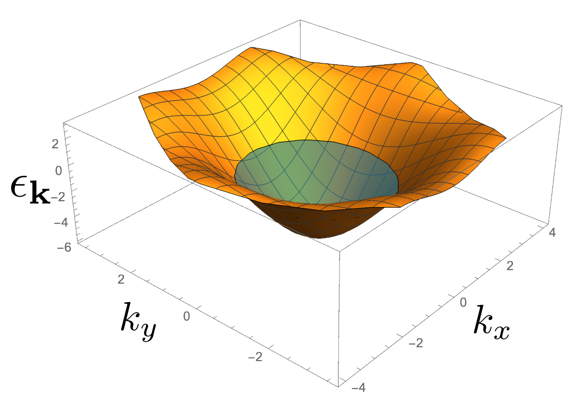


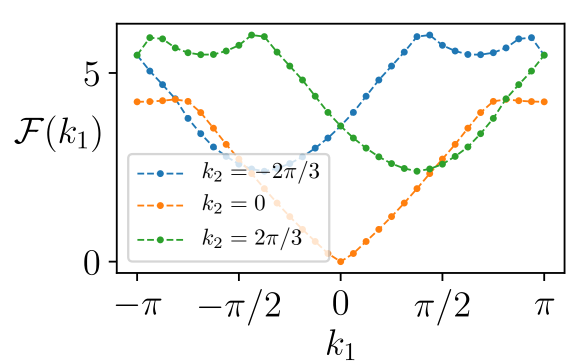


AK, Lucile Savary, Leon Balents, SciPost 2019

- **Quarter filling**

Numerical results on finite circumference cylinders are consistent with a gapless liquid state with an emergent Fermi surface





AK, Bela Bauer, Cenke Xu, Chao-Ming Jian, PRL 2020