Spin-orbital quantum liquid on the honeycomb lattice

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Collaborators

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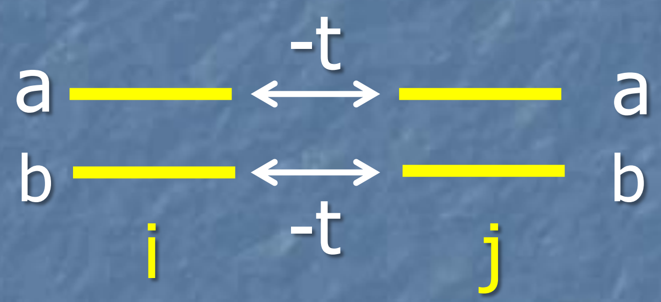
Scope

- Introduction: the spin-orbital symmetric Kugel-Khomskii model as SU(4) quantum permutation
- SU(4) on honeycomb lattice
  - → Hartree
  - → Flavour-wave theory
  - → iPEPS
  - → Gutzwiller projected wavefunctions
- Conclusion: no LRO, algebraic correlations

Mott insulator with orbital degeneracy



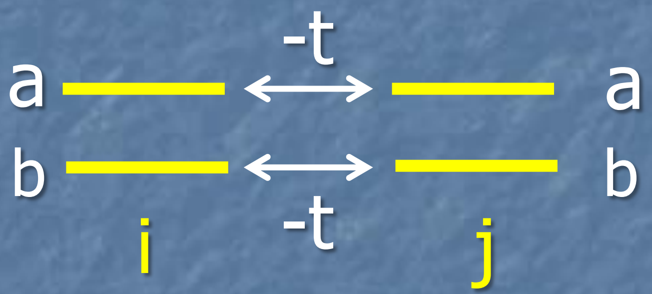
- 1 electron per site
- on-site repulsion U

spin orbital

$$\mathcal{H} = \frac{2t^2}{U} \sum_{\langle i,j \rangle} (2\mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{2})(2\mathbf{T}_i \cdot \mathbf{T}_j + \frac{1}{2})$$

Symmetric Kugel-Khomskii model

SU(4) formulation



- 1 electron per site
- on-site repulsion U

$$\mathcal{H} = -t \sum_{\langle i,j\rangle,\alpha} (c^{\dagger}_{i,\alpha} c_{j,\alpha} + \mathrm{H.c.}) + U \sum_{i,\alpha<\beta} n_{i,\alpha} n_{i,\beta}$$

$$\alpha = |a\uparrow\rangle,\ |a\downarrow\rangle,\ |b\uparrow\rangle,\ |b\downarrow\rangle$$

$$\mathcal{H} = \frac{2t^2}{U} \sum_{\langle i,j\rangle} P_{ij}$$

Permutations

Quantum permutations

- Objects with N flavours on a lattice
- Hilbert space = {$|\sigma_1\ \sigma_2\ \dots\ \sigma_L\ \rangle$}

  σ_i = 1,2, …,N or σ_i = A, B, C,… or ●, ●, ●…

$$\mathcal{H} = \sum_{\langle i,j \rangle} P_{ij}$$

$$P_{ij} |\sigma_1 \dots \sigma_i \dots \sigma_j \dots \sigma_N\rangle = |\sigma_1 \dots \sigma_j \dots \sigma_i \dots \sigma_N\rangle$$

SU(N) formulation

$$H = \sum_{\langle i,j \rangle} S_m^n(i) S_n^m(j)$$

$$S_m^n |\mu\rangle = \delta_{n,\mu} |m\rangle$$

$$[S_m^n, S_k^l] = \delta_{n,k} S_m^l - \delta_{m,l} S_k^n$$

S_m^n → generators of SU(N)

At each site: fundamental N-dimensional representation

Physical realizations

- N=2 → spin-1/2 Heisenberg $P_{ij} = 2\vec{S}_i \cdot \vec{S}_j + 1/2$
- N=3 → S=1 biquadratic $P_{ij} = \vec{S}_i \cdot \vec{S}_j + (\vec{S}_i \cdot \vec{S}_j)^2 - 1$
- N=4 → symmetric Kugel-Khomskii model

$$H = \sum_{ij} J_{ij}\left(2\vec{s}_i \cdot \vec{s}_j + \frac{1}{2}\right)\left(2\vec{\tau}_i \cdot \vec{\tau}_j + \frac{1}{2}\right)$$

- Any N → N-flavour fermions in optical lattices

General properties

- Soluble in 1D with Bethe Ansatz
  → algebraic correlations with periodicity 2π/N
  Sutherland, 1974

- Equivalent of SU(2) dimer singlet: N sites
  $$| S > = \frac{1}{\sqrt{N!}} \sum_P \mathrm{sgn}(P) \, | \sigma_{P(1)} \sigma_{P(2)} \dots \sigma_{P(N)} >$$
  with $\{\sigma_1 \sigma_2 \cdots \sigma_N\}$=$\{1\ 2\ \cdots \mathrm{N}\}$
  Li, Ma, Shi, Zhang, PRL'98

Hartree approximation

$$|\psi\rangle = \prod_i |\varphi_i\rangle$$

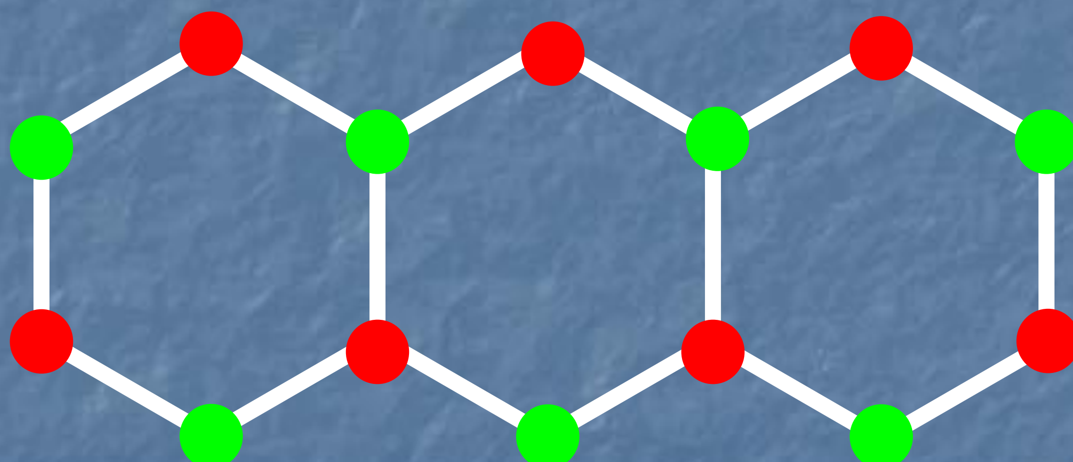
$$\langle \varphi_1 \varphi_2 | P_{12} | \varphi_1 \varphi_2 \rangle = \langle \varphi_1 \varphi_2 | \varphi_2 \varphi_1 \rangle = |\langle \varphi_1 | \varphi_2 \rangle|^2$$

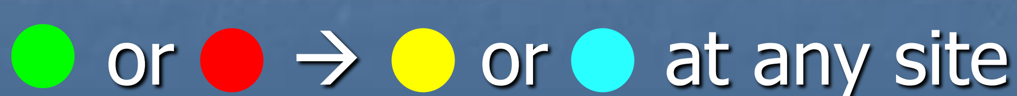
→ on 2 sites, energy minimal if $\langle \varphi_1 | \varphi_2 \rangle = 0$

→ on a lattice, Hartree energy certainly minimal if colors on nearest neighbors are different

SU(4) on honeycomb lattice

Bipartite lattice → infinite number of ‘Hartree’ ground states for more than 2 colors





Flavour-wave theory

- Schwinger bosons

$$\mathcal{P}_{ij} = \sum_{\mu,\nu\in\{A,B,C,D\}} a^{\dagger}_{\mu,i} a^{\dagger}_{\nu,j} a_{\nu,i} a_{\mu,j}$$

$$\sum_{\nu} a^{\dagger}_{\nu,i} a_{\nu,i} = 1$$

- Local condensation

$$a^{\dagger}_{\mu,i}, a_{\mu,i} \to \sqrt{1 - \sum_{\nu\neq\mu} a^{\dagger}_{\nu,i} \tilde{a}_{\nu,i}}$$

Harmonic theory

$$\mathcal{H} = \sum_{\substack{\alpha,\beta = A,B,C\ldots \\ \alpha \neq \beta}} \mathcal{H}_{\alpha\beta}$$

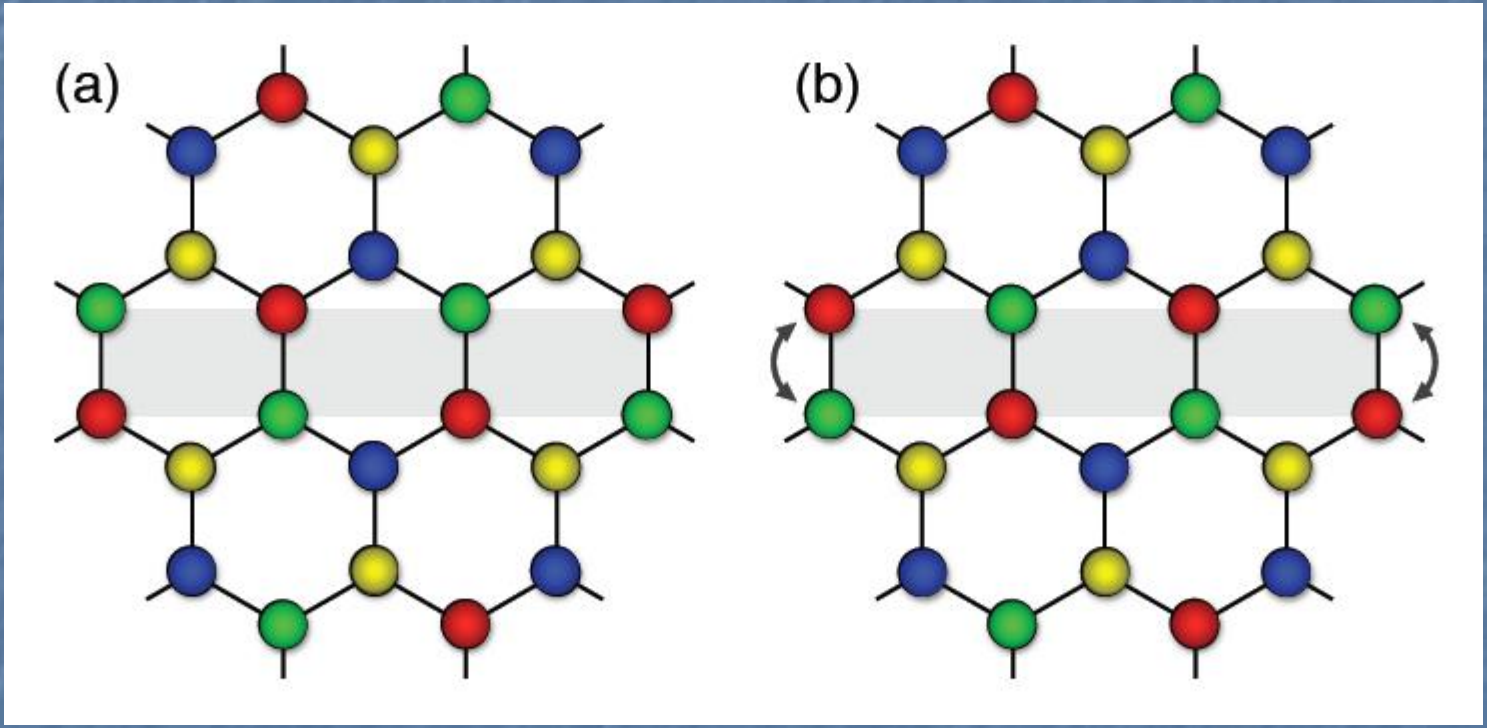
$$\mathcal{H}_{\alpha\beta} = \sum_{\substack{\text{disconnected} \\ \text{clusters } \mathcal{C}}} \sum_{\substack{\langle i,j\rangle \in \mathcal{C} \\ i \in \beta, j \in \alpha}} \mathcal{H}_{\alpha\beta}(i,j)$$

$$\mathcal{H}_{\alpha\beta}(i,j) = (\alpha_i^\dagger + \beta_j)(\alpha_i + \beta_j^\dagger) - 1$$

$$\langle(\alpha_i^\dagger + \beta_j)(\alpha_i + \beta_j^\dagger)\rangle \geq 0 \;\Rightarrow\; \langle \mathcal{H}_{\alpha\beta}(i,j)\rangle \geq -1$$

Lower bound saturated for two-site cluster

Harmonic ground states



Degeneracy still infinite!

iPEPS

- iPEPS = infinite Projected Entangled Pair States
- Variational method based on a tensor product wave-function
- Becomes exact if the dimension D of the tensors → ∞
- Can be seen as a generalization of DMRG

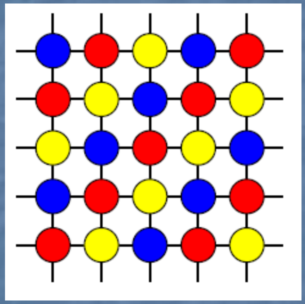
Verstraete and Cirac, 2004

iPEPS and symmetry breaking

- SU(3) on square lattice: stripe color order

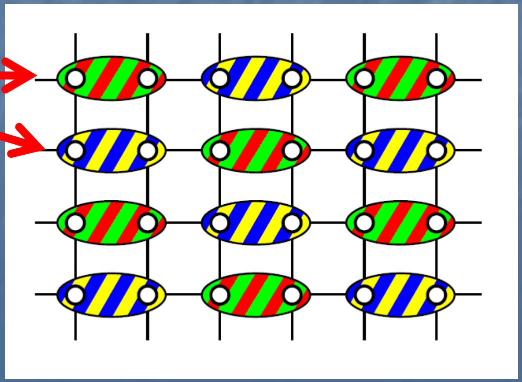
Toth, Läuchli, FM, Penc, PRL 2010

Bauer et al, PRB 2011



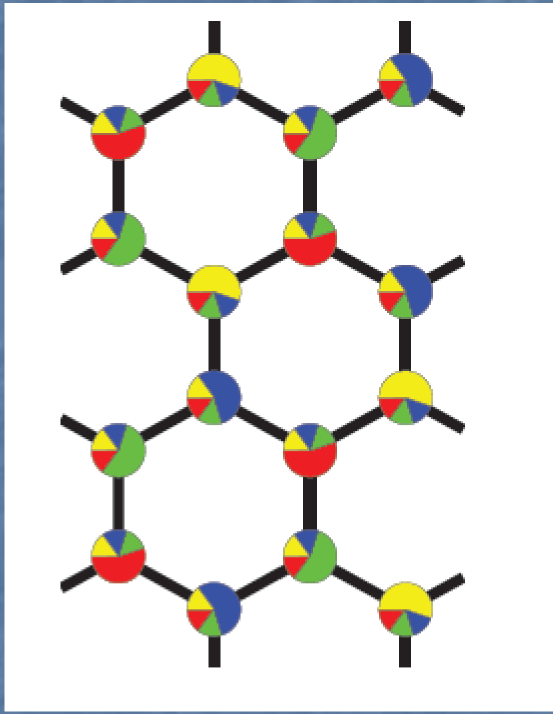
- SU(4) on square lattice: dimerization

IRREP dim=6



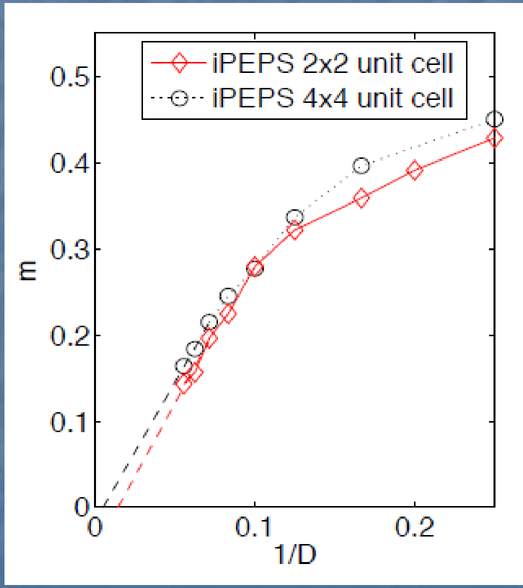
Corboz, Läuchli, Penc,
Troyer, FM, PRL 2011

iPEPS for SU(4) on honeycomb

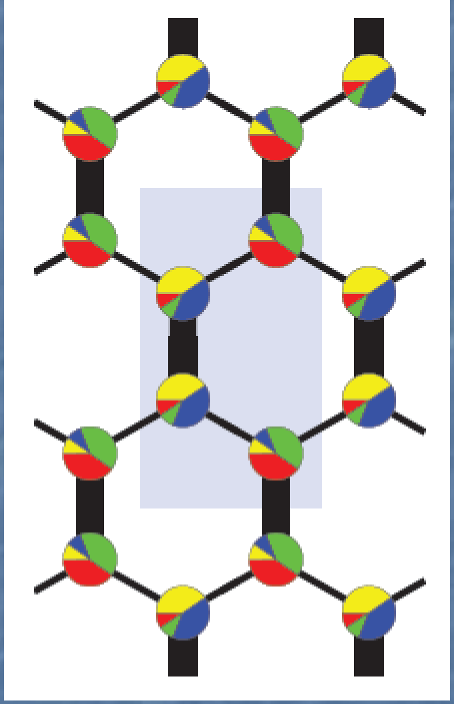


4x4 unit cell

- All bond energies equal
- No color order

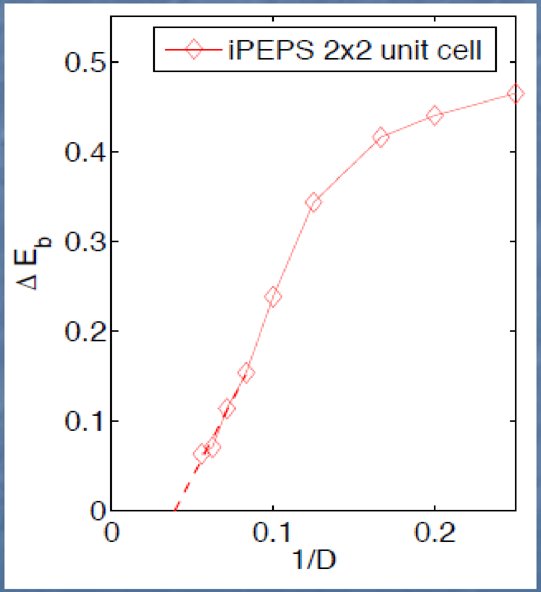


Absence of dimerization



2x2 unit cell

Difference between bond energies



SU(N) quantum liquids

- RVB? Not very likely (no closed 4-site plaquettes)
- Chiral liquid (N large, N/k atoms per site, k≥5)

  Hermele, Gurarie, Rey, PRL 2009
- Algebraic liquid for SU(4) on square lattice

  Wang and Vishwanath, PRB 2009

  → Majorana fermion representation

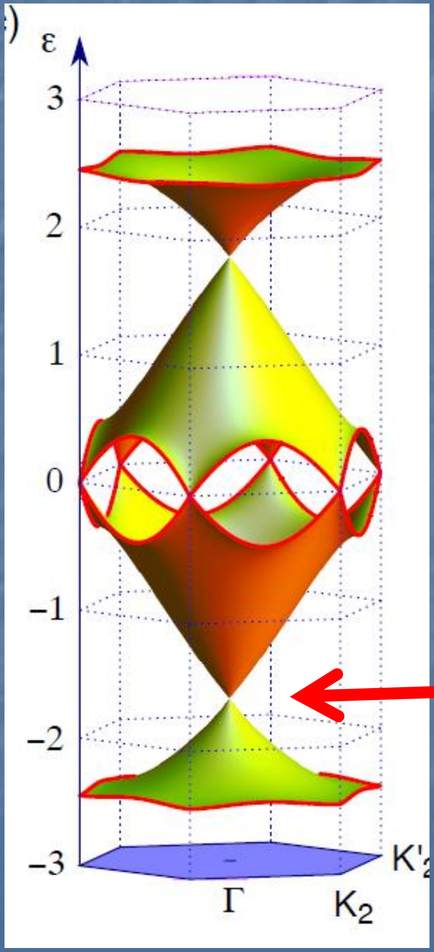
  → Half-filled band

  → Dirac spectrum for π -flux state

Fermionic approach for SU(4) on honeycomb

- Schwinger fermions
  → quarter filling
  → No flux: Fermi surface
  → π-flux: Dirac spectrum
- Majorana fermions
  → as for square lattice

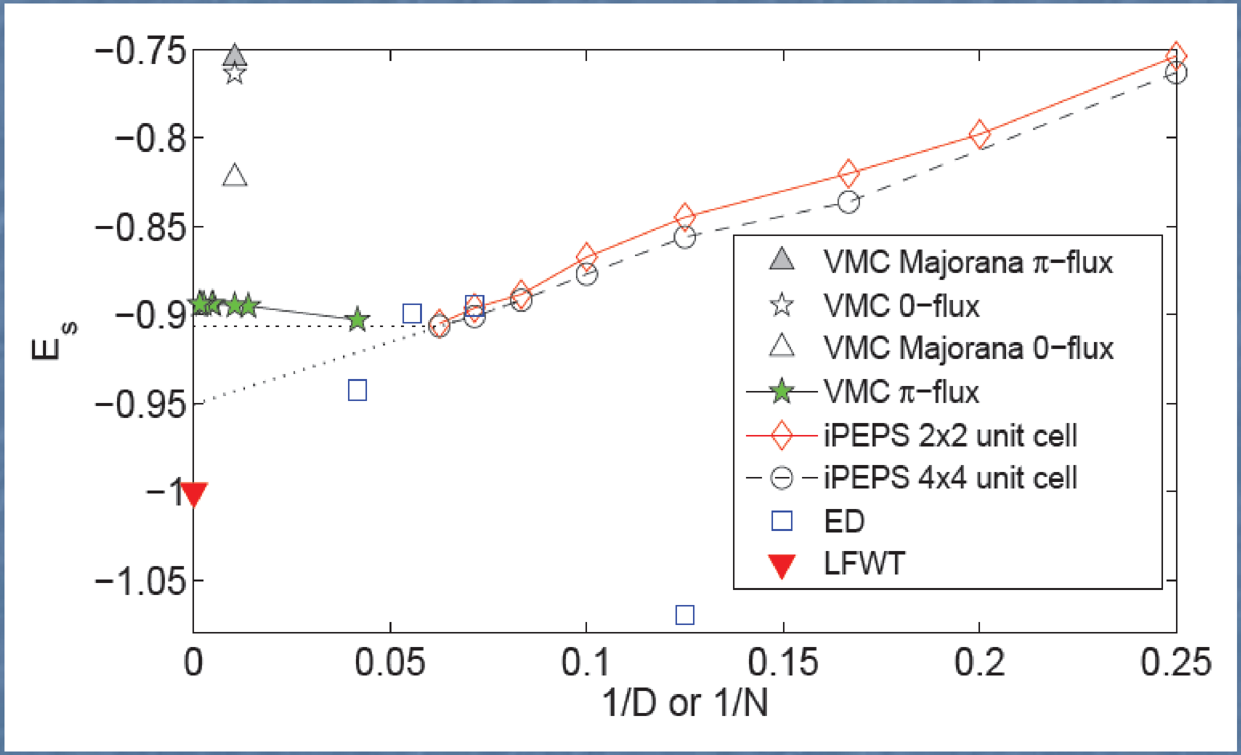
π-flux with Schwinger fermions



- π-flux per hexagonal plaquette
- $\Downarrow$

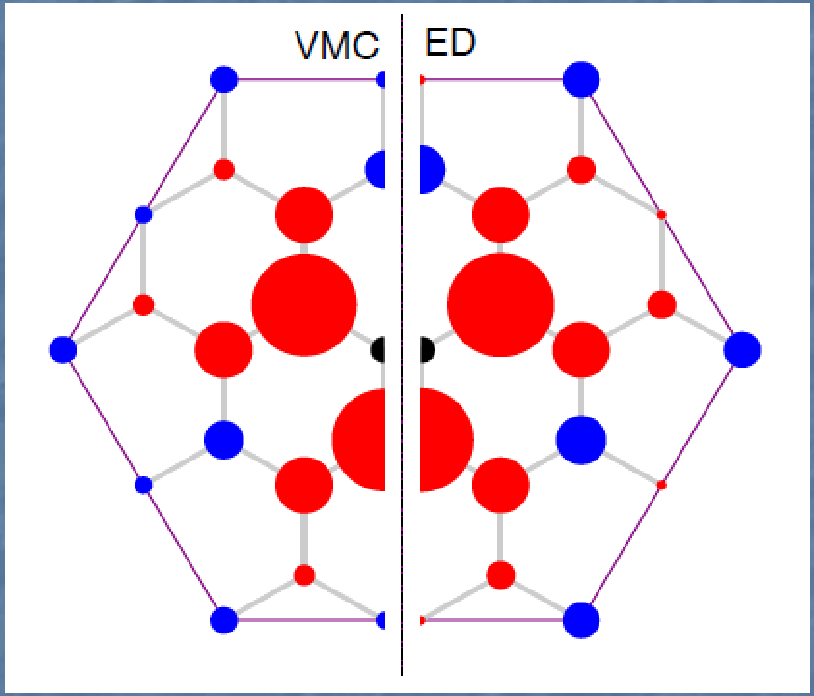
Dirac point at quarter filling

Ground-state energy



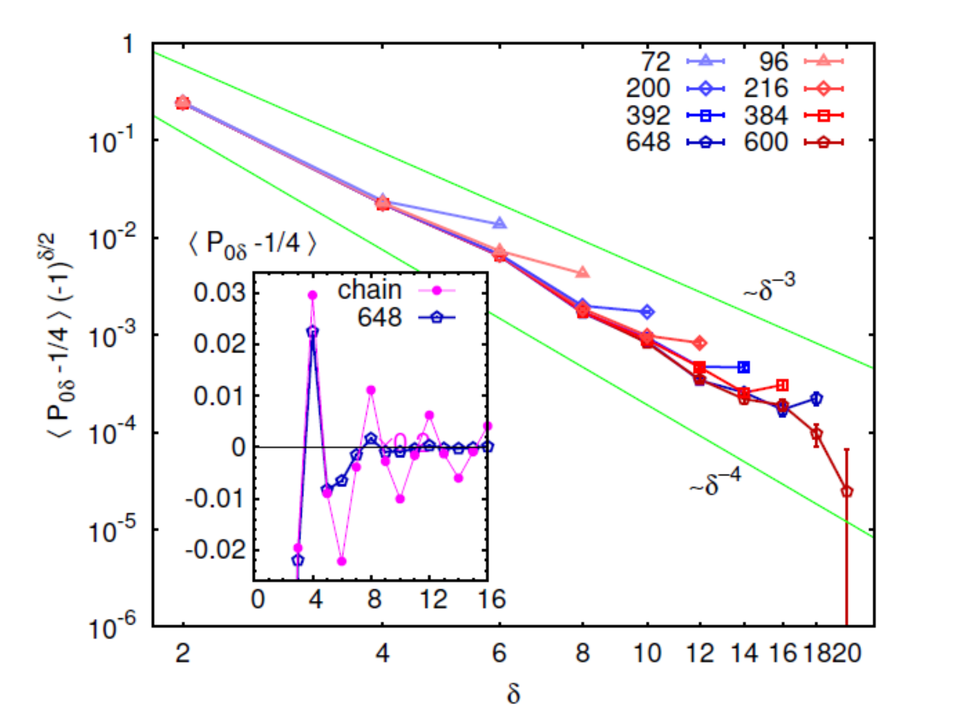
➔ Gutzwiller projected Schwinger fermion π-flux

Comparison ED / π -flux



Short-range color-color correlations: very good

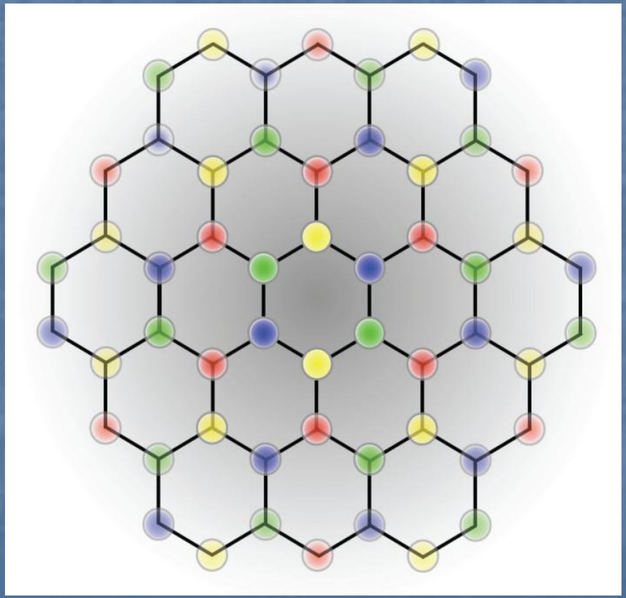
Long-distance correlations



$\langle P_{ij} - 1/4 \rangle \sim |\mathbf{r}_{ij}|^{-\alpha}$, with an exponent α between 3 and 4.

Discussion

- SU(4) in 1D: algebraic correlations with slow decay (exponent 3/2)
- Coupling between chains
  → no LRO
  → faster decay of correlations



Conclusion

- Symmetric Kugel-Khomskii on honeycomb lattice

  → no lattice symmetry breaking

  → no spin or orbital long-range order

  → evidence in favour of an algebraic liquid
- Related to $Ba_3CuSb_2O_9$?