Spin-orbital quantum liquid on the honeycomb lattice

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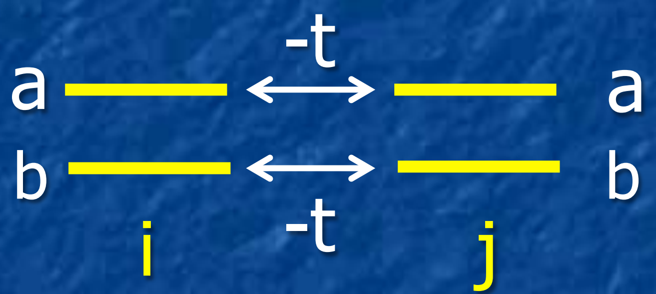
Scope

- 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

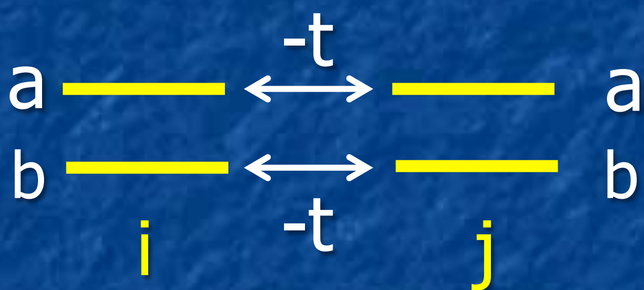
spin

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 = {| $\sigma_1\ \sigma_2 \ldots \sigma_L$ >}

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

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

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

SU(N) formulation

$$H = \sum_{\langle i,j \rangle} S^n_m(i) S^m_n(j)$$

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

$$[S^n_m, S^l_k] = \delta_{n,k} S^l_m - \delta_{m,l} S^n_k$$

S^n_m → 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

$$| S > = (1/\sqrt{N!}) \sum_P (-1)^P | \sigma_{P(1)} \sigma_{P(2)} \ldots \sigma_{P(N)} >$$

with $\{\sigma_1 \ \sigma_2 \ldots \sigma_N\} = \{1 \ 2 \ldots N\}$

Li, Ma, Shi, Zhang, PRL'98

Hartree approximation

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

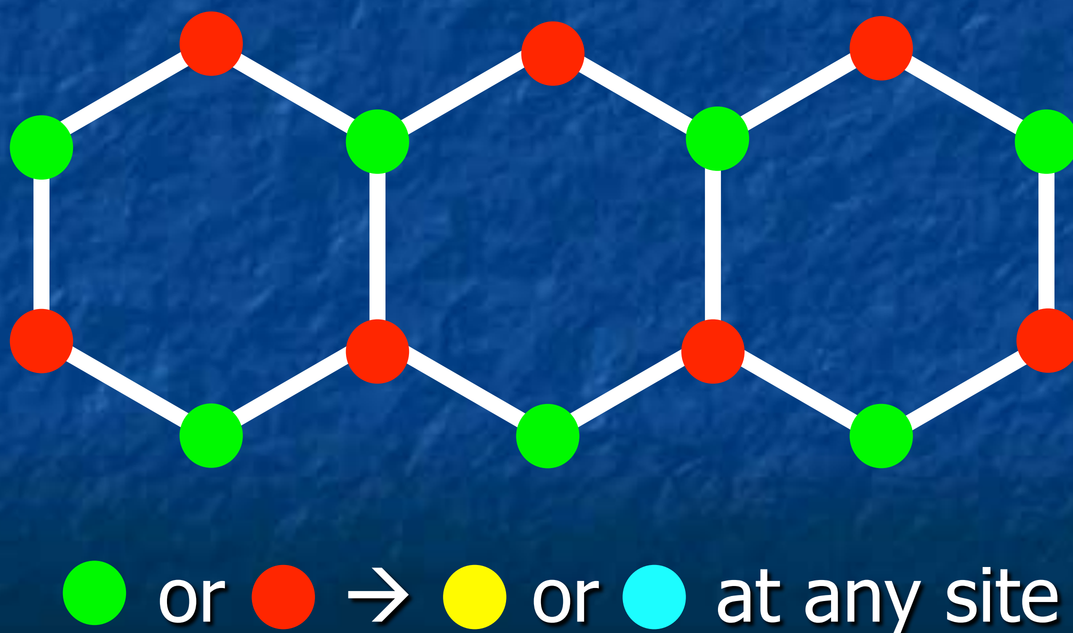
$$\langle\varphi_1\varphi_2|P_{12}|\varphi_1\varphi_2\rangle = \langle\varphi_1\varphi_2|\varphi_2\varphi_1\rangle = |\langle\varphi_1|\varphi_2\rangle|^2$$

→ 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

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

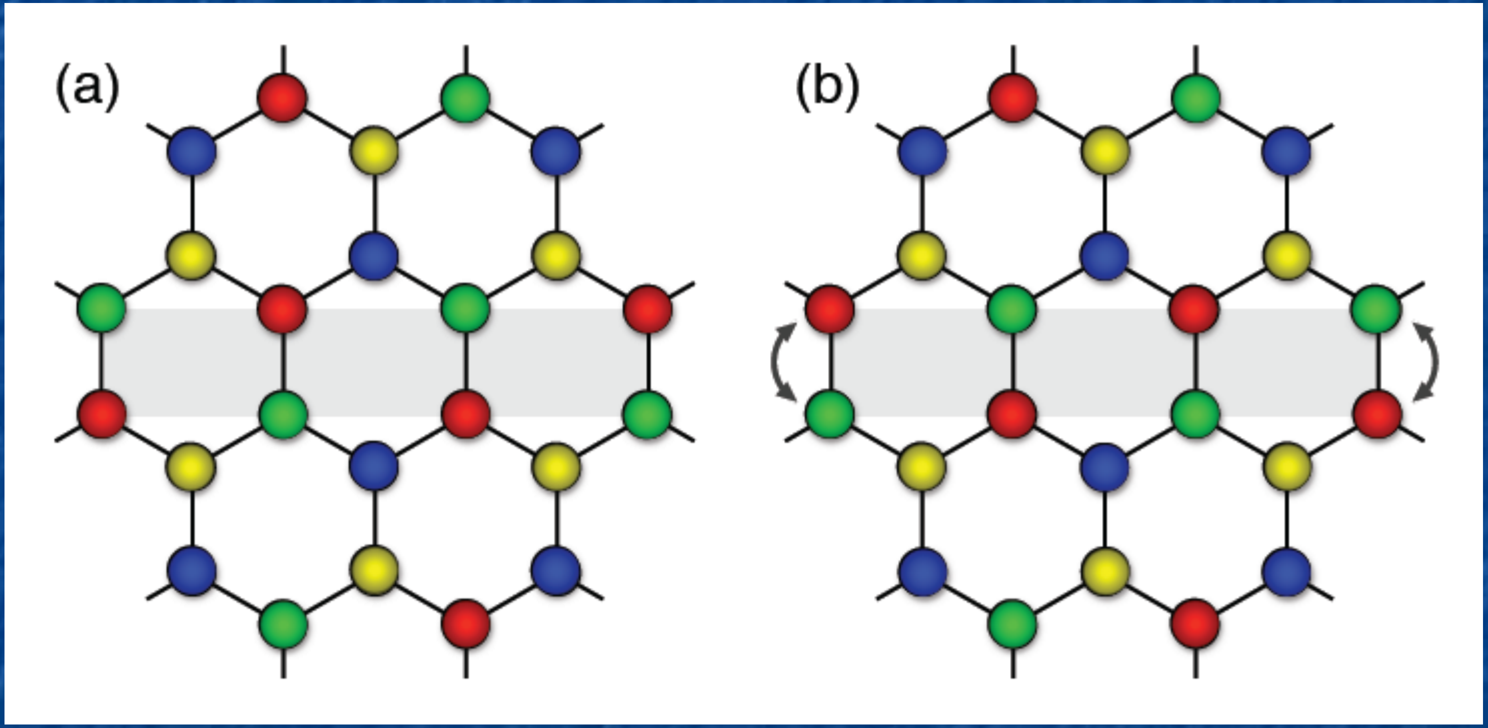
$$\mathcal{H}_{\alpha\beta} = \sum_{\substack{\text{disconnected} \\ \text{clusters } \mathcal{C}}} \sum_{\substack{\langle i,j \rangle \in \mathcal{C} \\ i \in \beta, j \in \alpha}} \mathcal{H}_{\alpha\beta}(i,j)$$

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

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

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

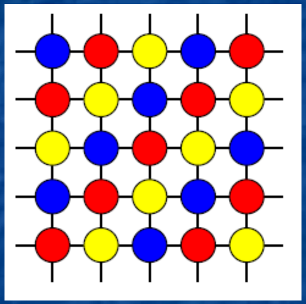
Verstraete and Cirac, 2004

iPEPS and symmetry breaking

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

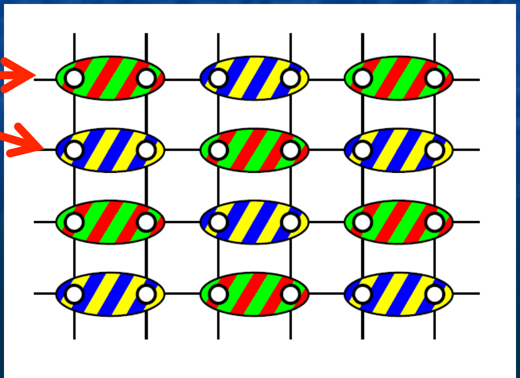
Toth, Läuchli, FM, Penc, PRL 2010

Bauer et al, PRB 2011



- SU(4) on square lattice: dimerization

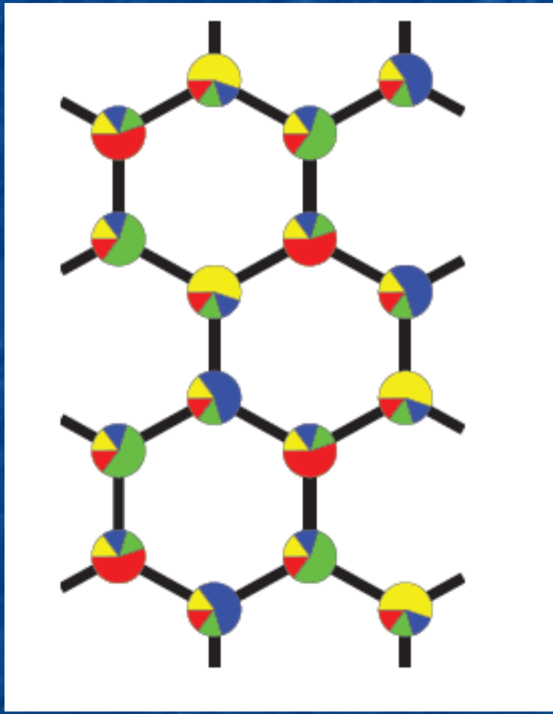
IRREP dim=6



Corboz, Läuchli, Penc,

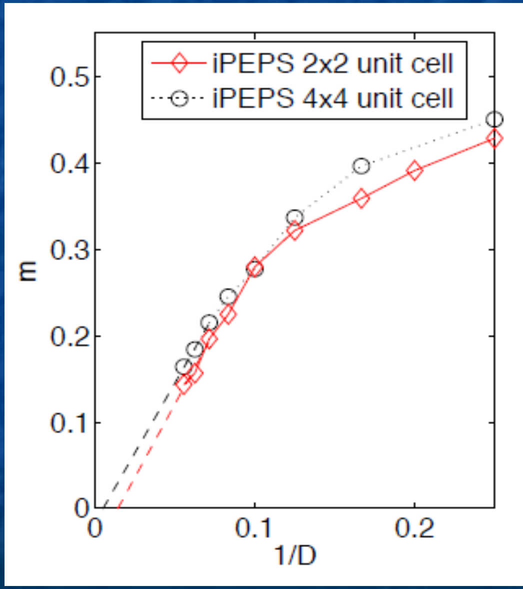
Troyer, FM, PRL 2011

iPEPS for SU(4) on honeycomb

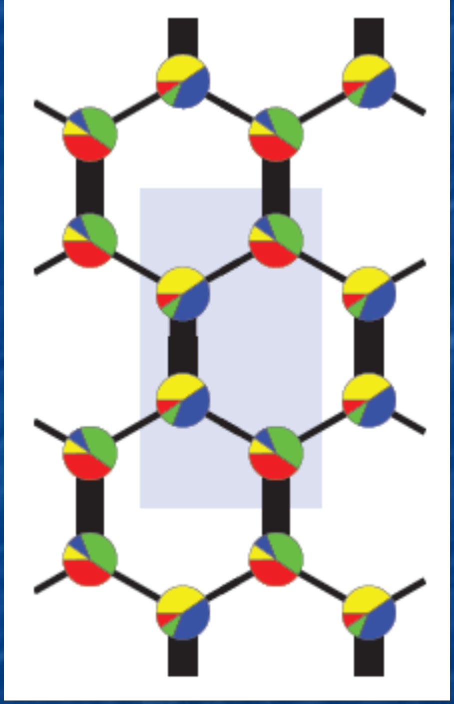


4x4 unit cell

- All bond energies equal
- No color order

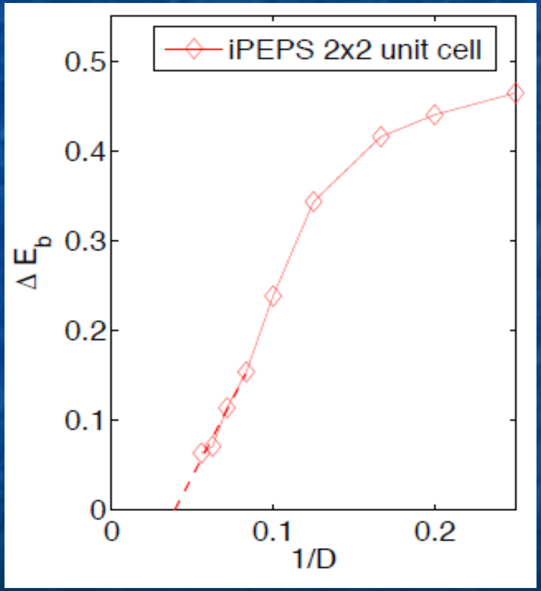


Absence of dimerization



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

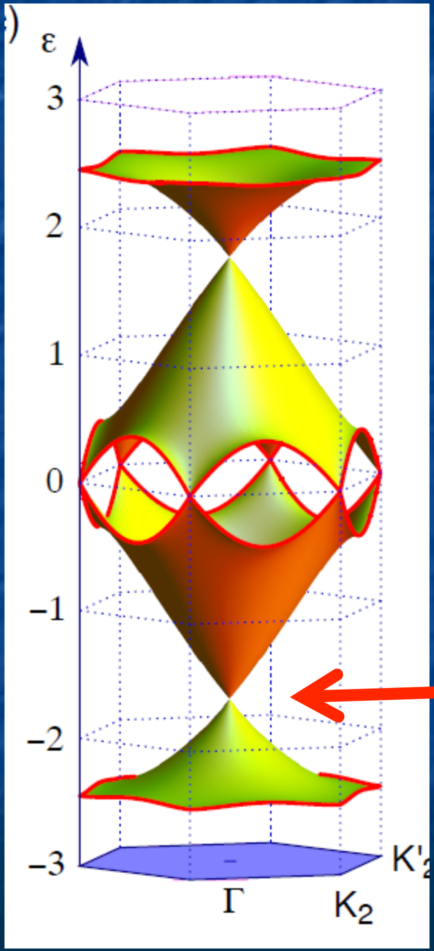
  → Half-filled band

  → 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

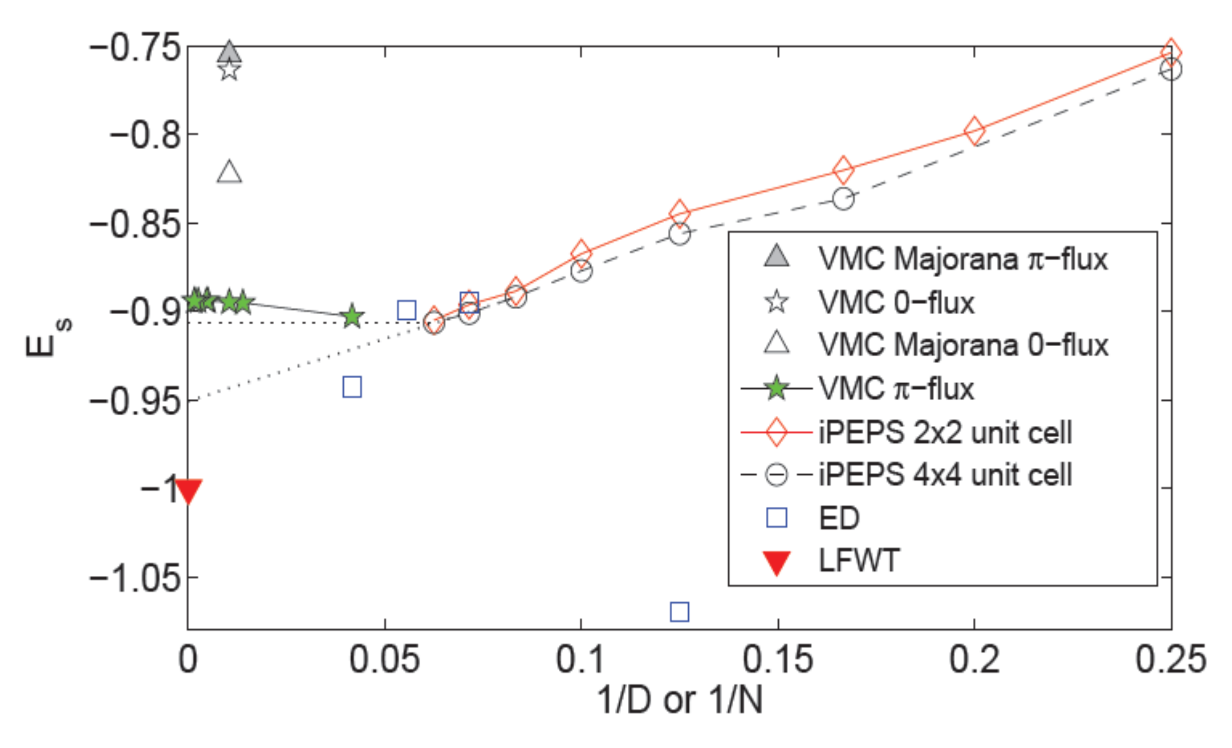


π-flux per hexagonal plaquette

$\Downarrow$

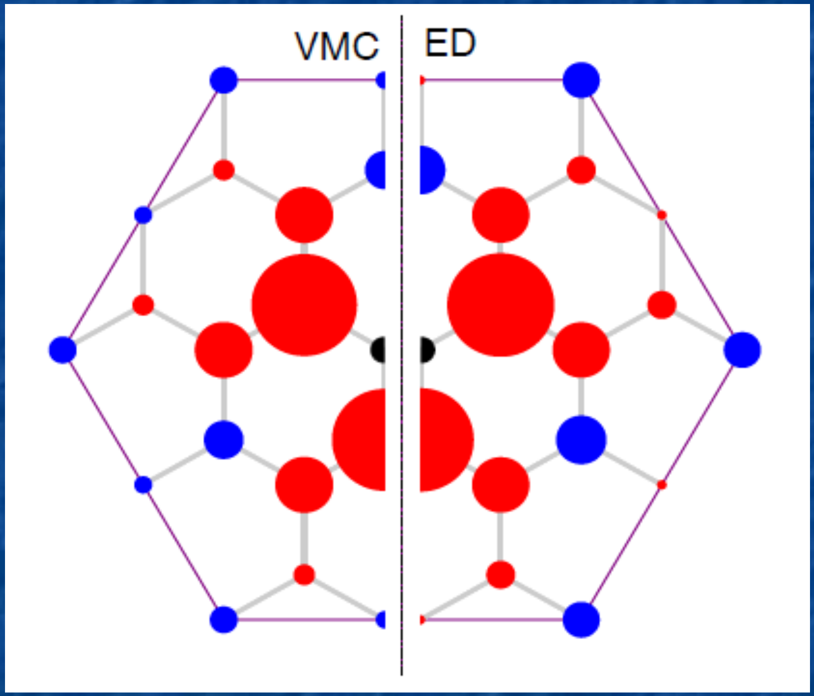
Dirac point at quarter filling

Ground-state energy



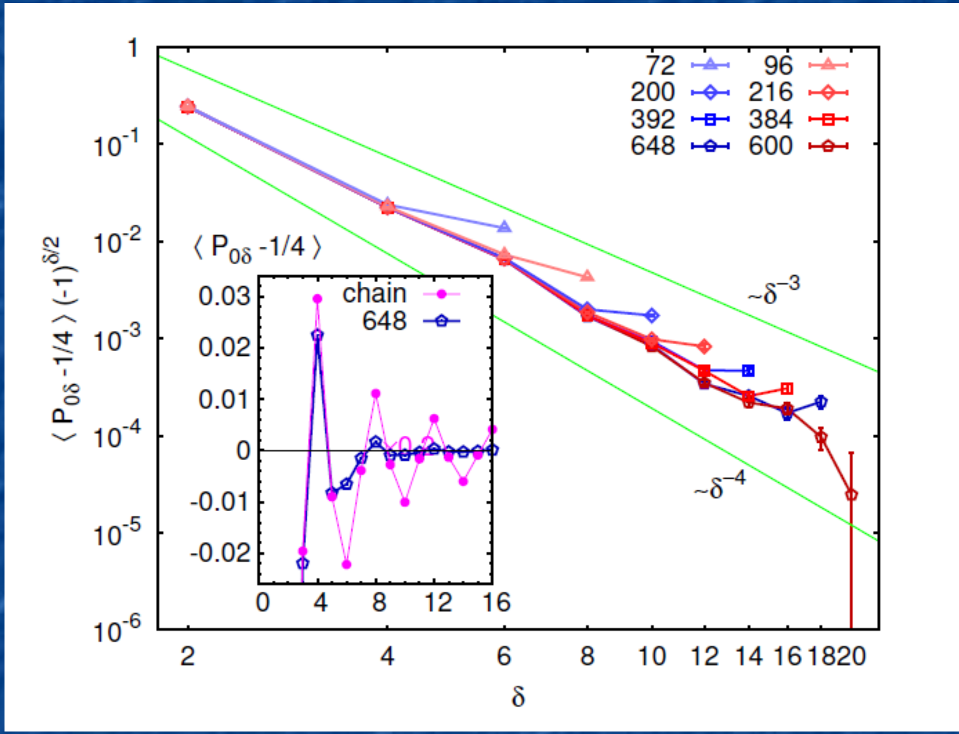
→ Gutzwiller projected Schwinger fermion π-flux

Comparison ED / π-flux



Short-range color-color correlations: very good

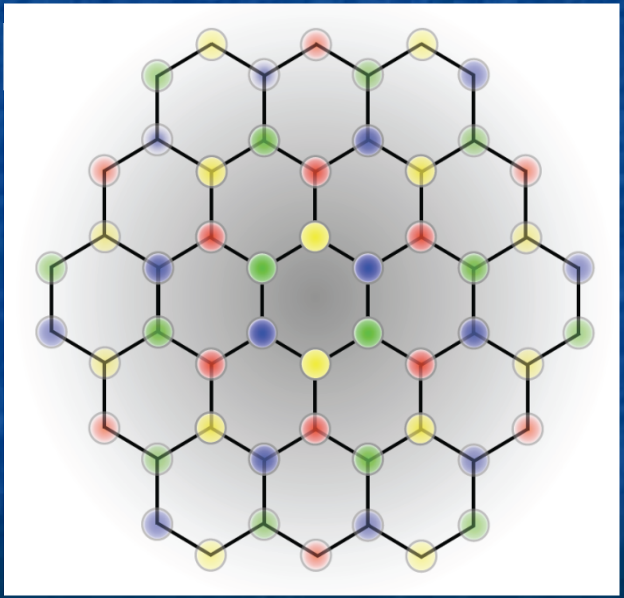
Long-distance correlations



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

Discussion

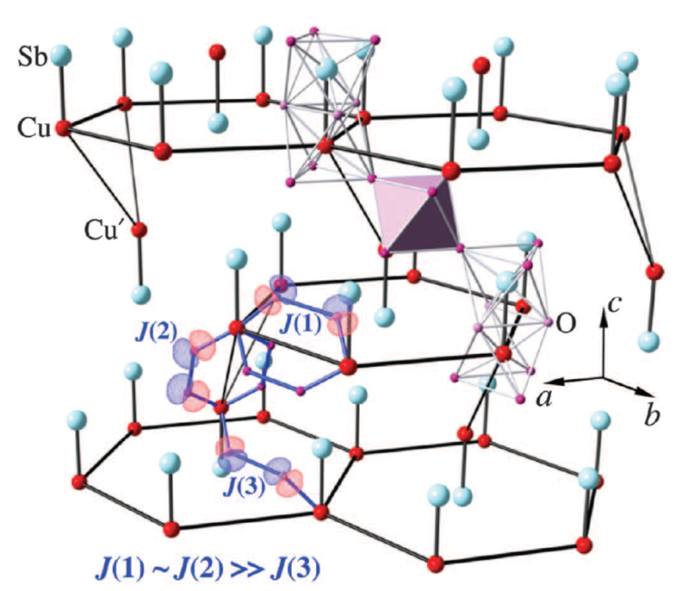
- SU(4) in 1D: algebraic correlations with slow decay (exponent 3/2)
- Coupling between chains
  → no LRO
  → faster decay of correlations



Experimental realization?

- $Ba_3CuSb_2O_9$:
  → hexagonal lattice of Cu^{2+} with orbital degeneracy
  → neither magnetic nor orbital order

  S. Nakatsuji et al, Science 2012



- Problems:
  → additional magnetic sites
  → unknown but probably disordered distribution

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 $Ba_3CuSb_2O_9$?