Kinetic Energy Frustration as a New Paradigm for Correlated Metals

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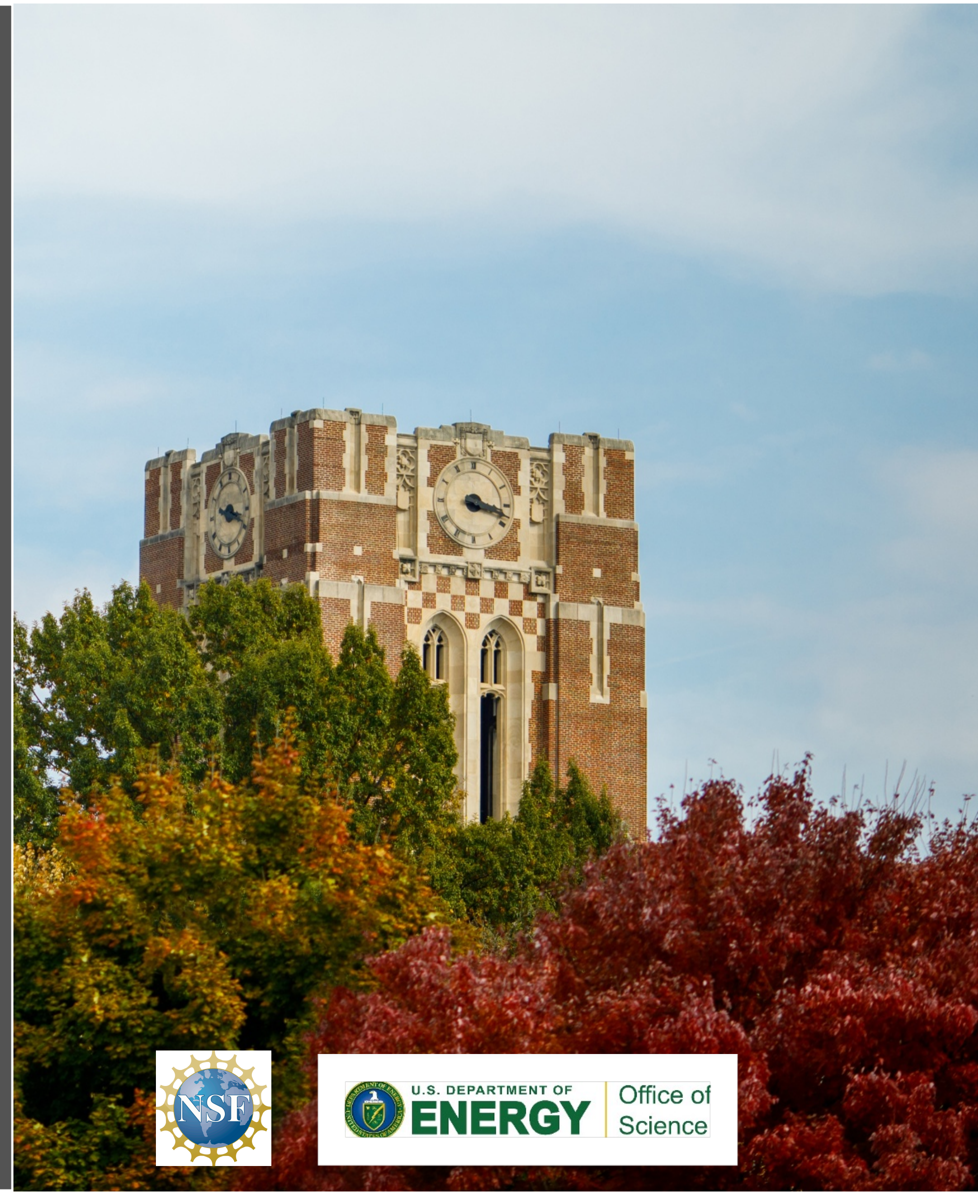
Quantum Spin Liquids 2025



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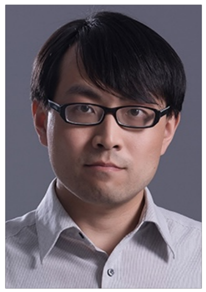
Shang-shun Zhang



Wei Zhu

Cecilie Glittum

Claudio Castelnovo

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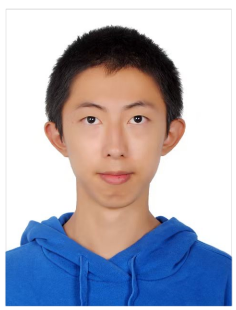
Yang Zhang



Yixin Zhang

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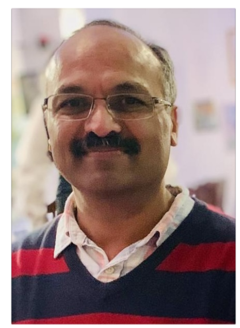

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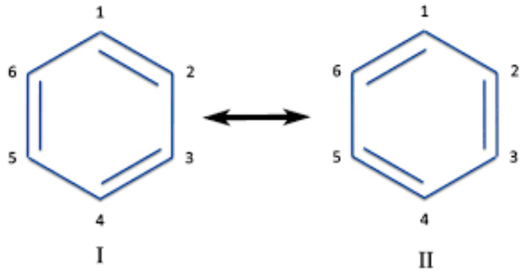
UNITED KINGDOM

S-S Zhang, Wei Zhu and CDB, Phys. Rev. B **97**, 140507(R) (2018)

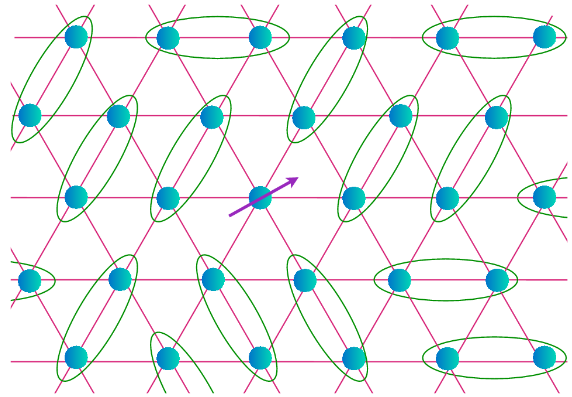
Cecilie Glittum et al, Nature Physics 2025, https://doi.org/10.1038/s41567-025-02923-8

RVB wave function

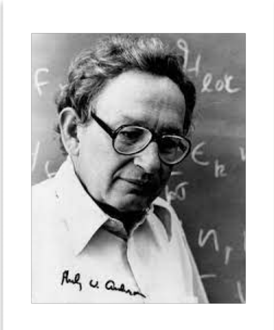
Linus Pauling
(1901-1994)



RVB in Benzene



(spinons : S = 1/2)



P. W. Anderson
(1923-2020)

P. Fazekas
(1945-2007)

Proposal: Frustration of AFM exchange favors a spin liquid state

P.W. Anderson, Mater. Res. Bull. **8,** 153 (1973)

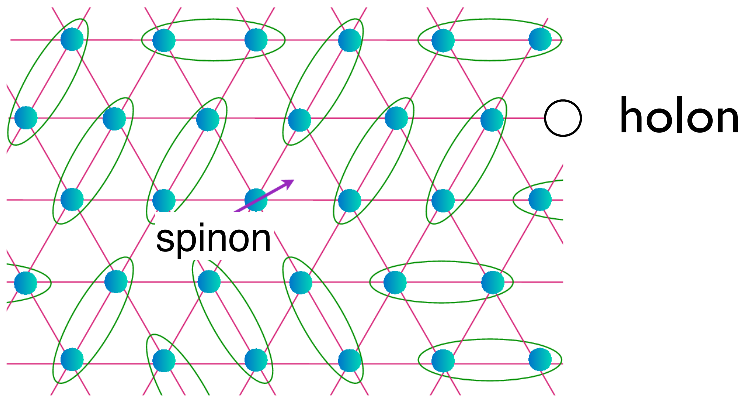
P. Fazekas and P.W. Anderson, Phil. Mag. **30**, 423 (1974)

Doped Mott Insulator

Spin-Charge Separation

Superconductivity?

RVB as Gutzwiller projection of BCS state



P.W. Anderson, Science **235,** 1196 (1987)

Baskaran, Zou and Anderson, Solid State Comm. 63 973(1987)

Kivelson, Roksar, Sethna PRB 35, 8865 (1988)

RVB Spin Liquids

Decades of searches, yet scarce evidence of RVB behavior in realistic Mott insulator Hamiltonians ...

Guiding principle: interactions + geometric frustration

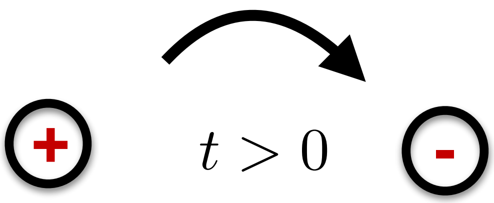
- **Quantum Dimer Models** Kivelson, Roksar, Sethna 1988-1989 **topological structure becomes transparent**
- **Short-range RVB liquid in QMD on triangular lattice** Moessner and Sondhi 2001
- **Vertex Models (e.g. spin ice)** Book by Udagawa and Jaubert 2021
- **Klein Related Models** CDB and Trugman 2004 Normand & Nussinov 2014-16

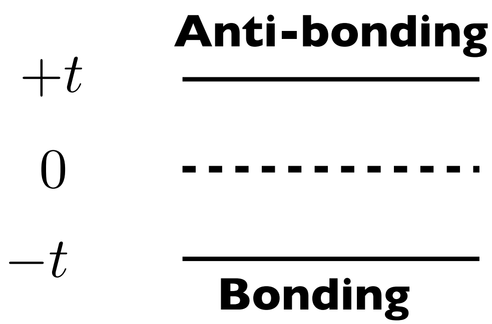
P.W. Anderson, Science **235,** 1196 (1987)

Kinetic energy frustration and superconductivity

Kinetic energy frustration

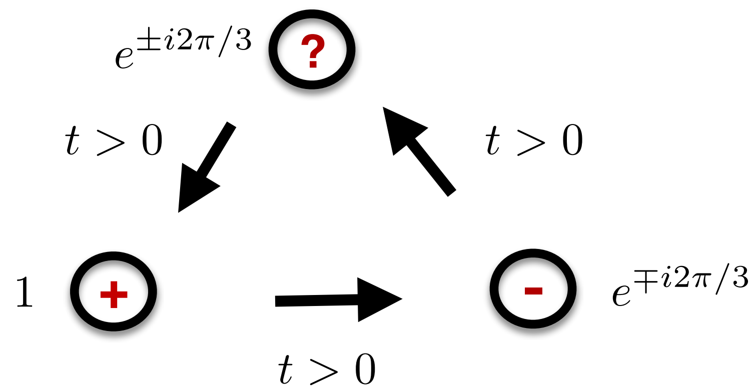
Diatomic molecule

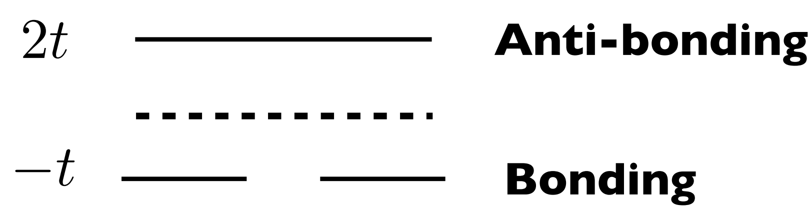




$$E_g = -|t|$$

Triatomic molecule





$$E_g = \begin{cases} -|t| & \text{for } t > 0 \\ -2|t| & \text{for } t < 0 \end{cases}$$

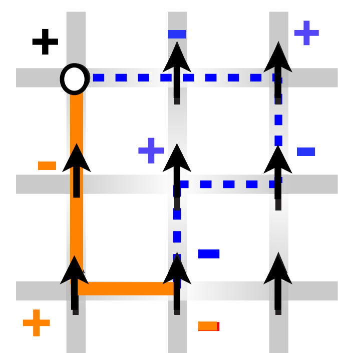
Frustration!

Nagaoka's Theorem

$$\mathscr{H} = -\sum_{\langle ij\rangle\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i n_i \quad \xrightarrow{\text{Large U/t}} \quad \hat{\mathscr{H}} = -t \sum_{\langle i,j\rangle\sigma} \left[\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + h.c. \right] + J \sum_{\langle i,j\rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j$$

d>1 bipartite lattice: FM ground state for infinite U Hubbard model when one hole added to the half-filled state.

Constructive interference



$$\min\left(E_{\mathbf{k}}\right) = -z\,|\,t\,| = -4\,|\,t\,|$$

D. J. Thouless, Proc. Phys. Soc. London **86**, 893 (1965).

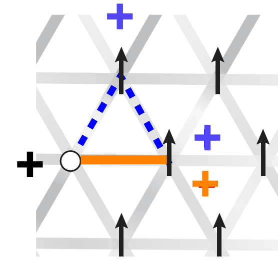
Y. Nagaoka, Phys. Rev. **147**, 392 (1966).

Single-hole on Triangular Hubbard Mott Insulator

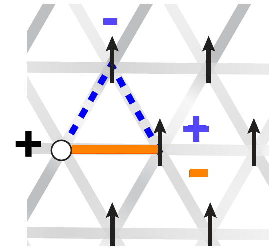
$$U \to \infty$$

FM background

$$\min\left(\epsilon_k\right) = \begin{cases} -6\left|t_1\right|, & t_1 < 0 \\ -3\left|t_1\right|, & t_1 > 0 \end{cases}$$

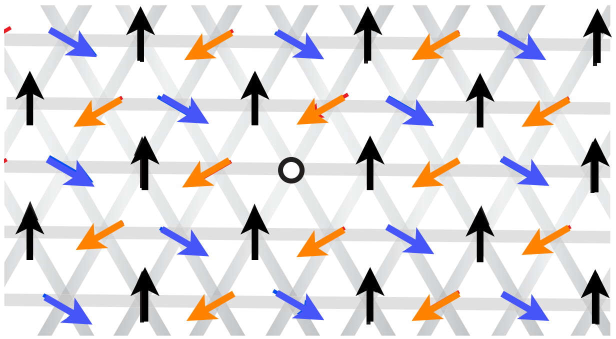


Nagaoka's Theorem
$t_1 < 0$



Destructive Interference!
$t_1 > 0$

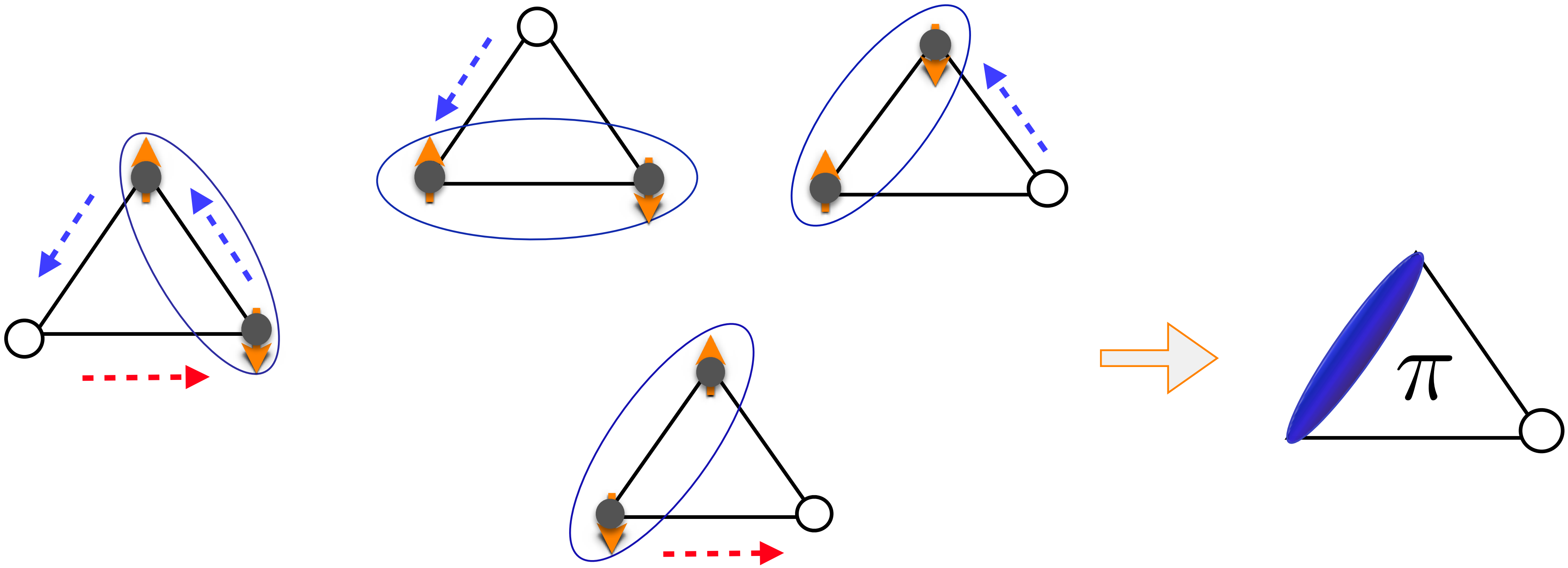
Solution: 120°
AFM ordering!



Frustrated Kinetic Energy favors AFM!

J. O. Haerter and B. S. Shastry, Phys. Rev. Lett. **95**, 087202 (2005)

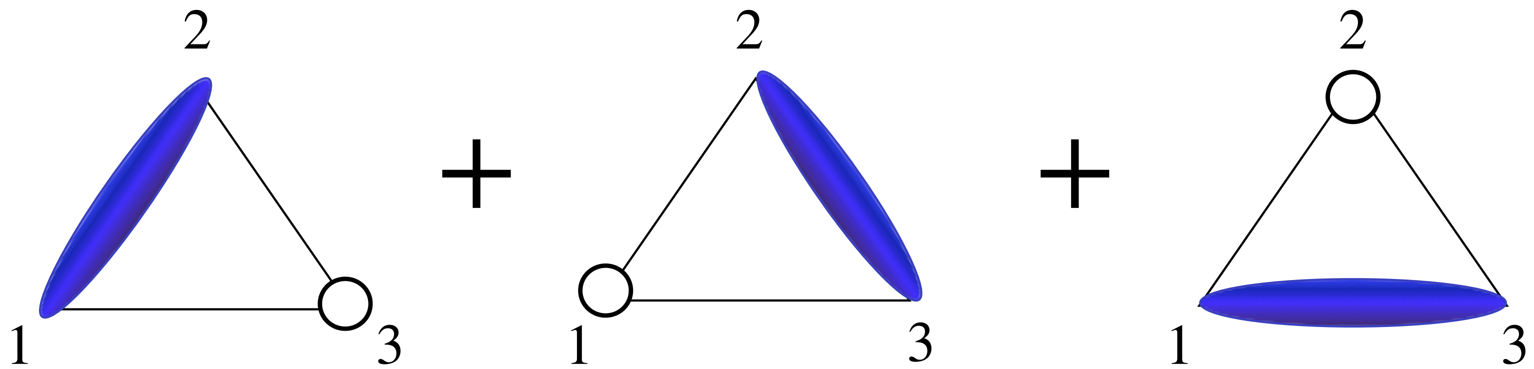
Single Triangle



The presence of the singlet turns the destructive interference for $t > 0$ into constructive interference!

The singlet inserts a π-flux

Ground State of Single Triangle



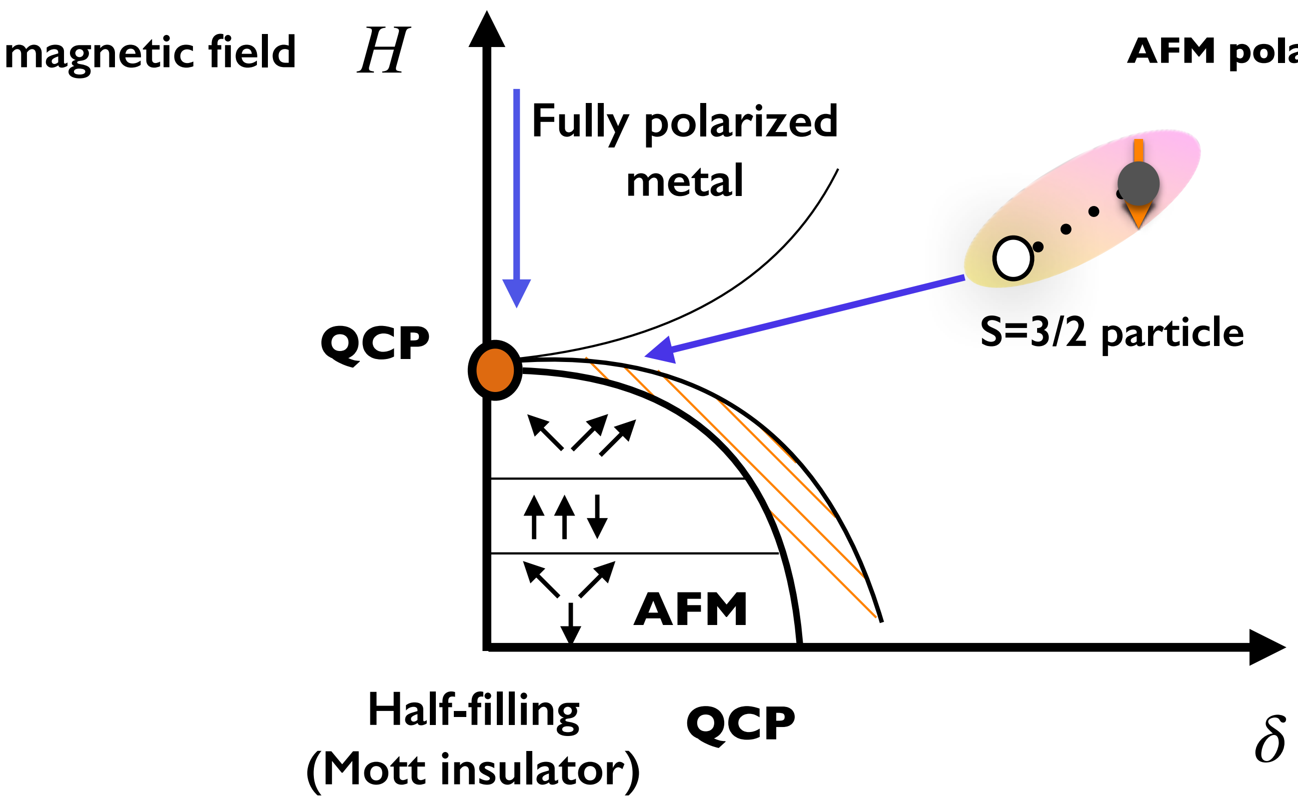
$$\Psi_0 = \frac{1}{\sqrt{3}}(\hat{d}^\dagger_{12} + \hat{d}^\dagger_{23} + \hat{d}^\dagger_{31})\,|0\rangle$$

$$E_g = -2\,|t|$$

$$\hat{d}^\dagger_{ij} = \frac{1}{\sqrt{2}}(\hat{c}^\dagger_{i\uparrow}\hat{c}^\dagger_{j\downarrow} - \hat{c}^\dagger_{i\downarrow}\hat{c}^\dagger_{j\uparrow})$$

The singlet inserts a π-flux

Hole-magnon Bound State

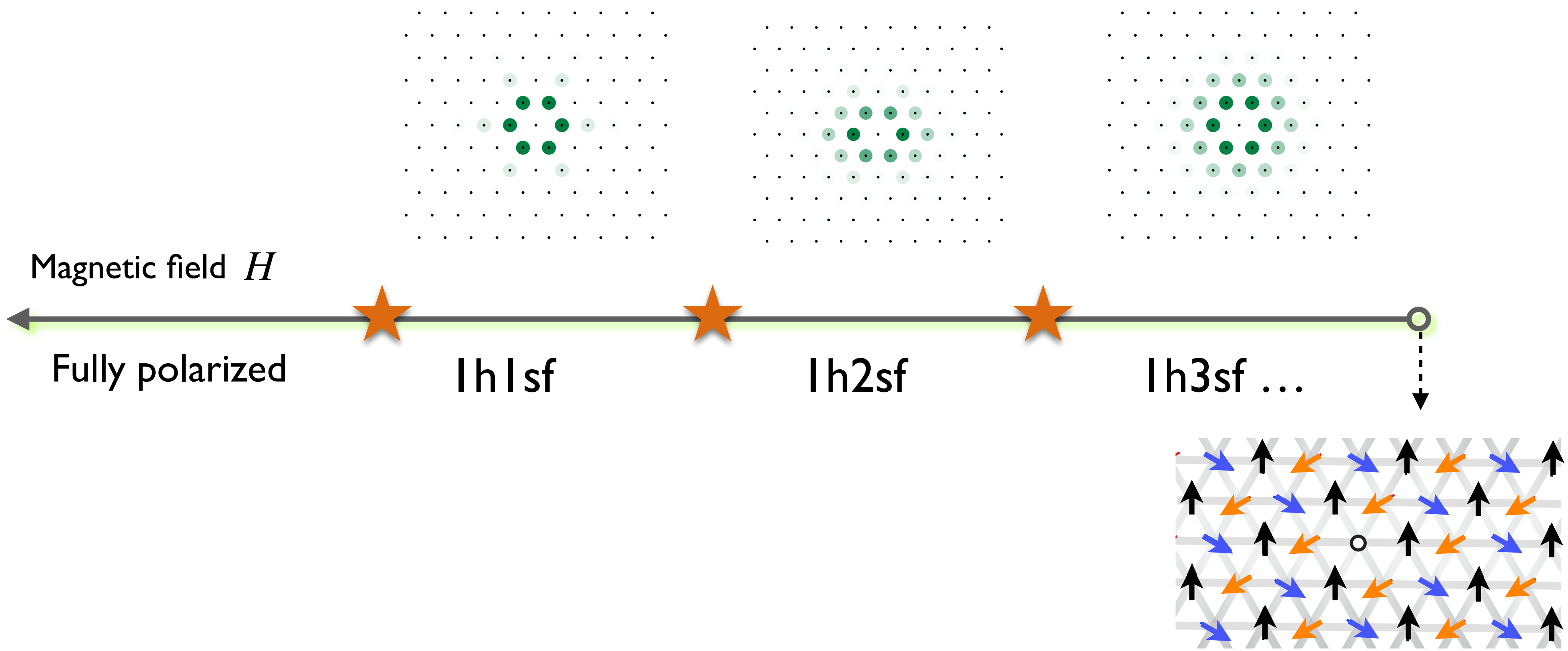


$$H < H_{\text{sat}} = \Delta_b^{h-m}$$

$$U \to \infty : \Delta_b^{h-m} \simeq |t|/2$$

S-S Zhang, Wei Zhu and CDB, Phys. Rev. B **97**, 140507(R) (2018)

Hole-magnon Bound States



S-S Zhang, Wei Zhu and CDB, Phys. Rev. B **97**, 140507(R) (2018)

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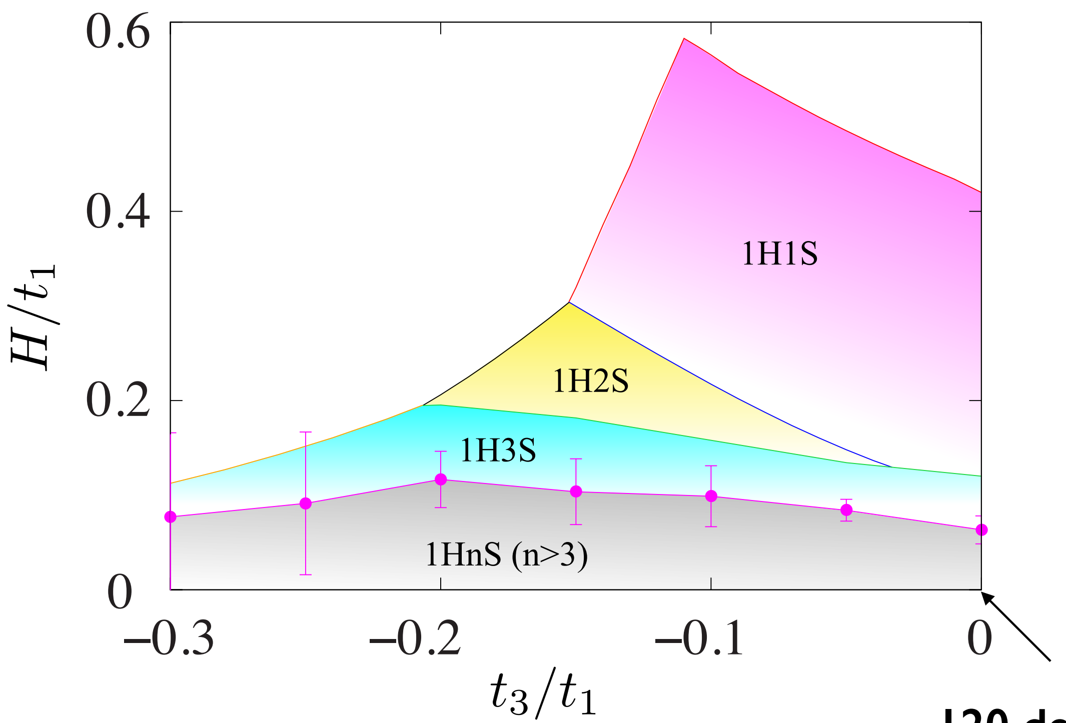
Phase Diagram of single hole



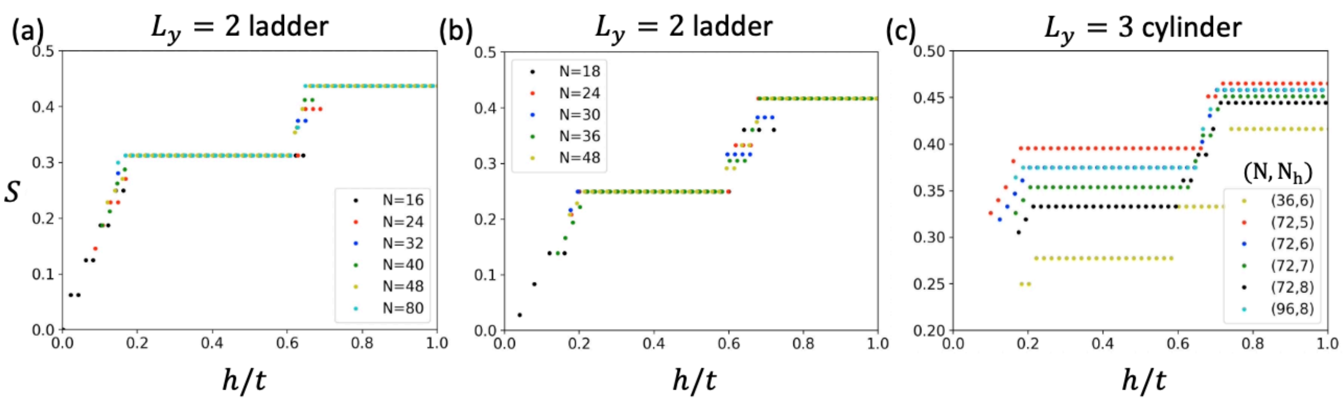
120 degree ordering

J. O. Haerter and B. S. Shastry, Phys. Rev. Lett. **95**, 087202 (2005)

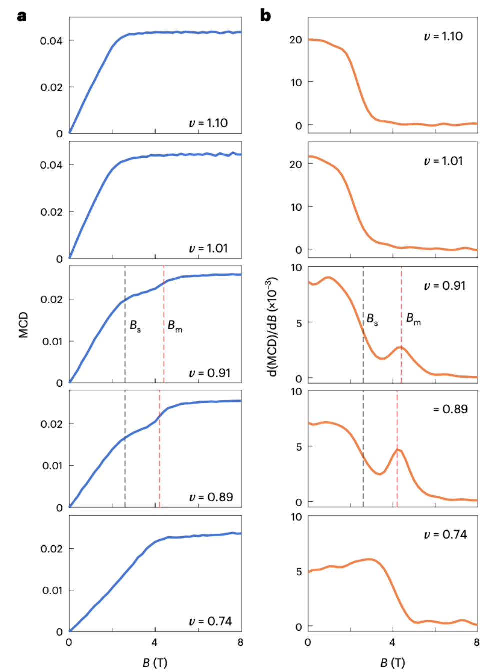
Experimental Confirmation of AFM Polarons in TMD moire Superlattices

MoTe$_2$/WSe$_2$ moiré bilayers

$\delta = 1/8$ $\delta = 1/6$

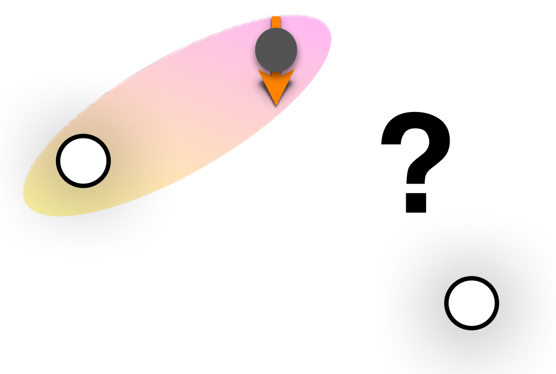


$$S_p = N(1 - 3\delta)/2$$

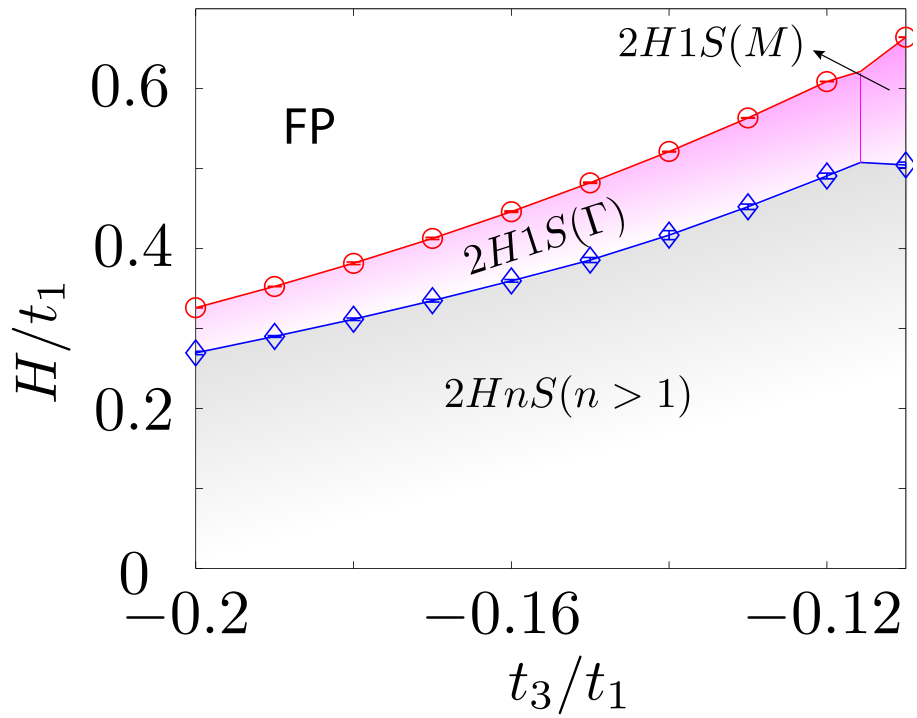


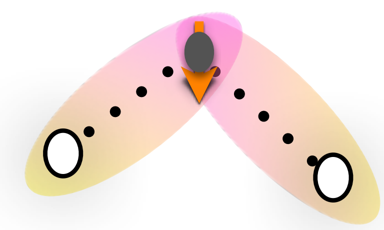
“Observation of spin polarons in a frustrated moiré Hubbard system”

Binding of a secondary hole?



Phase diagram of two holes





AFM polaron
($t_3, t_2 \neq 0$)

"Magnonic superconductivity"

S-S Zhang, Wei Zhu and CDB, Phys. Rev. B **97**, 140507(R) (2018)

K. Nazaryan & Liang Fu, Science Adv. **10,** eadp5681 (2024)

Repulsive interaction between bipolarons

Order Parameter $\Delta = \langle h_i^\dagger h_j^\dagger S_k^- \rangle$

B_2 irrep of D_6 space group f-wave

U(1) symmetry in charge or spin sector is broken individually, but has a combined U(1) symmetry

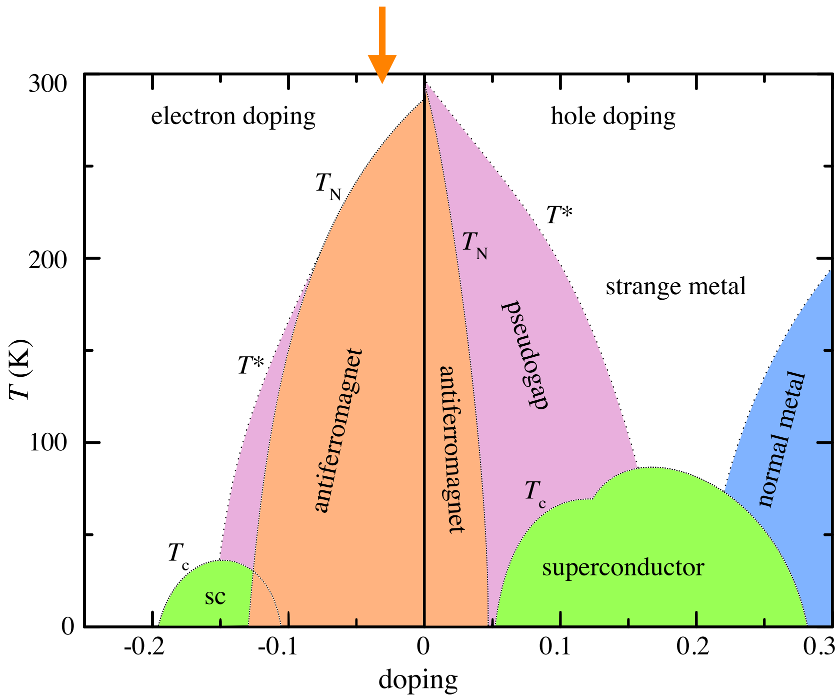
$$h_i^\dagger \to h_i^\dagger e^{-i\phi}, S_i^- \to S_i^- e^{2i\phi},$$

- No AFM magnetic order (AFM correlation length ~ coherence length).
- Ground state carries both charge and spin supercurrent.

AFM and pairing induced by Kinetic Frustration on Square Lattice

Infinite U limit of $t_1 - t_2$ Hubbard model

Frustrated Kinetic Energy



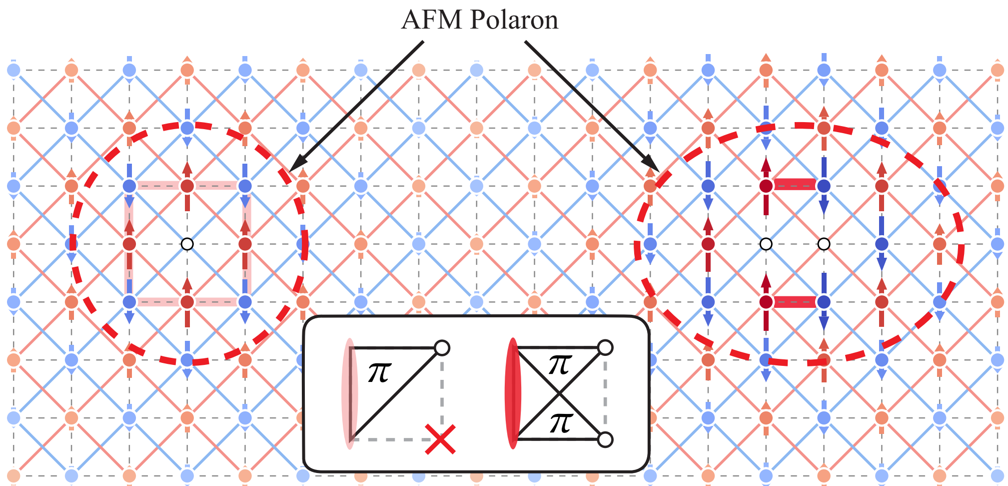
Ground state of one added electron is AFM for

$$t_2 \gtrsim t_1/2$$

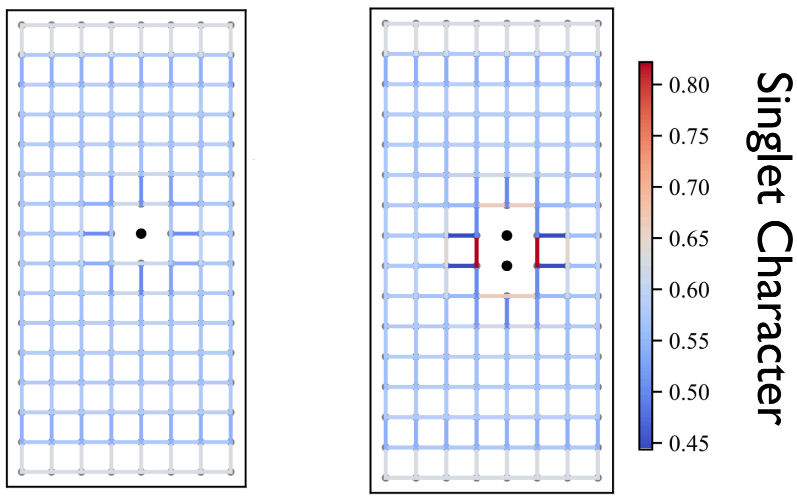
Yixin Zhang, CDB, and Yang Zhang **Arxiv 2506.16464** (2025)

AFM and pairing induced by Kinetic Frustration on Square Lattice

Large U regime of $t_1 - t_2$ Hubbard model



Strong d-wave pairing due to polaronic effect!



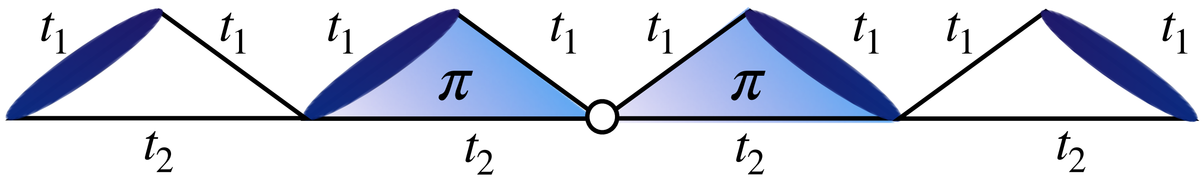
8-leg cylinder

DMRG results for $t_2/t_1 = 0.6, U = 10t_1$

Phase segregation is avoided

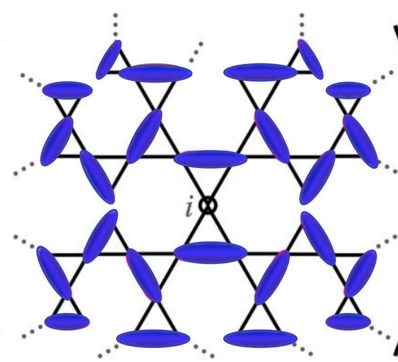
Kinetic energy frustration and RVB state

“Counter-Nagaoka theorem” for Saw-tooth Chain and Husimi Cactus



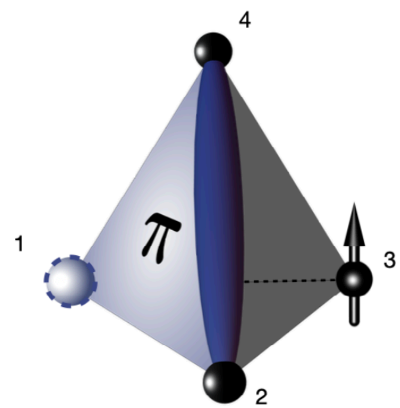
Exact group state: domain wall of VBC ordering attached to hole

$$|\Psi_0\rangle = \sum_i a(i) \left| \quad \right\rangle$$



Similar solution for triangular Husimi Cactus

Single Tetrahedron



Static unpaired spin

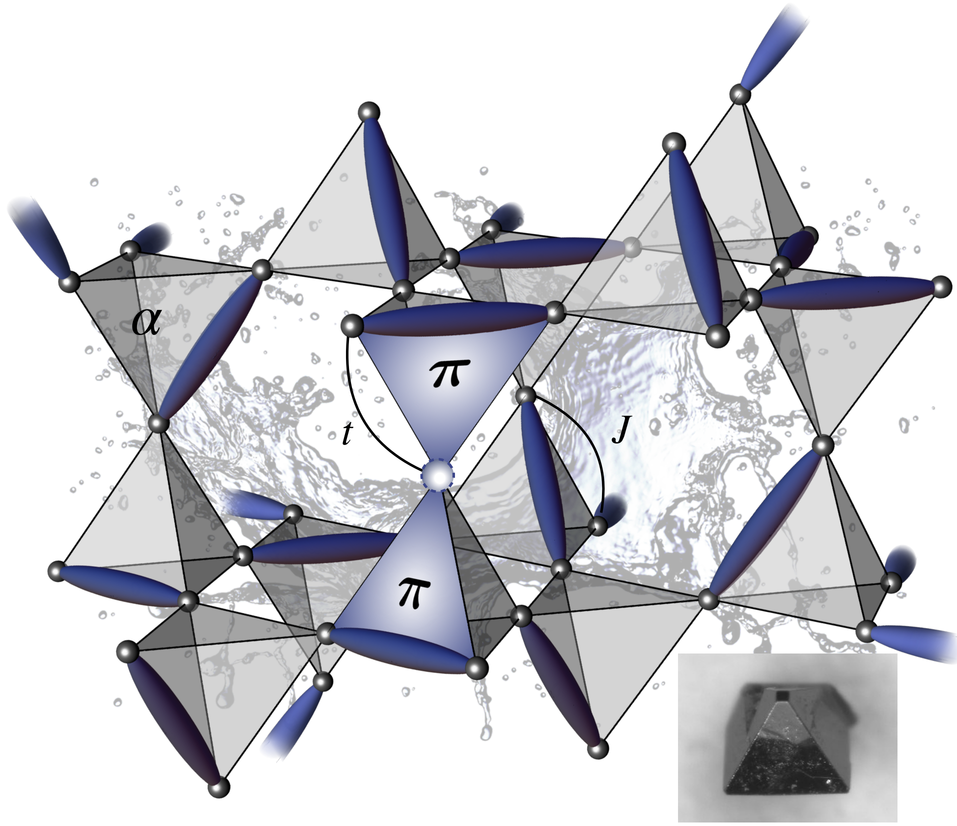
(Destructive Interference)

$$\left|\Psi_{\mathrm{GS}}\right\rangle \propto \left(\hat{d}^{\dagger}_{12} + \hat{d}^{\dagger}_{24} + \hat{d}^{\dagger}_{14}\right) \hat{c}^{\dagger}_{3,\uparrow} |0\rangle$$

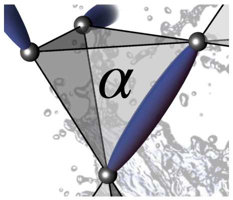
$$E^{\mathrm{one-treta}}_{\mathrm{min}} = -2|t|$$

(4 wavefunctions but only 3 linearly independent)

What is the “counter-Nagaoka theorem” for a Pyrochlore Lattice?



Cecilie Glittum et al, Nature Physics 2025, https://doi.org/10.1038/s41567-025-02923-8



Lower Bound for single-Hole Energy

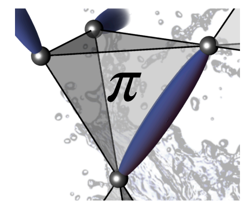
$$\hat{\mathscr{H}} = \sum_{\alpha} \hat{\mathscr{H}}^{\alpha}$$

$$|\Psi_0\rangle = \sum_{\boldsymbol{r}} |\phi_{\boldsymbol{r}}\rangle \qquad \langle \phi_{\boldsymbol{r}} | \phi_{\boldsymbol{r}'} \rangle = 0 \quad \boldsymbol{r} \neq \boldsymbol{r}' \quad \langle \Psi_0 | \Psi_0 \rangle = 1$$

$$|\chi_\alpha\rangle = \sum_{\boldsymbol{r}\in\alpha} |\phi_{\boldsymbol{r}}\rangle \qquad E_g = \sum_{\boldsymbol{r},\boldsymbol{r}'} \langle \phi_{\boldsymbol{r}} | \hat{\mathscr{H}} | \phi_{\boldsymbol{r}'} \rangle = \sum_{\langle \boldsymbol{r},\boldsymbol{r}' \rangle} \langle \phi_{\boldsymbol{r}} | \hat{\mathscr{H}} | \phi_{\boldsymbol{r}'} \rangle = \sum_{\alpha} \langle \chi_\alpha | \hat{\mathscr{H}}^{\alpha} | \chi_\alpha \rangle$$

Probability distribution over tetrahedra

$$p_\alpha = \frac{1}{2} \langle \chi_\alpha | \chi_\alpha \rangle \qquad E_g = \sum_{\alpha} p_\alpha 2 \frac{\langle \chi_\alpha | \hat{\mathscr{H}} | \chi_\alpha \rangle}{\langle \chi_\alpha | \chi_\alpha \rangle} \geq 2E_{\text{min}}^{\text{one-treta}}$$



$$\Downarrow$$

$$E_{\text{min}}^{\text{one-treta}} = -2|t|$$

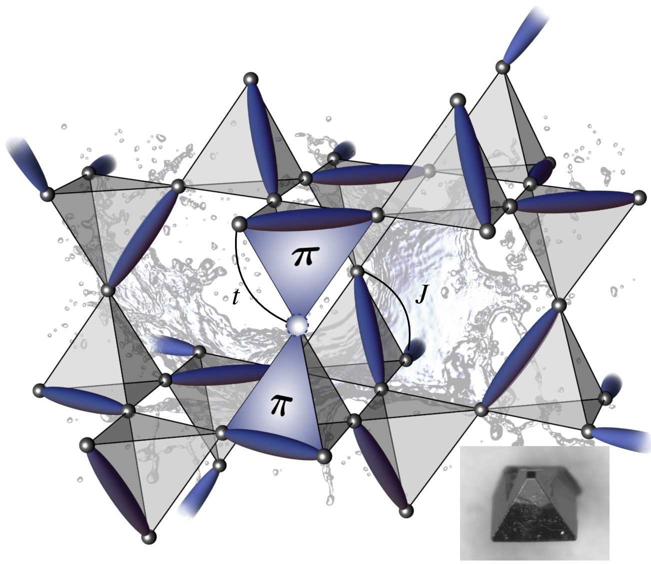
$$\langle \Psi_0 | \Psi_0 \rangle = 1 \implies \sum_{\alpha} p_\alpha = 1$$

$$\boxed{E_g \geq -4|t|}$$

Cecilie Glittum et al, Nature Physics 2025, https://doi.org/10.1038/s41567-025-02923-8

Exact RVB Ground State: one hole

Thermodynamic Limit



$$|\Psi^{1h}_{\rm RVB}\rangle = \frac{1}{\mathcal{N}_1} \sum_{\boldsymbol{r},\{a_{\boldsymbol{r}}\}} \prod_{\langle i,j\rangle \in a_{\boldsymbol{r}}} \hat{d}^{\dagger}_{ij} |0\rangle$$

$$\hat{d}^{\dagger}_{ij} = \frac{1}{\sqrt{2}}(\hat{c}^{\dagger}_{i\uparrow}\hat{c}^{\dagger}_{j\downarrow} - \hat{c}^{\dagger}_{i\downarrow}\hat{c}^{\dagger}_{j\uparrow})$$

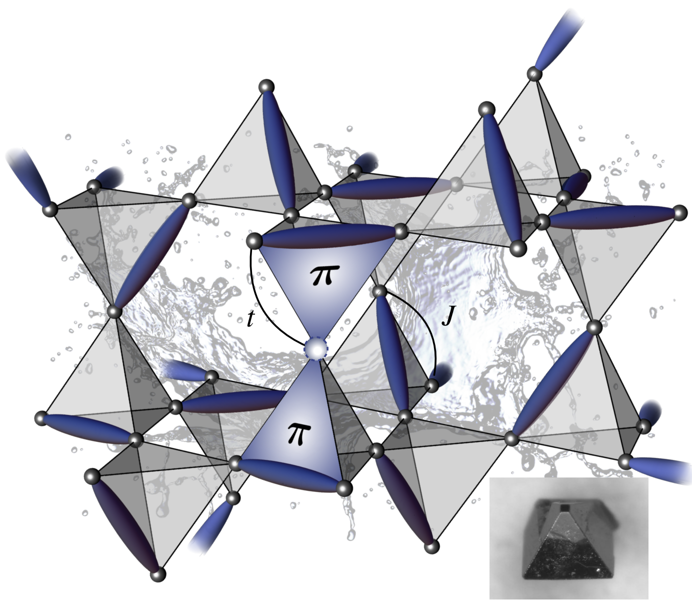
$$\langle \Psi^{1h}_{\rm RVB} | \hat{\mathscr{H}} | \Psi^{1h}_{\rm RVB} \rangle = -4|t|$$

The unpaired spin is localized while the hole is completely delocalized

Spin-charge separation in 3D

Exact RVB Ground State: two holes

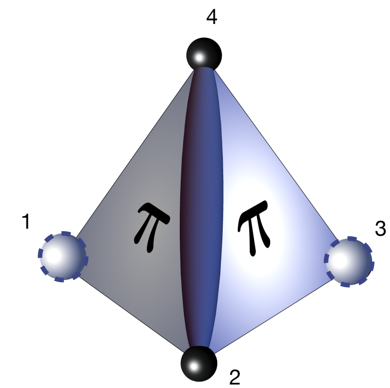
Thermodynamic Limit



$$|\Psi^{2h}_{\mathrm{RVB}}\rangle = \frac{1}{\mathcal{N}_2} \sum_{\boldsymbol{r},\boldsymbol{r}',\{a_{\boldsymbol{r},\boldsymbol{r}'}\}} \prod_{\langle i,j\rangle \in a_{\boldsymbol{r},\boldsymbol{r}'}} \hat{d}^{\dagger}_{ij} |0\rangle$$

$$\hat{d}^{\dagger}_{ij} = \frac{1}{\sqrt{2}} (\hat{c}^{\dagger}_{i\uparrow}\hat{c}^{\dagger}_{j\downarrow} - \hat{c}^{\dagger}_{i\downarrow}\hat{c}^{\dagger}_{j\uparrow})$$

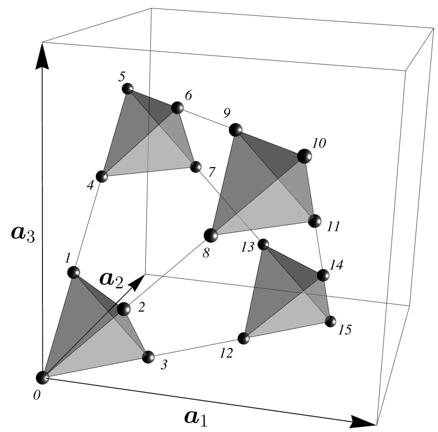
$$\langle \Psi^{2h}_{\mathrm{RVB}} | \hat{\mathscr{H}} | \Psi^{2h}_{\mathrm{RVB}} \rangle = -8|t|$$

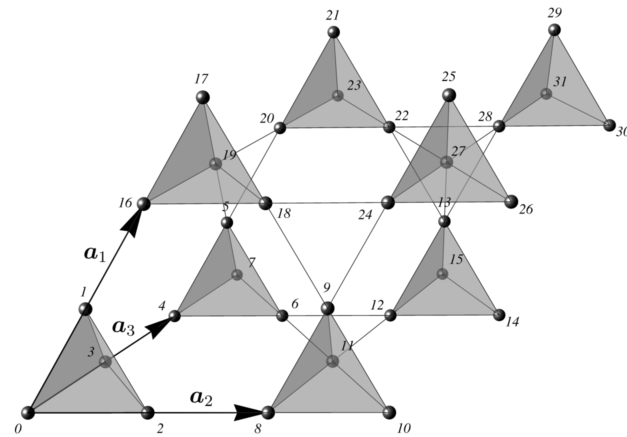


Cecilie Glittum et al, Nature Physics 2025, https://doi.org/10.1038/s41567-025-02923-8

Finite Size Clusters (PBC)

16 sites (ED)





32 sites (DMRG)

$$|\Psi^{1h,\sigma}_{\text{RVB}}\rangle = c^{\dagger}_{\boldsymbol{r}\sigma} \sum_{\boldsymbol{r},\{a_{\boldsymbol{r},\boldsymbol{r}'}\}} \prod_{\langle i,j\rangle\in a_{\boldsymbol{r},\boldsymbol{r}'}} \hat{d}^{\dagger}_{ij}|0\rangle$$

$$|\Psi^{2h}_{\text{RVB}}\rangle = \sum_{\boldsymbol{r},\boldsymbol{r}',\{a_{\boldsymbol{r},\boldsymbol{r}'}\}} \prod_{\langle i,j\rangle\in a_{\boldsymbol{r},\boldsymbol{r}'}} \hat{d}^{\dagger}_{ij}|0\rangle$$

$$\langle\Psi^{1h}_{\text{RVB}}|\hat{\mathscr{H}}|\Psi^{1h}_{\text{RVB}}\rangle = -4|t|$$

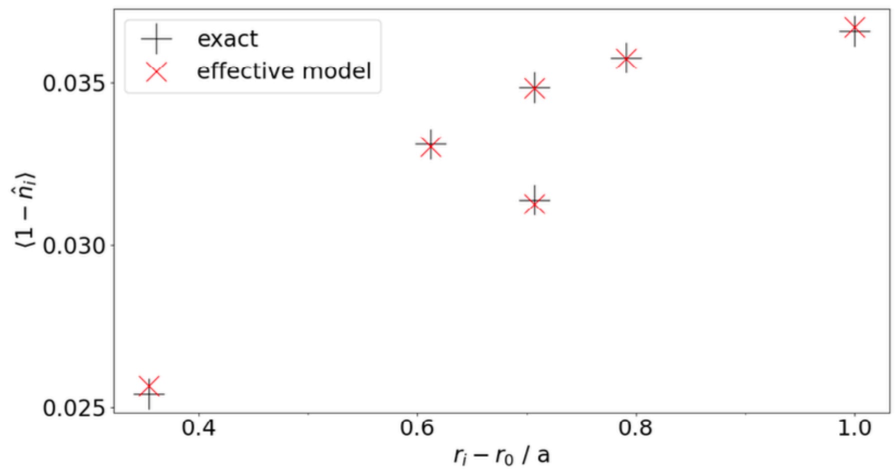
$$\langle\Psi_{\text{RVB}}|\hat{\mathscr{H}}|\Psi_{\text{RVB}}\rangle = -8|t|$$

Bosonic Holon Statistics

Effective hardcore boson model

$$H_{\text{eff}} = -\,t_{\text{eff}} \sum_{\langle ij \rangle} \left(b_i^\dagger b_j + b_j^\dagger b_i \right) + V \sum_{\langle ij \rangle} n_i n_j$$

$$t_{\text{eff}} = 2t/3, \quad V \simeq (-0.73 \pm 0.03)t$$



No bound pairs ⇒ charge-e condensation and SC?

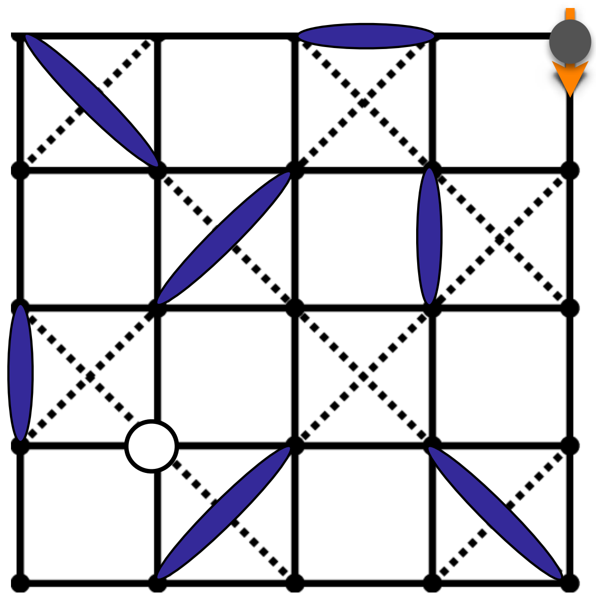
2*e* or not 2*e*: Flux Quantization in the Resonating Valence Bond State.

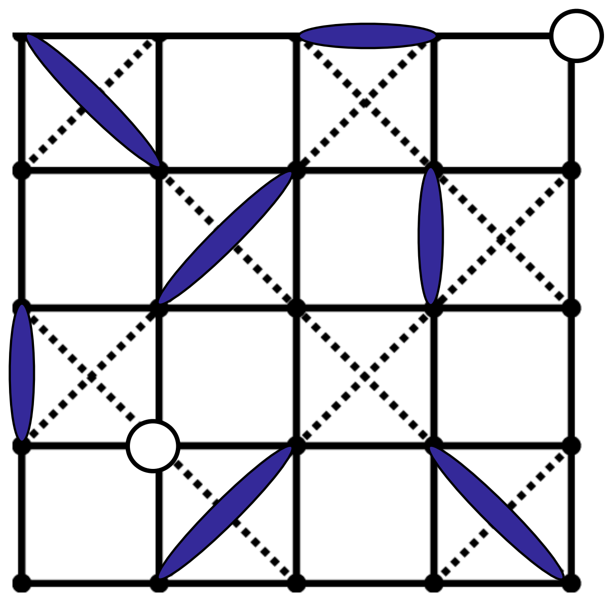
S. A. Kivelson (*), D. S. Rokhsar (**) ($) and J. P. Sethna

Cecilie Glittum et al, Nature Physics 2025, https://doi.org/10.1038/s41567-025-02923-8

The proofs hold for a checkerboard lattice

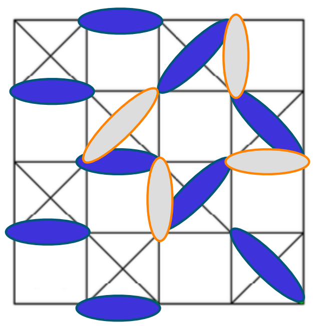
$$|\Psi^{1h,\sigma}_{\mathrm{RVB}}\rangle = c^\dagger_{\boldsymbol{r}\sigma} \sum_{\boldsymbol{r},\{a_{\boldsymbol{r},\boldsymbol{r}'}\}} \prod_{\langle i,j\rangle \in a_{\boldsymbol{r},\boldsymbol{r}'}} \hat{d}^\dagger_{ij}|0\rangle \qquad |\Psi^{2h}_{\mathrm{RVB}}\rangle = \sum_{\boldsymbol{r},\{a_{\boldsymbol{r},\boldsymbol{r}'}\}} \prod_{\langle i,j\rangle \in a_{\boldsymbol{r},\boldsymbol{r}'}} \hat{d}^\dagger_{ij}|0\rangle$$



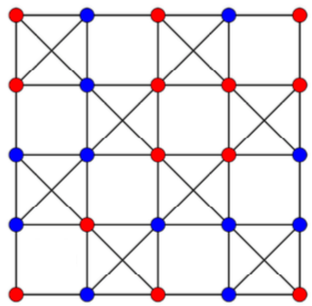


From singlets to product spin states

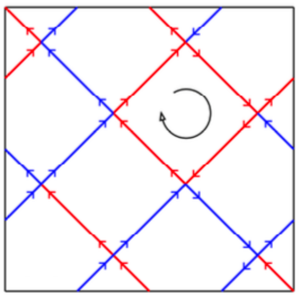
Need to understand the nature of the spin liquid background:



RK-loop



Graph Representation



Both coverings contribute the same Fock spin state with opposite signs

RBV superposition vanishes for zero hole concentration with PBC!

Conclusions

- **Kinetic energy frustration is a new paradigm to find new states of matter.**
- **Nagaoka's conditions (Mott insulator doped with one hole in $U \rightarrow \infty$ limit) lead to:**
  - **Ferromagnets** for bipartite lattices (Nagaoka's theorem)
  - **Antiferromagnet** for triangular lattice (Hearter and Shastry)
  - **Valence bond state** for Husimi Cactus (Kyung-Su Kim) and sawtooth chain (Theorem)
  - **RVB liquid** (spin charge separation) for pyrochlore and checkerboard lattices (Theorem)
- **AFM correlations are generated because a singlet generates a π-flux.**
- **The bound state between the hole and the singlet (AFM polaron) leads to unconventional pairing establishing a clear connection between KEF and SC.**

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