

Slater and Mott Physics of SU(N) Hubbard models

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1. D. Wang, Lei Wang, CW, arXiv:1907.01748.
2. Shenglong Xu, Julio Barreiro, Yu Wang, CW, Phys. Rev. Lett. 121, 167205 (2018)
3. D. Wang, Y. Li, Z. Cai, Z. Zhou, Yu Wang, CW, Phys. Rev. Lett. 112, 156403 (2014).
4. Z. C. Zhou, CW , Yu Wang, Phys. Rev. B 97, 195122 (2018).
5. Z. C. Zhou, D. Wang, Zi Yang Meng, Yu Wang, CW , Phys. Rev. B 93, 245157 (2016).
6. Hsiang-hsuan Hung, Yupeng Wang, CW, Phys. Rev. B 84, 054406 (2011).

Collaborators

Da Wang	(UCSD→ Nanjing Univ.)
Yi Li	(UCSD→ Princeton → Johns Hopkins)
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Collaborators on earlier works: S. C. Zhang (Stanford), J. P. Hu, S. Chen and Y. P. Wang (IOP, CAS).

Supported by NSF, AFOSR.



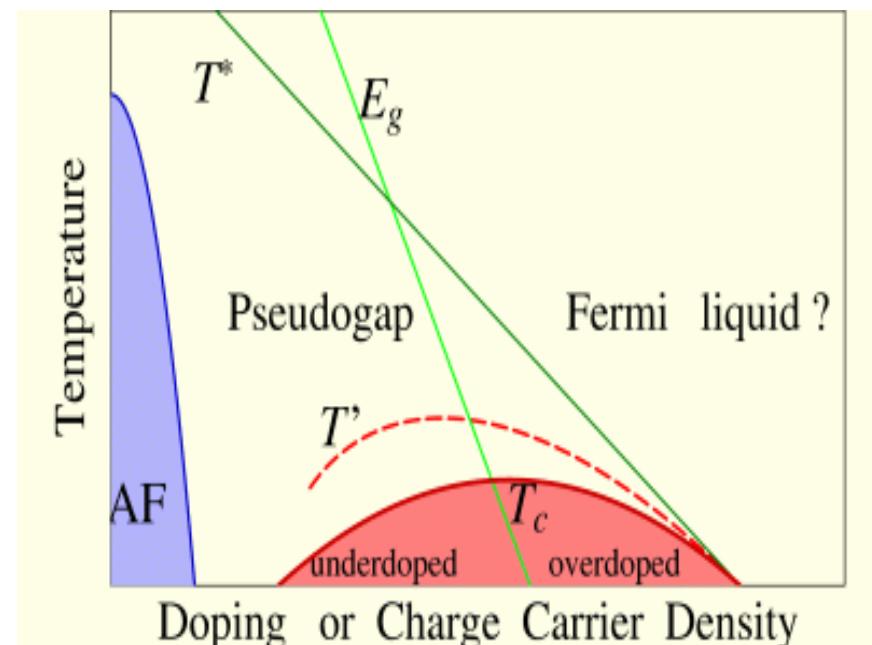
$SU(N)$



The Hubbard model

$$H = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^+ c_{j\sigma} + h.c. - \mu \sum_{i,\sigma} c_{i\sigma}^+ c_{i\sigma} + U \sum_{i,\sigma} n_{i\uparrow} n_{i\downarrow}$$

- Hubbard 1963: originally for itinerant ferromagnetism (FM) --- unsuccessful.
- Successful for metal-Mott insulator transitions.
- High T_c cuprates?
--- Still in debates.



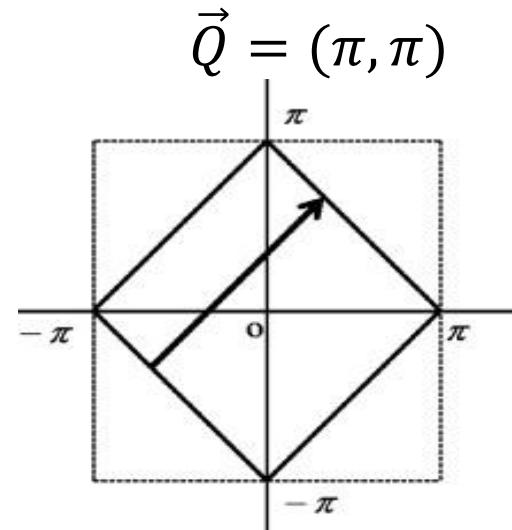
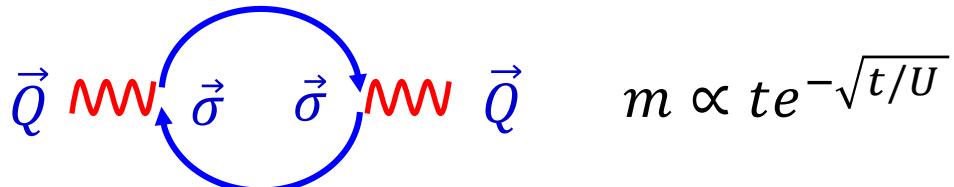
1D Mott state – Absence of long-range order

- Half-filled ($U>0$) – Lieb-Wu solution (Hubbard).
 1. Charge gap opens at $U \rightarrow 0$: Relevance of the Umklapp term
 2. Spin channel is critical \rightarrow no symmetry breaking
 3. Bosonization+Sine-Gordon, DMRG
- Bethe ansatz solution for the Heisenberg model.
 1. Ground state energy $E/N = \frac{1}{4} - \ln 2$
 2. Fractionalized gapless excitation: spinon

C. N. Yang, PRL 19, 1312 (1967); Lieb and F. Y. Wu, PRL 20, 1445, (1968).

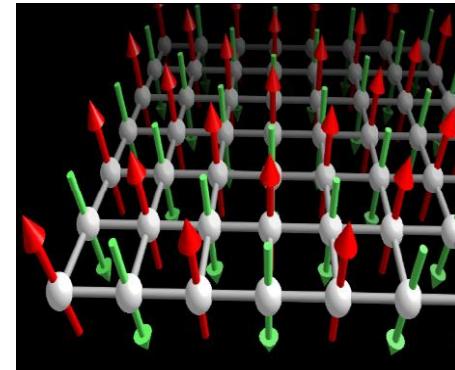
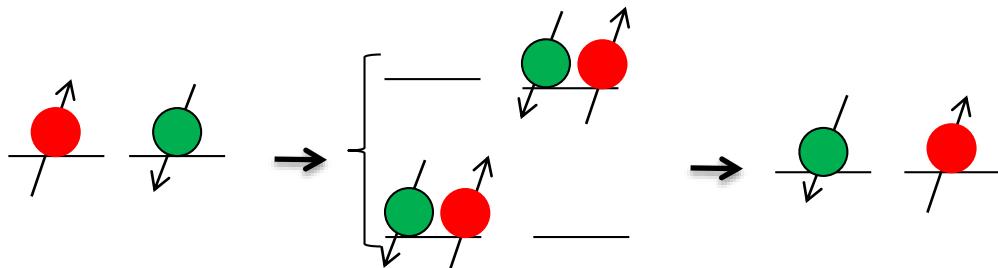
2D: Slater v.s. Mott (half-filling)

- Fermi surface nesting ($U/t \rightarrow 0$) : strong charge fluctuations.



- Local moments ($U/t \rightarrow \infty$) : AF super-exchange.

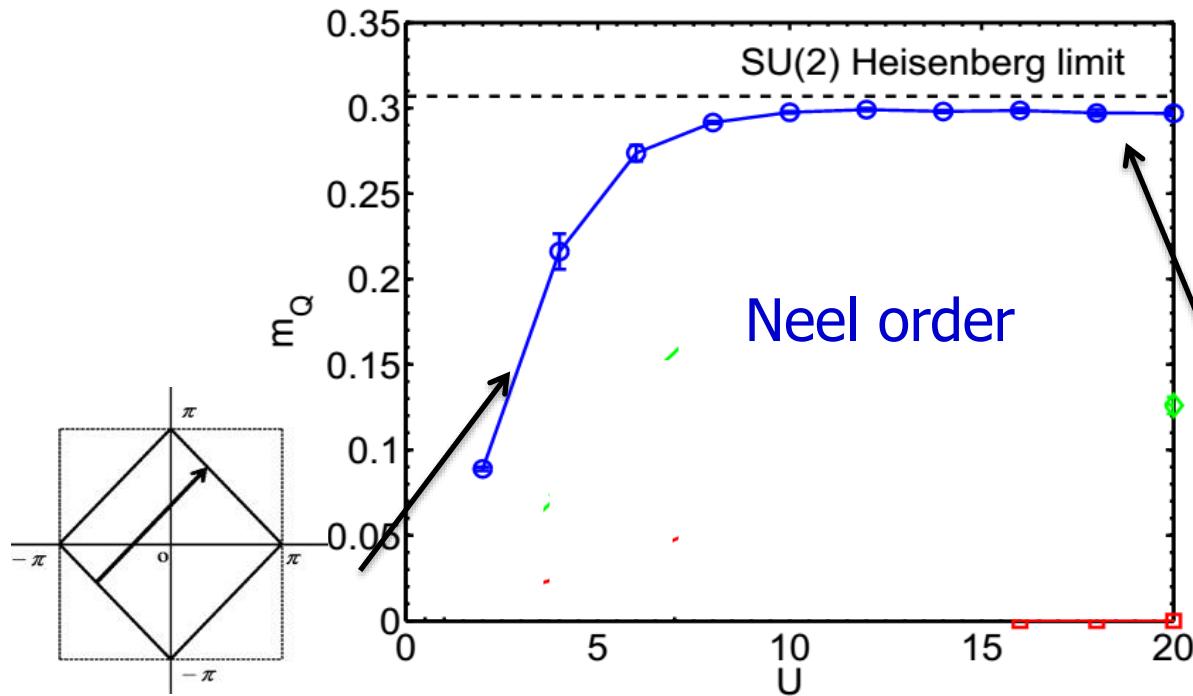
$$H = J \sum \vec{S}_i \cdot \vec{S}_j$$



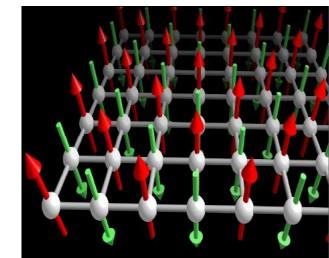
Crossover: Slater → Mott

- AF long-range order for all values of U.

Determinant QMC: J. Hirsch, 1985.



D. Wang, Y. Li, Z. Cai, Z. Zhou, Y. Wang, **CW**, Phys. Rev. Lett. 112, 156403 (2014).



Blackenbecler, Scalapino, Sugar, PRD (1981); J. Hirsch, PRB 31, 4403 (1985).

SO(4) symmetry – pseudo-spin SU(2)

- Yang and Zhang's η -pairing: the charge channel.

$$\eta^- = \sum_i (-)^i c_{i\downarrow} c_{i\uparrow}, \quad \eta^+ = \sum_i (-)^i c_{i\uparrow}^+ c_{i\downarrow}^+, \quad [\eta^-, \eta^+] = 2N,$$

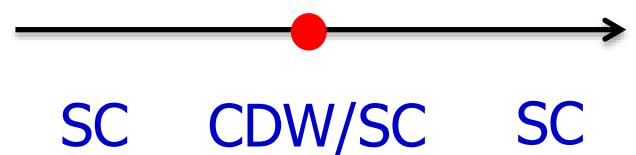
- Degeneracy between charge-density-wave (CDW) and superconductivity (SC) at half-filling ($U<0$)

$$O_{cdw} = \sum_i (-)^i n_i, \quad \Delta = \sum_i c_{i\uparrow} c_{i\downarrow}, \quad \Delta^+ = \sum_i c_{i\downarrow}^+ c_{i\uparrow}^+, \quad [\eta^+, \Delta] = O_{cdw},$$

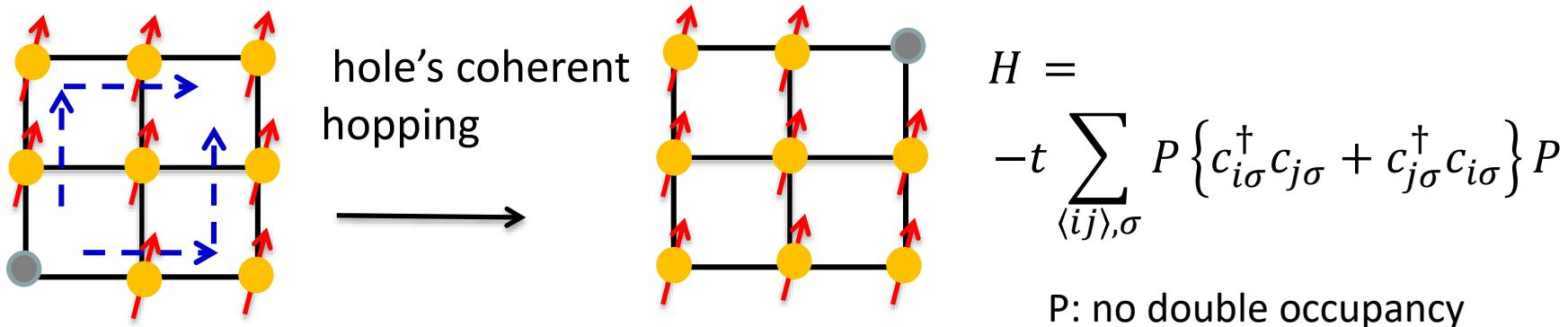
- Pseudo-Goldstone: η -mode

$\delta = 0$ doping

$$H(\eta^+ |G_{sc}\rangle) = (\mu - \mu_0) \eta^+ |G_{sc}\rangle,$$



Nagaoka FM: infinite-U + single hole

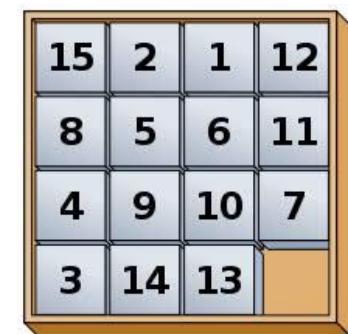


- Ground state WF positive definite – Perron-Frobenius

Bases: $|\psi(h_j, \{\sigma_i\})\rangle = (-)^j c_{\sigma_1}^\dagger(i_1) \dots c_{\sigma_2}^\dagger(j-1) c_{\sigma_2}^\dagger(j+1) \dots |vac\rangle$.

- Nearly arbitrary graph (e.g. honeycomb, diamond) -- 15 puzzle problem.

E. Bobrow, K. Stubis, Yi Li, Phys. Rev. B 98, 180101 (2018)



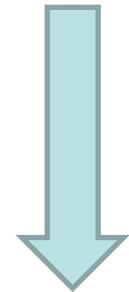
Phase string – hole's motion

- The Marshall sign can be absorbed.

$$H = -t \sum_{\langle ij \rangle, \sigma} P \left\{ c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right\} P$$

$$+ J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

$$c_{i\sigma} \rightarrow c_{i\sigma}, c_{j\sigma} \rightarrow (-)^\sigma c_{j\sigma}$$



- The hole exchanges with a spin $\downarrow \rightarrow$ a minus sign.

$$H = t \sum_{\langle ij \rangle, \sigma} P \left\{ -c_{i\uparrow}^\dagger c_{j\uparrow} + c_{i\downarrow}^\dagger c_{j\downarrow} + h.c. \right\} P$$

$$+ J \sum_{\langle ij \rangle} \{ -\vec{S}_x \cdot \vec{S}_x - \vec{S}_y \cdot \vec{S}_y + \vec{S}_z \cdot \vec{S}_z \}$$

- Hole's motion frustrates the WF.

D. Sheng, Chen, Z. Y. Weng, Phys. Rev. Lett. 98, 180101 (1996)
Z. Y. Weng, Front. Phys. 6, 370 (2011).

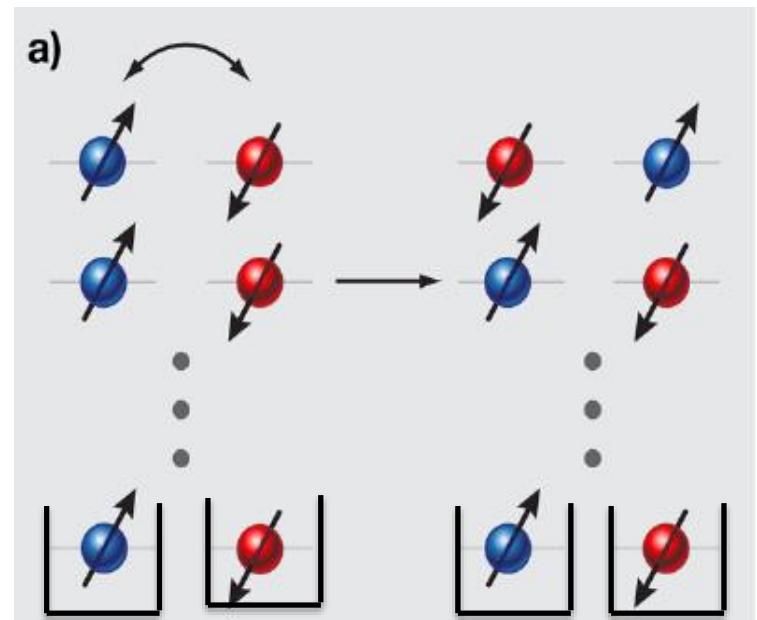
Transition metal oxides (**large S** → classical)

- **Large spin magnitude** from Hund's coupling.
- Inter-site coupling: exchange **a single pair** of electrons.

- **1/S-fluctuations:** $\Delta S_z = \pm 1$

- Bilinear exchange dominates

$$\frac{t^2}{U} \vec{S}_i \cdot \vec{S}_j + \frac{t^4}{U^3} (\vec{S}_i \cdot \vec{S}_j)^2 + \dots$$



C. Wu, Physics 3, 92 (2010).

C. Wu, Nature Physics 8, 784 (2012) (News and Views).

Large-spin cold fermions inaccessible in solids

- A new view point: high symmetries, Sp(2N), SU(2N).

Sp(4), SO(5), SU(4) : (spin $-\frac{3}{2}$) ^{132}Cs , ^9Be , ^{135}Ba , ^{137}Ba , ^{201}Hg

C. Wu, S. C. Zhang, S. Chen, Y. P. Wang, A. Tsvelik, G. M. Zhang, Lu Yu, X. W. Guan, Azaria, Lecheminant, et al. (2003 ---).

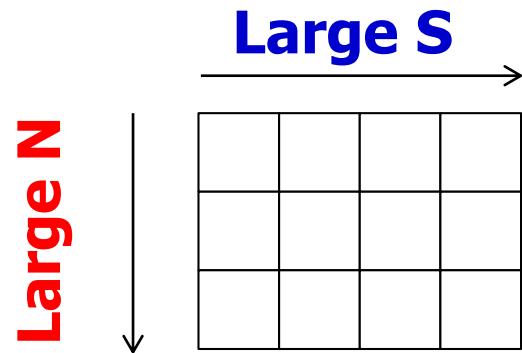
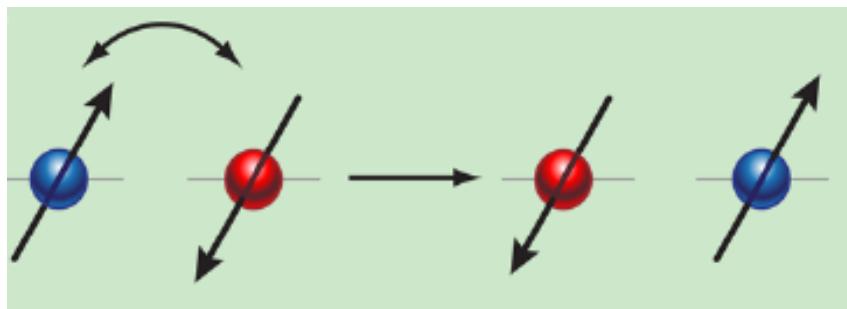
SU(2N): V. Guriare, M. Hermele, A. Rey, E. Demler, M. Lukin, P. Zoller, et al. (2010 ---).

- What is large? --- High symmetry (SU(2N), Sp(2N)) rather than large spin magnitude (large S).

Cold fermions: large N → enhanced fluctuations!

- One step of super-exchange can completely overturn spin configurations.

$$\Delta S_z = \pm 1, \pm 2, \dots \pm S$$



- Bilinear, bi-quadratic, bi-cubic terms, etc., → equal importance.

$$\vec{S}_i \cdot \vec{S}_j, (\vec{S}_i \cdot \vec{S}_j)^2, (\vec{S}_i \cdot \vec{S}_j)^3$$

Spin-3/2 Hubbard model

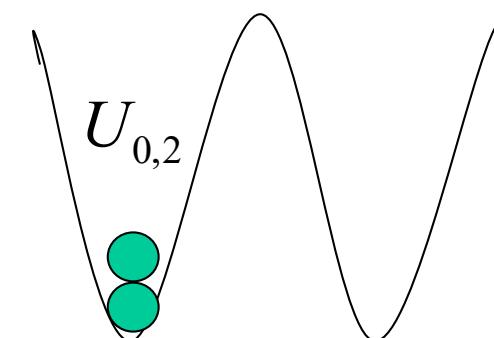
$$H = \sum_{\langle ij \rangle, \alpha} -t \{ c_{i,\alpha}^+ c_{j,\alpha} + h.c. \} - \mu \sum_i c_{i,\alpha}^+ c_{i,\alpha} \\ + U_0 \sum_i \eta^+(i) \eta(i) + U_2 \sum_{a=1 \sim 5} \chi_a^+(i) \chi_a(i)$$

$$\begin{array}{c} \uparrow \left| \frac{3}{2} \right\rangle \uparrow \left| \frac{1}{2} \right\rangle \\ \downarrow \left| -\frac{1}{2} \right\rangle \downarrow \left| -\frac{3}{2} \right\rangle \end{array}$$

- Fermi statistics: only $F_{\text{tot}}=0, 2$ are allowed.

singlet: $\eta^+(i) = \sum_{\alpha\beta} \langle 00 | \frac{3}{2} \frac{3}{2}; \alpha\beta \rangle c_\alpha^+(i) c_\beta^+(i)$

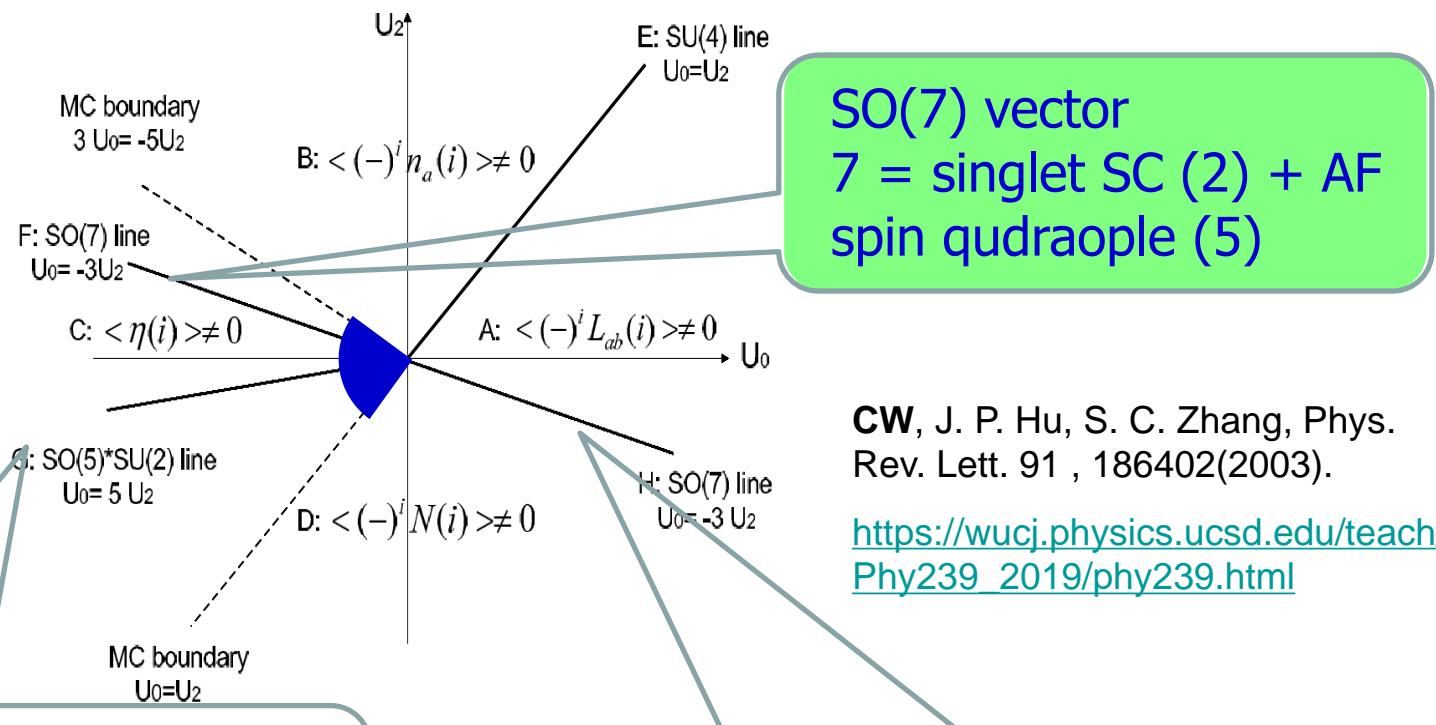
quintet: $\chi_a^+(i) = \sum_{\alpha\beta} \langle 2a | \frac{3}{2} \frac{3}{2}; \alpha\beta \rangle c_\alpha^+(i) c_\beta^+(i)$



- **Exact** Sp(4), or, SO(5) symmetry: arbitrary values of t, μ, U_0, U_2 and lattice geometry.

Grand unification under symmetry principle

- $4^2 = 1 + 3 + 5 + 7$: charge, spin, quadrupole, octupole
spin (3) + spin octupole (7) \rightarrow 10: Sp(4) or SO(5)



Pseudospin SO(3) vector
7 = singlet SC (2) + CDW (1)

"Grand unification" via SO(7) – adjoint
21 = CDW (1) + quintet SC (10) + AF
spin (3) and octupole (7)

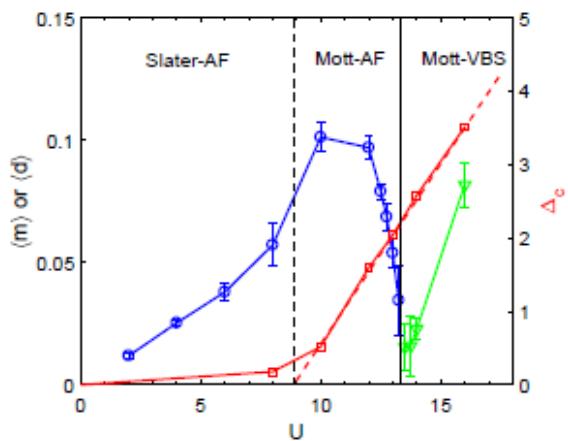
CW, J. P. Hu, S. C. Zhang, Phys.
Rev. Lett. 91 , 186402(2003).

[https://wucj.physics.ucsd.edu/teach/
Phy239_2019/phy239.html](https://wucj.physics.ucsd.edu/teach/Phy239_2019/phy239.html)

Slater v.s Mott
Neel v.s VBS

Convergence of
itinerancy and local
Mottness?

**SU(N)
Mott Physics**

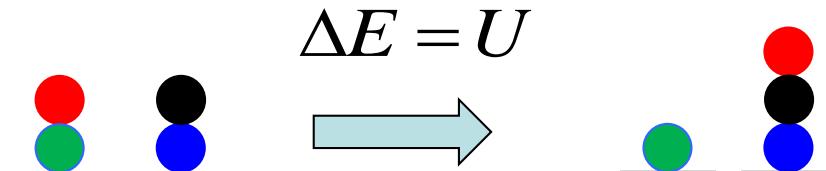


Color Magnetism

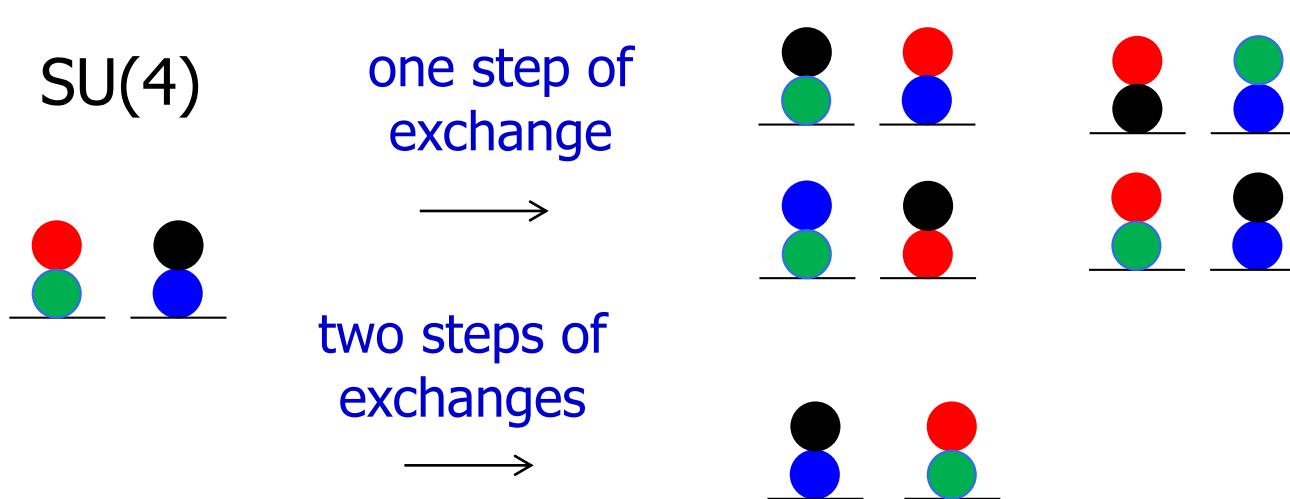
Half-filled SU(2N) Hubbard model

$$H = -t \sum_{\langle ij \rangle, \sigma=1}^N \{ c_{i\sigma}^+ c_{j\sigma} + h.c. \} + \frac{U}{2} \sum_{i,\sigma} (n_i - N)^2$$

- Atomic limit $t=0$.



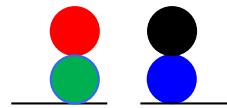
- # of super-exchange processes scales as N^2 .



Enhanced spin fluctuations

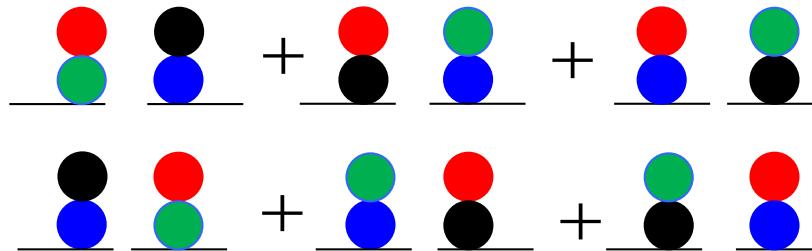
- Neel state unfavorable as N increases.

$$\Delta E = -2zN \frac{t^2}{U}$$



classic-Neel

$$\Delta E = -2zN(N+1) \frac{t^2}{U}$$

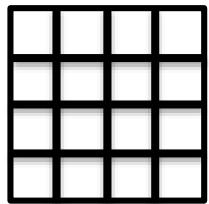


SU(2N)
singlet

- Dimer state consists of $\binom{2N}{N}$ resonating configurations.
- As $N > z$ (coordination number), valence bond dimerization favorable (Sachdev + Read).

Quantum Monte Carlo Simulations

Size L^2



Poll the
Hilbert space

Dimension of
Hilbert Space
 $\sim e^{\#L^2}$



Aesthetics of
brutal force

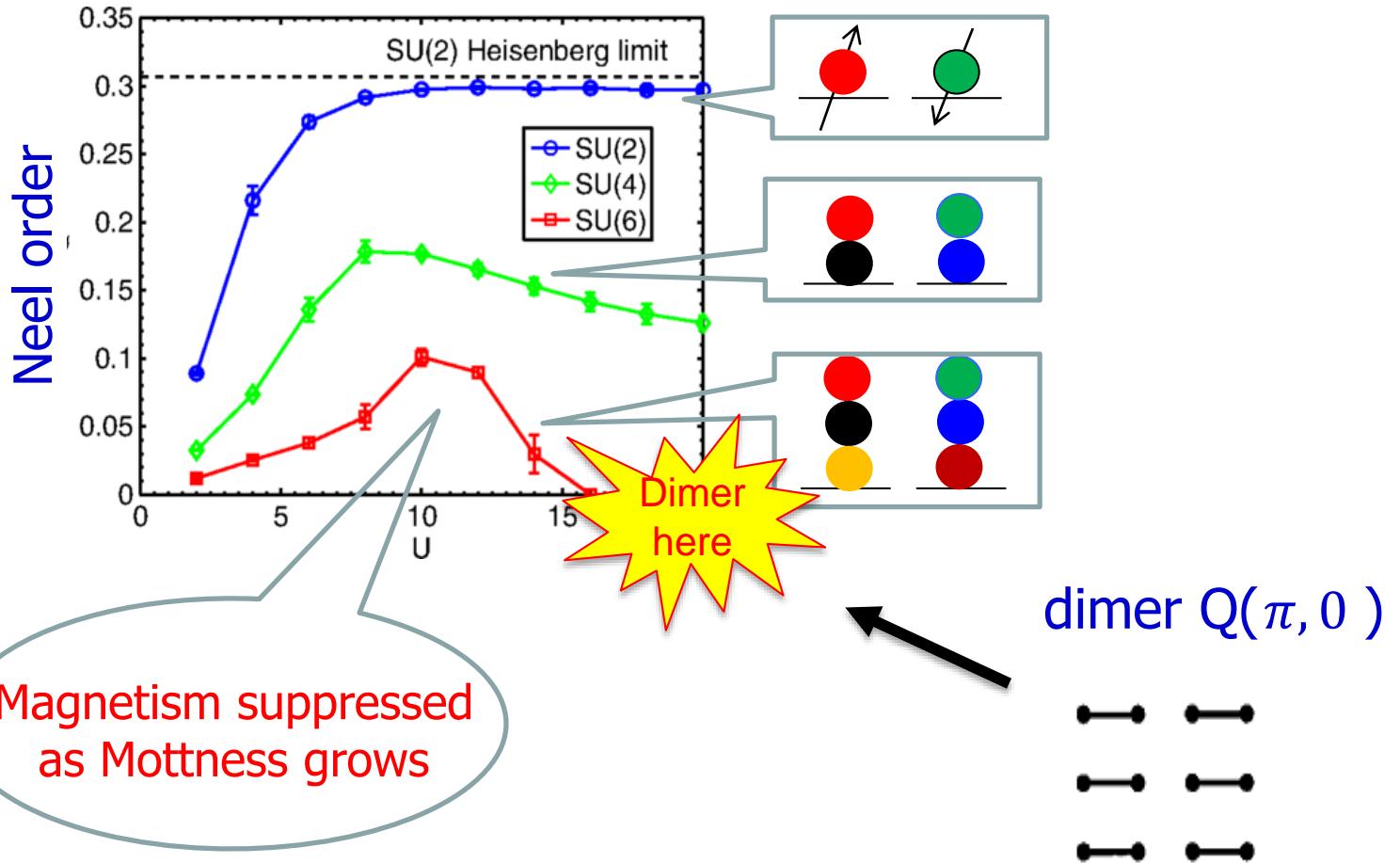
Numerical
exactness

Beautiful mathematical
structure

Quantum
Monte Carlo

- Condensed matter (**Magnetism and Superconductivity**),
high energy, nuclear physics

AFM: non-monotonic dependence on U



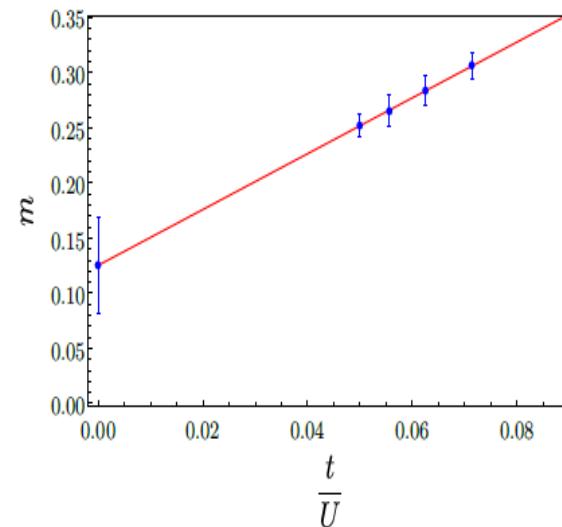
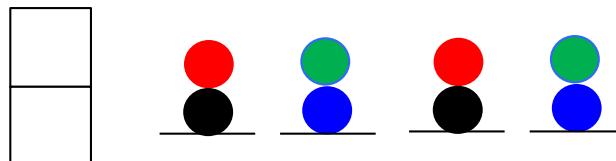
SU(4): Heisenberg model (self-conjugate)

- Stronger quantum fluctuations: AF long-range order with a smaller moment

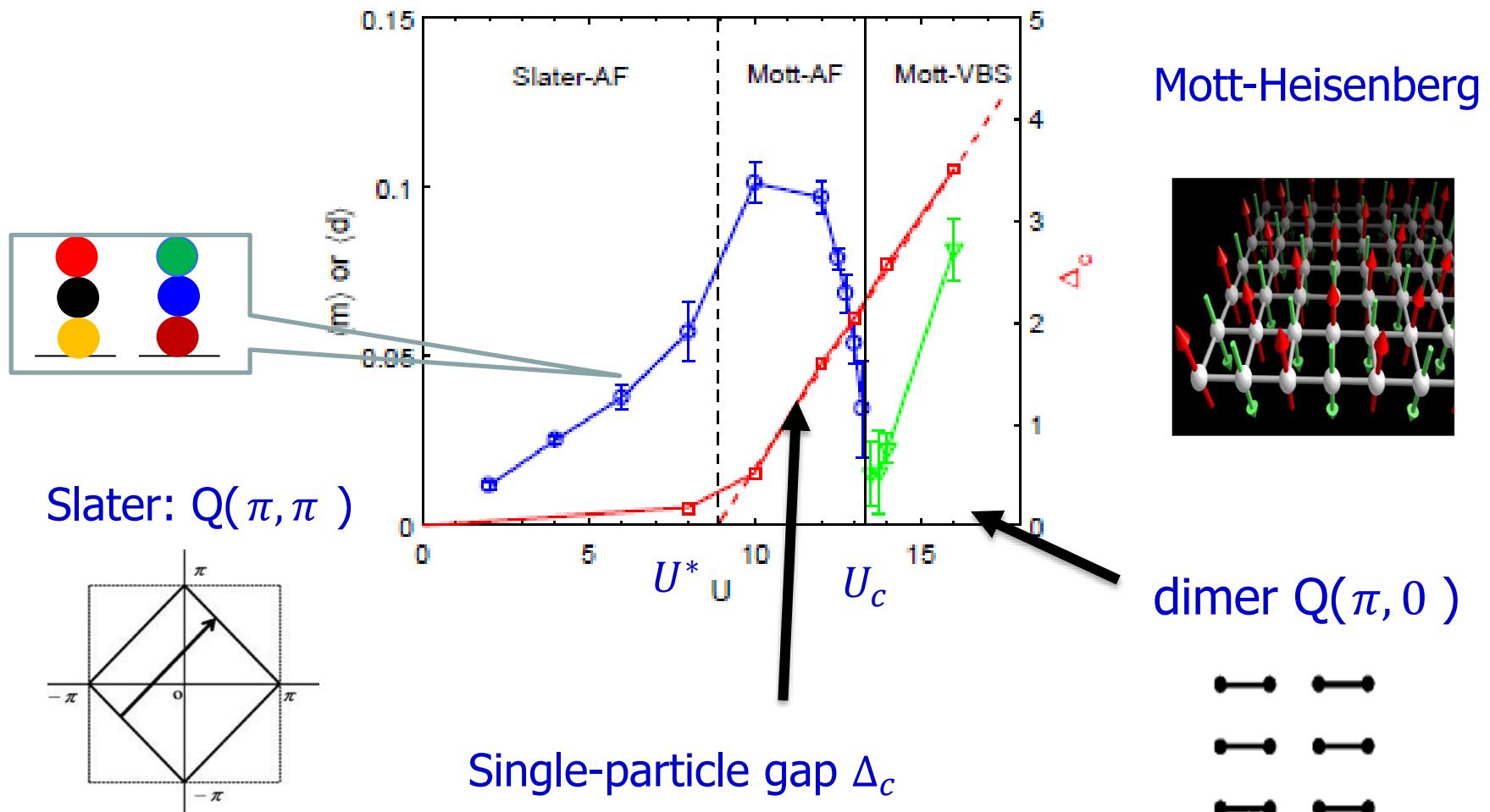
$$U \rightarrow \infty: m = \frac{1}{4} \langle (-)^i (n_1 + n_2 - n_3 - n_4) \rangle \approx 0.11 \pm 0.04$$

Assaad et al, arXiv 1906.06938

- Consistent with $1/U$ scaling of m based on our data.

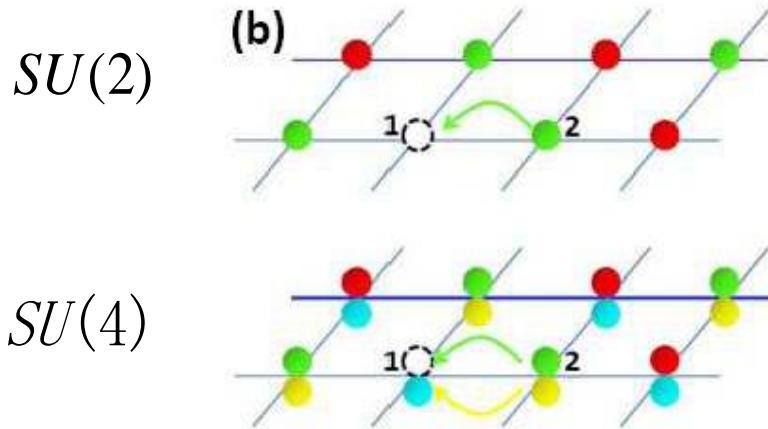
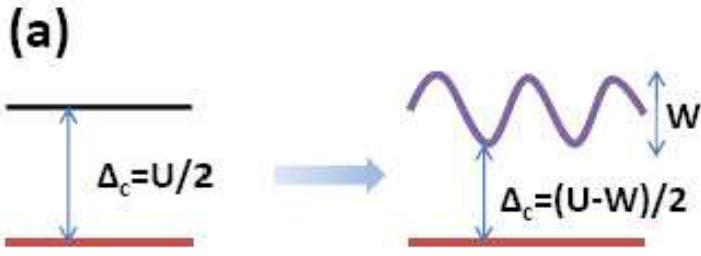


SU(6): Slater \rightarrow Mott, quantum phase transitions

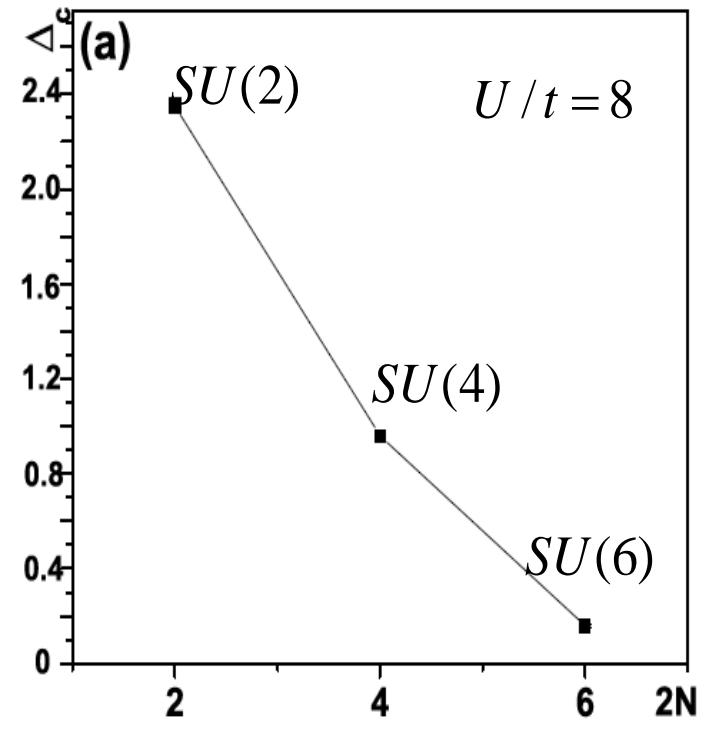


Single-particle gap softened as N increases

- Hole's band width $W \sim Nt$.



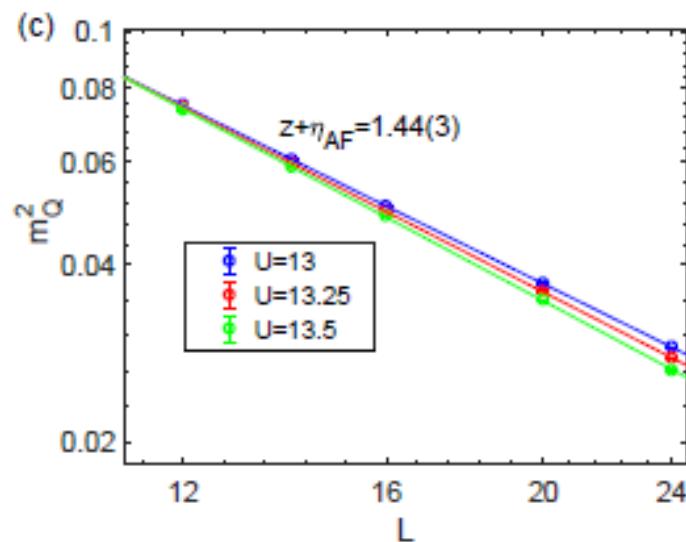
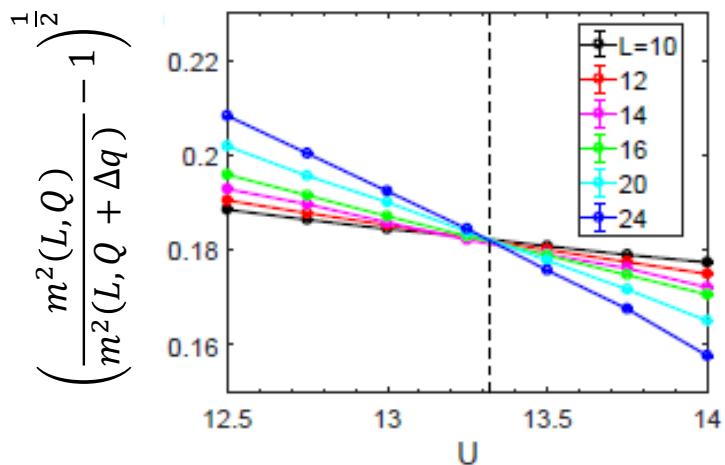
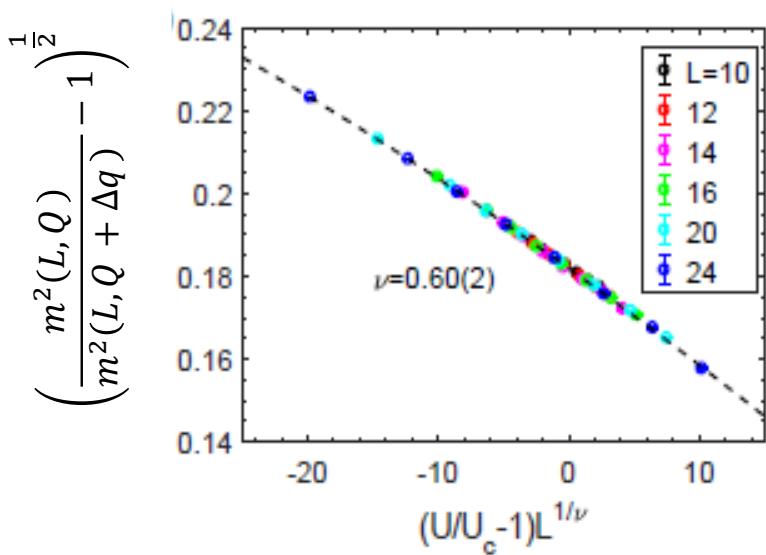
$$\Delta_{sg} = U - W \sim U - Nt$$



Critical exponents of the AF transition

- A continuous transition.

- $U_c = 13.3 \pm 0.05$,
- $\nu = 0.6 \pm 0.02$
- $\eta = 0.44 \pm 0.03$

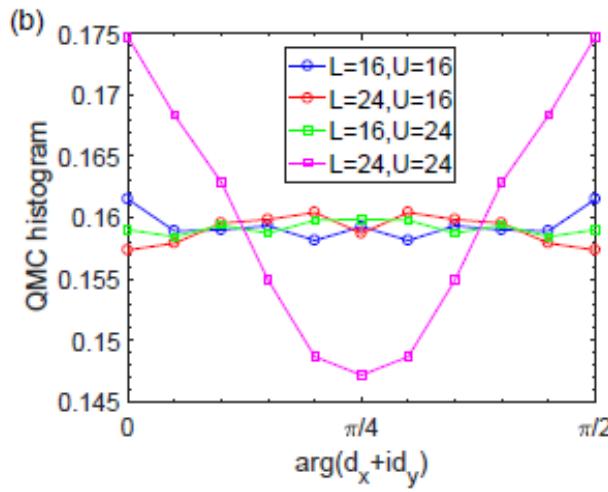
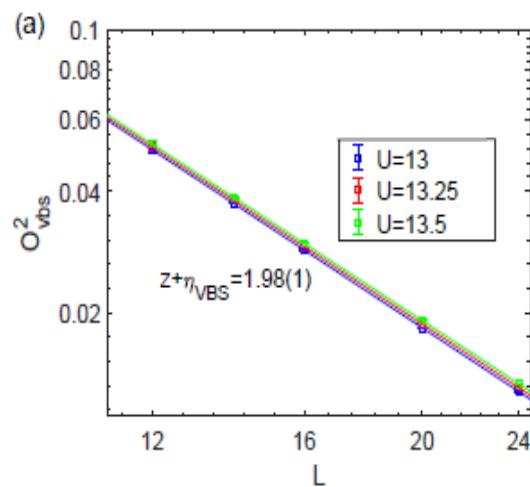
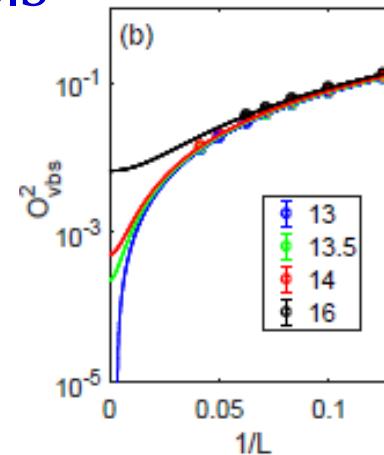


Dimerization -- VBS

- Structure factor fitting: $13 < U_c < 13.5$

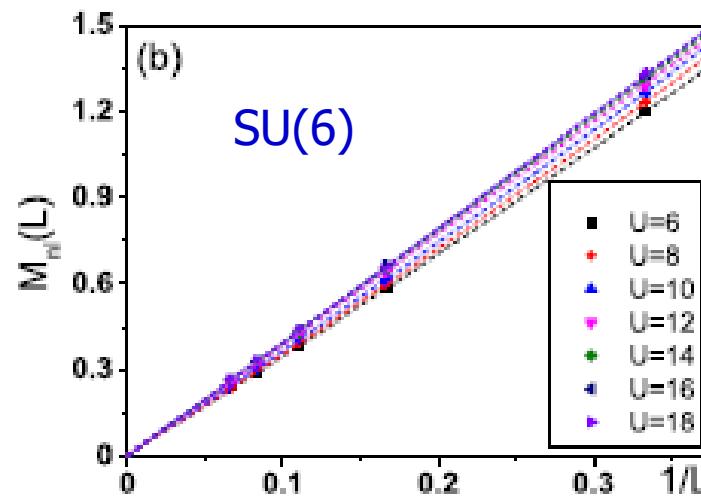
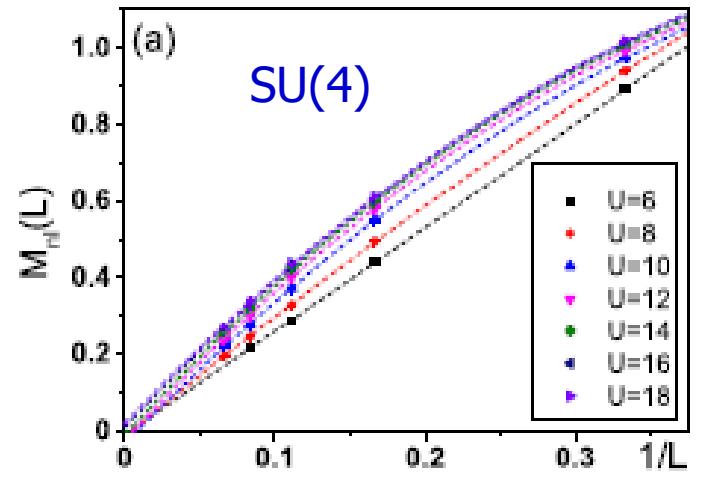
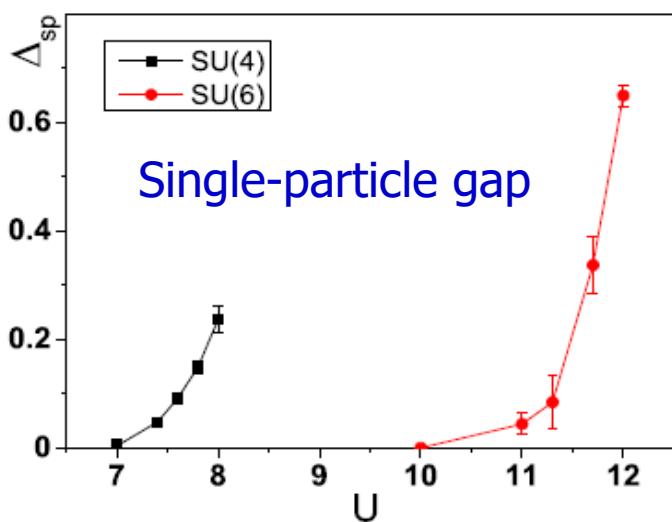
$$d_{i,\hat{e}_j} = \frac{1}{N} \sum c_{i\alpha}^+ c_{i+e_j,\alpha} + h.c.$$

- Columnar VBS when deep inside the VBS phase.
- Data insufficient to judge deconfined criticality or not



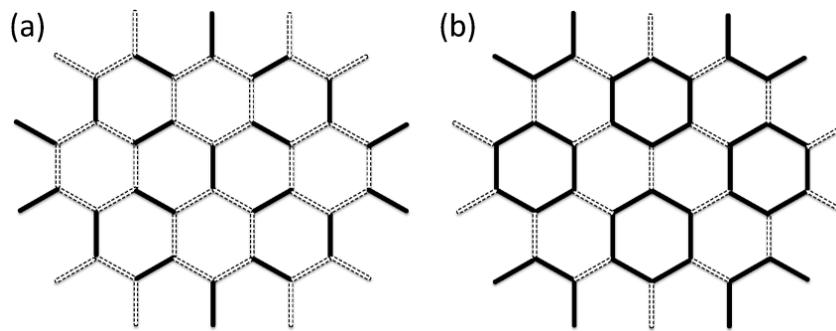
Mott transition of Dirac-fermion (honeycomb)

- $\text{AF} \rightarrow 0$ for all values of U .
- Mottness starts later than the case of square lattice:
 $U^* \approx 11$ for SU(6).



Dirac semi-metal → VBS transition

$$\psi = \frac{1}{L^2} \sum (d_{i,e_a} + \omega d_{i,e_b} + \omega^2 d_{i,e_c}) e^{i\vec{K} \cdot \vec{r}_i}$$



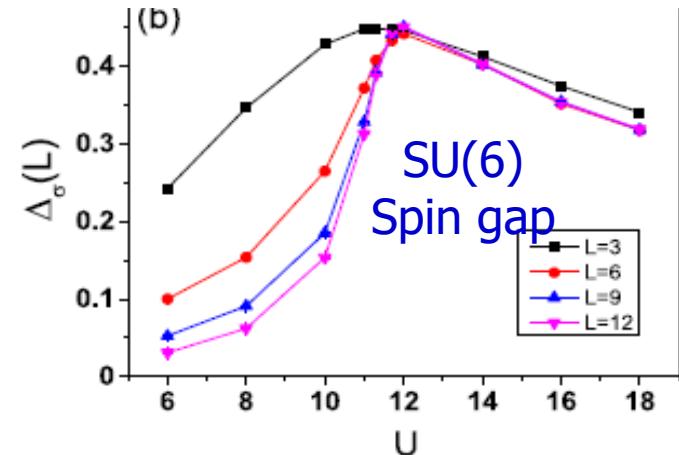
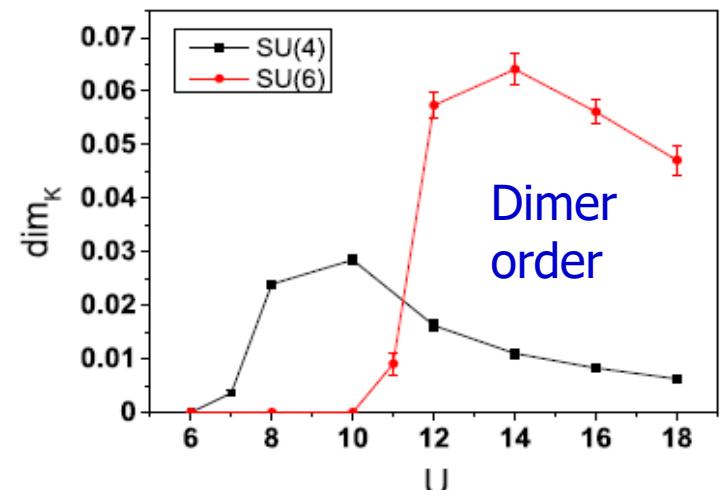
cVBS:

$$\arg \psi = 0, \frac{2\pi}{3}, \frac{4\pi}{3}$$

pVBS:

$$\arg \psi = \pi, \frac{\pi}{3}, \frac{5\pi}{3}$$

$$f_A(\psi, \psi^*) = r_2 |\psi|^2 - r_3 (\psi^{*3} + \psi^3) + r_4 |\psi|^4.$$



Z. C. Zhou, D. Wang, Zi Yang Meng, Yu Wang, **CW**, Phys. Rev. B 93, 245157 (2016).

Hong Yao et al, Nature Communications 8, 314 (2017)

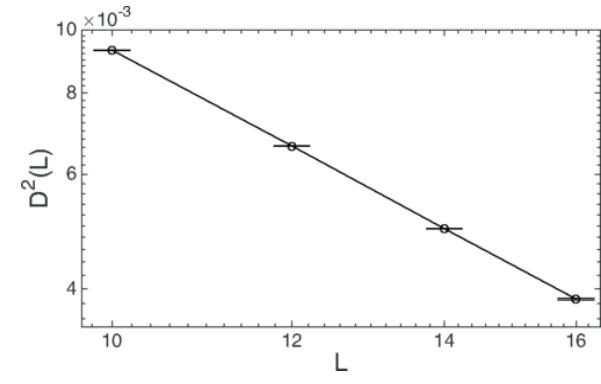
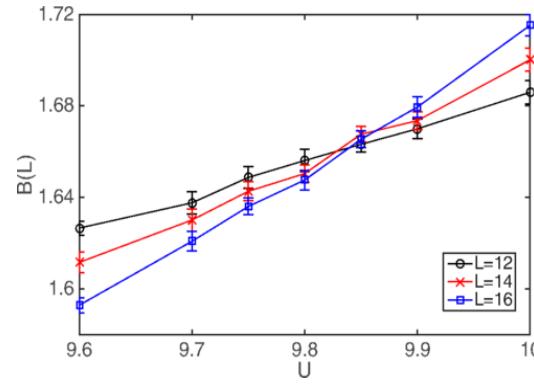
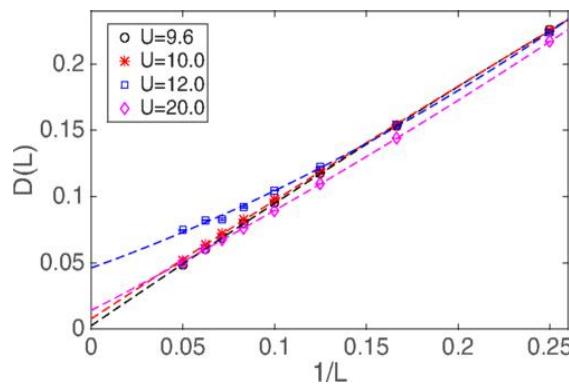
SU(4) Hubbard model (π -flux square lattice)

- Absence of the AF order at until $U \leq 20$, but expect to appear at $U \rightarrow \infty$
- VBS order appears at $U_c \approx 9.8 \sim 9.9$ via Binder ratio scaling. Non-monotonic dependence on U .

$$B_{1,2}^{x,y} = \chi_{x,y}(L, Q_{x,y}) / \chi_{x,y}(L, Q_{x,y} + \Delta q_{1,2})$$

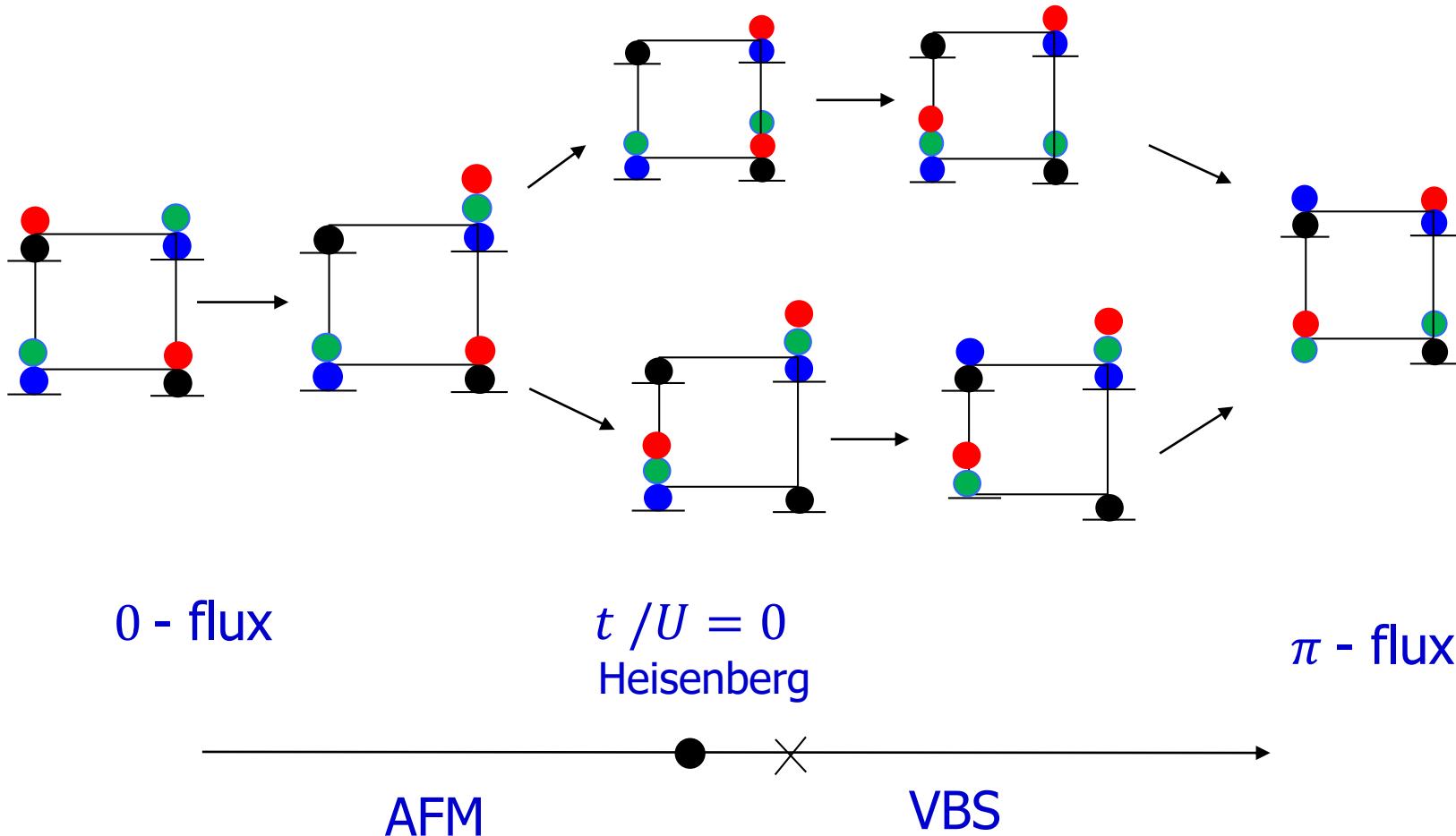
- Anomalous dimension via structural factor scaling

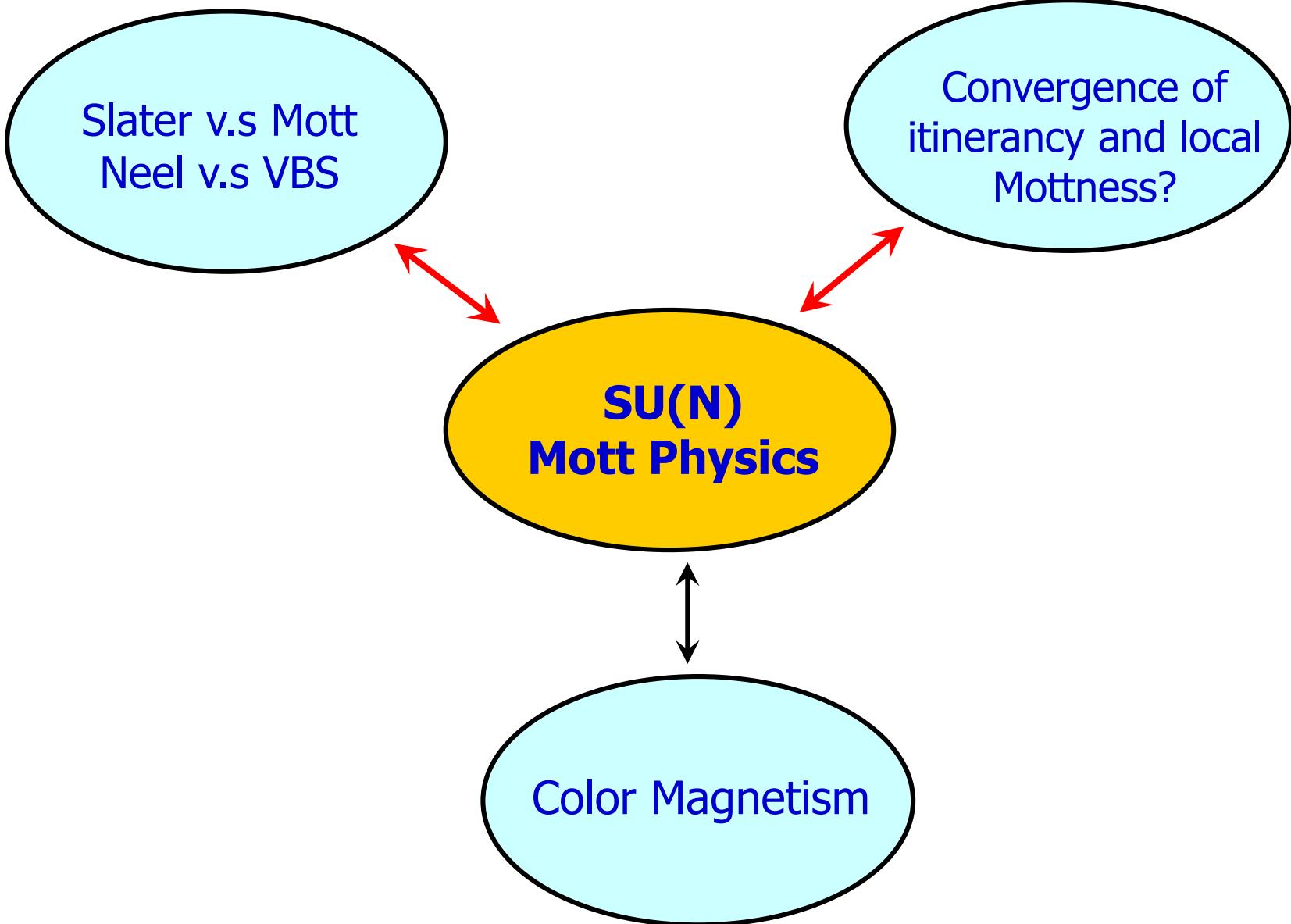
$$D^2(L) = L^{-z-\eta} f\left(|U - U_c| L^{\frac{1}{\nu}}\right) \rightarrow z + \eta = 1.86 \pm 0.04$$



Ring exchange

- Difference between 0 and π -flux SU(4) Hubbard model starts from the ring-exchange process: the order of t^4/U^3 .



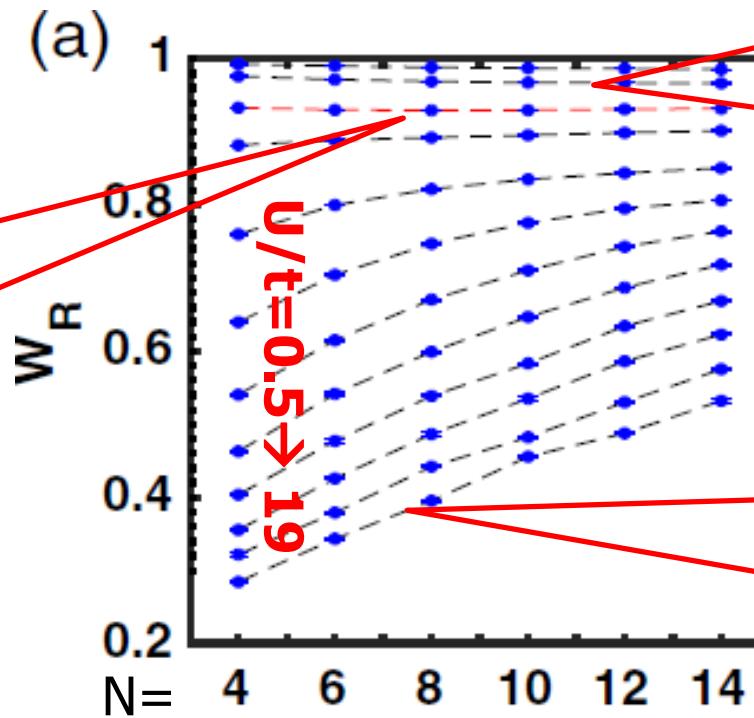


Convergence of itinerancy and locality

1D half-filled SU(N) Hubbard model: QMC study

relative band width: $W_R = \langle E_K(U) \rangle / \langle E_k^0 \rangle$

Hint:
an interacting
large-N limit?



weak coupling:
enhancement of
collision as $N \rightarrow \infty$

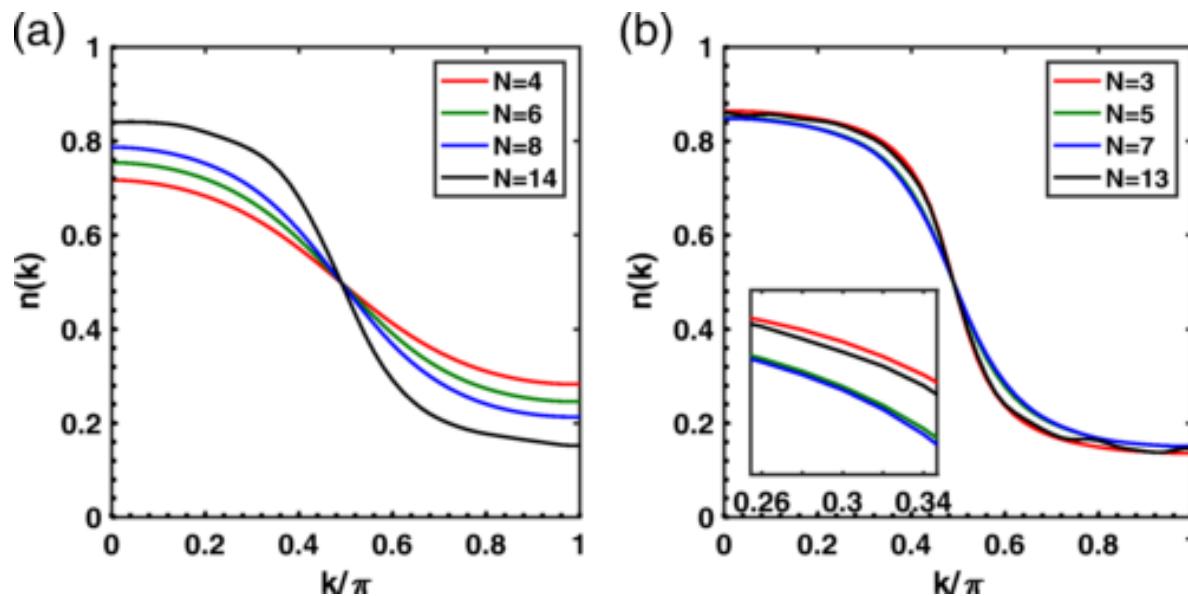
$$\frac{\Delta E_k}{N} \approx (N - 1)U$$

strong coupling:
softening of
Mottness

$$\frac{\Delta E_k}{N} \approx -Nt^2/U$$

Fermi distribution in the strong coupling regime

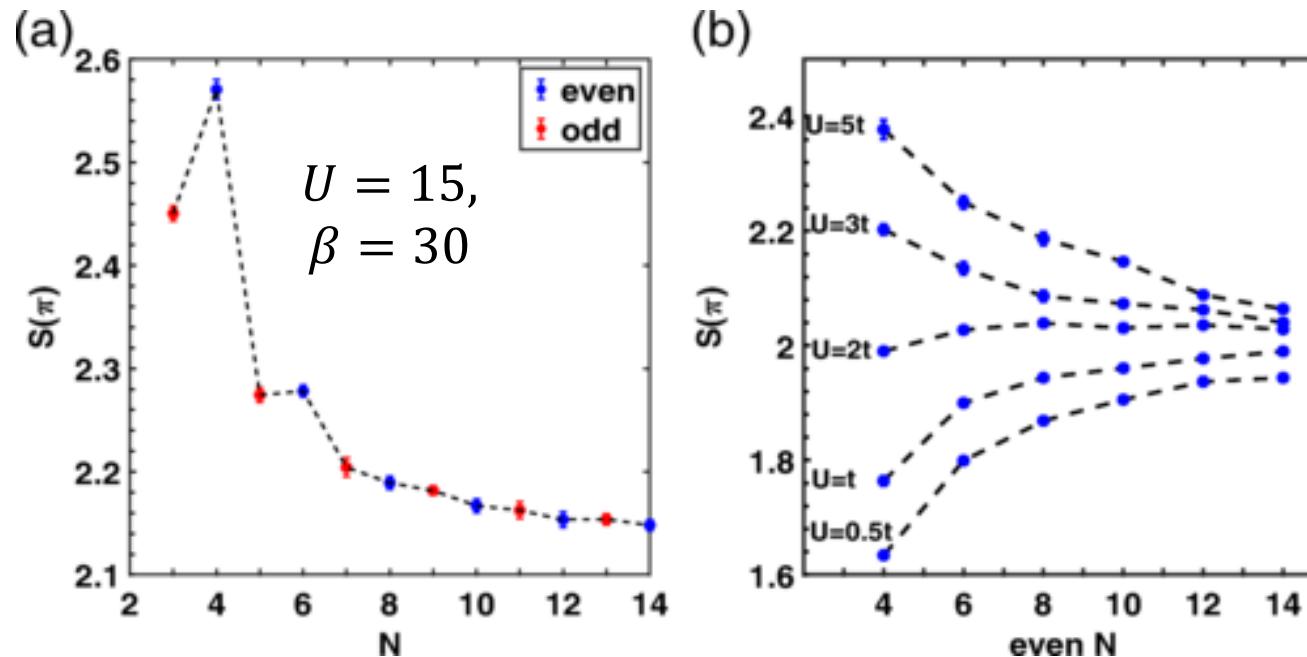
- Sharpening $n_f(k)$ as N (even) increases
- $n_f \neq$ the ideal Fermi distribution as $N \rightarrow \infty$

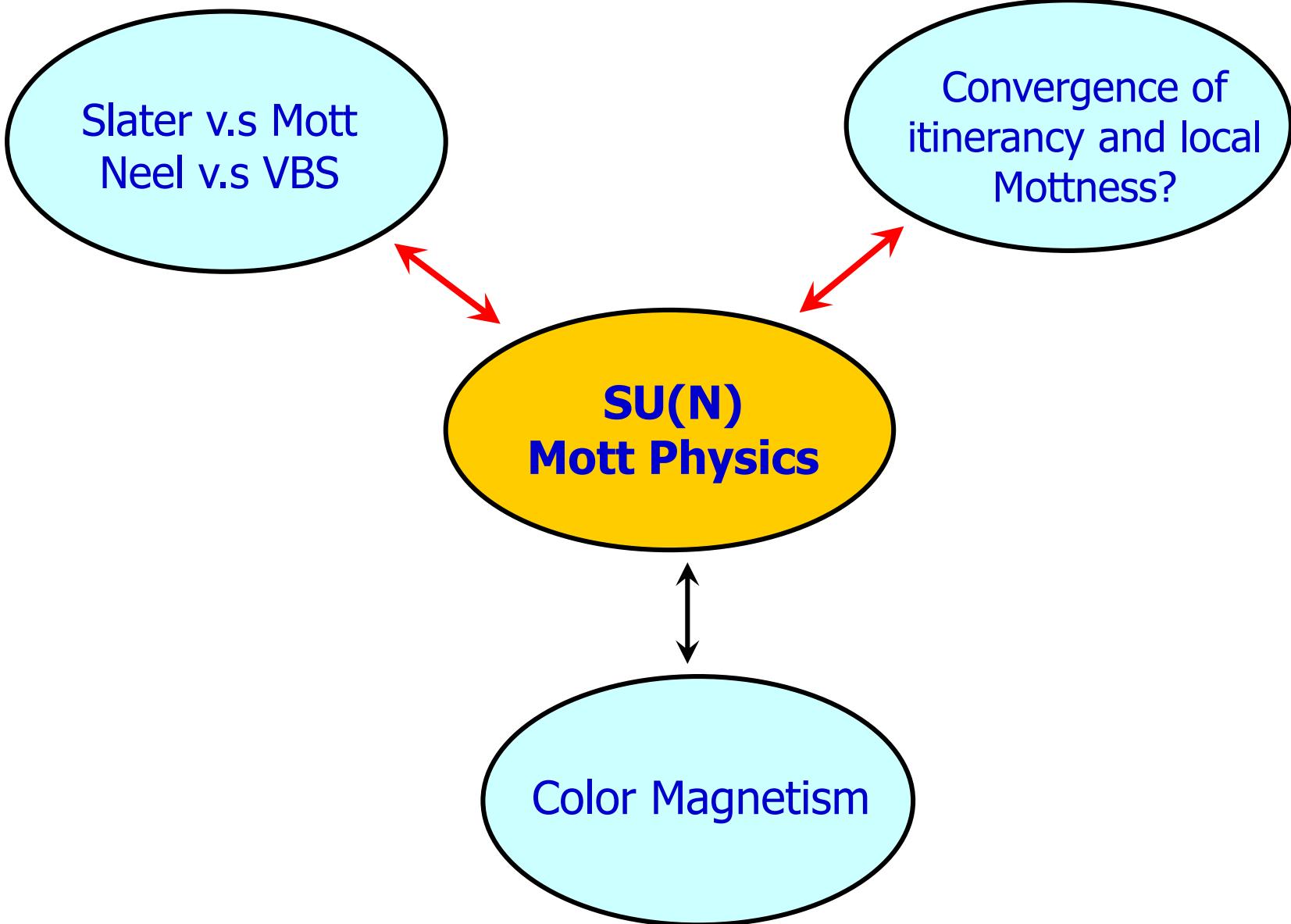


$$U = 15, \quad \beta = 30$$

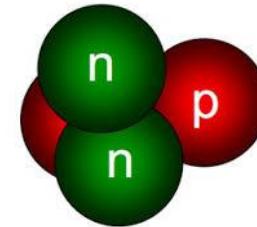
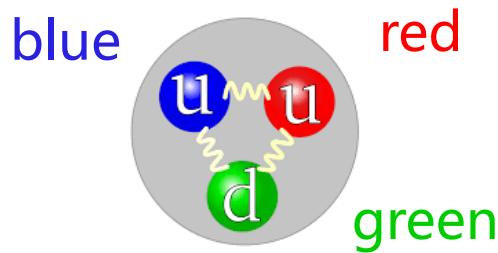
The AF structure factor

- Opposite dependences of $S(\pi)$ on N from the strong (local moment) and weak (itinerancy) interaction regimes.





$\frac{1}{4}$ -filling of SU(4) -- “color magnetism”



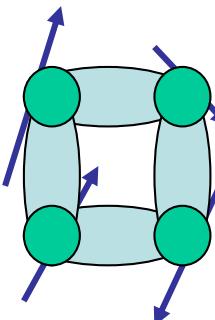
高能: 重子 (质子) -
3夸克色单态

核物理: α -粒子 (两
质子, 两中子)。

- 4 sites → an SU(4) singlet (Each site belongs to the fundamental Rep.)

baryon-like
$$\frac{\epsilon_{\alpha\beta\gamma\delta}}{4!} \psi_\alpha^+(1) \psi_\beta^+(2) \psi_\gamma^+(3) \psi_\delta^+(4) |0\rangle$$

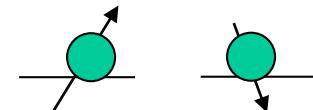
Bossche et. al., Eur. Phys. J. B 17, 367 (2000).



Sp(4) Heisenberg model at 1/4-filling

- Spin exchange: bond singlet (J_0), quintet (J_2).

$$H_{ex} = \sum_{\langle ij \rangle} -J_0 Q_0(ij) - J_2 Q_2(ij)$$



$$J_0 = 4t^2 / U_0, J_2 = 4t^2 / U_2, J_1 = J_3 = 0 \quad \frac{3}{2} \times \frac{3}{2} = \textcolor{red}{0+2+1+3}$$

- SO(5) or Sp(4) explicitly invariant form:

$$H_{ex} = \sum_{ij} \frac{J_0 + J_2}{4} L_{ab}(i)L_{ab}(j) + \frac{-J_0 + 3J_2}{4} n_a(i)n_b(j) \quad a, b = 1 \sim 5$$

L_{ab} : 3 spins + 7 spin-octupole tensors; n_a : spin-quadrupole operators;
 L_{ab} and n_a together form the 15 SU(4) generators.

1D lattice (one particle per site)

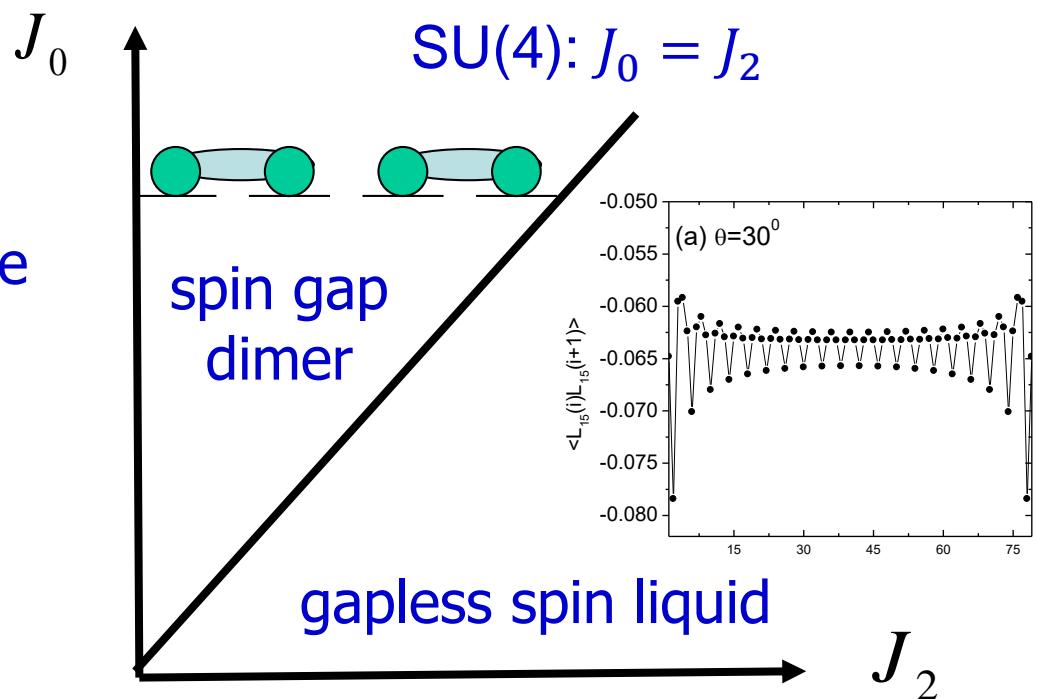
- Phase diagram obtained from bosonization + DMRG.

- Gapped spin dimer phase

at $J_0 > J_2$.

- Gapless spin liquid phase
at $J_0 \leq J_2$.

- Spin correlation exhibits
4-site periodicity of
oscillations.



Sp(4) magnetism: a four-site problem

- Bond spin singlet:

- Plaquette SU(4) singlet:

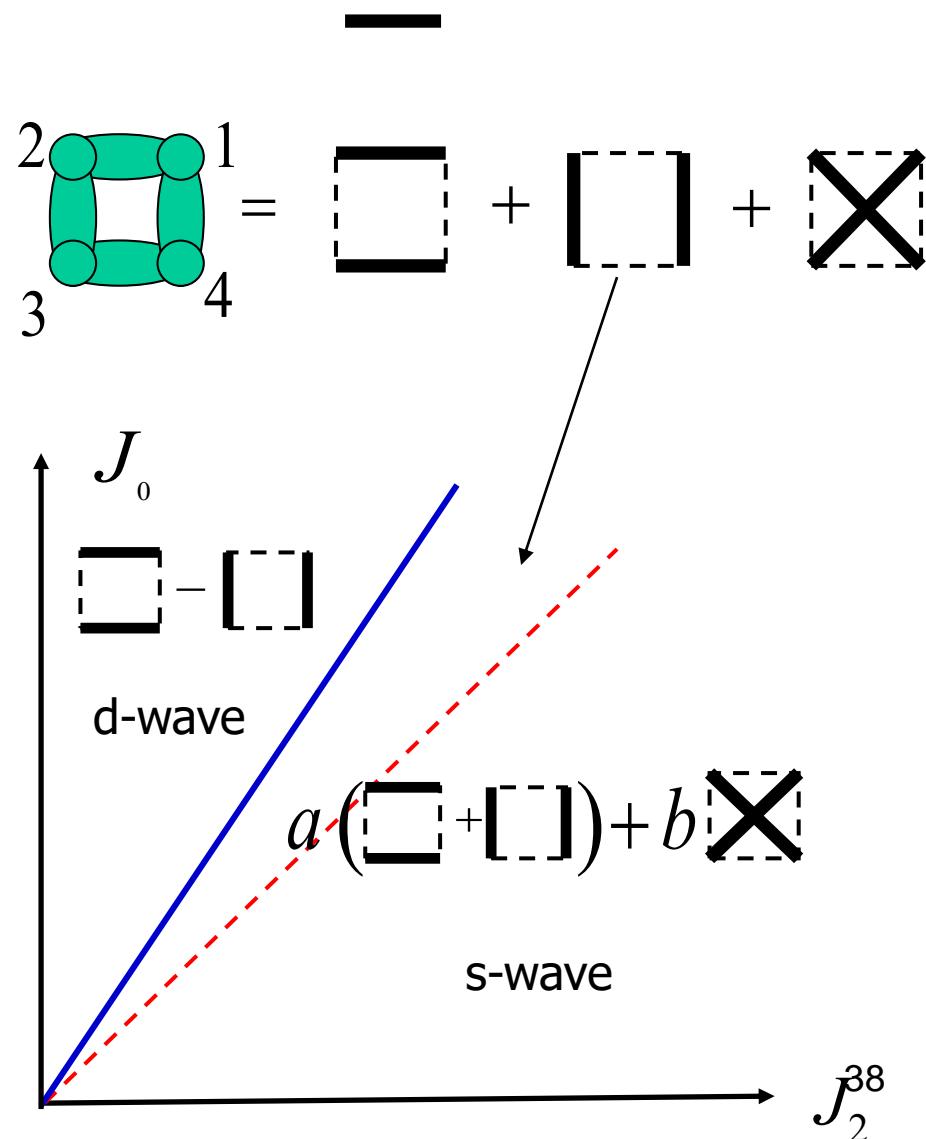
$$\frac{\epsilon_{\alpha\beta\gamma\delta}}{4!} \psi_\alpha^+ \psi_\beta^+ \psi_\gamma^+ \psi_\delta^+ |0\rangle$$

4-body EPR state; no bond orders

- Level crossing:

d-wave to s-wave

- Hint to 2D?



Unsolved difficulty: 2D phase diagram

- $J_2=0$, Neel ordering obtained by QMC.

K. Harada et. al. PRL 90, 117203, (2003).

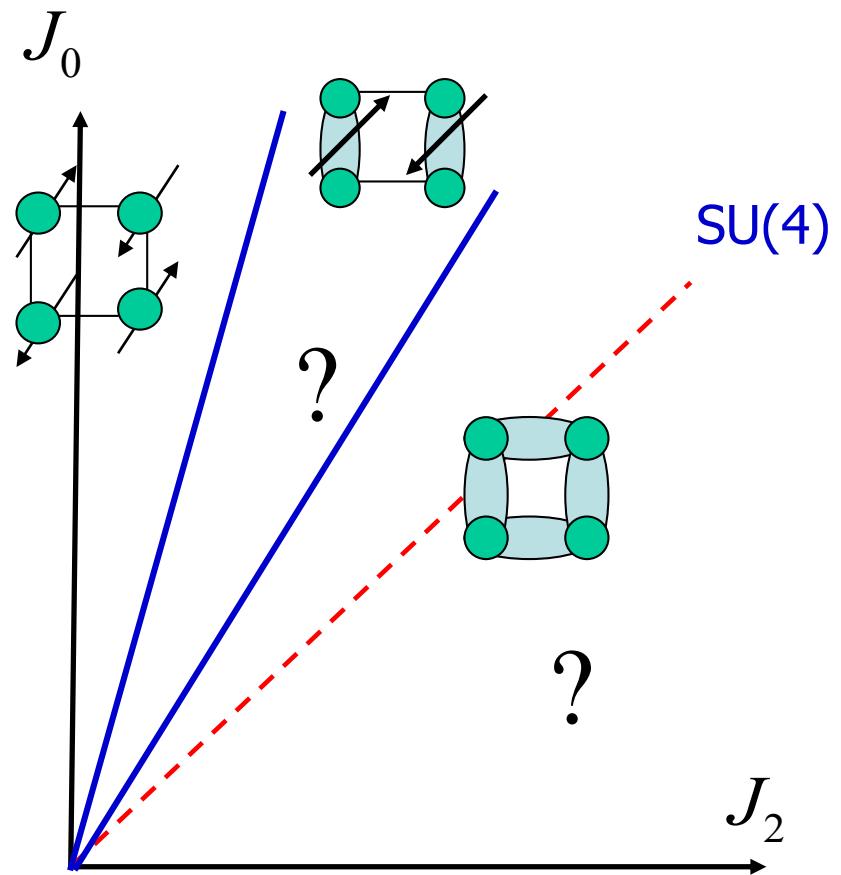
- $J_2>0$, no conclusive results!
Difficult both analytically and numerically.

2D Plaquette ordering at
the SU(4) point?

Exact diagonalization on a 4×4
lattice

Bossche et. al., Eur. Phys. J. B 17, 367 (2000).

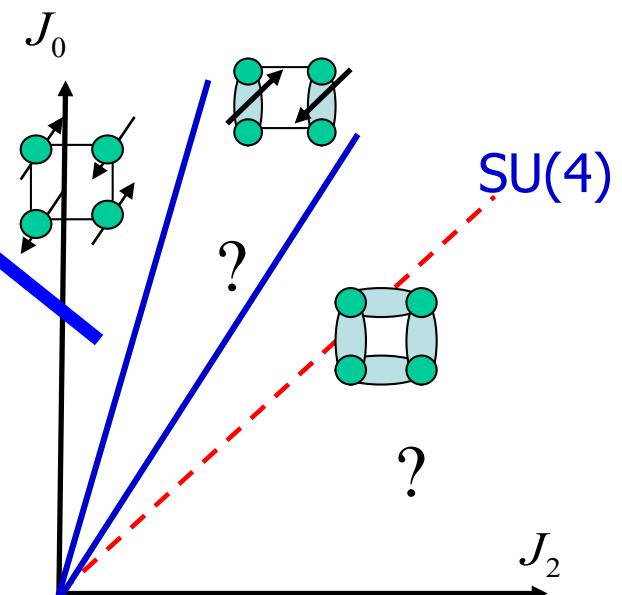
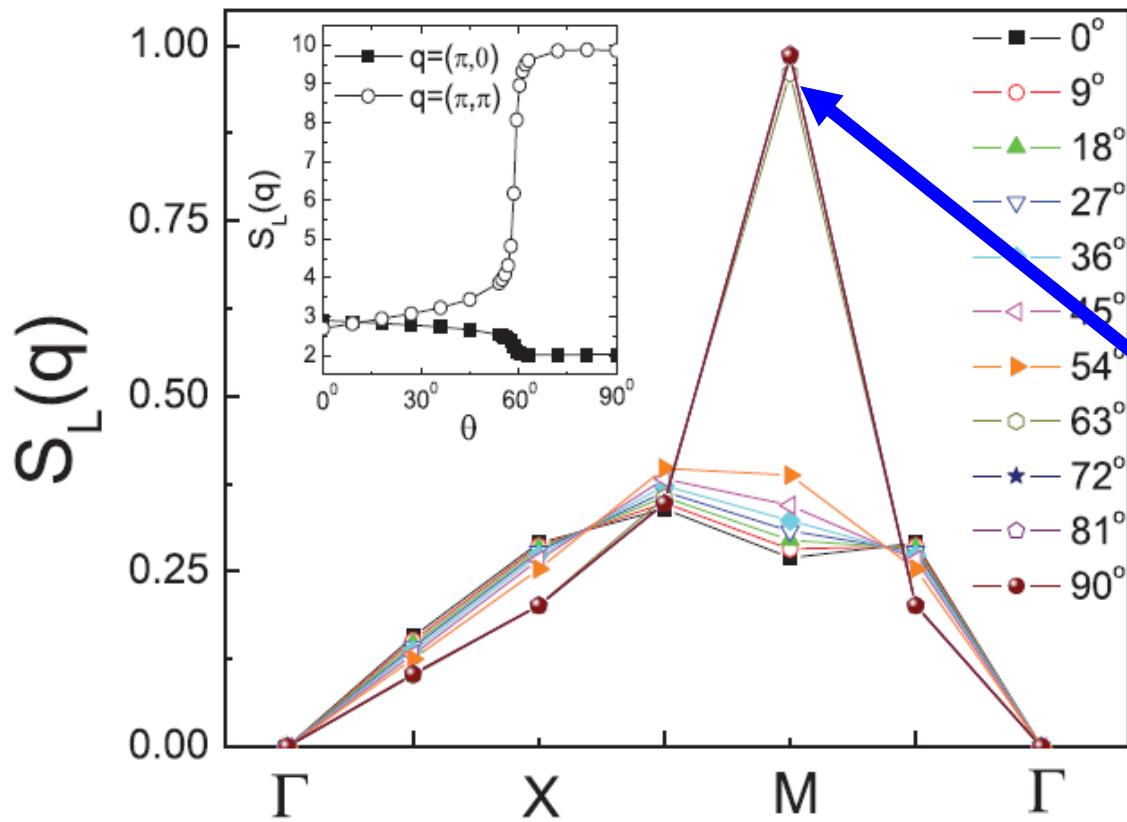
- Phase transitions as J_0/J_2 ?



4x4 Exact diag. (I): Neel correlation

- Spin structure form factor peaks at (π, π) at $\theta > 60^\circ$, indicating strong Neel correlation.

$$S_L(q) \sim \sum_{1 \leq a < b \leq 5} \sum_{i,j} \langle L_{ab}(i)L_{ab}(j) \rangle e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)}$$

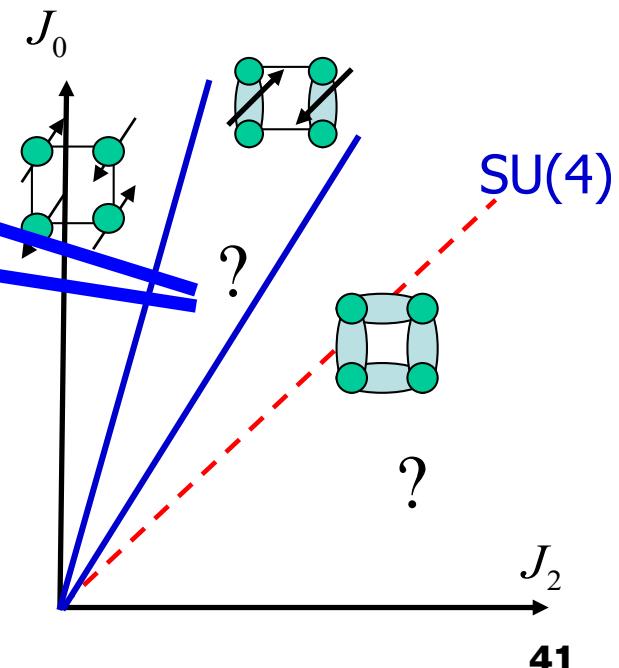
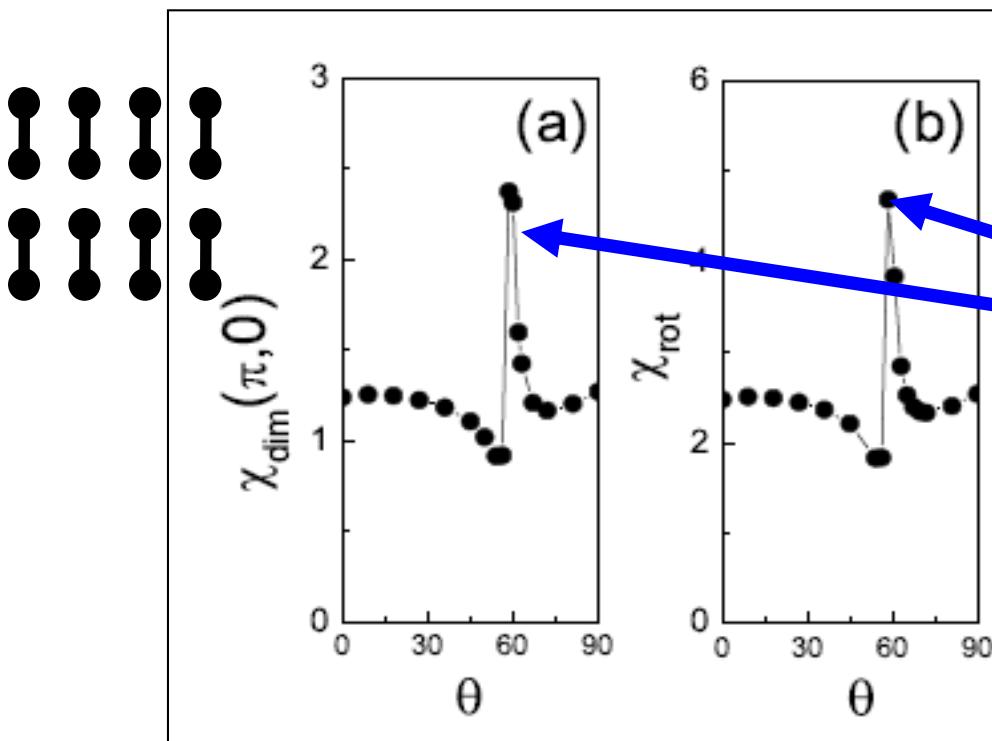


40

4x4 Exact Diag. (II): Dimer correlation

- Susceptibility: $H(\delta) = H_{exc} + \delta * H_{pert}$ $E(\delta) = E(0) - \frac{1}{2} \chi \delta^2,$
- a) Break translational symm: b) Break rotational symm:

$$H_{pert} = \sum_i \cos(\vec{Q} \cdot \vec{r}_i) H_{ex}(i, i+x), \quad H_{pert} = \sum_i H_{ex}(i, i+x) - H_{ex}(i, i+y)$$



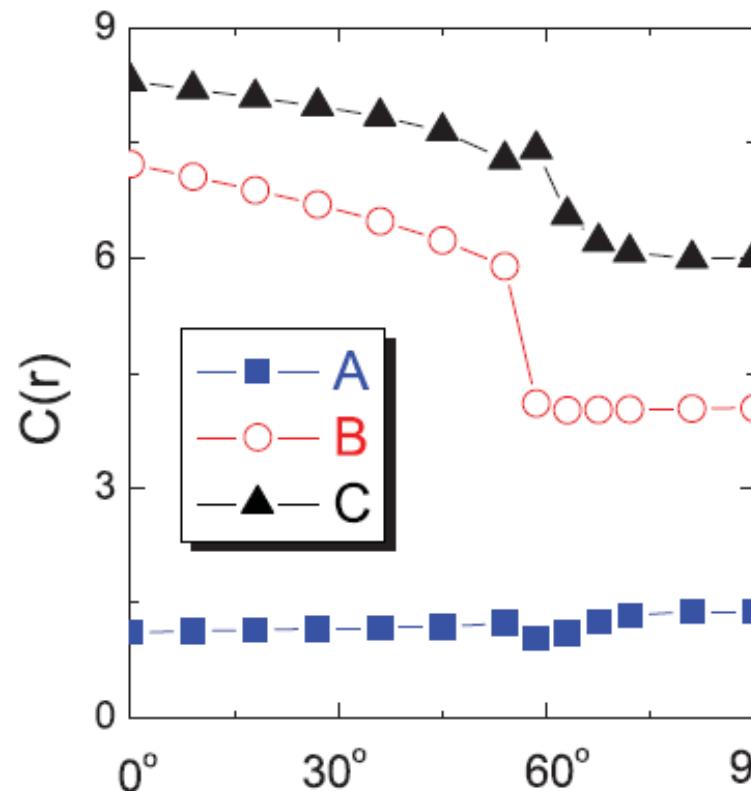
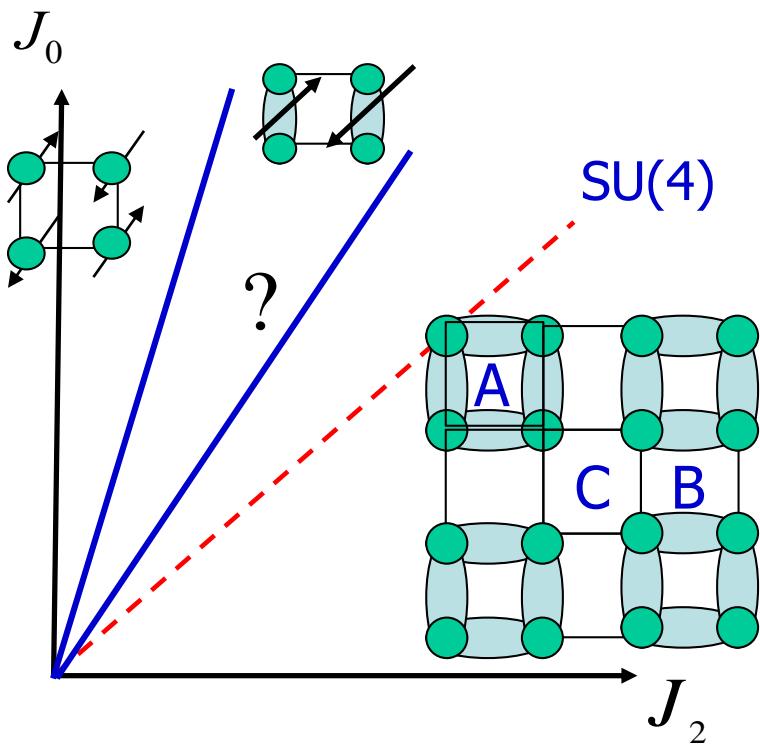
4x4 Exact Diag. (III): Plaquette formation?

- Local Casimir; analogy to total spin of SU(2).

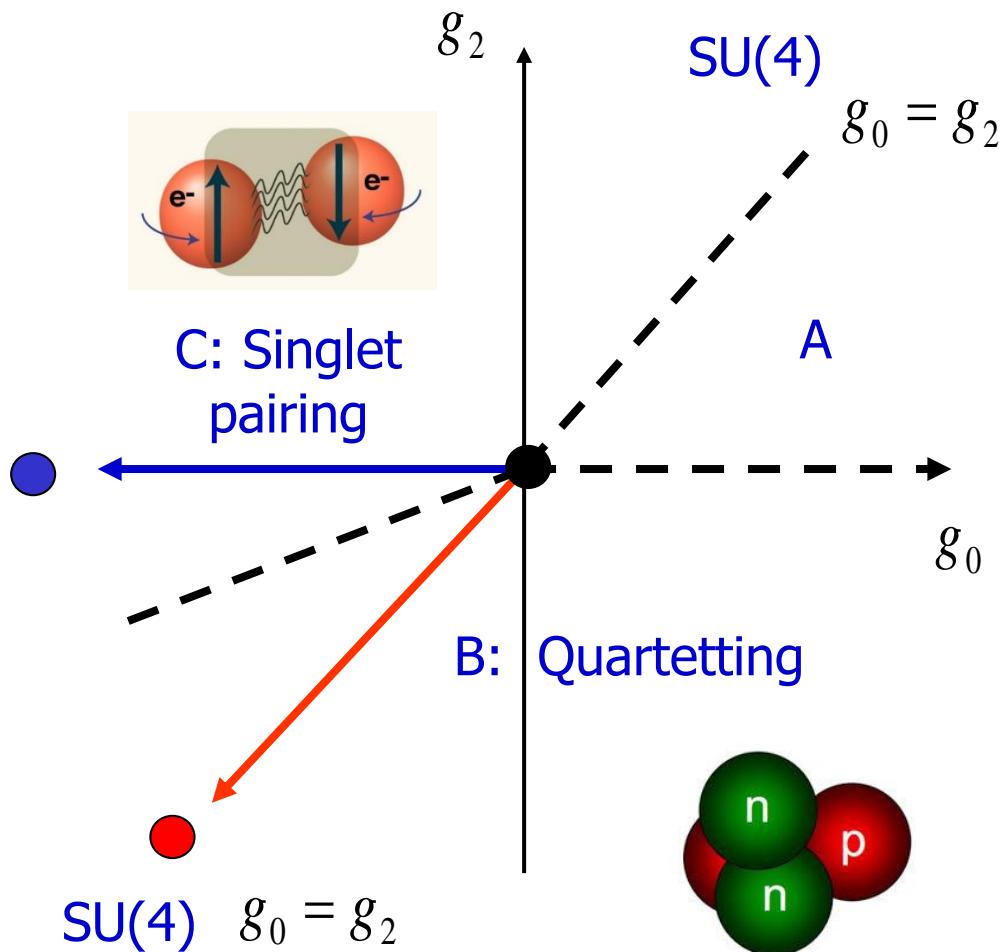
$$C(r) \sim \left\langle \sum_{1 \leq a < b \leq 5} \left\{ \sum_{i \in \text{plaquette } r} L_{ab}(i) \right\}^2 \right\rangle$$

$C(r) \rightarrow 0$: singlet

Open boundary condition



Pairing v.s. quartetting (RG 1 loop)



- (A) Luttinger liquid, spin-charge separation.
- Two spin gap phases: (B) quartetting, (C) pairing.
- Ising duality between (B) and (C).

Digression: itinerant FM based on Hubbard model

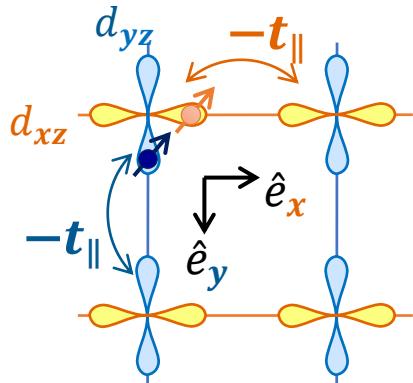
An entire phase of ground state itinerant FM

Y. Li, E. H. Lieb, **CW**, PRL 112, 217201 (2014).

QMC study to Curie-Weiss metal (sign problem-free)

The first proof to our knowledge.

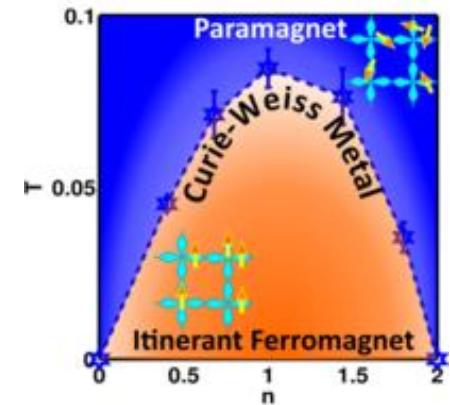
A simple and quasi-realistic model



1. Strong correlation
2. Hund's rule

Mechanism and Experiments

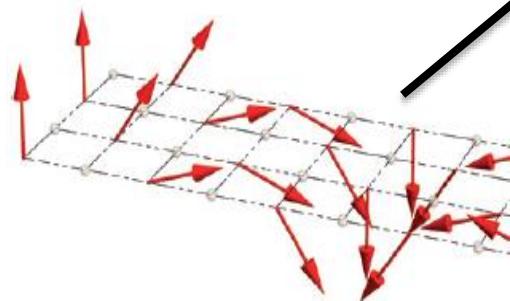
S. Xu, Y. Li, and **CW**, PRX 5, 021032, (2015).



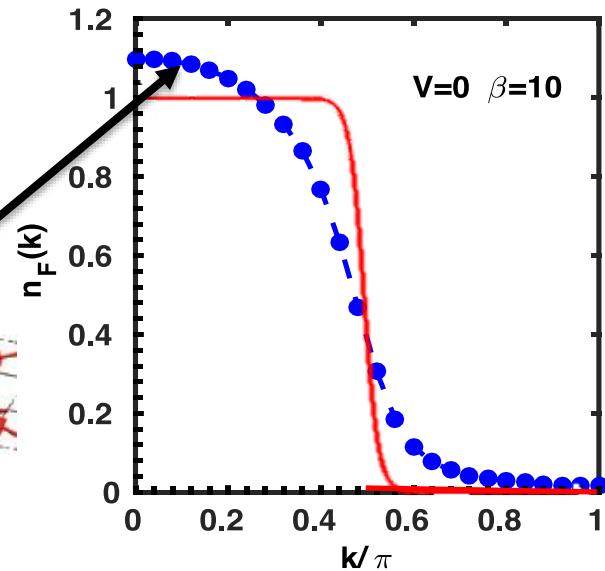
Curie-Weiss susceptibility v.s. metallic compressibility

Momentum space picture for CW metal

Domain fluctuations
c.f. pseudogap phase
of high T_c



$$n_F(k) = n_{\uparrow}(k) + n_{\downarrow}(k)$$



$$T_0/t \approx 0.08$$

At $k \rightarrow 0$, $n_{\uparrow}(k) = n_{\downarrow}(k) \approx 0.54 \ll 1$

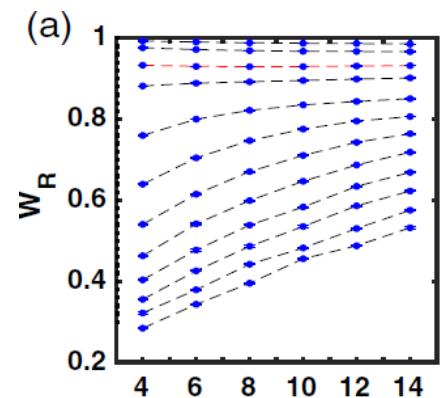
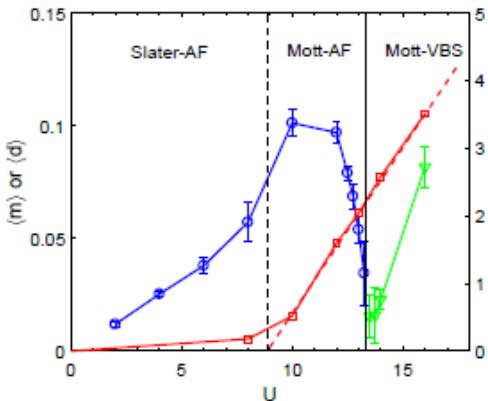
- Exclusion in momentum space $\langle n_{k\uparrow} n_{k\downarrow} \rangle \approx 0$
- Large entropy capacity \rightarrow Wilson ratio $\chi T/C = ?$

Summary

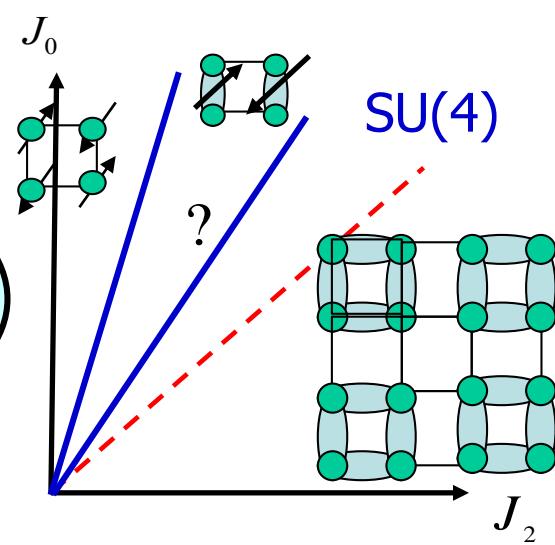
Slater v.s Mott
Neel v.s VBS

Convergence of
itinerancy and local
Mottness?

**SU(N)
Mott Physics**



Color Magnetism

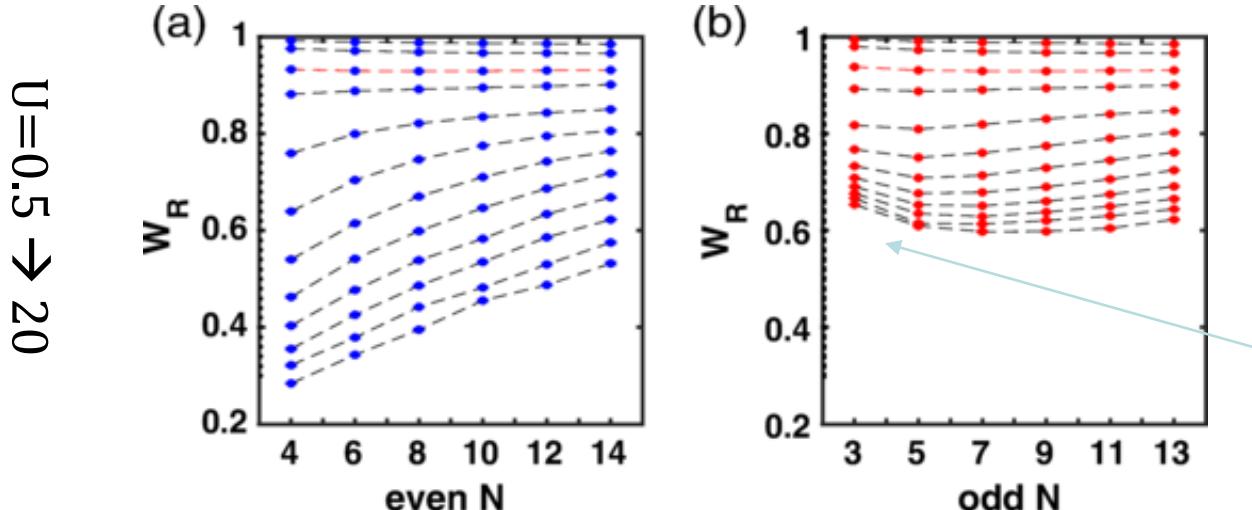


How do interaction effects scale with N?

- 1D SU(N) Hubbard models: U fixed, particle # per site $N/2$, i.e., $(k_f = \pi/2$, half-filling).
- Large U limit \rightarrow softening of Mottness $\rightarrow \frac{\Delta E_k}{N} \approx -Nt^2/U$
Small U limit \rightarrow enhance of collision $\rightarrow \frac{\Delta E_k}{N} \approx (N - 1)U$

- Relative band width:

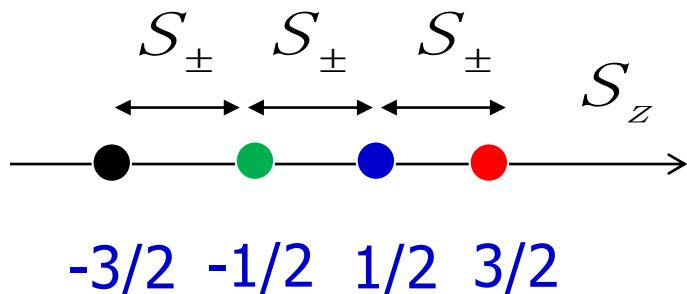
$$W_R = \frac{E_K(U)}{E_K(U = 0)}$$



Preexisting
charge
fluctuation
at odd N's

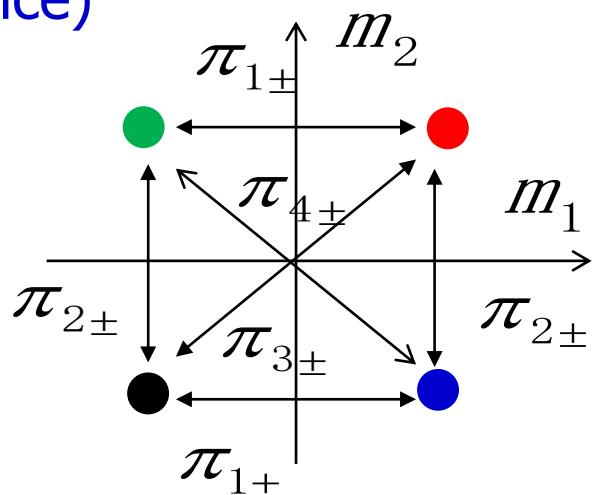
Two views of spin quartet (weight diagrams of Lie algebra)

Solid: SU(2) (1D lattice)



- A high rank spinor Rep. of a small group.
- Off-diagonal operator: (fluctuation) S_{\pm}

Cold fermions Sp(4) or SO(5)
(2D lattice)



- The fundamental spinor Rep of a large group.
- Much more off-diagonal operators.

$$\pi_{1\pm}, \pi_{2\pm}, \pi_{3\pm}, \pi_{4\pm}$$