Revisit of single-hole problem in Mott insulators: A DMRG study

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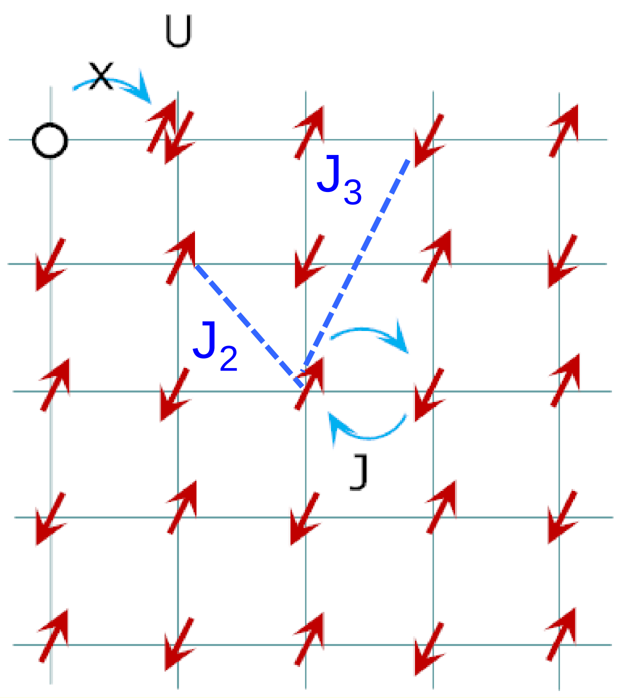
KITP “Frustrated Magnetism and Quantum Spin Liquids”

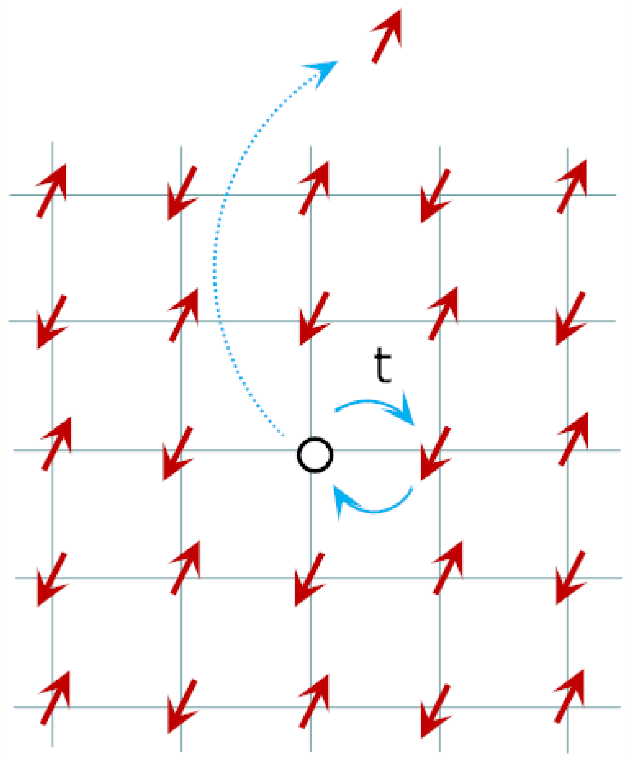
Santa Barbara 2012.10.16

frustrated Mott antiferromagnets



geometric frustrations

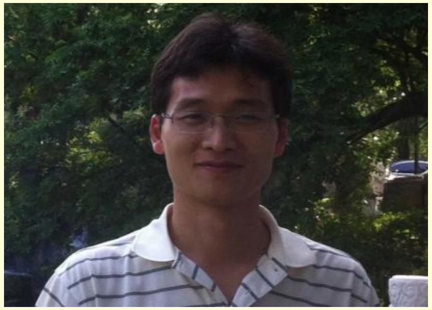
doped antiferromagnets



dynamic frustrations

Collaborators

Zheng Zhu (IAS, Tsinghua)



Hong-Chen Jiang (KITP/UCSB)

Yang Qi (IAS, Tsinghua)

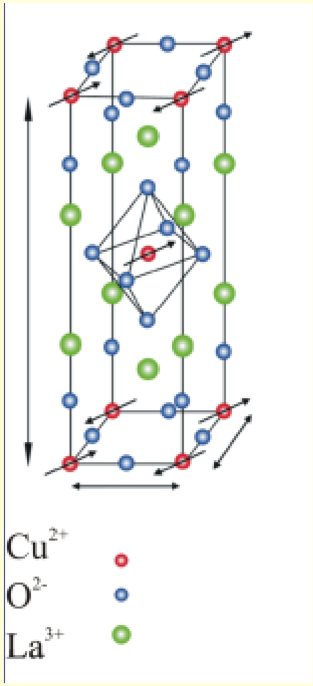
Chushun Tian (IAS, Tsinghua)

Outline

- Overview (after two decades…)
- DMRG results
- Implications

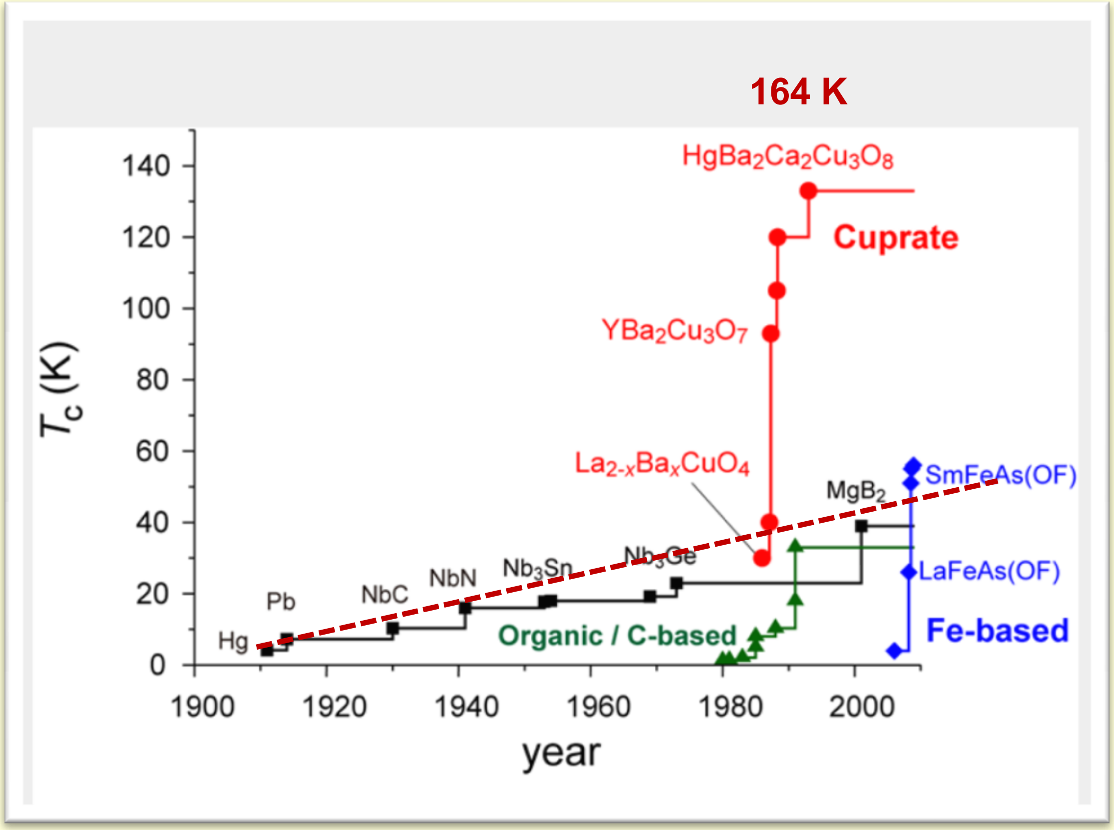
High-T_c cuprates: doped Mott insulators?

Science 1987

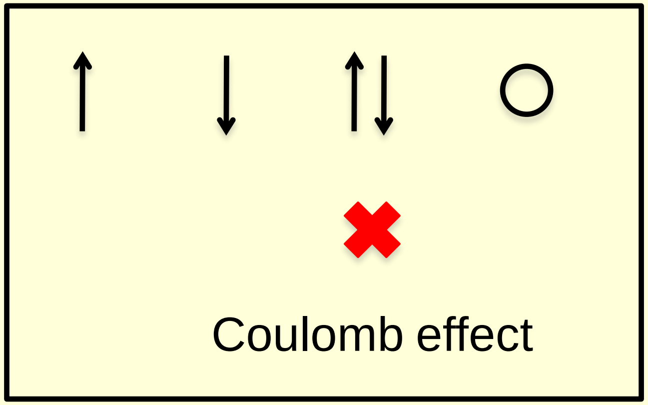


Mueller

Bednorz



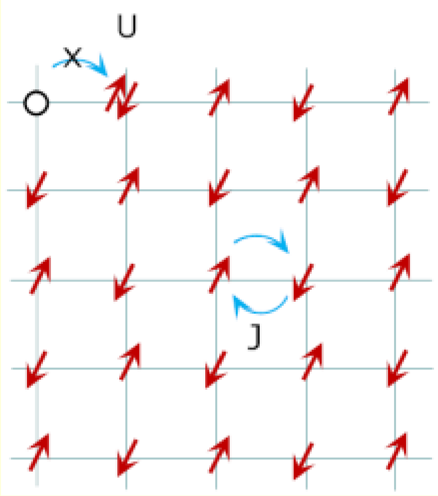
Problem of single hole doped into a Mott insulator



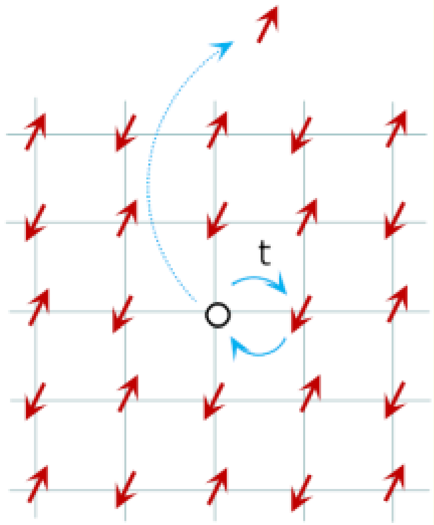
Coulomb effect

Half-filling:

A Mott insulator antiferromagnet



Question: How a single hole behaves?



Theoretical debate in one-hole problem

- Spin polaron picture (self-consistent Born approximation)

  S. Schmitt-Rink, C. M. Varma, and A. E. Ruckenstein (1988);

  C. L. Kane, P. A. Lee, and N. Read (1989); ….

  → Quasiparticle

- ED result

  P.W. Leung and R. J. Gooding (1995);…

  → Quasiparticle

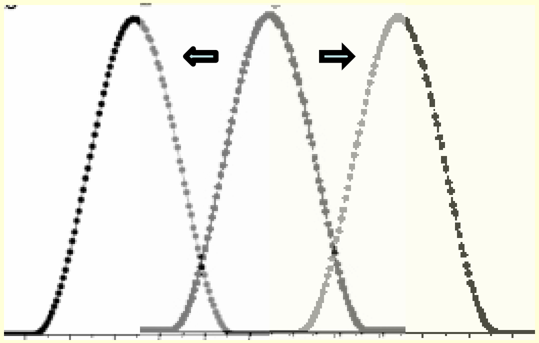
- P. W. Anderson's unrenormalizable phase shift argument (1990)

  → Non-quasiparticle

- Phase string effect *(D.N. Sheng, Y. C. Chen, ZYW (1996))*

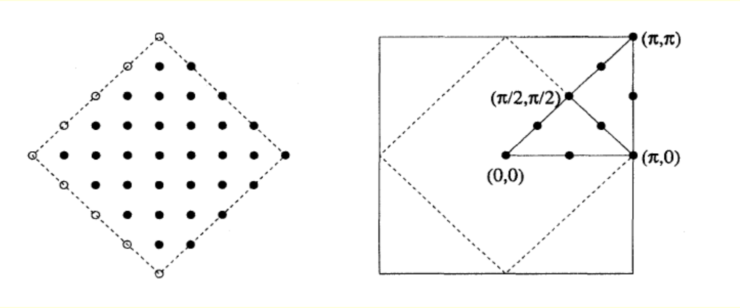
  → Localization (non-quasiparticle) (ZYW, et al. (2001))

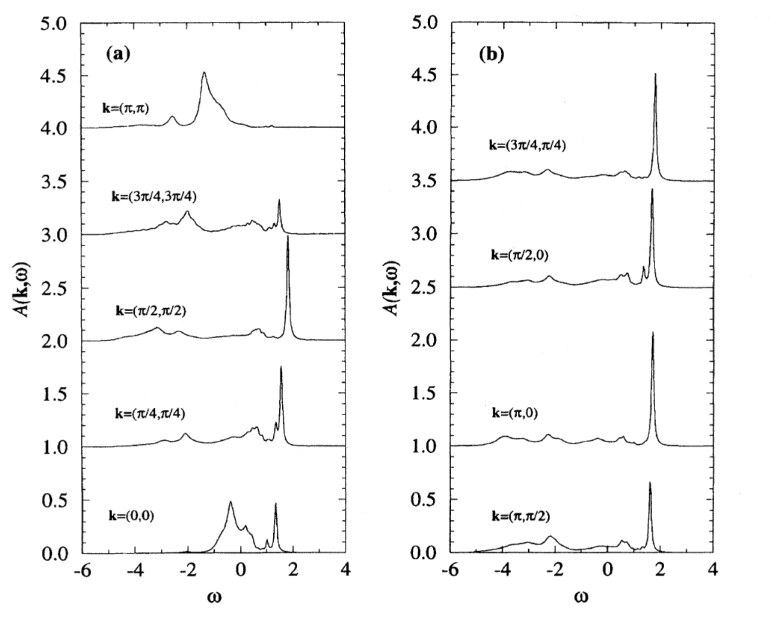
Quasiparticle (spin-polaron) picture



Bloch theorem holds
for a many-body system?

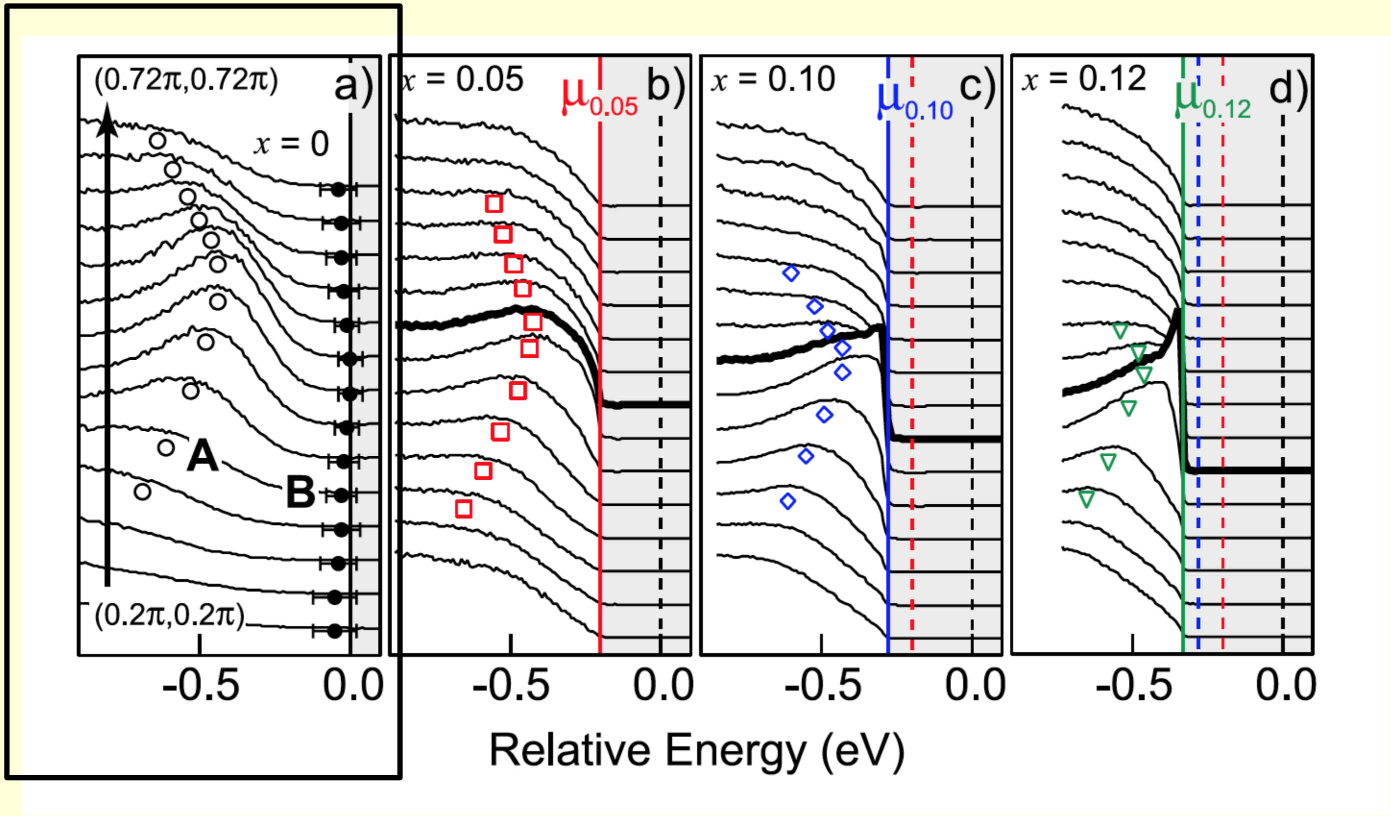
S^z (Ising)-strings can be destroyed by quantum spin flips (*C. L. Kane, P. A. Lee, and N. Read (1989)*)

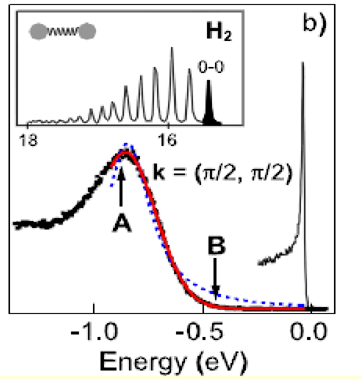




P.W. Leung and R. J. Gooding (1995)

ARPES result: A broad peak at x=0





$Ca_2CuO_2Cl_2$

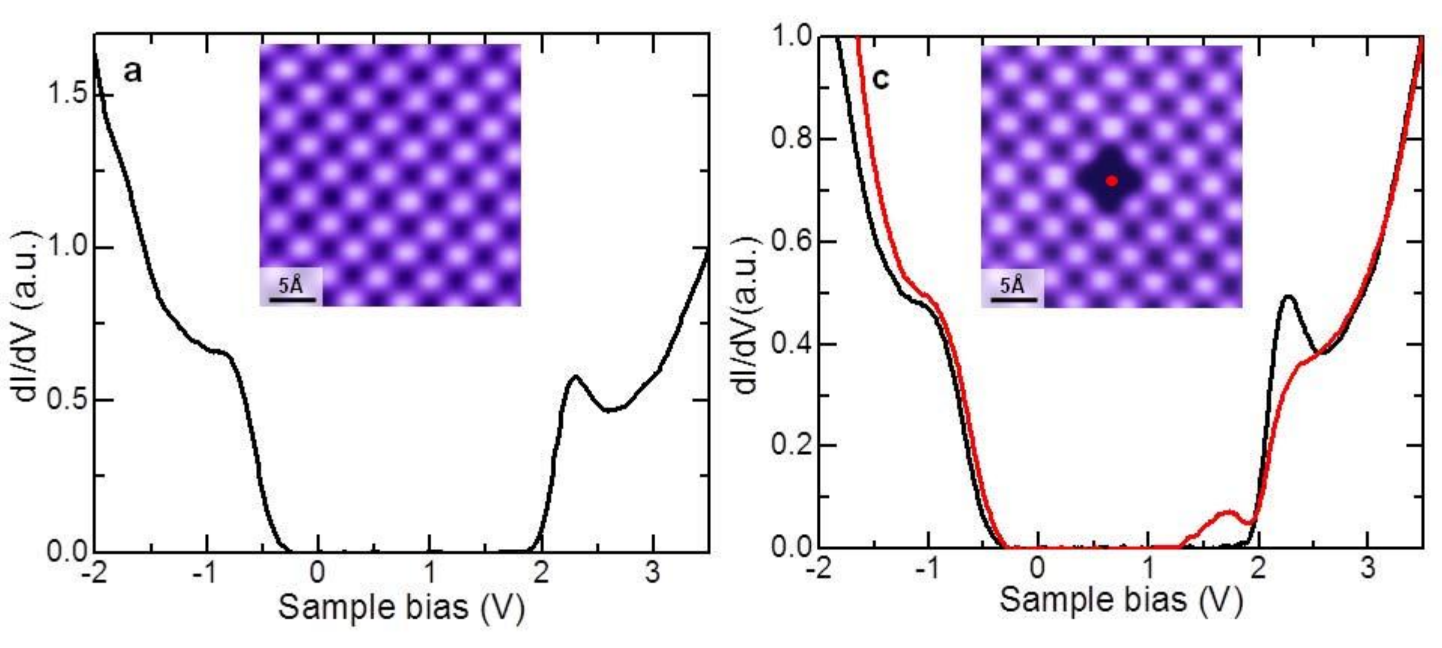
K. M. Shen et al, PRL 93, 267002 (2004)

Experimental Results (STM)

Localization

C. Ye, et. al., arXiv:1201.0342v1
(Yayu Wang's group in Tsinghua)

$Ca_2CuO_2Cl_2$



Strong localization of a single electron donated by a Cl defect

Theoretical debate in one-hole problem

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  → Quasiparticle

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  P.W. Leung and R. J. Gooding (1995);…

  → Quasiparticle

- P. W. Anderson’s unrenormalizable phase shift argument (1990)

  → Non-quasiparticle

- Phase string effect *(D.N. Sheng, Y. C. Chen, ZYW (1996))*

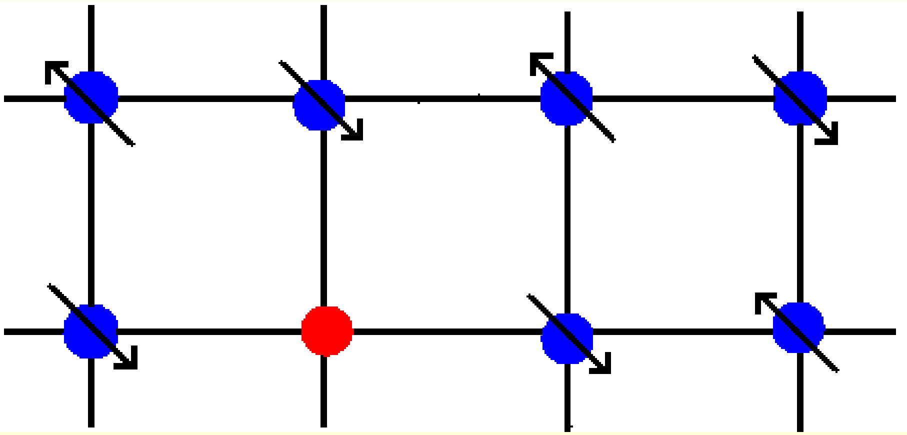
  → Localization (non-quasiparticle) (ZYW, et al. (2001))

A minimal model for doped Mott insulators: t-J model

$$H = -t\sum_{\langle ij\rangle}\left(c^\dagger_{i\sigma}c_{j\sigma} + h.c.\right) + J\sum_{\langle ij\rangle}\left(\mathbf{S_i}\cdot\mathbf{S_j} - \frac{1}{4}n_i n_j\right)$$

hopping

superexchange



constrained by

$$\sum_{\sigma} c^{+}_{i\sigma} c_{i\sigma} \leq 1$$

1-hole propagator : Phase string effect

$$G(j,i,E) = \langle \psi_0 | c^\dagger_{js} G(E) c_{is} | \psi_0 \rangle \propto \sum_c \tau_c W[c;E]$$

$$G(E) = \frac{1}{E - H_{t-J} - 0^+}$$

$$\tau_c \equiv (+1) \times (-1) \times (-1) \times \ldots\ldots$$

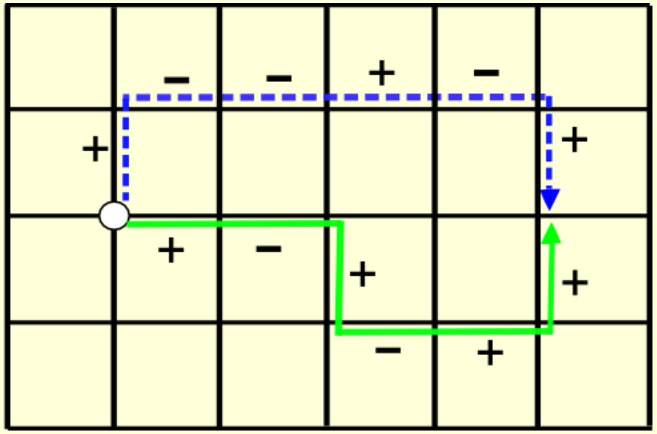
$$= (-1)^{N_h^{\downarrow}(c)}$$

$$W[c;E] = \left(\frac{t}{-E}\right)^{M_h} \left(\frac{J}{-2E}\right)^{M_{\uparrow\downarrow}+M_Q} \geq 0$$

Partition function :

$$Z = \sum_{\text{loop c}} \tau_c W(c)$$

$$W(c) = \underbrace{\frac{2t}{J} \times \frac{2t}{J} \cdots \frac{2t}{J}}_{M_h(C)} \sum_n \frac{(\beta J/2)^n}{n!} \delta_{M_h+M_{\uparrow\downarrow},n} \geq 0$$



D.N. Sheng, Y.C. Chen, ZYW, PRL (1996); K. Wu, ZYW, J. Zaanen, PRB (2008)

Removing the phase string: A sign-free model

$$H = -t \sum_{\langle ij \rangle} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + h.c. \right) + J \sum_{\langle ij \rangle} \left(\mathbf{S_i} \cdot \mathbf{S_j} - \frac{1}{4} n_i n_j \right)$$

σ

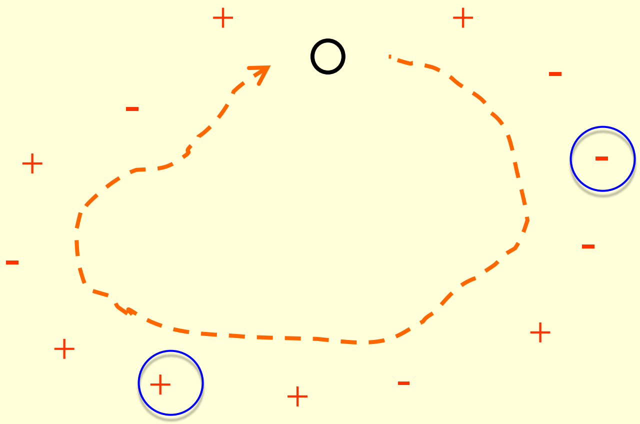
$$Z = \sum_{loop\ c} \tau_c W(c)$$

$$\boxed{\tau_c \equiv 1}$$

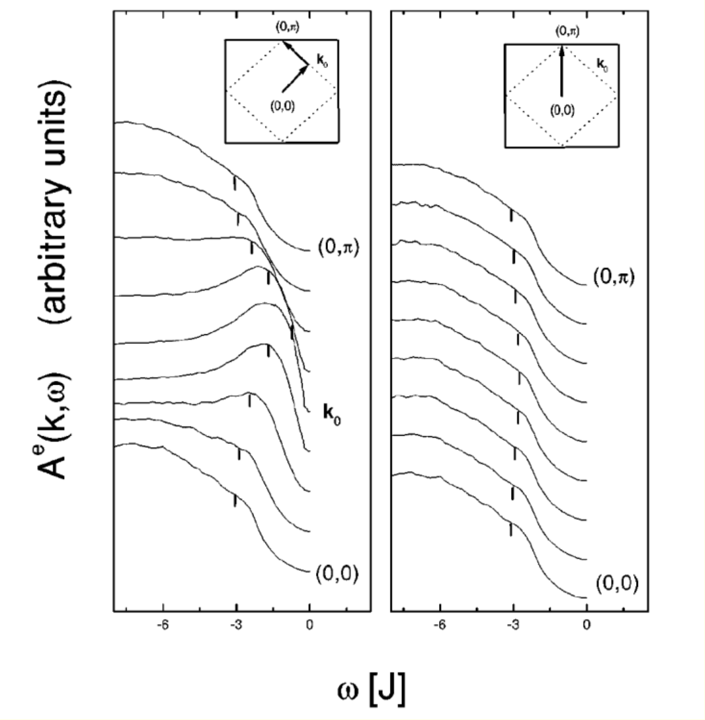
for one-hole case

$$W(c) = \underbrace{\frac{2t}{J} \cdot \frac{2t}{J} \cdots \frac{2t}{J}}_{M_h(C)} \sum_n \frac{(\beta J/2)^n}{n!} \delta_{M_h + M_-, n} \geq 0$$

Prediction: self-localization of the one-hole



AFM state



ZYW, V. N. Muthukumar, D.N. Sheng, C.S. Ting (2001)

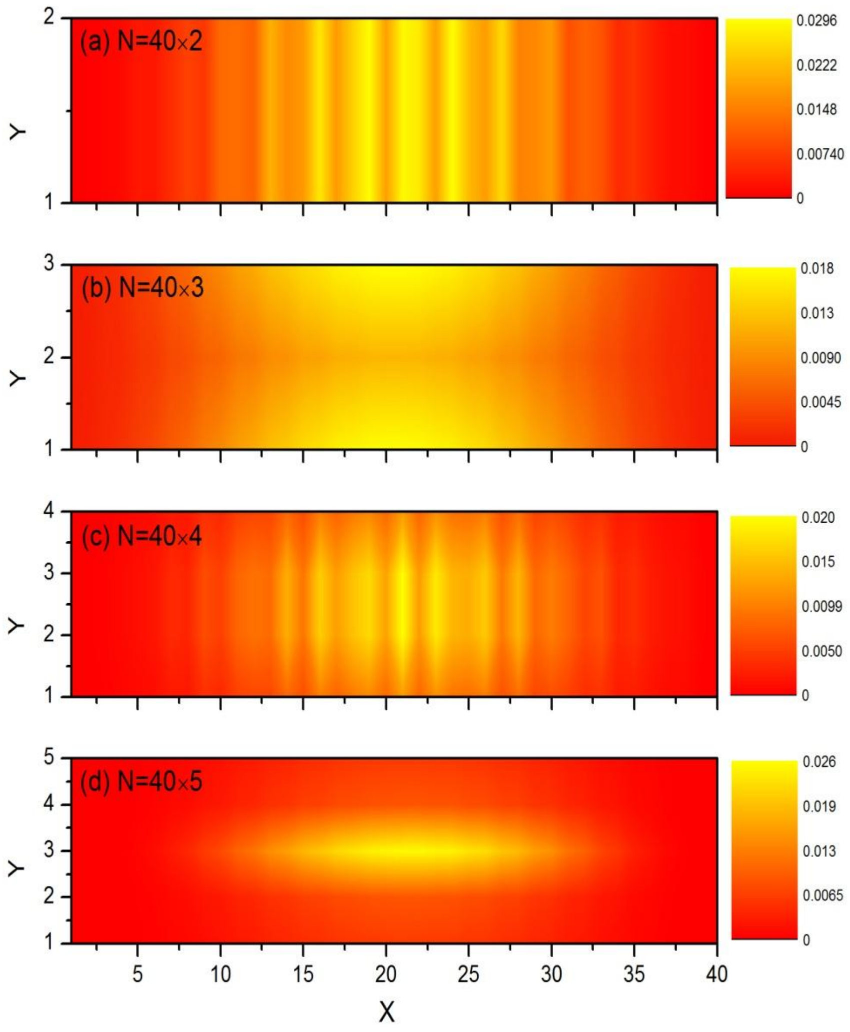
Holon localization at low doping: S.P. Kou, ZYW, PRL (2003)

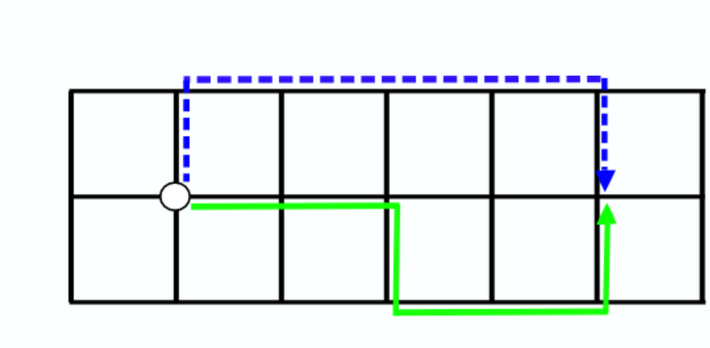
P. Ye and Q.R. Wang, arXiv:1206.0258

DMRG results

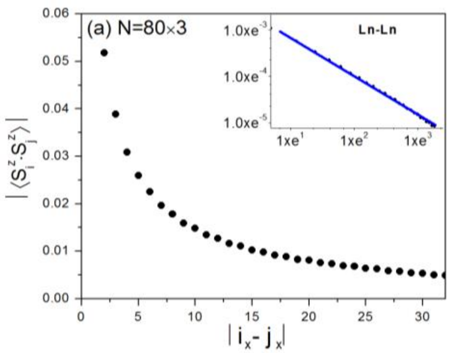
Real space distribution of a single hole in t-J ladders

Z. Zhu, H.C. Jiang, Y. Qi, C.S.Tian, ZYW (2012)

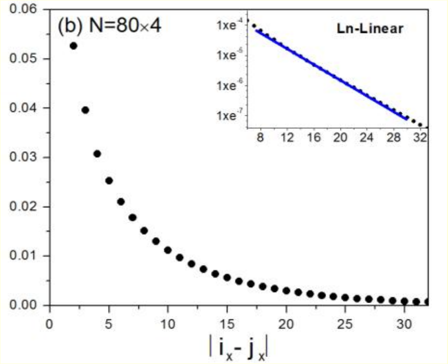




t-J ladders: $t = 3J$

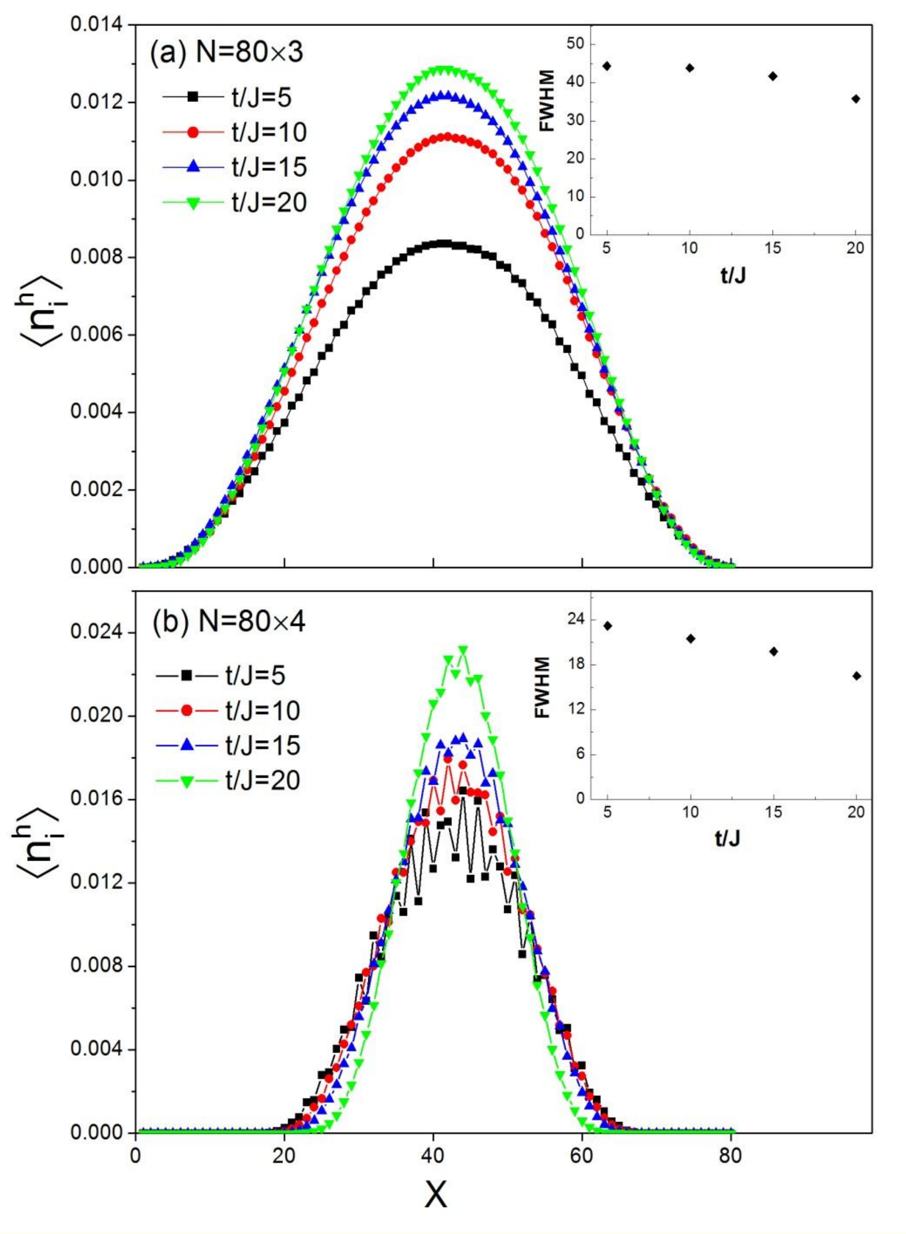


odd (3-legs)



even (4-legs)

Localization with the ratio t/J



$$\sum_i \langle n_i^h \rangle = 1$$

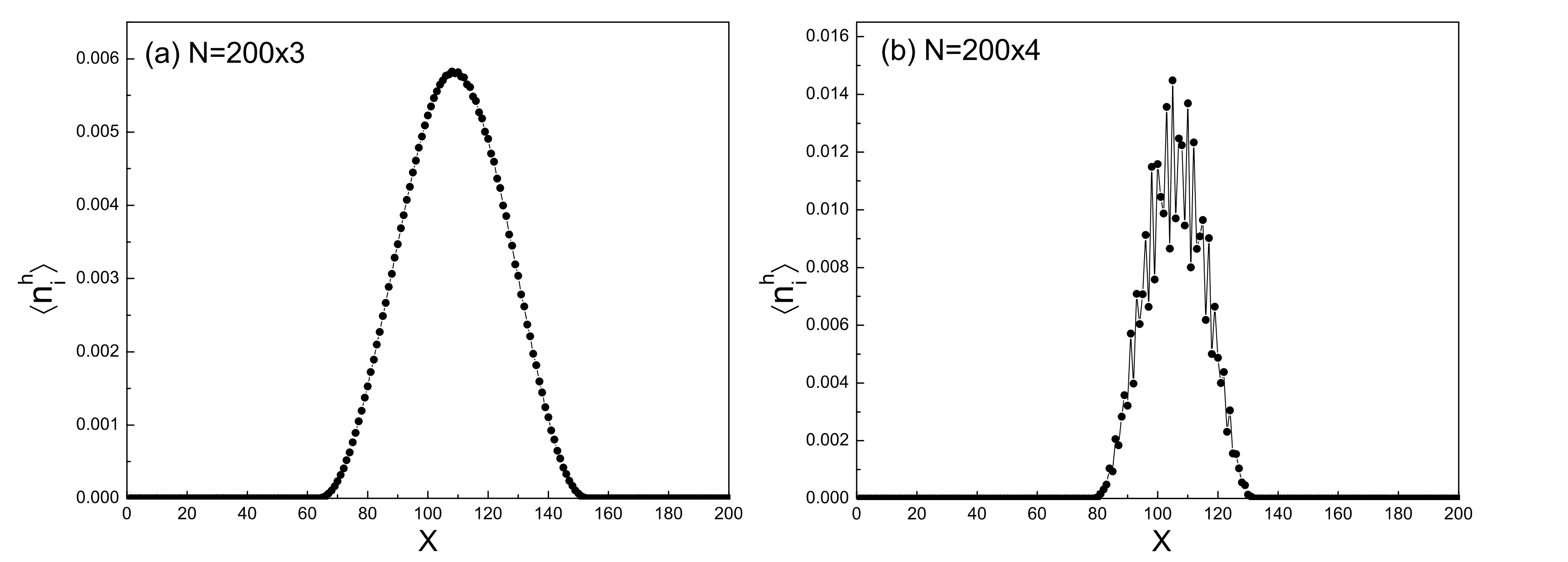
1. Localization length is monotonically reduced as t/J increases

- ➢ **spin dynamics is not essential to the hole localization.**

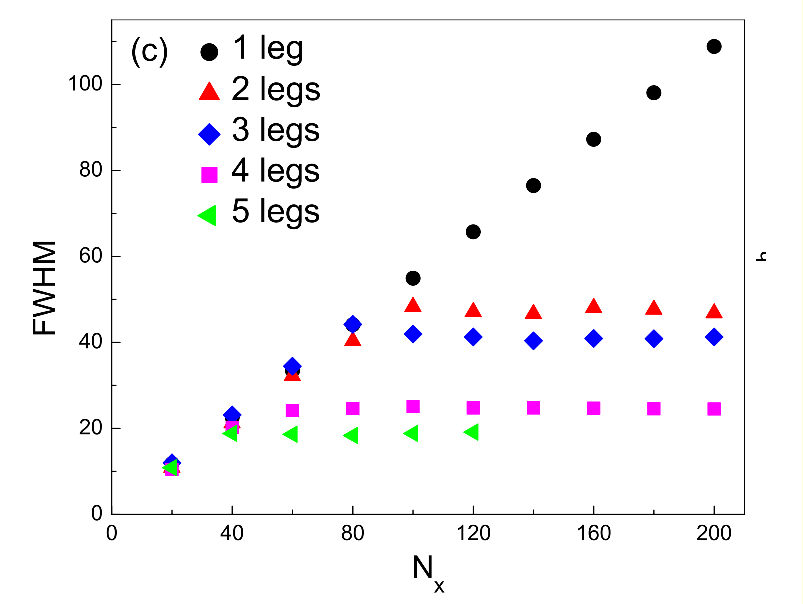
2. Oscillation for the even-leg ladders diminish as t/J increases

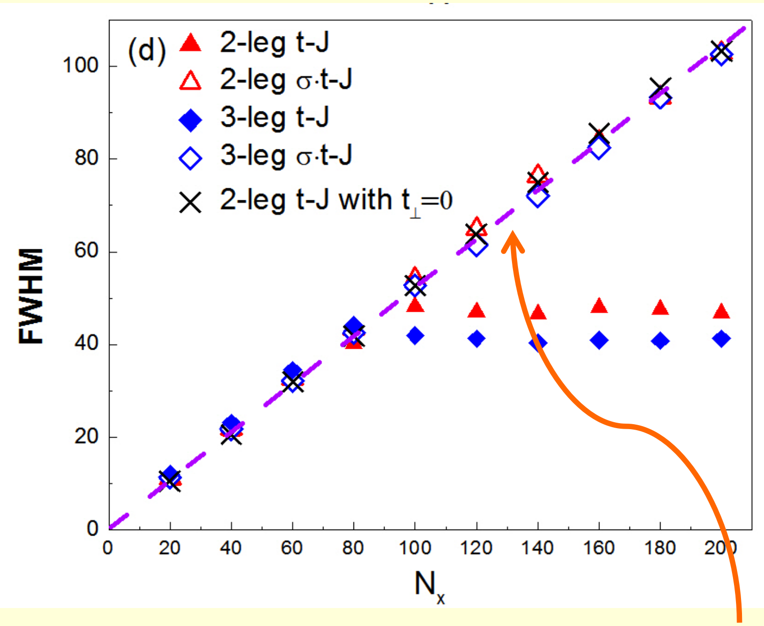
- ➢ **the spin-gap effect will be gradually reduced with the increase of t/J**

Single-hole problem: A DMRG calculation

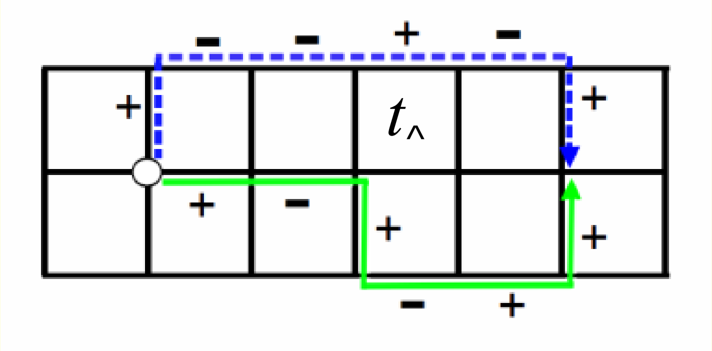


Effect of phase string effect



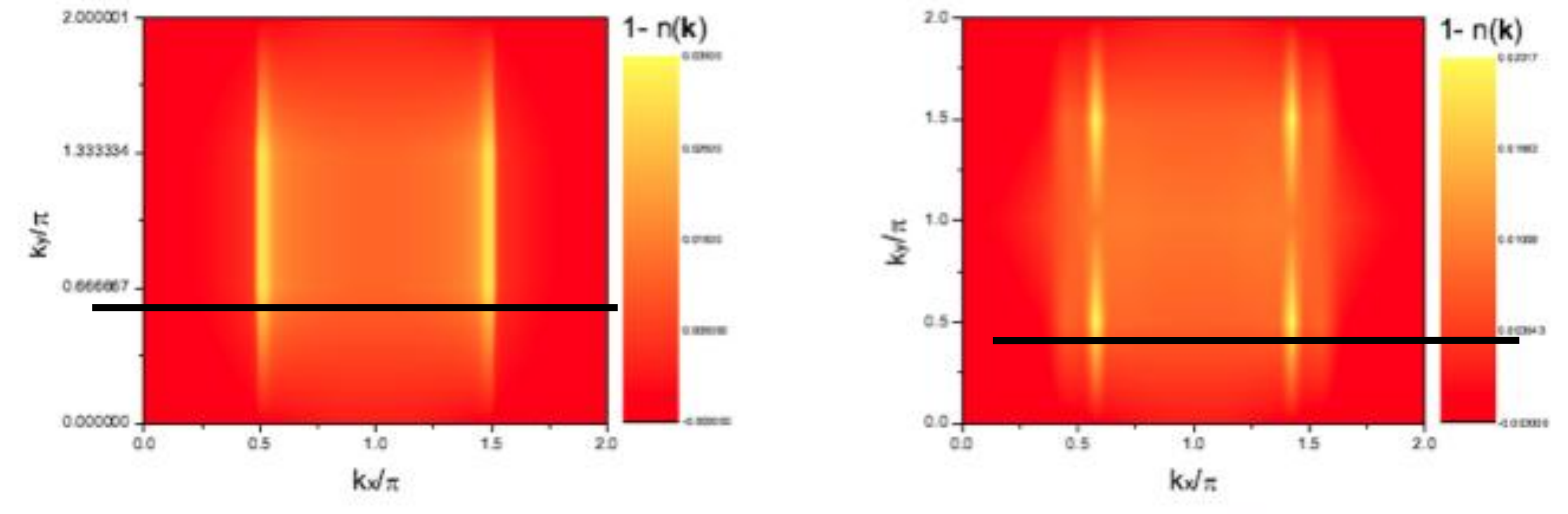


no phase string effect



Self-localization of the hole!

Picturing the Fermi surface

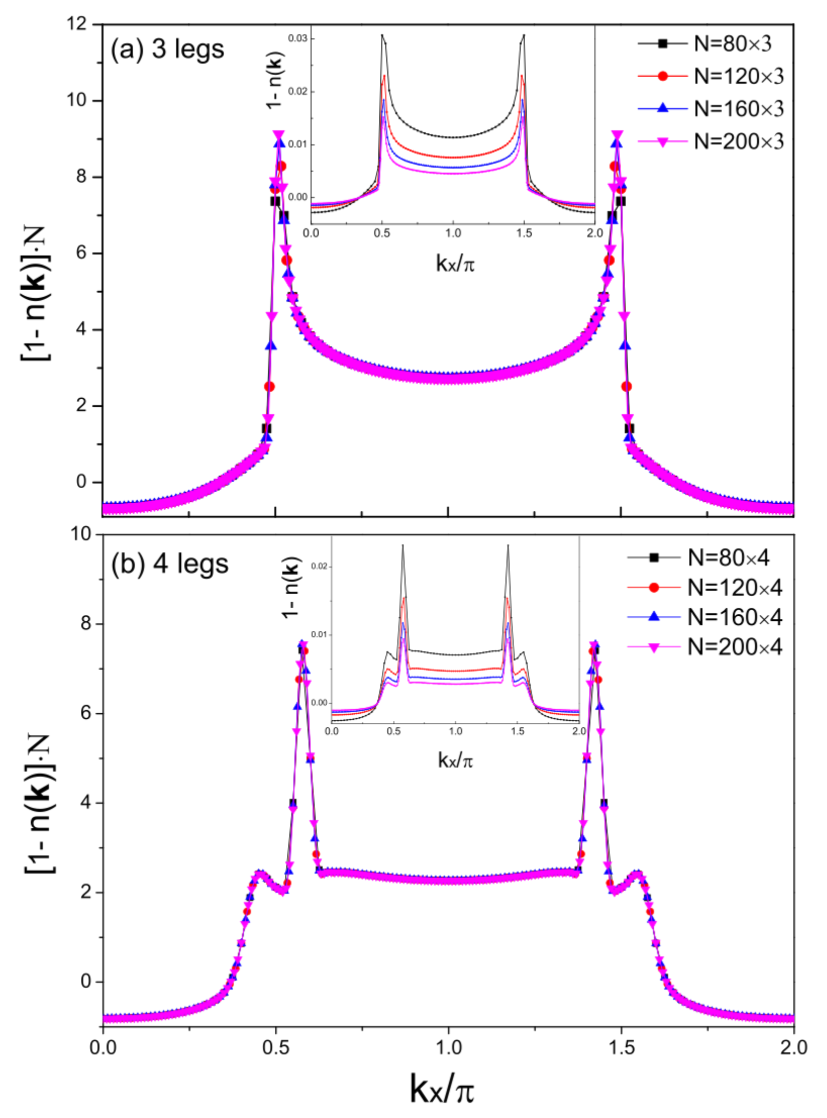


(a) N=80×3

(b) N=80×4

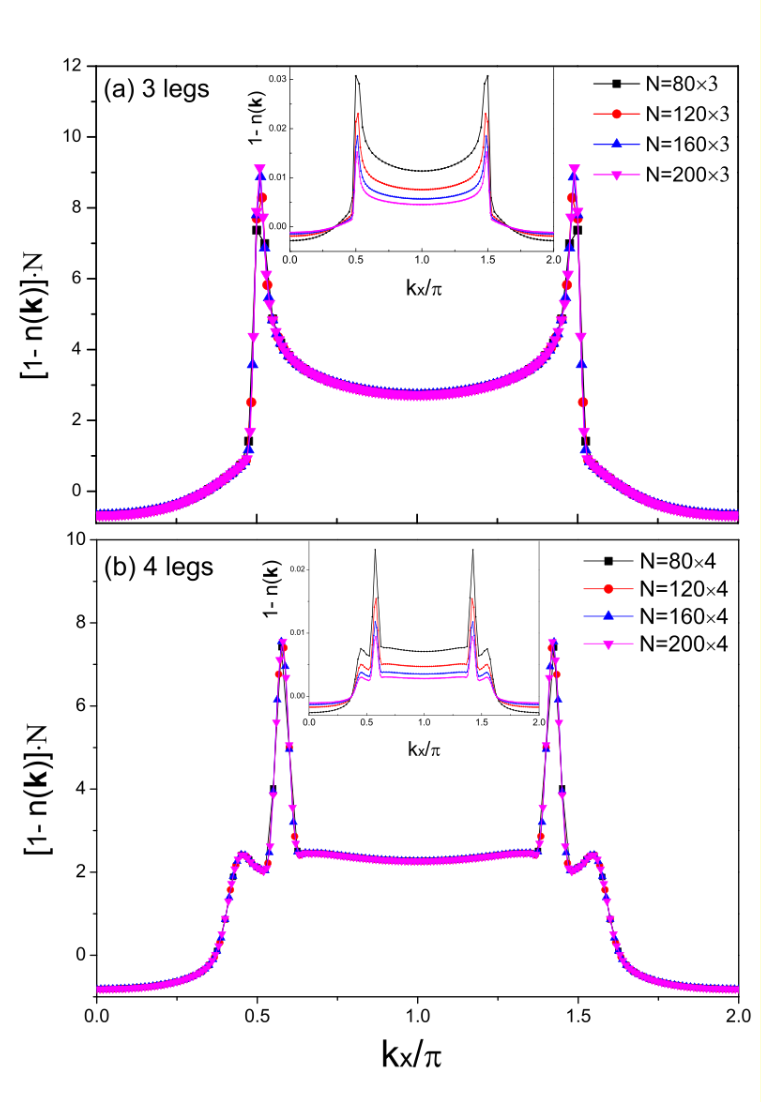
- DMRG gives n(k) of the ground state
- Jump in n(k) → Fermi surface

Vanishing quasiparticle weight

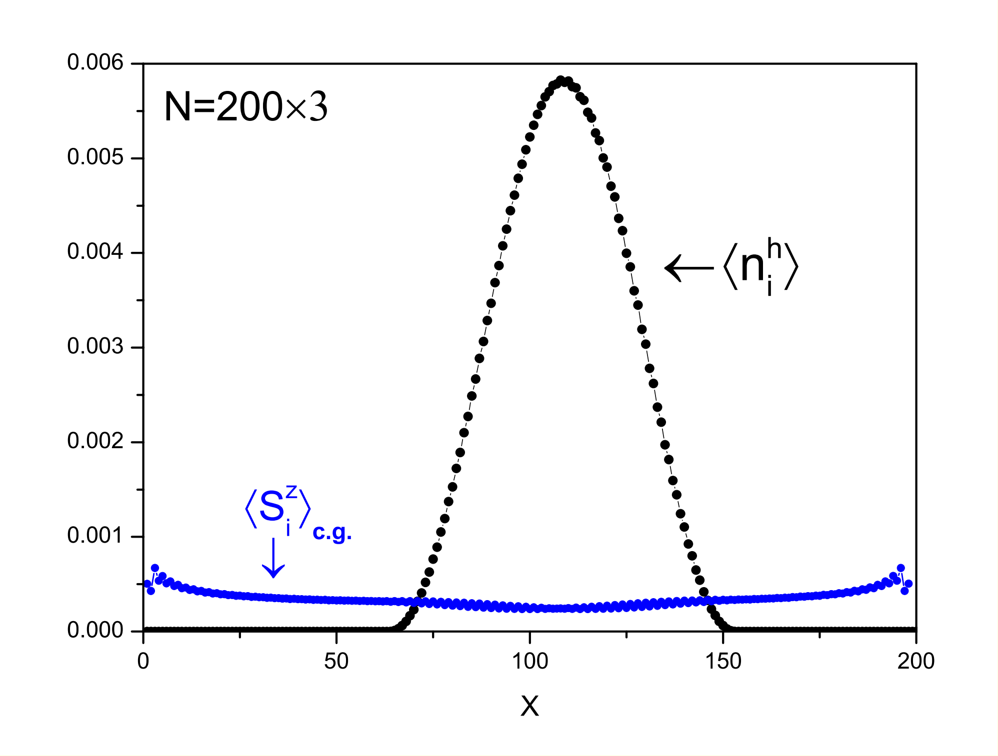


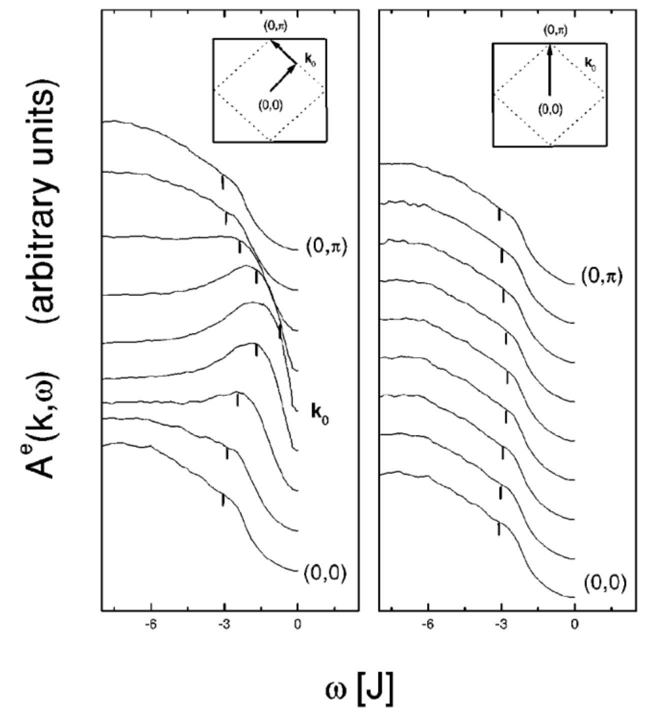
- 1-n(k) ~ 1/N
- peak height ~ 1/N
- peak width ~ const
- quasiparticle within the localized region

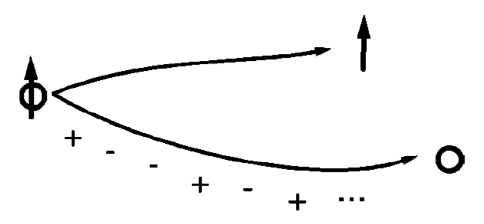
Momentum distribution



Spin-charge separation





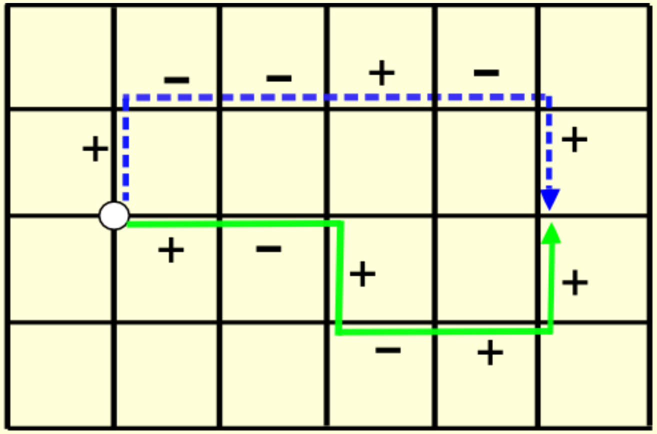


ZYW, V. N. Muthukumar, D.N. Sheng, C.S. Ting (2001

Implications

Emergent gauge force in doped Mott insulators!

$$(+1)\times(-1)\times(-1)\times\ldots\ldots \equiv \tau_c$$



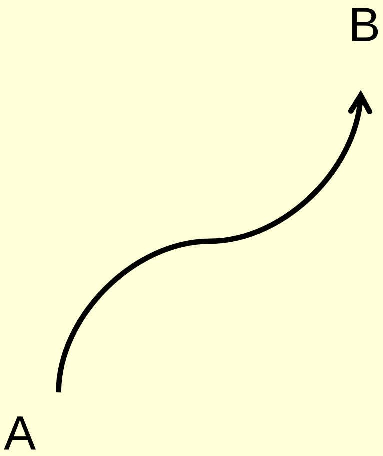
Partition function

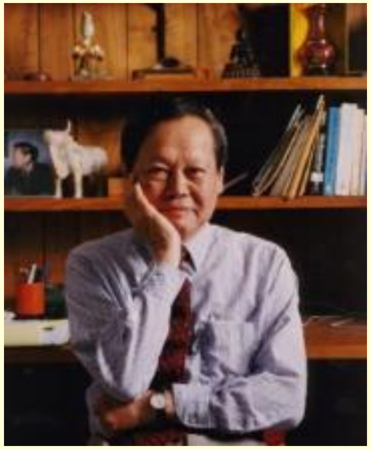
$$Z = \sum_{loop\ c} \tau_c W(c) \qquad W(c) \geq 0$$

C. N. Yang (1974) , Wu and Yang (197

Nonintegrable phase factor:

$$\boxed{Pe^{i\frac{e}{\hbar c}\int_A^B A_\mu dx^\mu}}$$





“An intrinsic and complete description of electromagnetism”

“Gauge symmetry dictates the form of the fundamental forces in nature”

At arbitrary doping, dimensions, temperature: t-J model

$$Z = \sum_c \tau_c \mathcal{Z}(c)$$

$$\tau_c = (-1)^{N_h^{\downarrow}(c)} \times (-1)^{N_h^{h}(c)}$$

$$\mathcal{Z}[c] = \left(\frac{2t}{J}\right)^{M_h[c]} \sum_n \frac{(\beta J/2)^n}{n!} \delta_{n, M_h + M_{\uparrow\downarrow} + M_Q}$$

$M_h(C)$ = total steps of hole hoppings

$M_{\uparrow\downarrow}(C)$ = total number of spin exchange processes

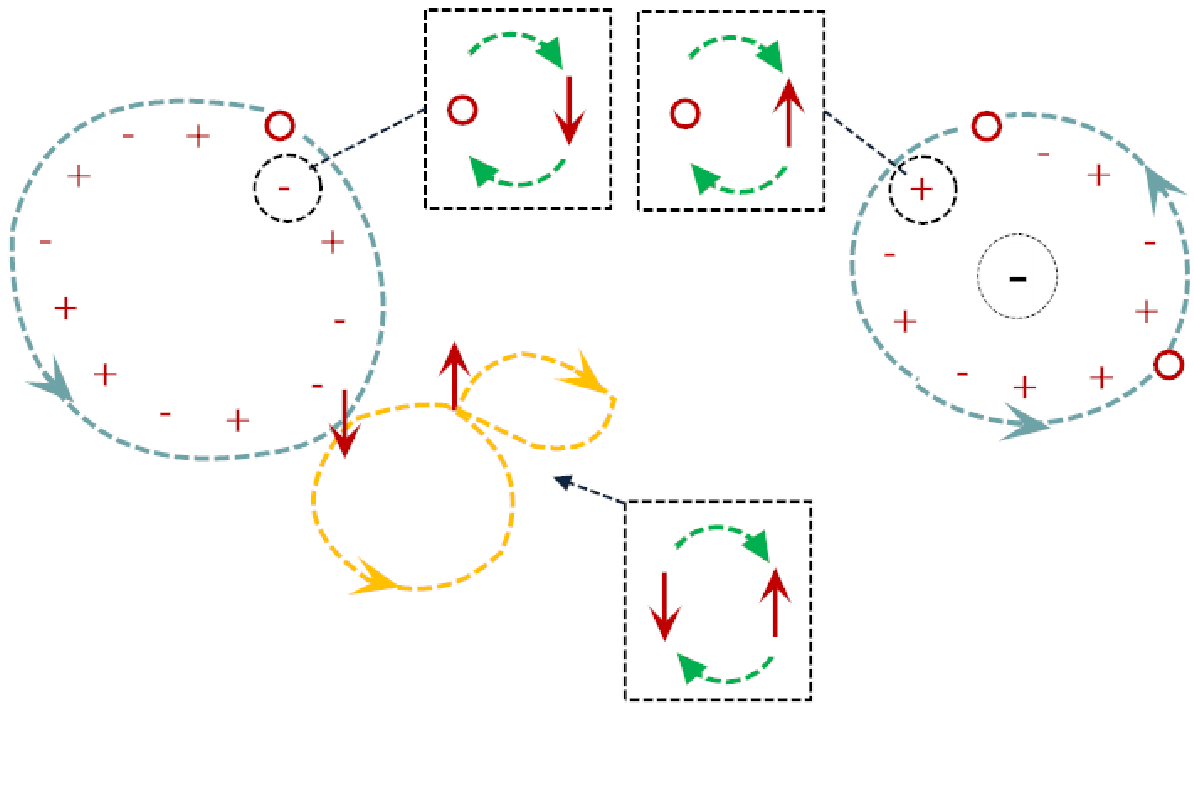
$M_Q(C)$ = total number of opposite spin encounters

$$\mathcal{Z}(c) \geq 0$$

Wu, Weng, Zaanen, PRB (2008)

General sign struture rule:

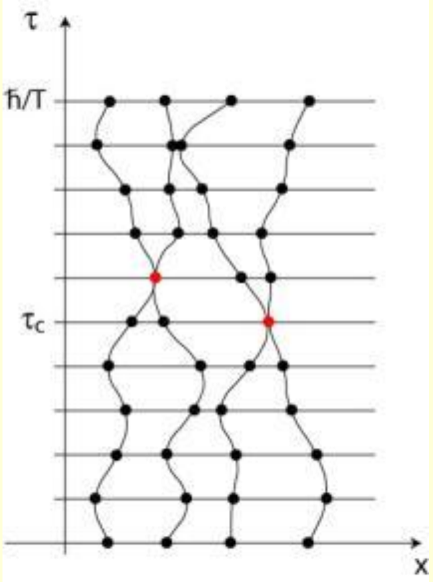
$$\tau_c = (-1)^{N_h^{\downarrow}(c)} \times (-1)^{N_h^h(c)}$$



Feynman‘s path-integral

$$\mathcal{Z} = \mathrm{Tr}\exp(-\beta\hat{\mathcal{H}}) = \int \mathrm{d}\mathbf{R}\,\rho(\mathbf{R},\mathbf{R};\beta)$$

Fermion signs



$$\mathbf{R} = (\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

$$\rho_{B/F}(\mathbf{R},\mathbf{R};\beta) = \frac{1}{N!}\sum_{\mathcal{P}}(\pm 1)^{\mathcal{P}}\rho_D(\mathbf{R},\mathcal{P}\mathbf{R};\beta) = \frac{1}{N!}\sum_{\mathcal{P}}(\pm 1)^{\mathcal{P}}\int_{\mathbf{R}\to\mathcal{P}\mathbf{R}}\mathcal{D}\mathbf{R}(\tau)\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar/T}\mathrm{d}\tau\left(\frac{m}{2}\dot{\mathbf{R}}^2(\tau)+V(\mathbf{R}(\tau))\right)\right\}$$

t-J model:

$$Z = \sum_c \tau_c \mathcal{Z}(c)$$

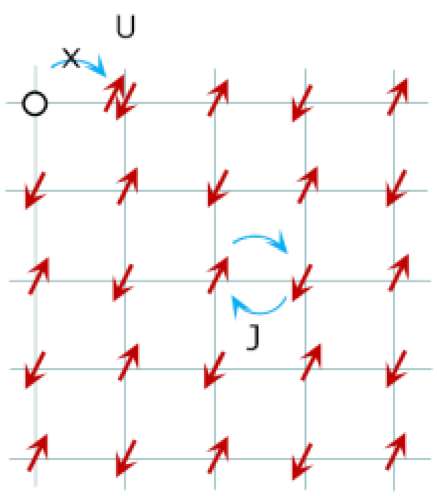
$$\tau_c = (-1)^{N_h^{\downarrow}(c)} \times (-1)^{N_h^{h}(c)}$$

Mott physics = ↑↓ + new statistical signs

✖ (nonintegrable phase factor)

Trivial limits of phase string effect

Half-filling:



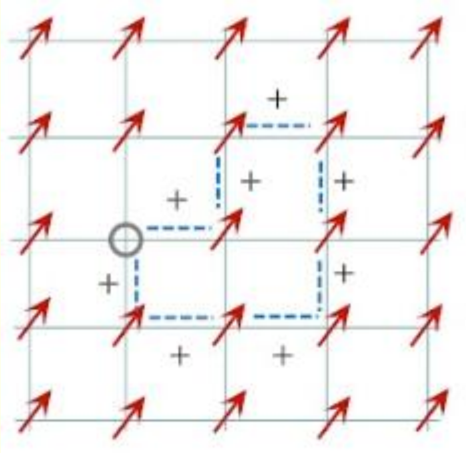
$$Z_{t-J} = \sum_c \tau_c \mathcal{Z}[c]$$

$$t_c = 1$$

no sign problem $N_h^-(c) = 0$

antiferromagnetic ground state

Nagaoka state (J=0)

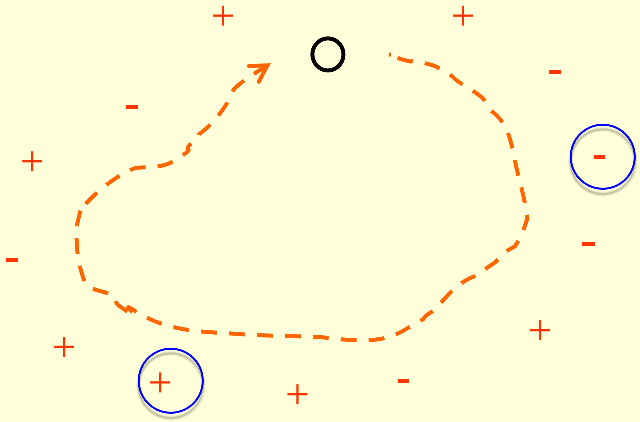


$$N_h^-(c) = 0$$

$$t_c = 1$$

no sign problem

Long-range entanglement between charge and spin!



one hole

self-localization

Perspective

- Mott physics = $\uparrow\downarrow$ ✖ **+ sign structure**
- ⟹ electron fractionalization
- ⟺ ODLROs for sub-systems (rigidity)
- True ODLRO: sign structure/mutual statistics

Z.Y. Weng, New J. Phys. 13 (2011) 103039

Conclusion

- Nonintegral phase factor (sign structure) dictates (1-hole) doped Mott physics:

emergent gauge symmetry

$$e^{i\frac{e}{\hbar c}\int_A^B A_m dx^m} \Longrightarrow (+1)\times(-1)\times(-1)\times\ldots\ldots$$

mutual statistics （geometric/topological)

- Examples:

1) Half-filling: antiferromagnet (no sign problem)

2) One-hole (J=0): Nagaoka state (no sign problem)

3) One-hole (J finite): self-localization (DMRG)

4) One-dimensional case: Luttinger liquid (non-trivial signs)

5) 2D finite doping: origin of high-T_c superconductivity