

High-Temperature Superconductivity and Strong Correlations (II)

Zheng-Yu Weng

Institute for Advanced Study
Tsinghua University, Beijing

ICAM-2011-Tsinghua Summer School 2014.7.25

Outline

- High- T_c superconductivity: A general survey
- High- T_c cuprates as strongly correlated electron systems
- Mott physics: Basic organizing principles
- Examples
- Understanding of the phase diagram
- Summary and conclusion

Mechanism of superconductivity in high- T_c cuprates: What is the most essential issue?

Ground state wavefunction = Cooper pair condensation + additional structure

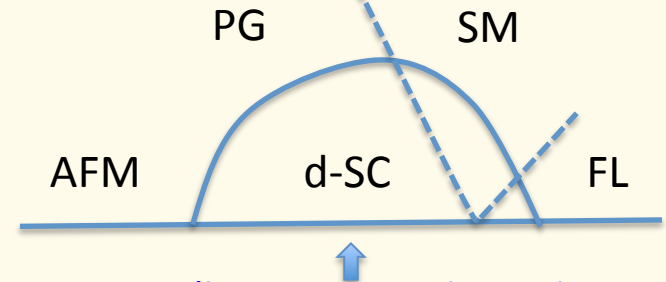
➤ Cooper pair condensation

BCS like: d-wave pairing symmetry;

Bogoliubov nodal quasiparticle; GL equation (low-energy, long distance)

➤ additional structure (short-range, high-energy)

non-FL-like: pseudogap, AF, strange metal, ...

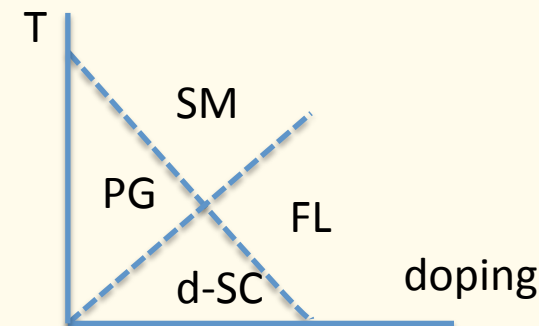


quantum order? long-range entanglement? fractionalization? competing order?

➤ Example: Anderson's RVB theory:

P_G : Gutzwiller projection $|\Psi_{RVB}\rangle = P_G |\text{BCS}\rangle$

doped Mott insulator picture: on-site Coulomb repulsion
no double occupancy



Baskaran, Zou, Anderson; ...



Cuprates = doped Mott Insulator

Anderson, Science 1987

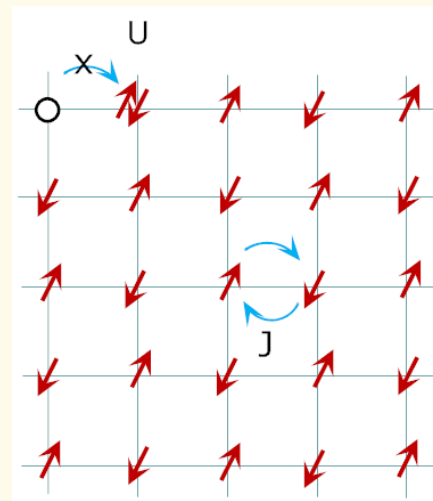
one-band large-U Hubbard/t-J model:

$$H_t = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + H.c.$$

$$H_J = \sum_{\langle ij \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right)$$

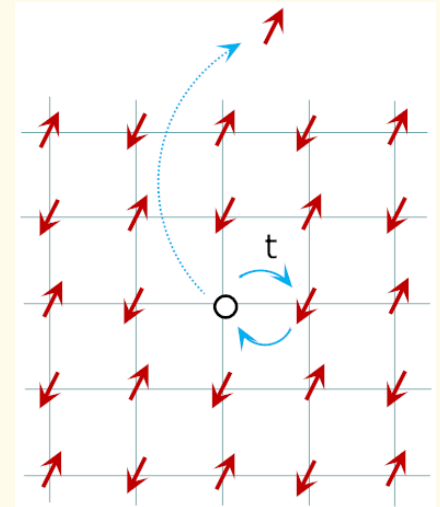
$$\sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} \leq 1$$

Mott insulator



Heisenberg model

doped Mott insulator



t-J model

Half-filling

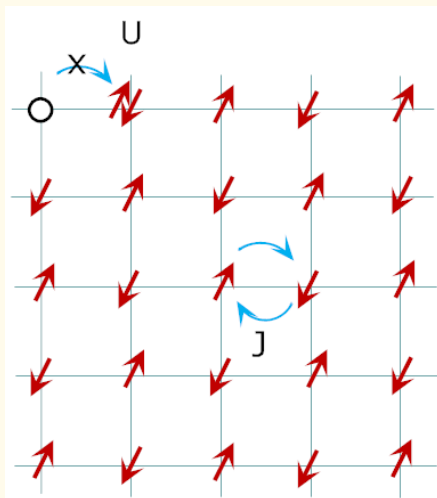
How to construct the ground state at finite doping?

Guiding principles:

- No double occupancy constraint

Anderson's RVB ansatz: $|\Psi_{RVB}\rangle = P_G |\text{BCS}\rangle$ P_G : Gutzwiller projection

- Accurate AFM ground state at half-filling limit



Heisenberg model:

well describes antiferromagnetism in the cuprate

《Quantum Phase Transitions》 S. Sachdev

Ground state at Half-filling:

Liang –Docout-Anderson wave function

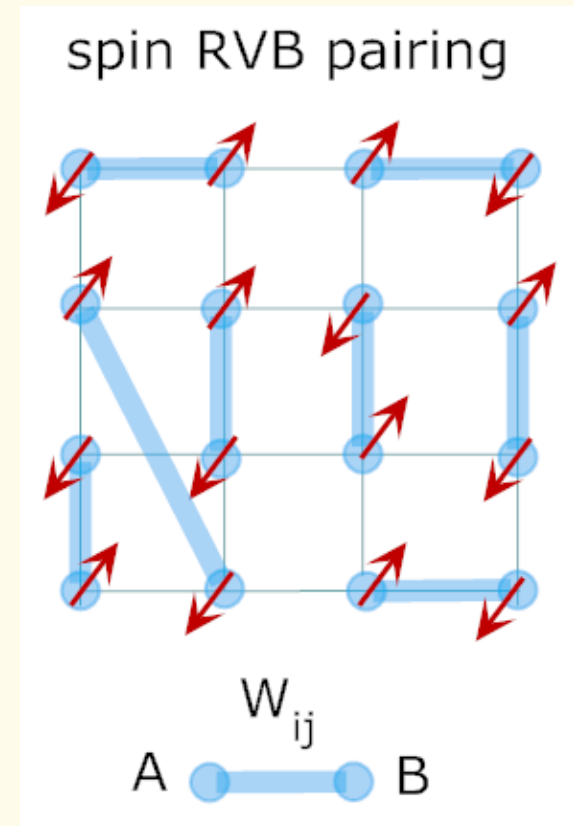
$$|b - \text{RVB}\rangle = \sum_{\{\sigma_s\}} \Phi_{\text{RVB}}(\sigma_1, \sigma_1, \dots, \sigma_N) c_{1\sigma_1}^\dagger c_{2\sigma_2}^\dagger \cdots c_{N\sigma_N}^\dagger |0\rangle$$

$$\Phi_{\text{RVB}}(\{\sigma_s\}) \equiv \sum_{\text{partition}(ij)} \prod (-1)^i W_{ij} \quad i : \uparrow \quad j : \downarrow$$

$$W_{ij} \propto \frac{1}{|\mathbf{r}_{ij}|^3} \quad ij \in A, B$$

bosonic resonating valence bond (b-RVB) state!

variational energy	$E_G = -0.3344$	$m = 0.30$
exact numerics	$E_G = -0.3346$	$m = 0.31$



Liang, Docout, Anderson (1988)

How to construct the ground state at finite doping?

Guiding principles:

- No double occupancy constraint
- Accurate AFM ground state at half-filling limit

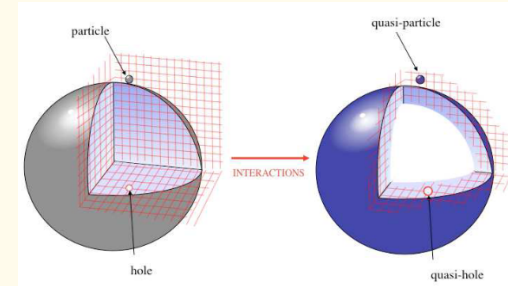
$$|\text{b-RVB}\rangle$$

- Emergent sign structure for the t-J/Hubbard model

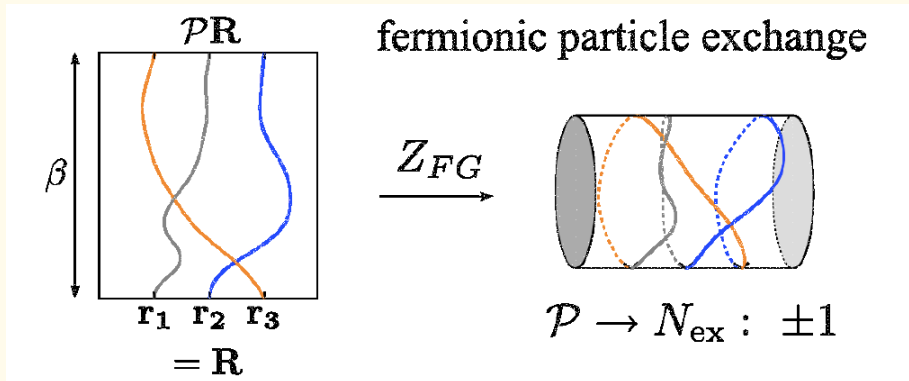
Statistical sign structure for Fermion systems

Fermion signs

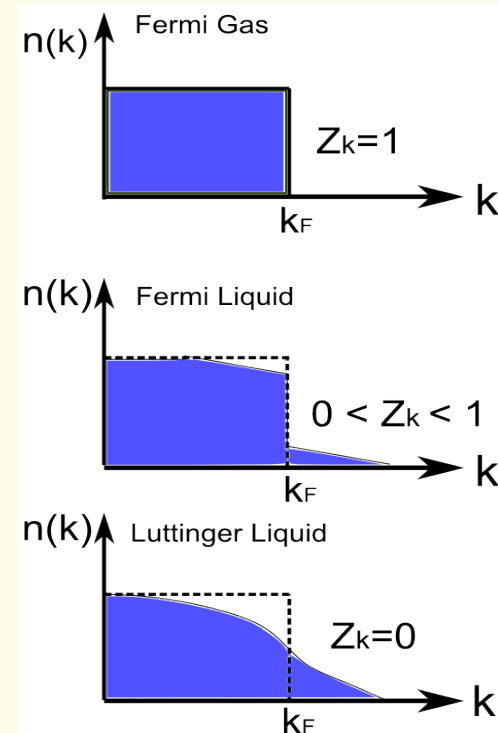
$$\psi(x_1, x_2, \dots) = -\psi(x_2, x_1, \dots)$$



Landau Fermi Liquid



$$Z_{FG} \equiv \text{Tr}(e^{-\beta H}) = \sum_{\text{loop } c} (-1)^{N_{ex}(c)} W(c), \quad W(c) \geq 0$$



(1) Fermi liquid: Fermion signs

$$Z_{FG} = \sum_{\text{loop } c} (-1)^{N_{ex}(c)} W(c) \quad W(c) \geq 0$$

(2) Off Diagonal Long Rang Order (ODLRO):
compensating the Fermion signs

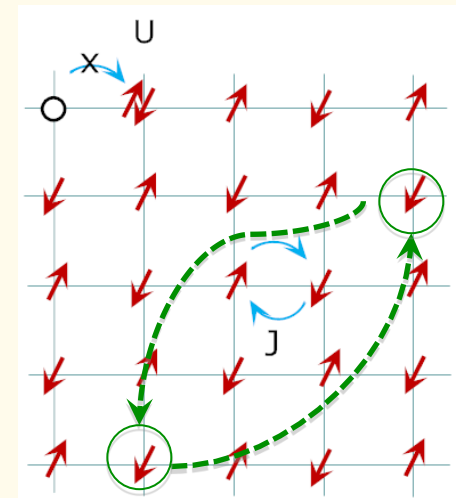
Bose condensation

Cooper pairing in SC state

CDW (“exciton” condensation)

SDW (weak coupling)

(3) Antiferromagnetic order (strong coupling)



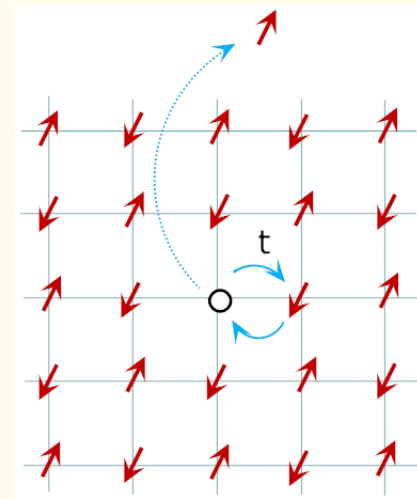
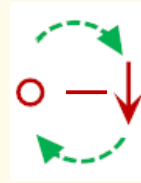
$$Z_{\text{Heisenberg}} = \sum_{\text{loop } c} W(c) \quad W(c) = \sum_n \frac{(\beta J / 2)^n}{n!} \delta_{M_{\uparrow\downarrow} + M_Q, n} \geq 0$$

Complete disappearance of Fermion signs!

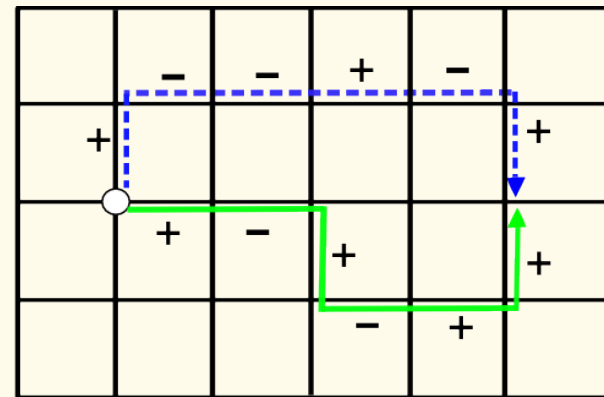
Single-hole-doped Heiserberg model:

$$Z_{1-hole} = \text{Tr}(e^{-\beta H}) = \sum_{\text{loop } c} \tau_c W(c)$$

$$\begin{aligned} \tau_c &\equiv (+1) \times (-1) \times (-1) \times \dots \\ &= (-1)^{N_h^\downarrow(c)} \end{aligned}$$



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



Phase string effect

General sign structure at arbitrary doping, dimensions, temperature for the t-J model

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

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

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

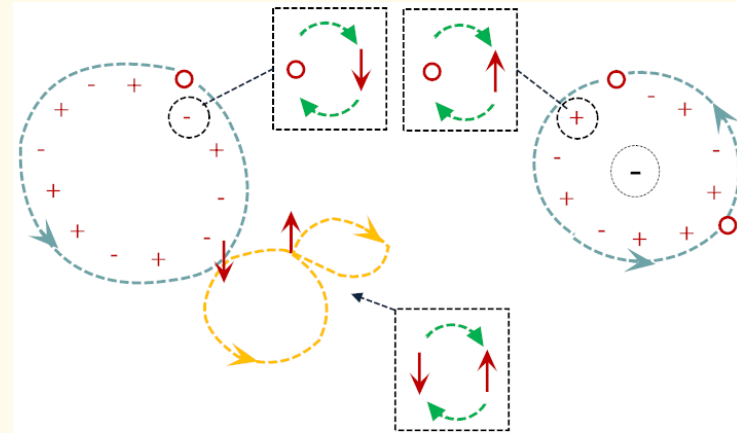
fermion signs

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

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

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

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



How to construct the ground state at finite doping?

Guiding principles:

- No double occupancy constraint
- Accurate AFM ground state at half-filling limit
- Emergent sign structure for the t-J/Hubbard model

Organizing principles for emergent physics of strongly correlated electrons!

New class of ground state wave function

$$|\Psi_G\rangle = e^{\hat{D}} |\text{b-RVB}\rangle$$

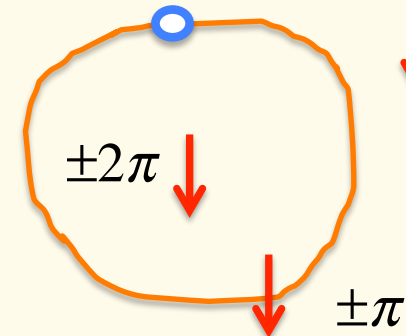
protected by Mott gap!

$$\Phi_{\text{RVB}}(\{\sigma_s\}) \equiv \sum_{\text{partition}(ij)} \prod (-1)^i W_{ij} \quad \hat{D} = \sum_{ij} g_{ij} \tilde{c}_{i\uparrow} \tilde{c}_{j\downarrow}$$

two-component RVB state

$$\tilde{c}_{i\sigma} = c_{i\sigma} e^{-i\hat{\Omega}_i}$$

$$\hat{\Omega}_i = -\sum_l \theta_i(l) n_{l\downarrow}^b, \quad \theta_i(l) = \theta_l(i) \pm \pi$$



sign structure of the t-J model

Anderson's one-component RVB ansatz:

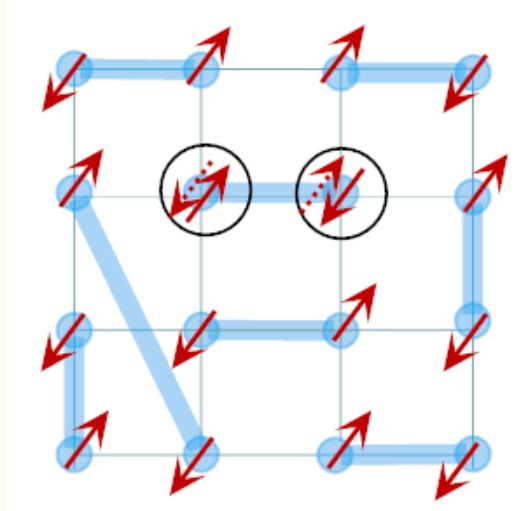
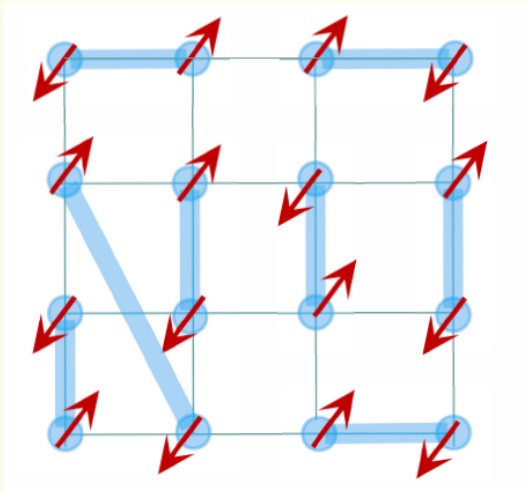
$$|\Psi_{\text{RVB}}\rangle = P_G |\text{BCS}\rangle$$

P_G : Gutzwiller projection

Z.Y. Weng, NJP (2011)

Wave function expression:

$$|\Psi_G\rangle = e^{\hat{D}} |\text{b-RVB}\rangle \quad \longrightarrow \quad |\Psi_G\rangle = \hat{\Lambda}_h \left(\exp \sum_{ij} g_{ij} c_{i\uparrow} c_{j\downarrow} \right) |\text{b-RVB}\rangle$$



$$\hat{\Lambda}_h = \left[\prod_l e^{-i\hat{\Omega}_l} \right] \phi_h(l_1, l_2, \dots, l_{N_h})$$

$$\Phi_{\text{RVB}}(\{\sigma_s\}) \equiv \sum_{\text{partition}(ij)} \prod (-1)^i W_{ij}$$

$$\Psi_G = K \Phi_a(l_1, l_2, \dots, l_{N_h}) \Phi_{\text{RVB}}(i_1 \dots; j_1 \dots)$$

$$K \equiv \prod_{hd} \frac{(z_{l_h}^* - z_{j_d}^*)}{|z_{l_h} - z_{j_d}|} \phi_h(l_1, l_2, \dots, l_{N_h}) = \prod_{hu} (z_{l_h} - z_{i_u})^{1/2} \prod_{hd} (z_{l_h}^* - z_{j_d}^*)^{1/2} \prod_{i \neq j} \frac{(z_i^* - z_j^*)^{1/2}}{|z_i - z_j|^{1/2}} \phi_h(l_1, l_2, \dots, l_{N_h})$$

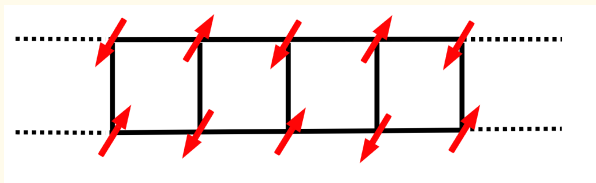
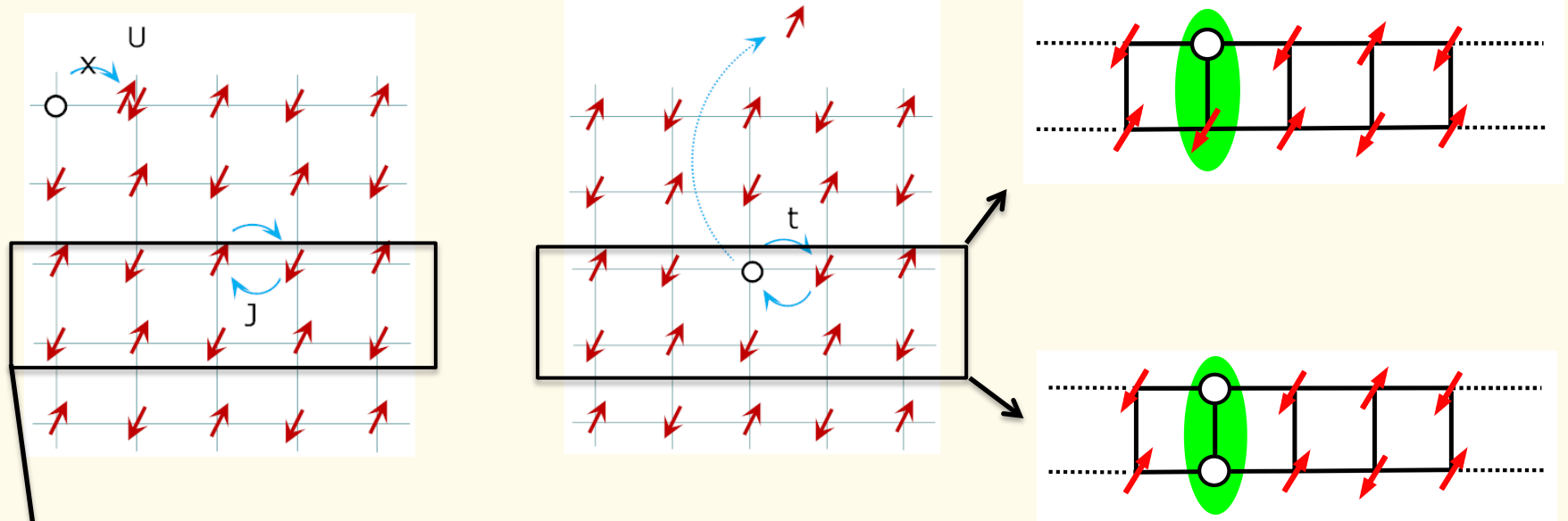


mutual statistics!

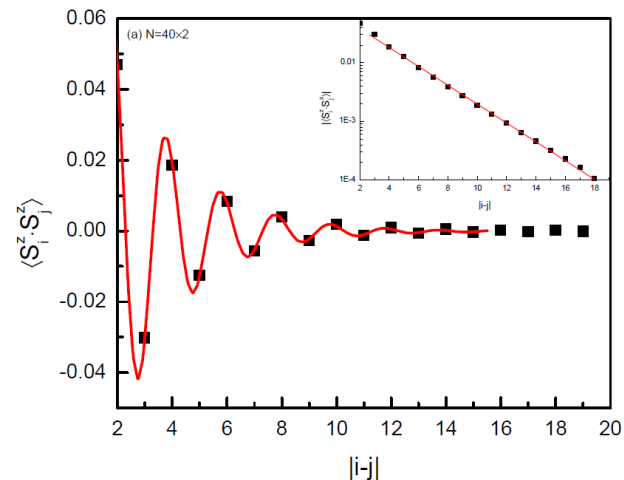
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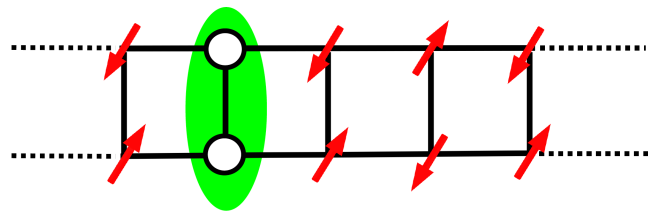
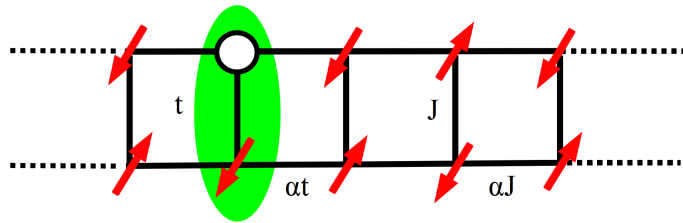
Example: Two-leg t-J ladder doped by one or two holes



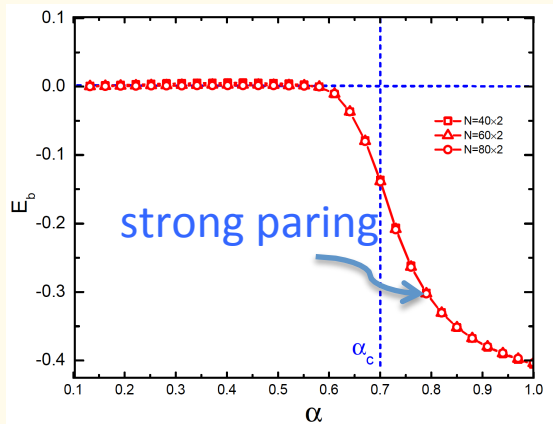
Half-filled 2-leg ladder is a Mott insulator with a spin gap



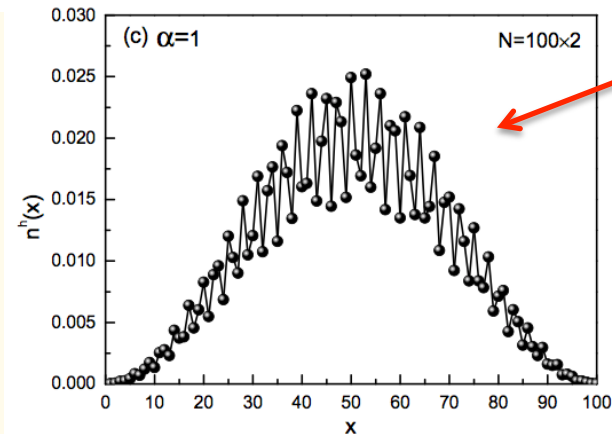
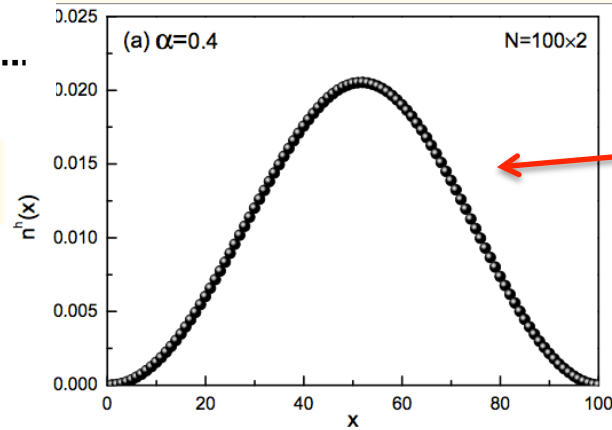
DMRG simulation



two hole binding energy ($t/J=3$)

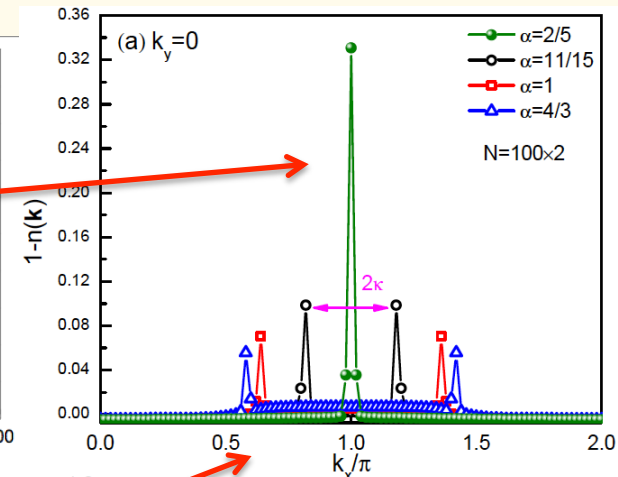


hole distribution

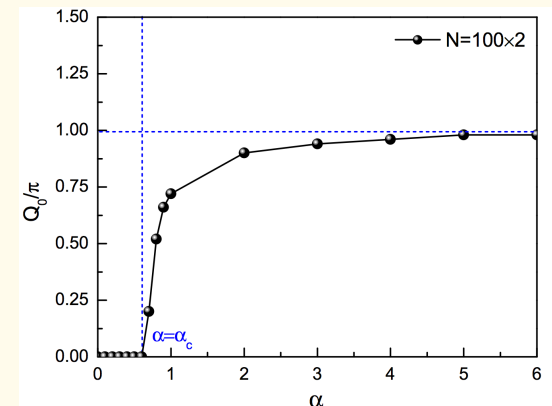


charge modulation

Fermi point reconstruction



wavevector $Q_0 = 2\kappa$



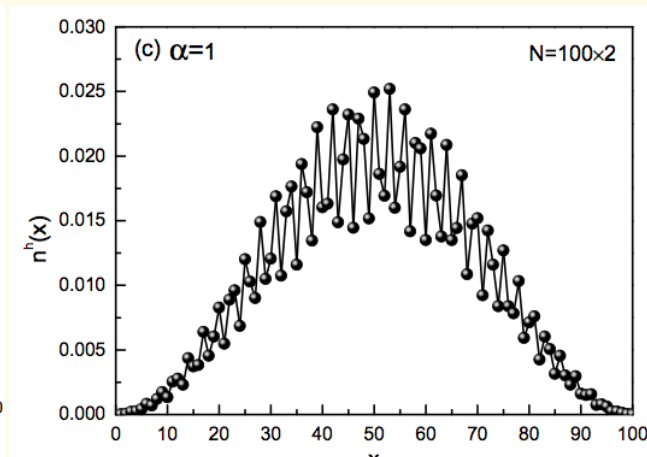
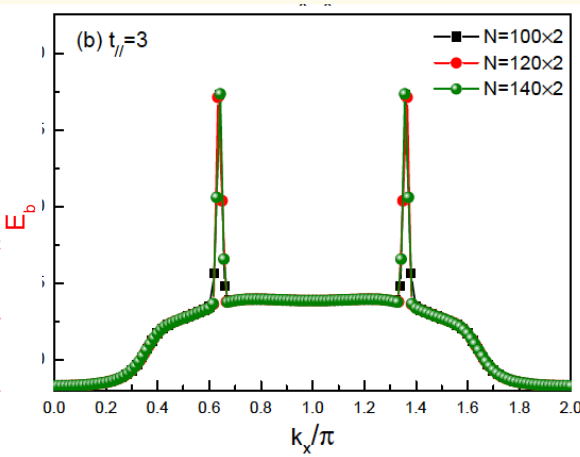
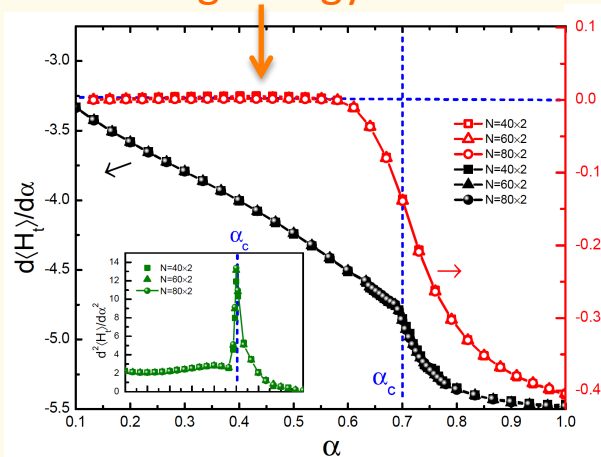
t-J model

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

$$H_t = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) \quad H_J = J \sum_{\langle ij \rangle} \left(\mathbf{s}_i \mathbf{s}_j - \frac{1}{4} n_i n_j \right)$$

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

binding energy

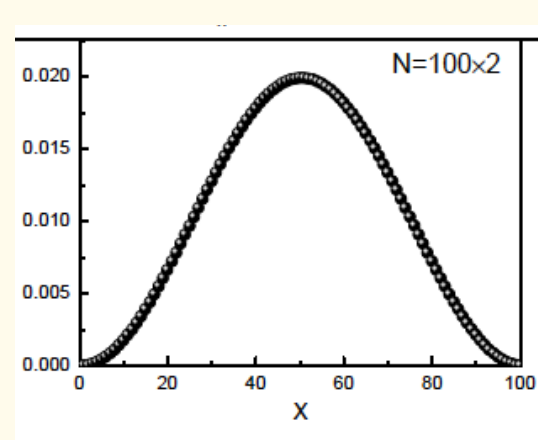
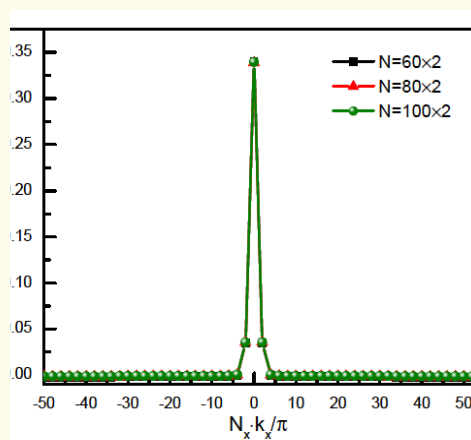
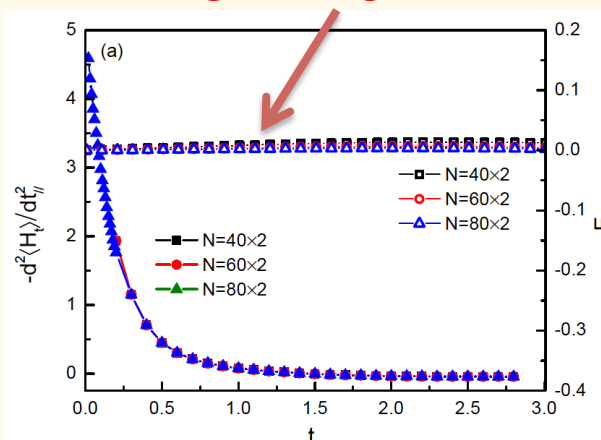


sigma t-J model

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

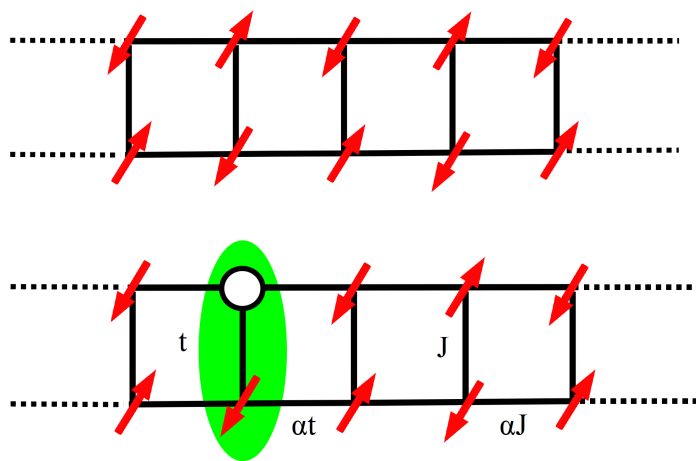
$$H_{\sigma,t} = -t \sum_{\langle ij \rangle \sigma} \sigma (c_{i\sigma}^\dagger c_{j\sigma} + h.c.)$$

vanishing binding

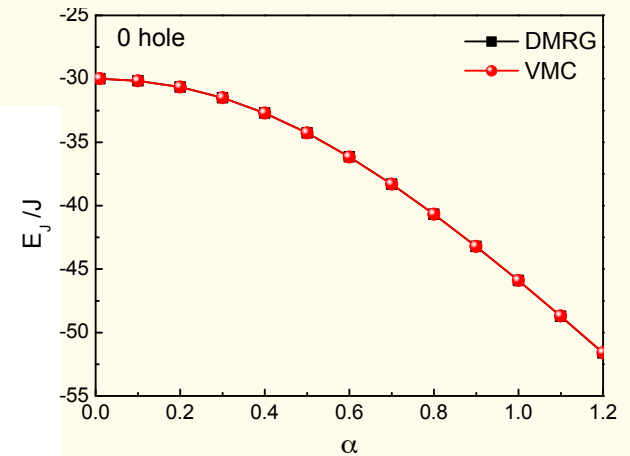


Variational Monte Carlo study

Q-R.Wang, Y. Qi, ZYW



$|\text{b-RVB}\rangle$



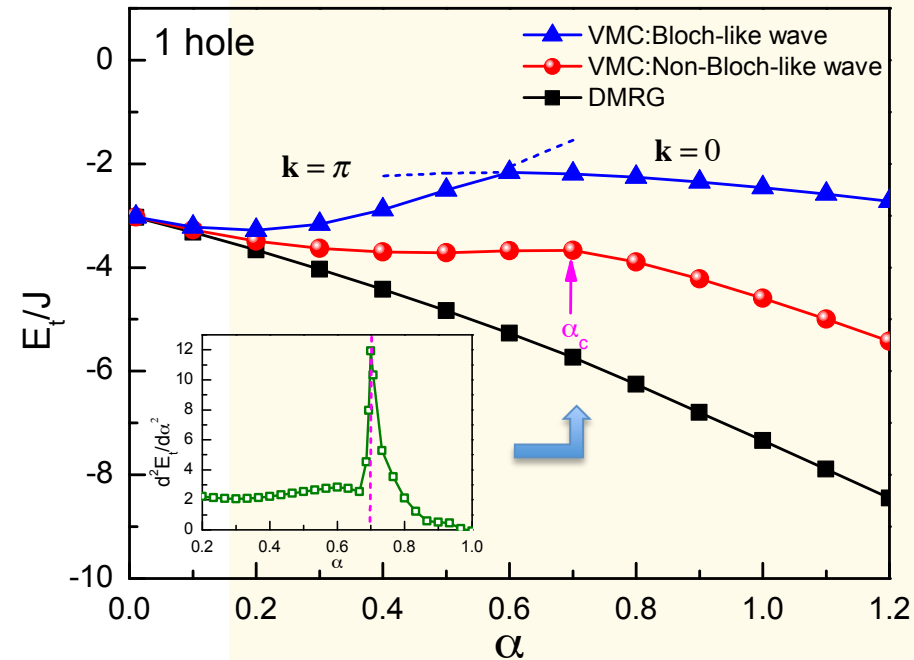
$$|\Psi_G\rangle_{1h} = \left(\sum_{ij} \phi_h(i) \tilde{c}_{i\uparrow} \right) |\text{b-RVB}\rangle$$

$$\tilde{c}_{i\sigma} = e^{-i\hat{\Omega}_i} c_{i\sigma}$$

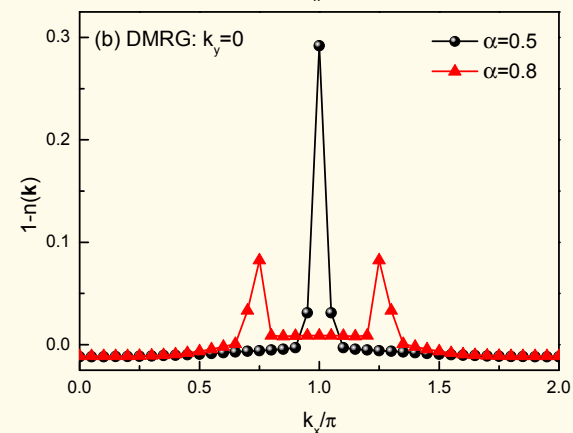
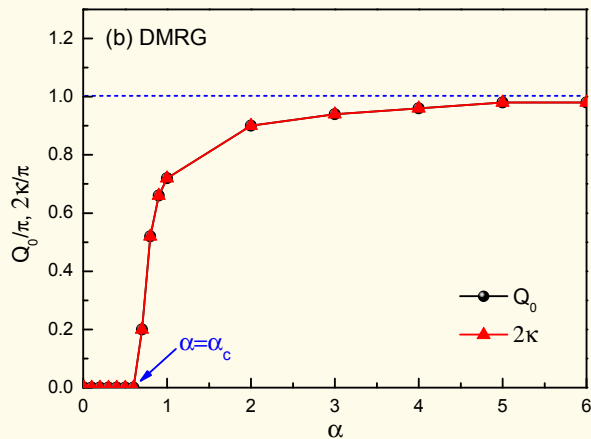
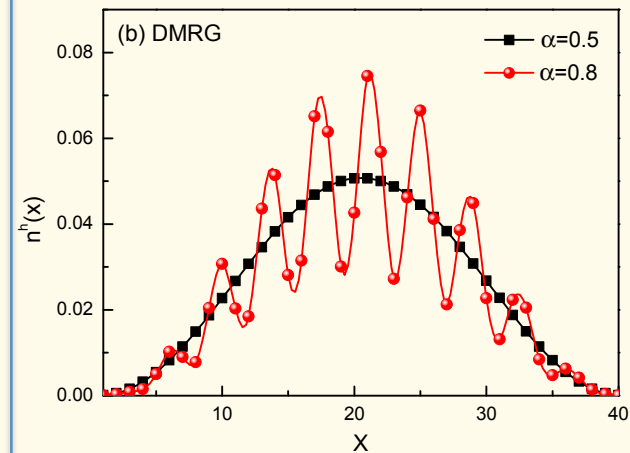
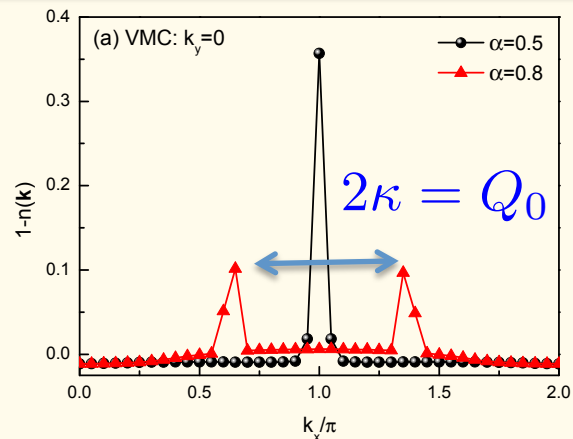
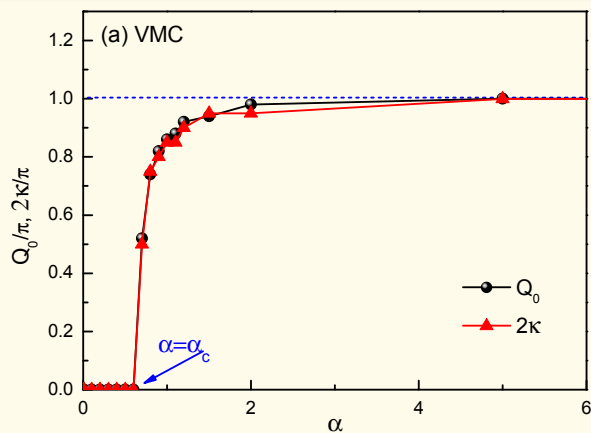
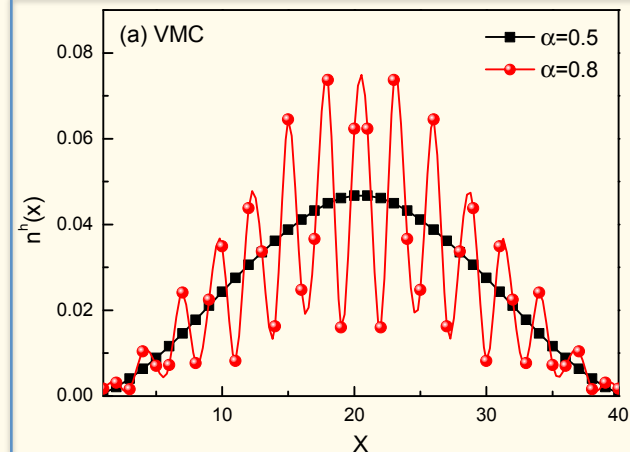
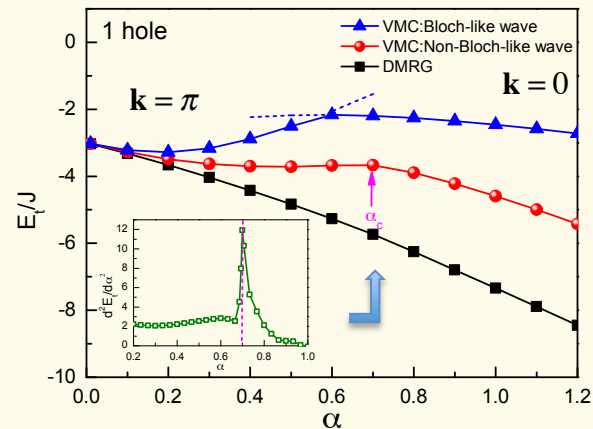
compare to

$$\phi_h(i) e^{-i\hat{\Omega}_i} \rightarrow \frac{1}{\sqrt{N}} e^{i\mathbf{k} \cdot \mathbf{r}_i}$$

$$|\mathbf{k}\rangle_{\text{BL}} = \left(\frac{1}{\sqrt{N}} \sum_{ij} e^{i\mathbf{k} \cdot \mathbf{r}_i} c_{i\uparrow} \right) |\text{b-RVB}\rangle$$



$$|\Psi_G\rangle = \left(\sum_{ij} \phi_h(i) e^{-i\hat{\Omega}_i} c_{i\uparrow} \right) |\text{b-RVB}\rangle$$



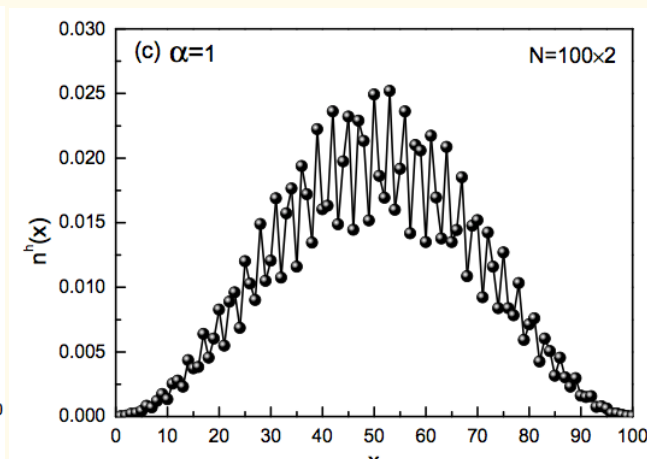
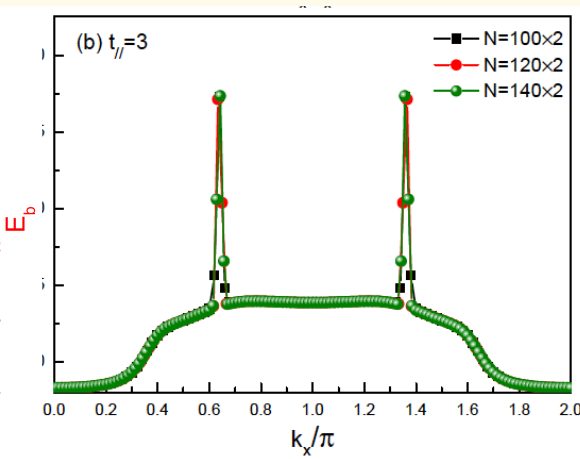
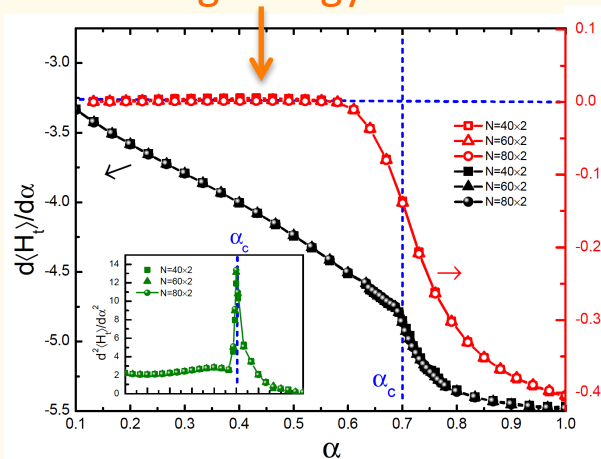
t-J model

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

$$H_t = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) \quad H_J = J \sum_{\langle ij \rangle} \left(\mathbf{s}_i \mathbf{s}_j - \frac{1}{4} n_i n_j \right)$$

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

binding energy

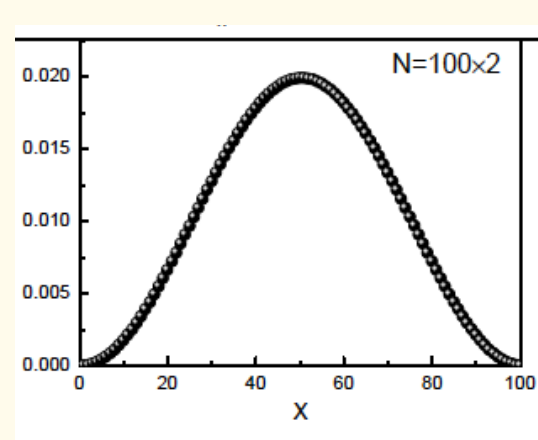
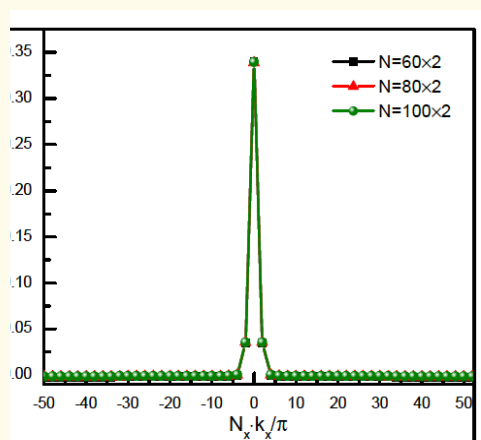
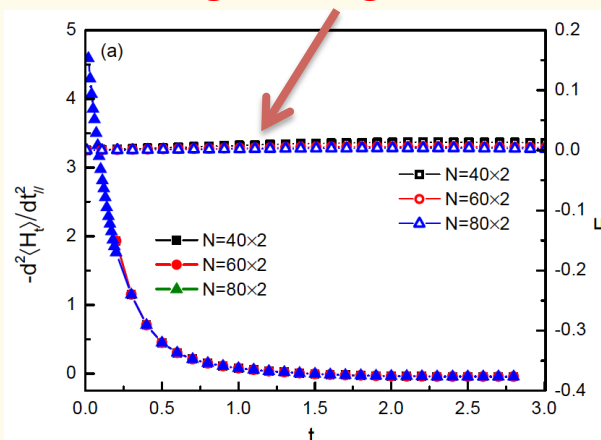


sigma t-J model

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

$$H_{\sigma,t} = -t \sum_{\langle ij \rangle \sigma} \sigma (c_{i\sigma}^\dagger c_{j\sigma} + h.c.)$$

vanishing binding



Moral of the story of the doped two-leg t-J/Hubbard ladder

“pseudogap phenomenon”:

- spin gapped background
- charge modulation
- Fermi point reconstruction
- charge modulation $\longleftrightarrow$ strong pairing

two sides of one coin!
- phase string effect is responsible

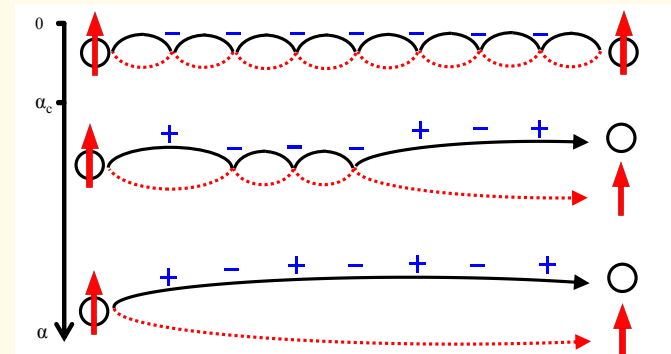
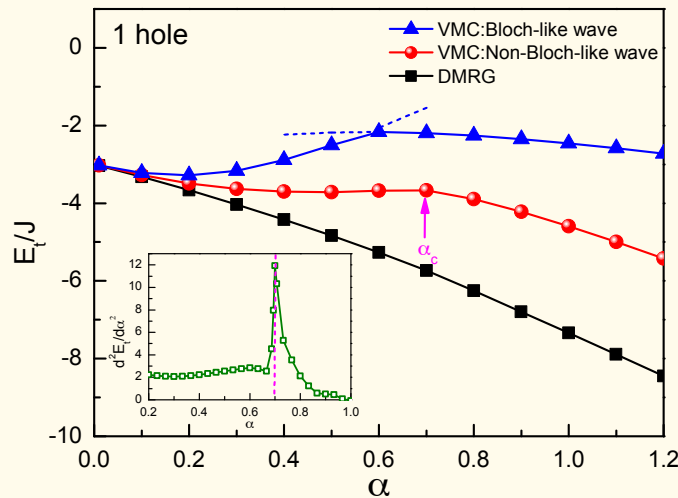
$$|\Psi_G\rangle = \left(\sum_{ij} \varphi_h(i) e^{-i\hat{\Omega}_i} c_{i\uparrow} \right) |\phi_0\rangle, \quad |\phi_0\rangle \equiv |\text{b-RVB}\rangle$$

$$\langle H_t \rangle = \langle \phi_0 | \hat{H}_h | \phi_0 \rangle$$

$$\hat{t}_{ji} \equiv t_{ji}^0 \hat{H}_{ji}$$

$$\hat{H}_h = - \sum_{\langle ij \rangle} \hat{t}_{ji} \varphi_h^\dagger(j) \varphi_h(i) + \text{h.c.} \quad t_{ji}^0 \equiv t_{ji} \left(\frac{1}{4} - \frac{1}{3} \langle \phi_0 | \mathbf{S}_i \cdot \mathbf{S}_j | \phi_0 \rangle \right)$$

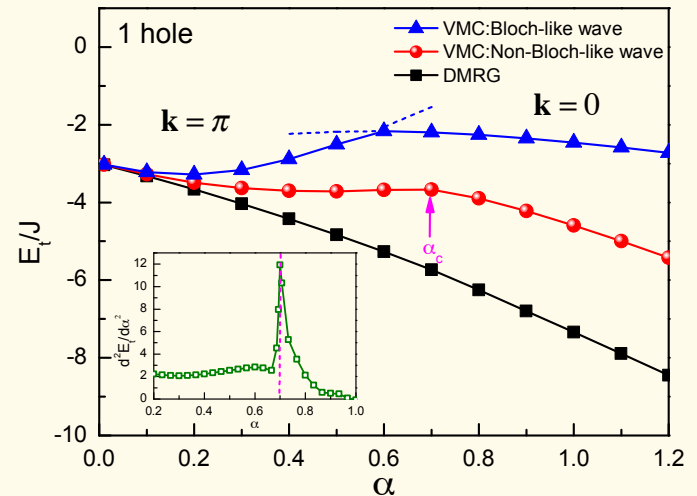
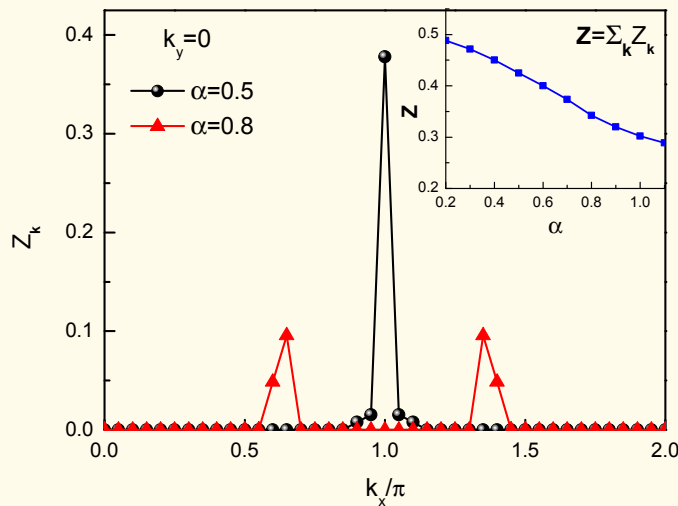
$$\hat{H}_{ji} \equiv e^{i(A_{ji}^s - \phi_{ji}^0)} \quad A_{ji}^s - \phi_{ji}^0 \equiv \sum_{l \neq j,i} (\theta_j(l) - \theta_i(l)) n_{j\downarrow}^b$$



$$|\Psi_G\rangle = \left(\sum_{ij} \phi_h(i) e^{-i\hat{\Omega}_i} c_{i\uparrow} \right) |\text{b-RVB}\rangle \quad \text{vs.} \quad |\mathbf{k}\rangle_{\text{BL}} \equiv \left(\frac{1}{\sqrt{N}} \sum_{ij} e^{i\mathbf{k}\cdot\mathbf{r}_i} c_{i\uparrow} \right) |\text{b-RVB}\rangle$$

$$|\Psi_G\rangle = a_{\mathbf{k}} |\mathbf{k}\rangle_{\text{BL}} + \dots$$

$$a_{\mathbf{k}} \equiv_{\text{BL}} \langle \mathbf{k} | \Psi_G \rangle \quad Z_{\mathbf{k}} \equiv |a_{\mathbf{k}}|^2$$



Breakdown of the Landau's one-to-one correspondence of qp picture
(Fermi surface reconstruction in violation of the Luttinger theorem)

2D case at finite doping:

$$|\Psi_G\rangle = e^{\hat{D}} |\text{b-RVB}\rangle$$

$$\hat{D} = \sum_{ij} g_{ij} \tilde{c}_{i\uparrow} \tilde{c}_{j\downarrow}$$

$$\tilde{c}_{i\sigma} = c_{i\sigma} e^{-i\hat{\Omega}_i}$$

$$\Phi_{\text{RVB}}(\{\sigma_s\}) \equiv \sum_{\text{partition } (ij)} \prod (-1)^i W_{ij}$$

two-component RVB state



$|\text{b-RVB}\rangle$

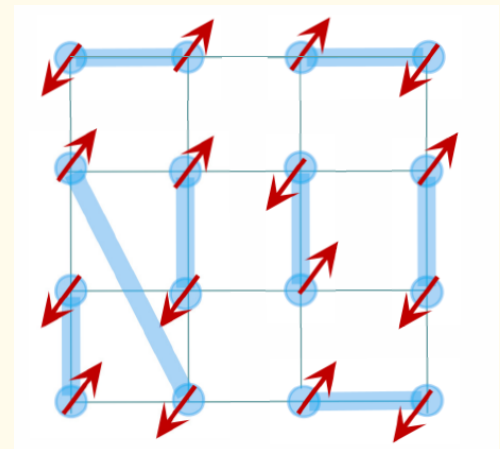
AFM

spin liquid

'Curie-Weiss'

doping

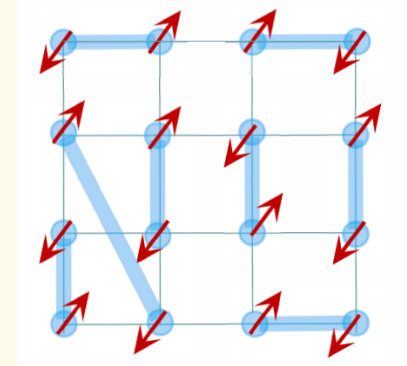
$$W_{ij} \propto \frac{1}{|\mathbf{r}_{ij}|^3} \quad |W_{ij}| \propto \exp\left[-\frac{|\mathbf{r}_{ij}|^2}{2\xi^2}\right] \quad W_{ij} \rightarrow W\delta_{ij}$$



$$|\Psi_G\rangle = e^{\hat{D}} |\text{b-RVB}\rangle$$

$$\hat{D} = \sum_{ij} g_{ij} \tilde{c}_{i\uparrow} \tilde{c}_{j\downarrow} \quad \Phi_{\text{RVB}}(\{\sigma_s\}) \equiv \sum_{\text{partition } (ij)} \prod (-1)^i W_{ij}$$

$$\tilde{c}_{i\sigma} = c_{i\sigma} e^{-i\hat{\Omega}_i} \quad \text{two-component RVB state}$$

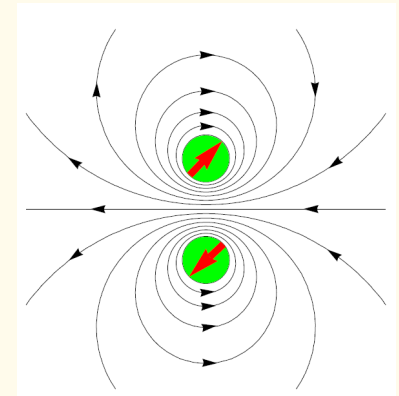


finite doping $\langle \hat{D} \rangle = \sum_{ij} g_{ij} \langle \tilde{c}_{i\uparrow} \tilde{c}_{j\downarrow} \rangle \neq 0 \longrightarrow \langle \tilde{c}_{i\uparrow} \tilde{c}_{j\downarrow} \rangle = \Delta_{ij}^0 \neq 0$

superconducting order parameter

$$\langle c_{i\uparrow} c_{j\downarrow} \rangle = \Delta_{ij}^0 \langle e^{i(\hat{\Omega}_i + \hat{\Omega}_j)} \rangle$$

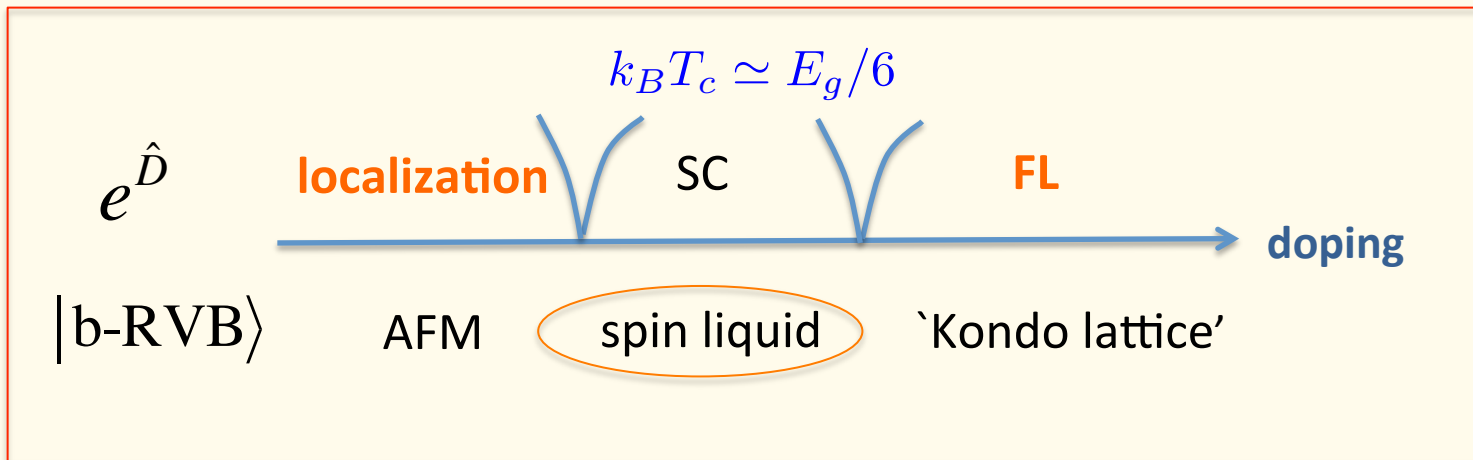
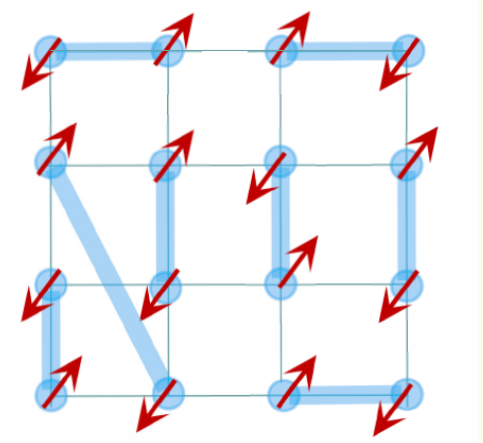
$$\begin{aligned} \hat{\Omega}_i &= - \sum_{l \neq i} \arg(i-l) [n_{l\downarrow}^b] \\ &= \frac{1}{2} \sum_{l \neq i} \arg(i-l) [n_{l\uparrow}^b - n_{l\downarrow}^b - 1] \end{aligned}$$



$$|\Psi_G\rangle = e^{\hat{D}} |\text{b-RVB}\rangle$$

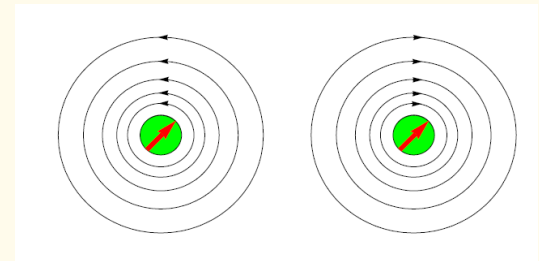
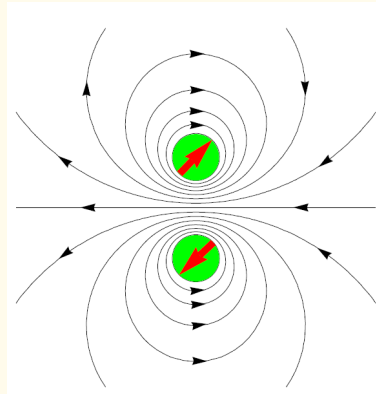
$$\hat{D} = \sum_{ij} g_{ij} \tilde{c}_{i\uparrow} \tilde{c}_{j\downarrow} \quad \tilde{c}_{i\sigma} = c_{i\sigma} e^{-i\hat{\Omega}_i}$$

$$|\text{b-RVB}\rangle =$$



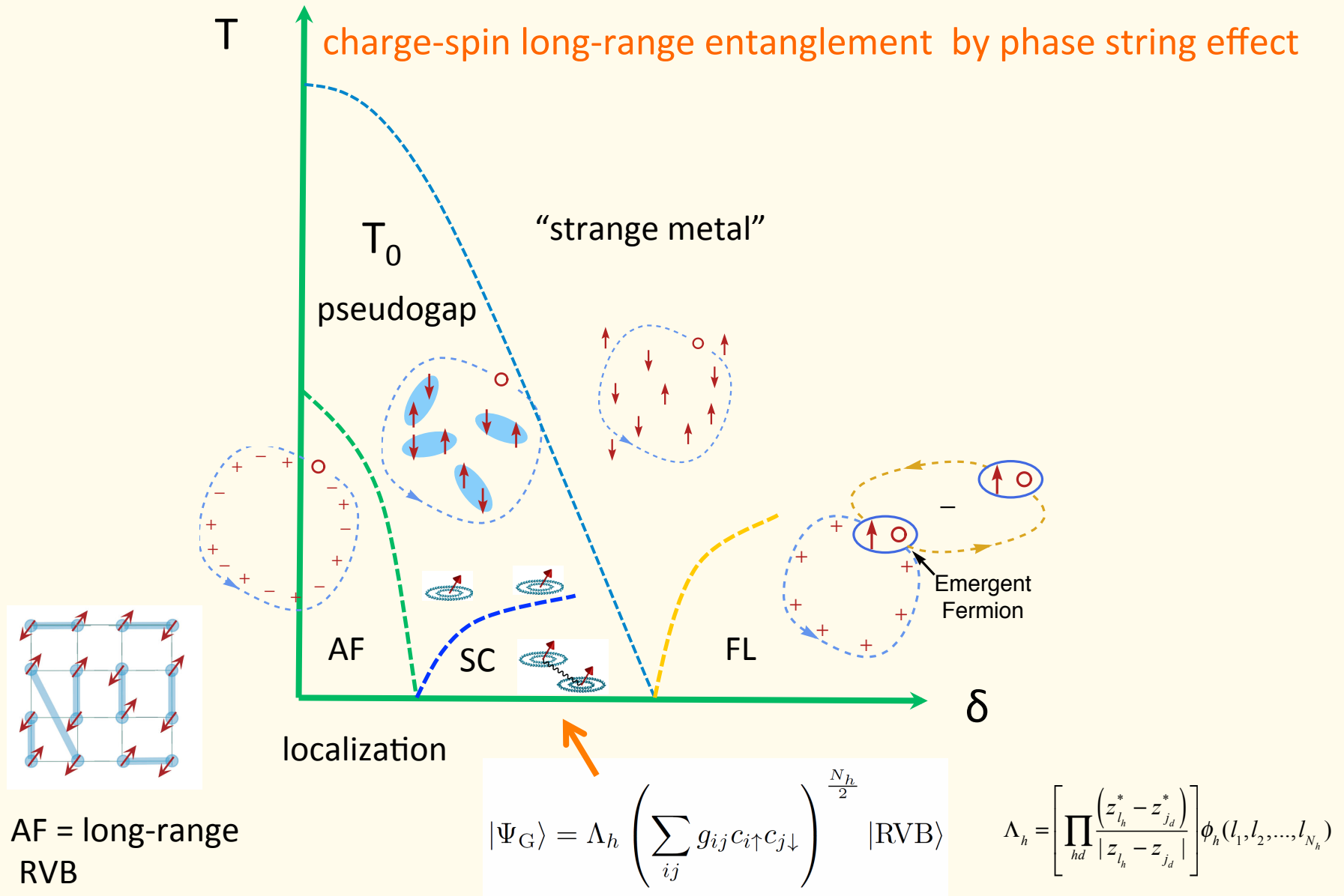
superconducting transition

$$\langle c_{i\uparrow} c_{j\downarrow} \rangle = \Delta_{ij}^0 \langle e^{i(\hat{\Omega}_i + \hat{\Omega}_j)} \rangle \rightarrow 0$$



J.W. Mei & ZYW, PRB (2010)

Global phase diagram



Fractionalization description of the ground state

$$|\Psi_G\rangle = \hat{\Lambda}_h \left(\exp \sum_{ij} g_{ij} c_{i\uparrow}^\dagger c_{j\downarrow} \right) |\text{b-RVB}\rangle \quad \hat{\Lambda}_h = \left[\prod_l e^{-i\hat{\Omega}_l} \right] \phi_h(l_1, l_2, \dots, l_{N_h})$$

$$c_{i\sigma} = h_i^\dagger a_{i-\sigma}^\dagger e^{i\hat{\Omega}_i}$$

$$|\Psi_G\rangle = \mathcal{P} [|\Phi_h\rangle \times |\Phi_a\rangle \times |\Phi_b\rangle]$$

$$|\Phi_h\rangle \equiv \sum_{\{l_h\}} \varphi_h(l_1, l_2, \dots) h_{l_1}^\dagger h_{l_2}^\dagger \cdots |0\rangle_h,$$

– holon condensation

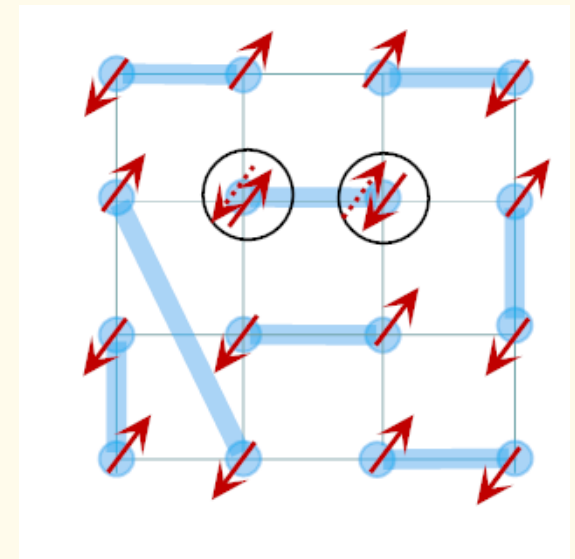
$$|\Phi_a\rangle \equiv \exp \left(\sum_{ij} \tilde{g}_{ij} a_{i\downarrow}^\dagger a_{j\uparrow}^\dagger \right) |0\rangle_a,$$

– backflow spinon: BCS-like

$$|\Phi_b\rangle \equiv \exp \left(\sum_{ij} W_{ij} b_{i\uparrow}^\dagger b_{j\downarrow}^\dagger \right) |0\rangle_b.$$

– bosonic spinon: b-RVB

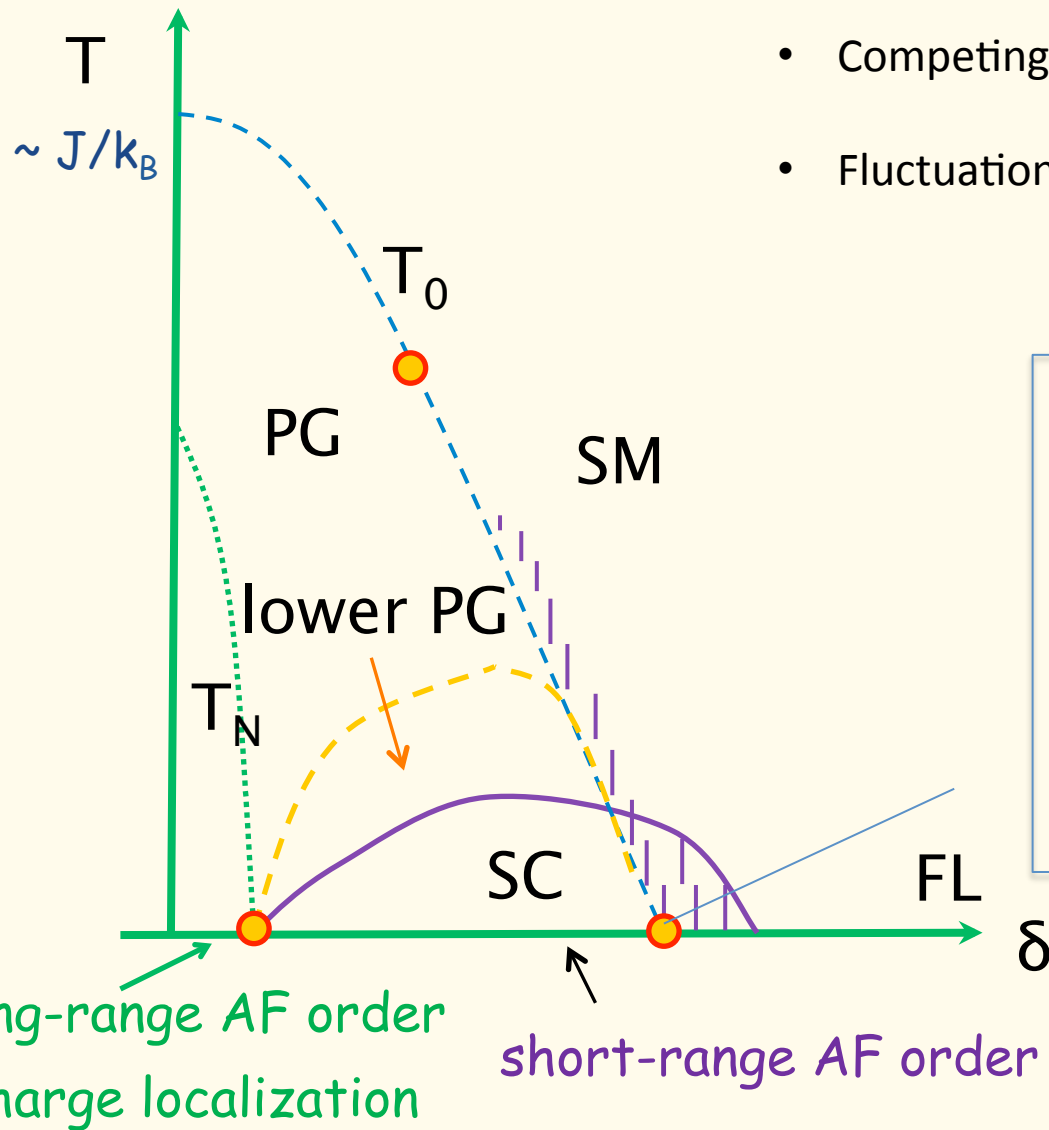
three hidden orders



two-dimensional limit, $T > 0$

Competing order or Fluctuating regime?

- Competing orders: generalized GL eq.
- Fluctuations: fractionalization of electron degrees of degree due to Mottness



$$|\Psi_G\rangle = \hat{P} \left[|\Phi_h\rangle \otimes |\Phi_a\rangle \otimes |\Phi_b\rangle \right]$$

three hidden orders:

- holon condensation
- bosonic spinon RVB
- backflow spinon RVB

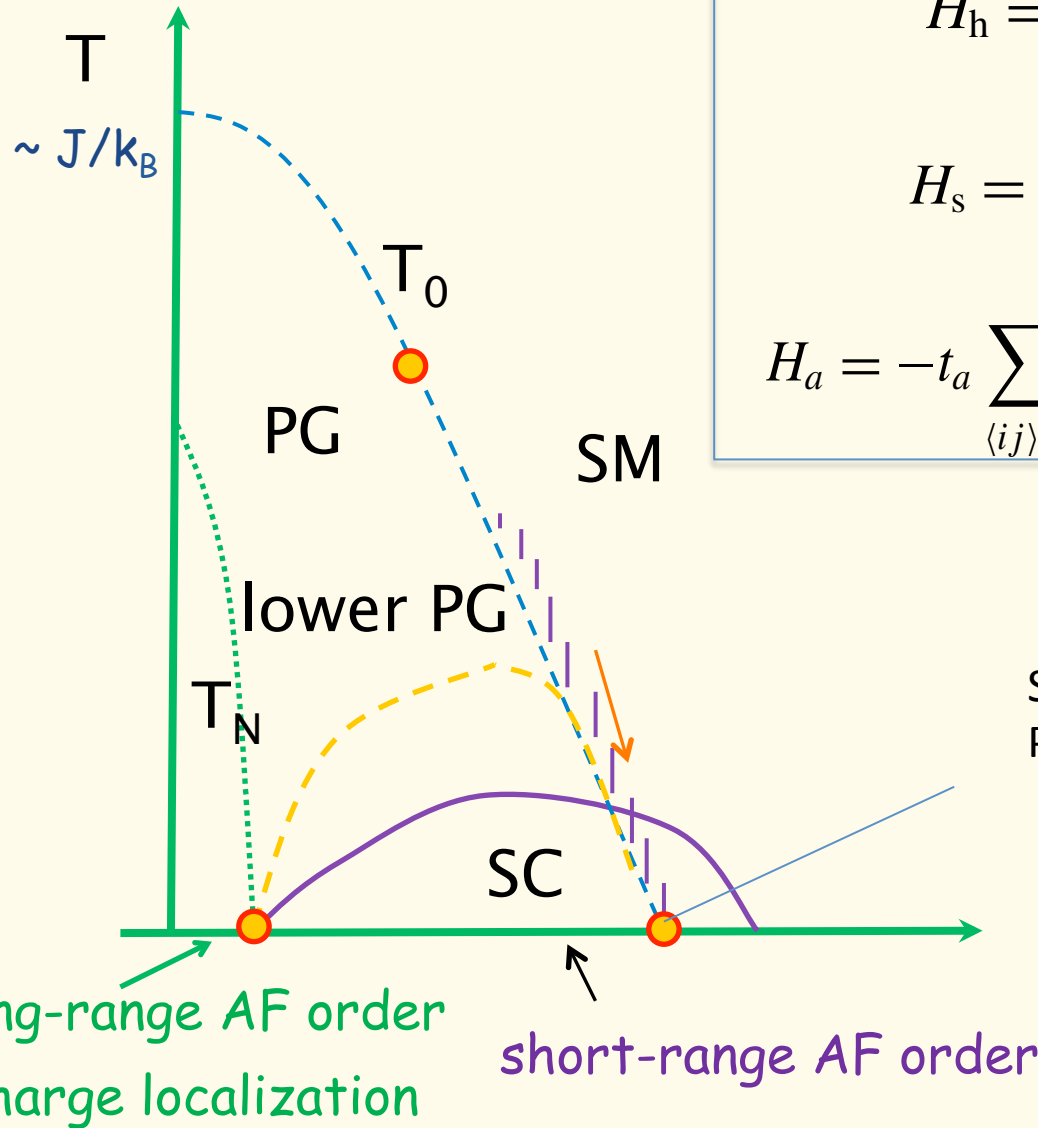
AF and SC instabilities at $T=0$

$$|\Psi_G\rangle = \mathcal{P} [|\Phi_h\rangle \times |\Phi_a\rangle \times |\Phi_b\rangle]$$

$$H_h = -t_h \sum_{\langle ij \rangle} (e^{iA_{ij}^s}) h_i^\dagger h_j + \text{h.c.},$$

$$H_s = -J_s \sum_{\langle ij \rangle \sigma} (e^{i\sigma A_{ij}^h}) b_{i\sigma}^\dagger b_{j-\sigma}^\dagger + \text{h.c.}$$

$$H_a = -t_a \sum_{\langle ij \rangle \sigma} e^{-i\phi_{ij}^0} a_{i\sigma}^\dagger a_{j\sigma} - J_a \sum_{\langle ij \rangle} \eta_{ij} \hat{\Delta}_{ij}^a + \text{h.c.}$$



mutual Chern-Simons theory

S.P. Kou, X.L. Qi, ZYW, PRB (2005)

P. Ye, C.S. Tian, X.L. Qi, ZYW, PRL (2011)

Mean-field theory

Y. Ma, P. Ye, ZYW, NJP (2014)

Strange metal behavior

Z.C. Gu, ZYW, PRB (2005)

Conclusion

- Constructed a ground state wavefunction based on three general principles:

$$|\Psi_G\rangle = e^{\hat{D}} |\text{b-RVB}\rangle$$

No double occupancy constraint;
Correct AFM state at half-filling;
Phase string sign structure at finite doping

- By VMC, the wavefunction reproduces the novel properties of one-hole-doped 2-leg t-J model by DMRG:

QCP, charge modulation, Fermi surface reconstruction etc.

- In 2D, the wavefunction predicts AFM, d-wave SC, and FL phases as a function of doping
- Fractionalization and mutual Chern-Simons gauge theory description of elementary excitations and finite-temperature phase diagram

Acknowledgements

Yi Zhou (Zhejiang U), V.N. Muthukumar (CCNY): wavefunction

Qing-Rui Wang, Yang Qi (Tsinghua/PI): VMC

Zheng Zhu (Tsinghua/MIT) , Hongchen Jiang (SLAC): DMRG

Kai Wu (SLAC), Jan Zannen (Leiden): Sign structure

Supeng Kou (BNU), , Xiaoliang Qi (Stanford), P. Ye (PI), Chushun Tian (Tsinghua):

Mutual Chern-Simons theory

Jia-Wei Mei (PI) : SC transition and T_c formula

Peng Ye (PI), Yao Ma (Tsinghua), Zhengcheng Gu (PI): Pseudogap phase