Superconductivity and bond order in a doped Mott insulator

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→ Oak Ridge Natl. Lab.

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D. C. Johnston, B. N. Harmon and Y. Lee (Ames)
C. Batista (LANL)

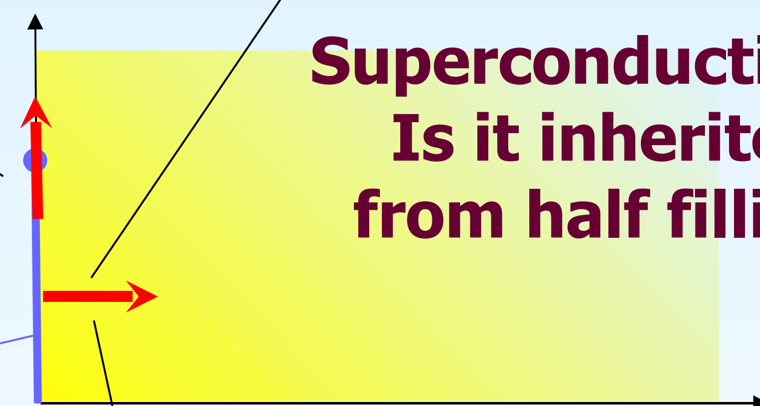
J. Liu, J. Schmalian, N. Trivedi, PRL 94, 127003 (2005))
J. Liu, N. Trivedi, B. N. Harmon, Y. Lee, J. Schmalian, cond-mat/0702118

Moving away from the Mott insulator

quasi two dimensional organic charge transfer salts
κ-(BEDT-TTF)$_2$X

$CuBO_3$-planes with Cu^{2+}-spins on a Shastry-Sutherland lattice
$SrCu_2(BO_3)_2$

pressure (band width)



Superconductivity?
Is it inherited from half filling?

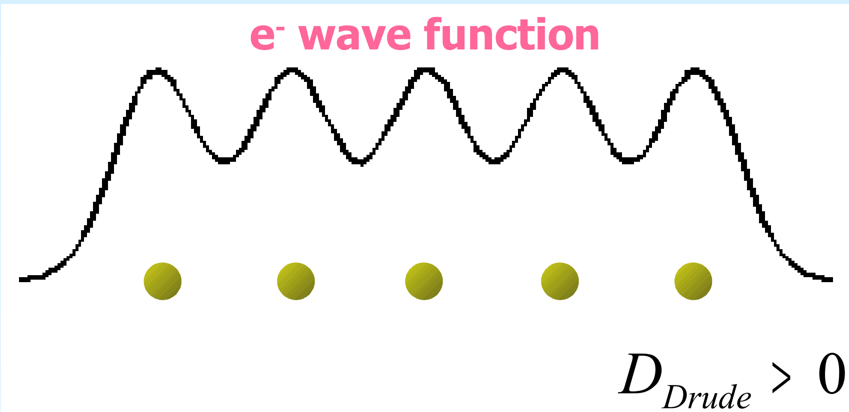
Mott insulator

carrier concentration

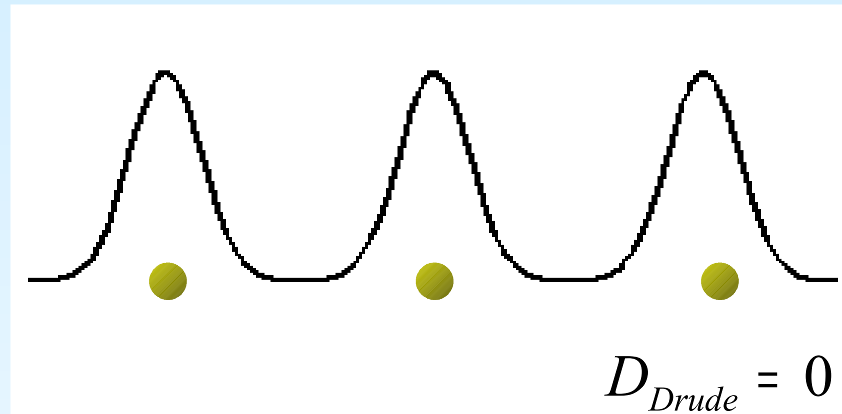
high temperature superconductors
$La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_{7-y}$, $Nd_{2-x}Ce_xCuO_4$ etc.

Mott insulator

periodic solid at commensurate filling (odd # of e^- per site)



weak interaction
metal



strong repulsion

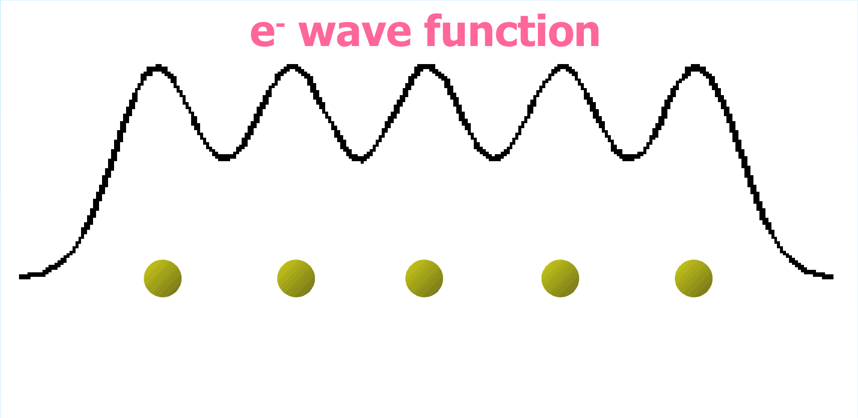
localization due to
strong Coulomb repulsion

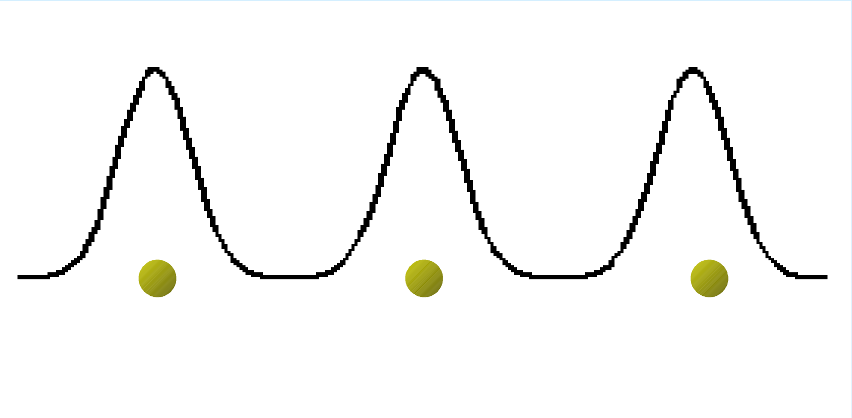
electric field changes boundary condition
W. Kohn, Phys. Rev. 133, A171 (1964)

$$\Psi\left(\mathbf{x}_i + L\right) = e^{i\phi}\Psi\left(\mathbf{x}_i\right) \qquad D_{Drude} \propto \frac{\delta^2 E}{\delta\phi^2} \qquad \sigma'(\omega) = \frac{D_{Drude}}{\pi}\frac{\tau}{1+(\omega\tau)^2}$$

Mott insulator

periodic solid at commensurate filling (odd # of e^- per site)





weak interaction
metal

strong repulsion

localization due to
strong Coulomb repulsion

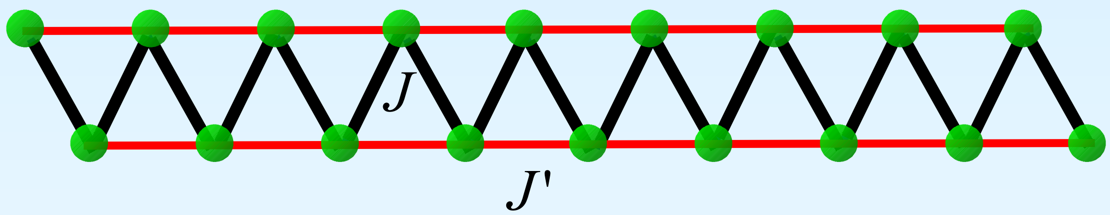
interesting consequences:

- what happens to the spin degree of freedom?
- coupling to orbital degrees + lattice
- transition tuned by changing overlap
- physics away from commensurate filling
- role of disorder
- …

Majumdar-Ghosh model

C. K. Majumdar, D. K. Ghosh, J. Math. Phys. 10 1388 (1969)

$$H = J\sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J'\sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+2}$$



$J' = \frac{1}{2}J$ ground state is exactly known: $\left|\Psi\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\Psi_1\right\rangle + \left|\Psi_2\right\rangle\right)$

$$\left|\Psi_1\right\rangle = \prod_{i=1}^{N/2} \frac{1}{\sqrt{2}}\left(\left|\uparrow_{2i},\downarrow_{2i+1}\right\rangle - \left|\downarrow_{2i},\uparrow_{2i+1}\right\rangle\right)$$

$$\left|\Psi_1\right\rangle = \prod_{i=1}^{N/2} \frac{1}{\sqrt{2}}\left(\left|\uparrow_{2i-1},\downarrow_{2i}\right\rangle - \left|\downarrow_{2i-1},\uparrow_{2i}\right\rangle\right)$$

Shastry-Sutherland model

1)

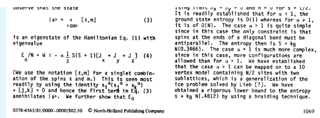
Physica 108B (1981) 1069-1070
North-Holland Publishing Company

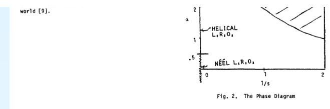
EXACT GROUND STATE OF A QUANTUM MECHANICAL ANTIFERROMAGNET

B. Sriram Shastry and Bill Sutherland

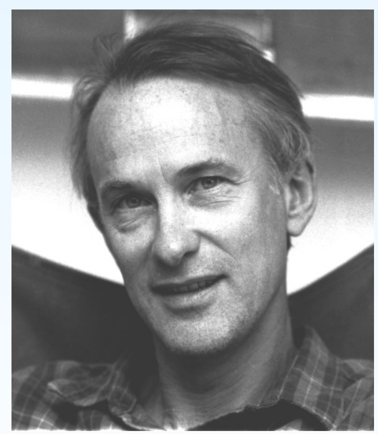
Department of Physics, University of Utah, Salt Lake City, UT 84112

We present some exact results for the ground state of a quantum mechanical antiferromagnetic model in the two dimensions with next-nearest neighbor interactions.





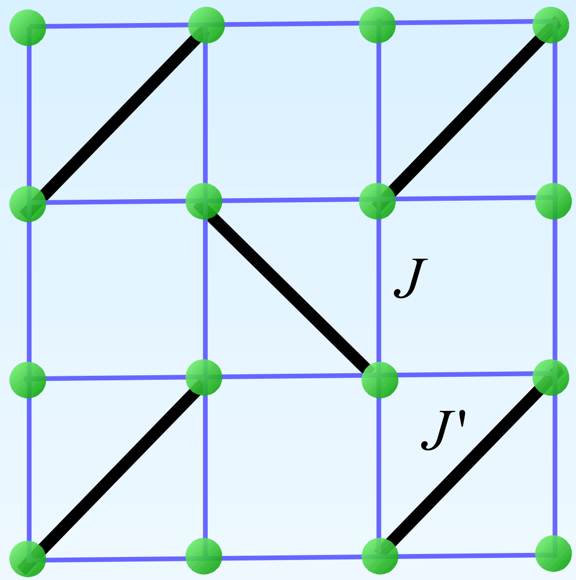
Sriram Shastry



Bill Sutherland

Shastry-Sutherland model

B. S. Shastry and B. Sutherland, Physica B **108**, 1069 (1981)



$$H = J\sum_{\langle ij\rangle} \mathbf{S}_i\cdot\mathbf{S}_j + J'\sum_{ij\in\,\mathrm{diag}} \mathbf{S}_i\cdot\mathbf{S}_j$$

ground state is exactly known:

$$|\Psi\rangle = \prod_{ij\in\,\mathrm{diag}} \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

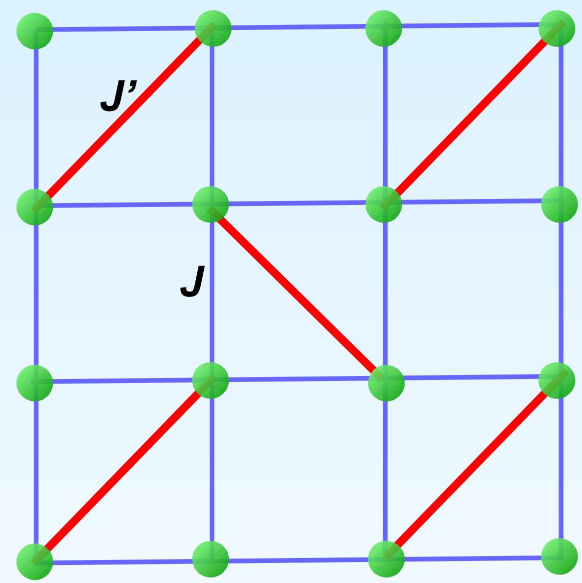
valence bond crystal

Shastry-Sutherland model

B. S. Shastry and B. Sutherland, Physica B **108**, 1069 (1981)

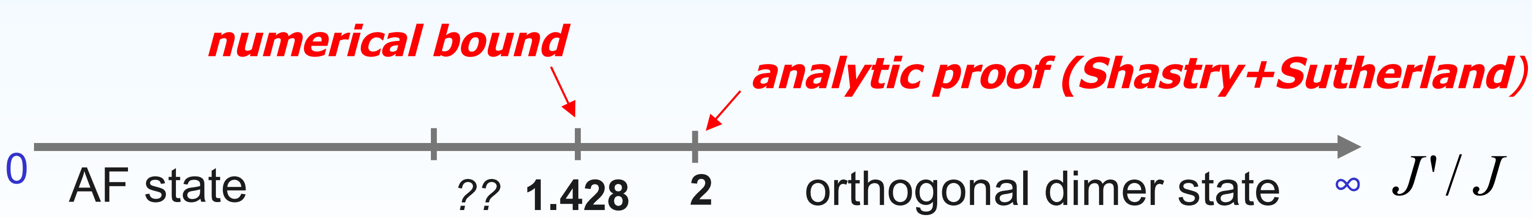
(1) $J'/J \to \infty$ → orthogonal dimer state

$$|\Psi_0\rangle = \prod_{ij \in \text{diag}} \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$$



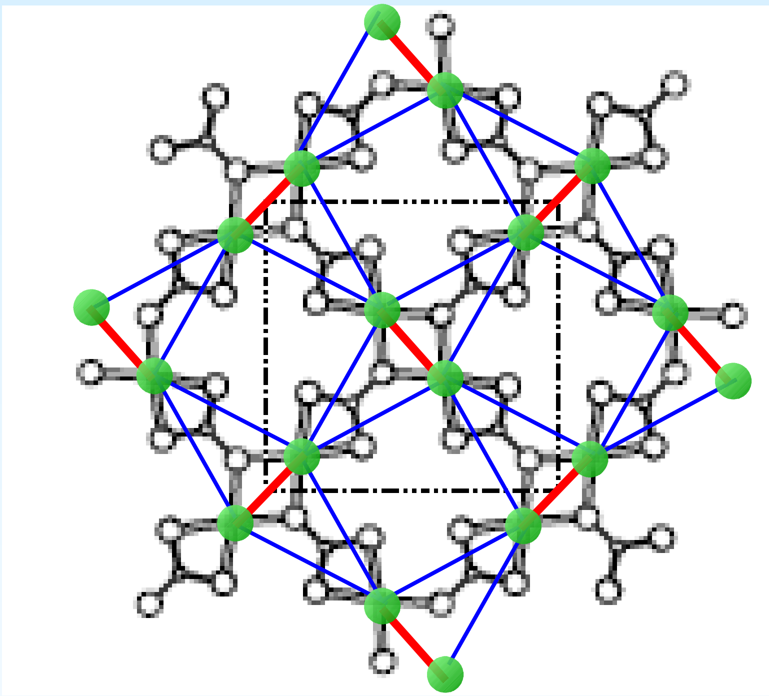
(2) $J'/J \to 0$ → antiferromagnet

(3) orthogonal dimer remains the **exact** ground state for some finite J'/J

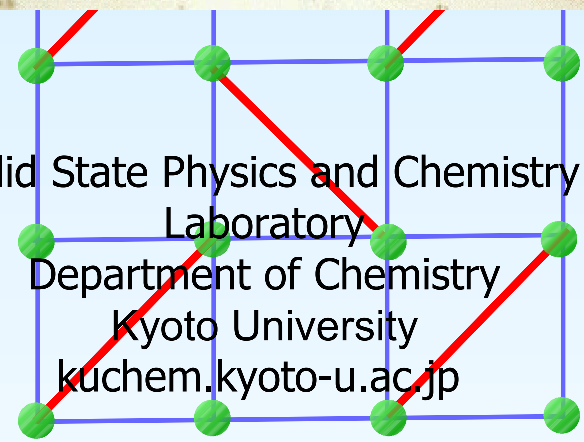


$CuBO_3$-planes in $SrCu_2(BO_3)_2$

H. Kageyama, K. Yoshimura, R. Stern, N. V. Mushnikov, K. Onizuka, M. Kato, K. Kosuge, C. P. Slichter T. Goto, Y. Ueda, Phys. Rev. Lett. **82** 3168 (1999)



Shastry-Sutherland lattice



Solid State Physics and Chemistry Laboratory
Department of Chemistry
Kyoto University
kuchem.kyoto-u.ac.jp

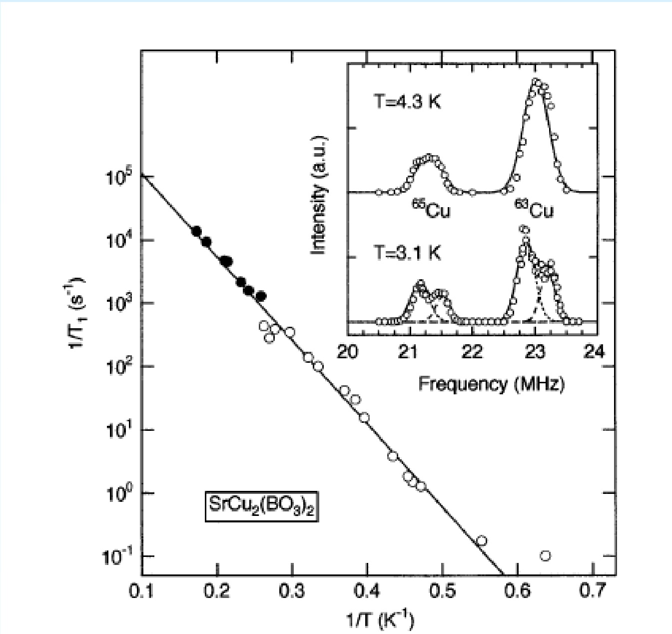
● Cu^{2+} sites → exchange interactions: J' (red line)

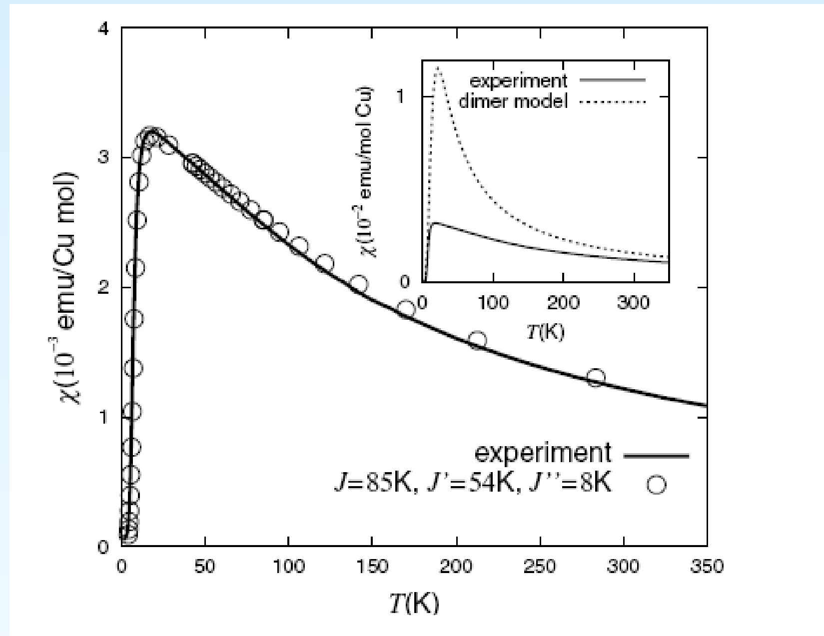
J (blue line)

CuBO$_3$-planes in SrCu$_2$(BO$_3$)$_2$

H. Kageyama, K. Yoshimura, R. Stern, N. V. Mushnikov, K. Onizuka, M. Kato, K. Kosuge, C. P. Slichter T. Goto, Y. Ueda, Phys. Rev. Lett. **82** 3168 (1999)

spin gap seen in NMR + susceptibility





Shin Miyahara and Kazuo Ueda
J. Phys.: Condens. Matter 15 (2003) R327–R366

$J'/J \approx 1.56$ $\quad$ $SrCu_2(BO_3)_2$

0 AF state ?? **1.428** **2** orthogonal dimer state ∞ J'/J

→ valence bond crystal is fragile

adding charge carriers to $SrCu_2(BO_3)_2$

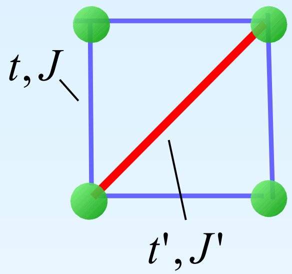
Heisenberg model

$$H = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \longrightarrow$$

t-J model

$$H_{tJ} = \sum_{ij} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + \sum_{ij} J_{ij} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4} n_i n_j \right)$$

$$\text{with} : \sum_{\sigma} c^{+}_{i\sigma} c_{i\sigma} \le 1$$



super exchange

$$J_{ij} = 4t_{ij}^2 / U$$

We know:

$$J, J' \longrightarrow t'^2 / t^2$$

We don't know:

$$t', t \text{ (relative sign?)}$$

- sign of t is irrelevant
- if t'>0 for hole doping, electron doping is described by t'<0 and vice versa

LDA calculation:

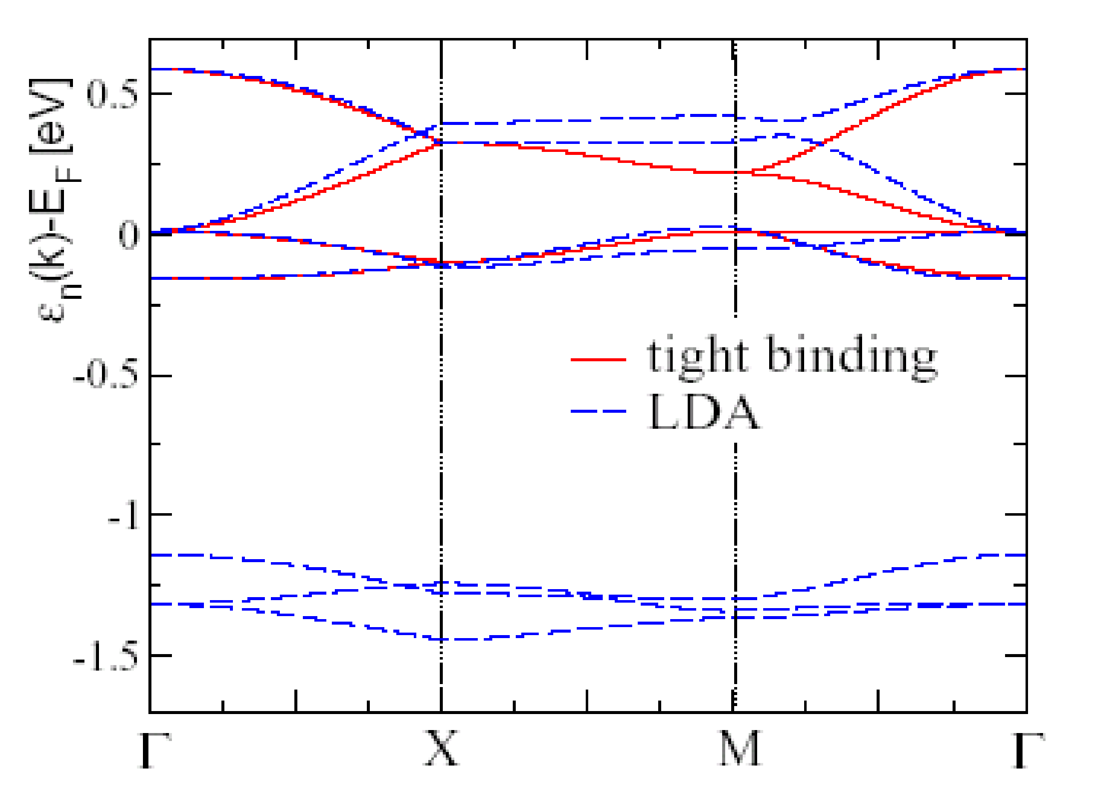
- experimets at half filling

$$J'/J \approx 1.56 \Rightarrow \quad t'/t \approx 1.25$$

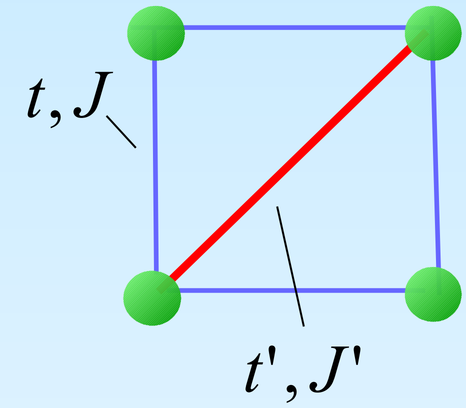
- tight binding fit

$$t'/t \approx 1.2$$

$$t' > 0$$



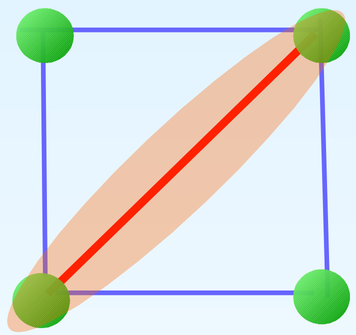
adding one hole to 4 sites

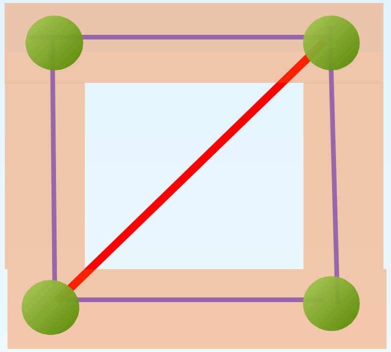


electron doping: (t’<0)

hole doping: (t’>0)

single
doped
carrier





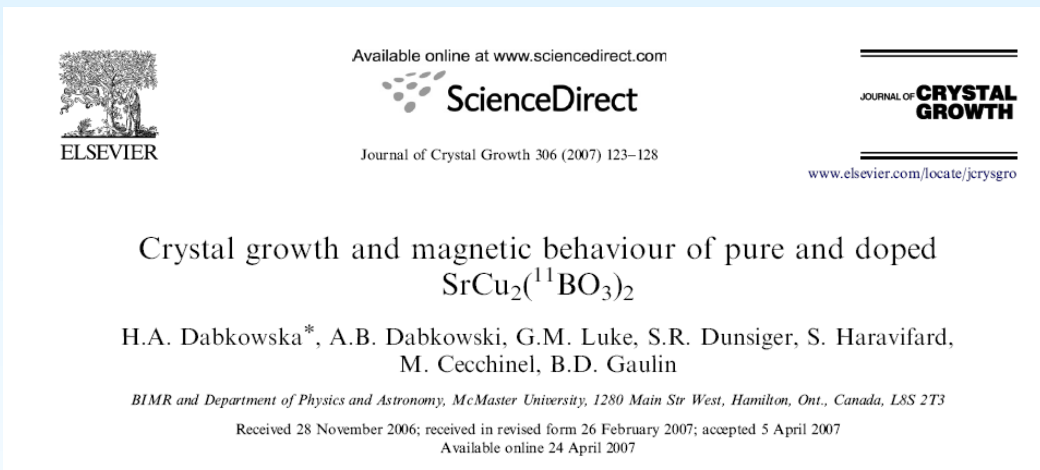
electron is localized on the dimer bond

hole delocalizes

expect strong asymmetry between electron and hole doping

experimental situation

- several groups are trying very hard to add carriers to $SrCu_2(BO_3)_2$
- recently: 2%+2.5% electron doping + 2.5% hole doping



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Journal of Crystal Growth 306 (2007) 123–128

JOURNAL OF CRYSTAL GROWTH

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Crystal growth and magnetic behaviour of pure and doped $SrCu_2(^{11}BO_3)_2$

H.A. Dabkowska*, A.B. Dabkowski, G.M. Luke, S.R. Dunsiger, S. Haravifard, M. Cecchinel, B.D. Gaulin

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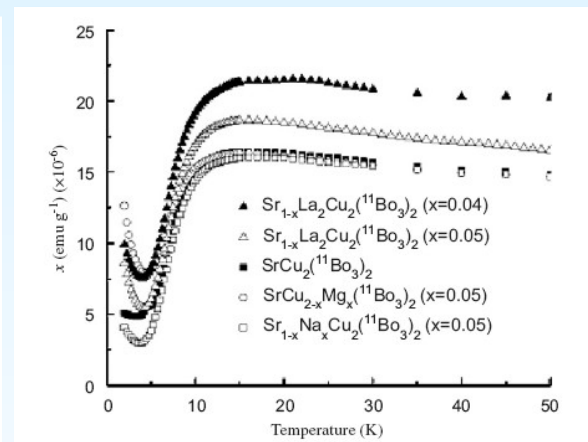
Available online 24 April 2007



Mean field approach to the t-J model

(Baskaran, Zou, Anderson (1988); Kotliar + Liu (1988))

$$H_{tJ} = \sum_{ij} t_{ij} c_{i\sigma}^{+} c_{j\sigma} + \sum_{ij} J_{ij} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4} n_i n_j \right) \qquad \text{with} : \sum_{\sigma} c_{i\sigma}^{+} c_{i\sigma} \le 1$$

slave boson: $c_{i\sigma} = f_{i\sigma} b_i^{+}$ $\qquad \sum_{\sigma} f_{i\sigma}^{+} f_{i\sigma} = 1 - b_i^{+} b_i$

Mean field ground state

$$\left| \Psi_{\text{mf}} \right\rangle = \left(b_{q=0}^{+} \right)^{N_h} \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} f_{\mathbf{k}\uparrow}^{+} f_{-\mathbf{k}\downarrow}^{+} \right) \left| 0 \right\rangle$$

Bose-condensate **BCS-wave function**

$\left| \Psi_{\text{mf}} \right\rangle \neq \left| \Psi_{\text{exact}} \right\rangle$ mean field theory poorly reproduces the exact valence bond crystal at half filling

proper projection

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

$$|\Psi\rangle = \prod_i \left(1 - n_{i\uparrow} n_{i\downarrow}\right) |\Phi_{\mathrm{BCS}}\rangle$$

projection to states

with $\sum_\sigma n_{i\sigma} \leq 1$

fermion mean field state

$$H_{\mathrm{mf}} = \sum_{ij,\sigma} t_{ij}^{*} c_{i\sigma}^{+} c_{j\sigma} + \sum_{ij} \left(\Delta_{ij} c_{i\uparrow}^{+} c_{j\downarrow}^{+} + h.c.\right)$$

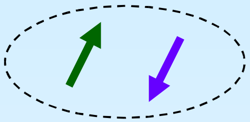
variational approach:

- minimize: $E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$ w.r.t. $\Delta_{ij}, t_{ij}^{*}, \mu_i \ldots$

D. M. Ceperley, G. V. Chester, M. H. Kalos, Phys. Rev. B 16, 3081 (1977)

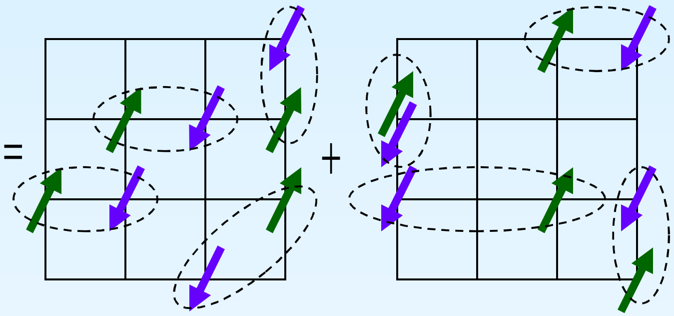
proper projection in real space

$$\left|\Psi_{BCS}\right\rangle = \frac{1}{N!}\sum_P (-1)^P \prod_{i=1,\ldots,N} \varphi\left(r_{i,\uparrow} - r_{P_i,\downarrow}\right)$$



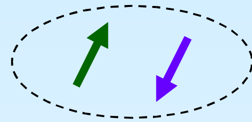
$: \varphi\left(r_\uparrow - r_\downarrow\right)$

$\left|\Psi_{BCS}\right\rangle =$

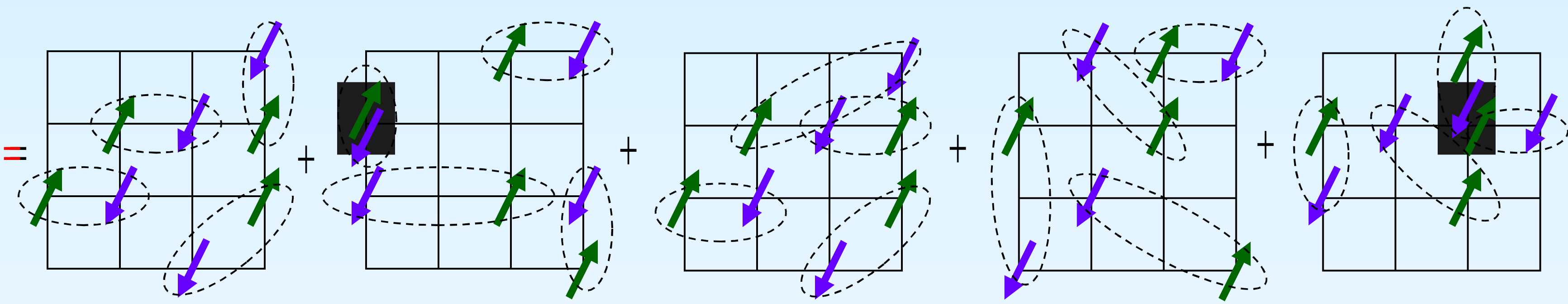


proper projection in real space

$$|\Psi_{BCS}\rangle = \frac{1}{N!}\sum_{P}(-1)^{P}\prod_{i=1,\dots,N}\varphi\left(r_{i,\uparrow} - r_{P_i,\downarrow}\right)$$

 $: \varphi\left(r_{\uparrow} - r_{\downarrow}\right)$

$|\Psi_{BCS}\rangle =$



- exact ground state included → at half filling $|\Psi\rangle = |\Psi_{\text{exact}}\rangle$
- allows distinction between ODLRO + singlet gap Δ_{ij}

$$F_{i'j'}(i-j) = \langle B^{+}_{ii'} B_{jj'} \rangle \qquad B^{+}_{ij} = c^{+}_{i\uparrow} c^{+}_{j\downarrow}$$

superconducting order parameter $|\psi|^2 = F_{i'j'}(i-j \to \infty)$

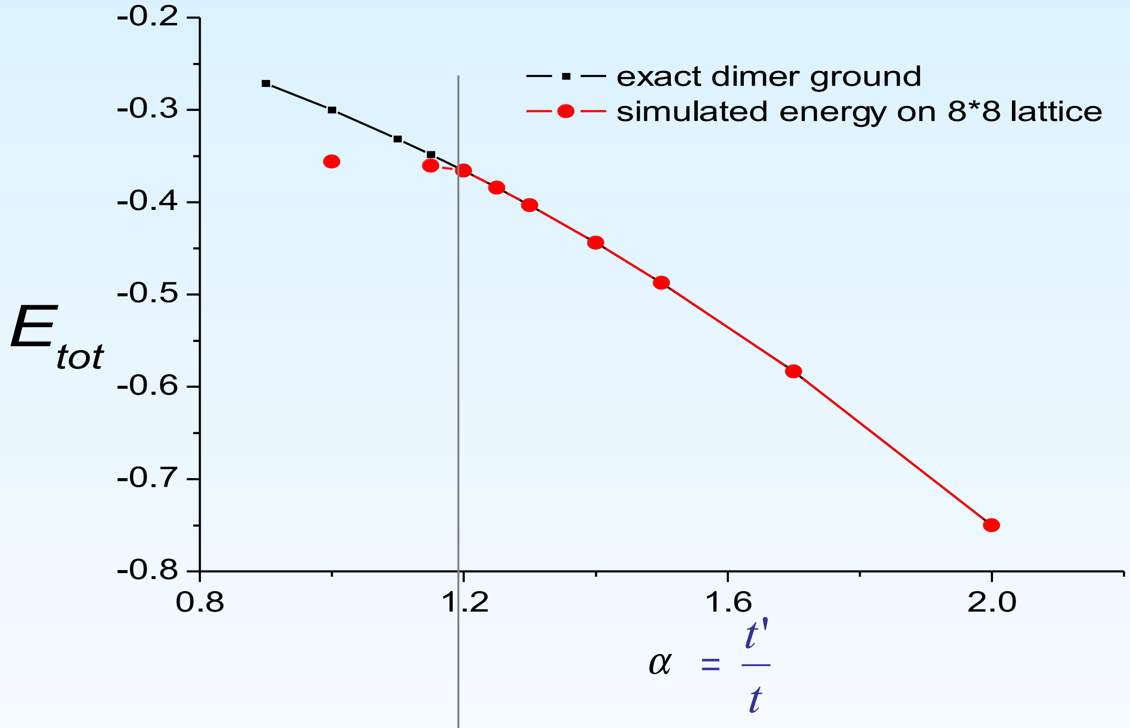
Meissner effect
flux quantization

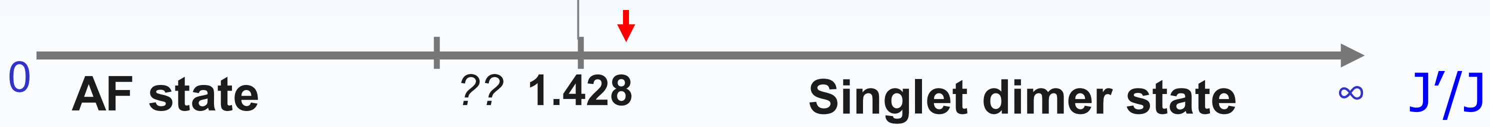
half filling

- $|\Psi_{RVB}\rangle$ yields the exact ground state energy and the exact spin correlations at half filling!

$$\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = -\frac{3}{4} \text{ or } = 0$$

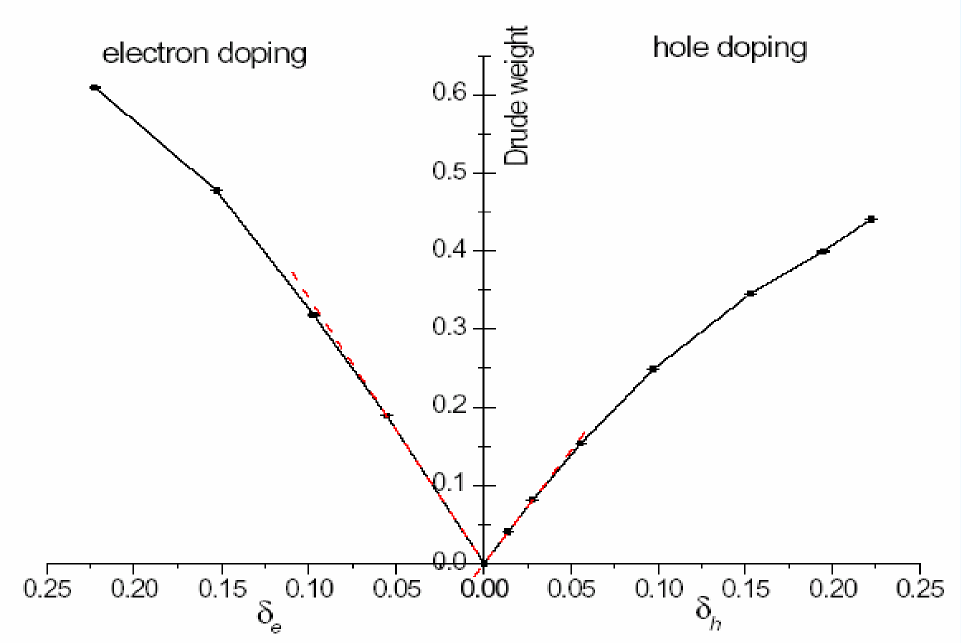
theory & simulated energy v.s. *t'/t*





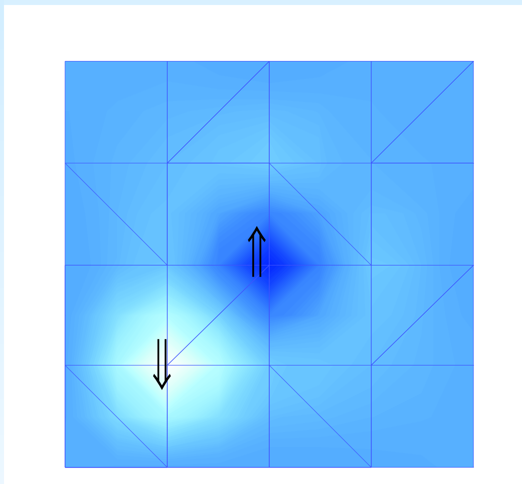
finite doping

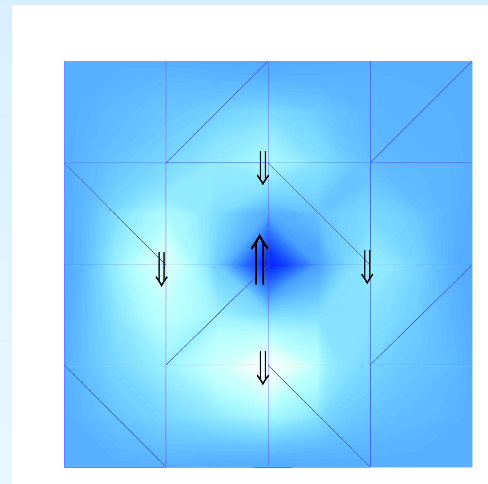
Low frequency Drude weight $\sigma'(\omega) = \frac{D_{Drude}}{\pi} \frac{\tau}{1+(\omega\tau)^2}$



metallic or superconducting !

spin correlations $\langle \mathbf{S}_{i=0} \cdot \mathbf{S}_j \rangle$





$$|\Psi\rangle = |\diagdown\rangle|\diagup\rangle|\diagdown\rangle|\diagup\rangle\cdots|\diagdown\rangle|\diagup\rangle$$

valence bond crystal

$$|\Psi\rangle = \sum_{\alpha} |=\rangle|\shortparallel\rangle|=\rangle|\shortparallel\rangle\cdots|=\rangle|\shortparallel\rangle$$

resonating valence bond state

electron doping

hole doping

singlets localize

singlets delocalize

superconductivity (ODLR)

$$F_{i'j'}(i-j) = \langle B^{+}_{ii'} B_{jj'} \rangle$$

$$(B_{ij} = c_{i\uparrow} c_{j\downarrow})$$

$$|\psi|^2 = F_{i'j'}(i-j \to \infty)$$

no superconductivity
in the valence bond crystal**!**

$\Delta_{ij} \neq 0$ in $|\Phi_{BCS}\rangle$

$z_{\mathbf{k}} = 0$ (discontinuity in $n_{\mathbf{k}}$)

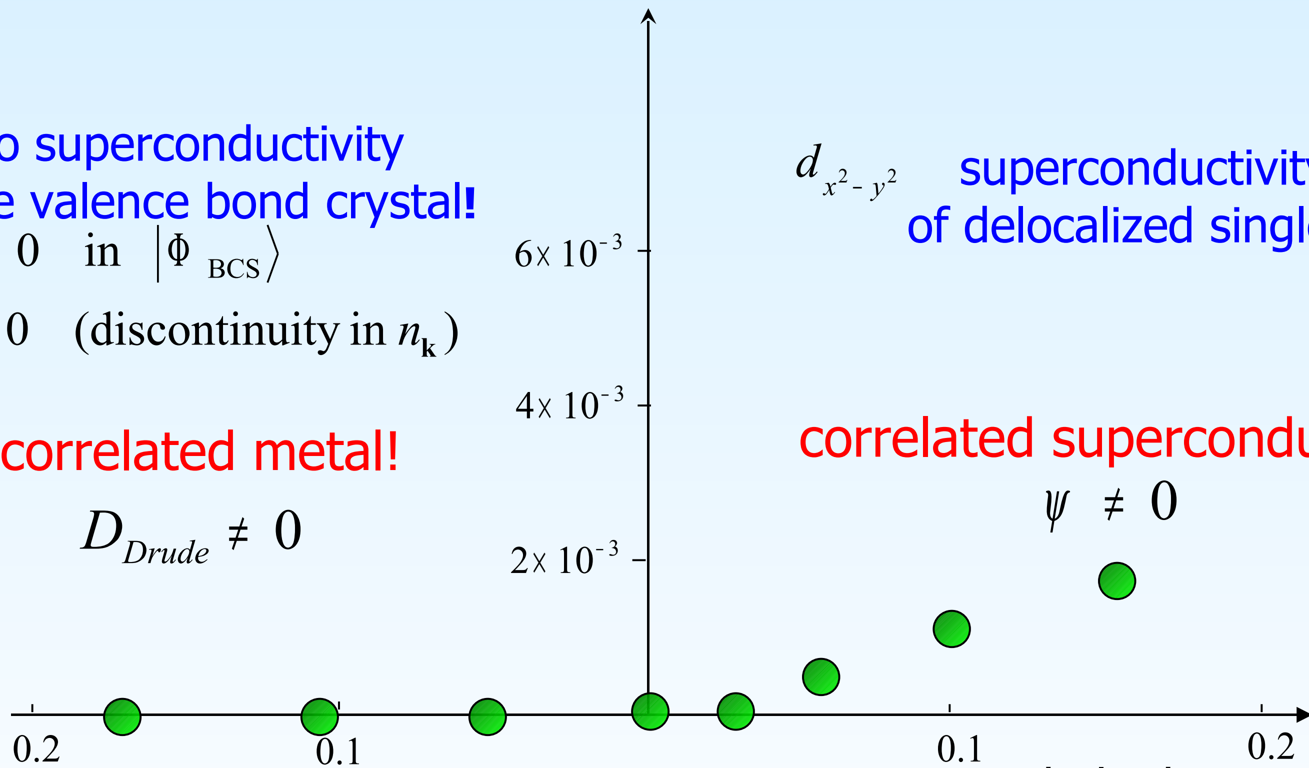
correlated metal!

$D_{Drude} \neq 0$

$d_{x^2-y^2}$ superconductivity
of delocalized singlets

correlated superconductor!

$\psi \neq 0$



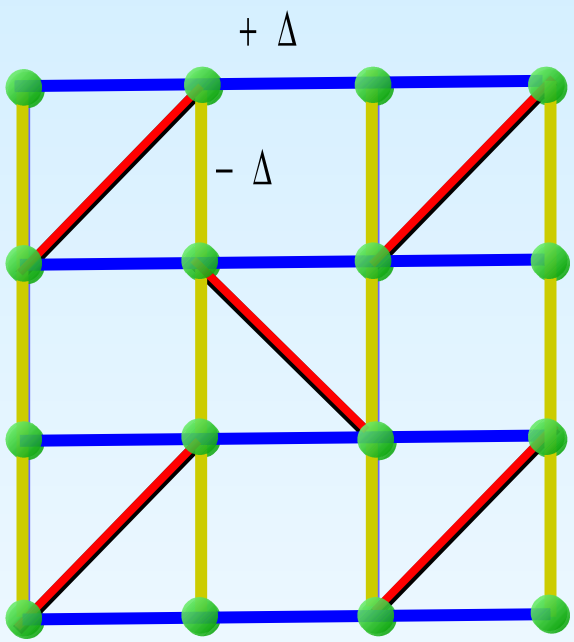
electron doping

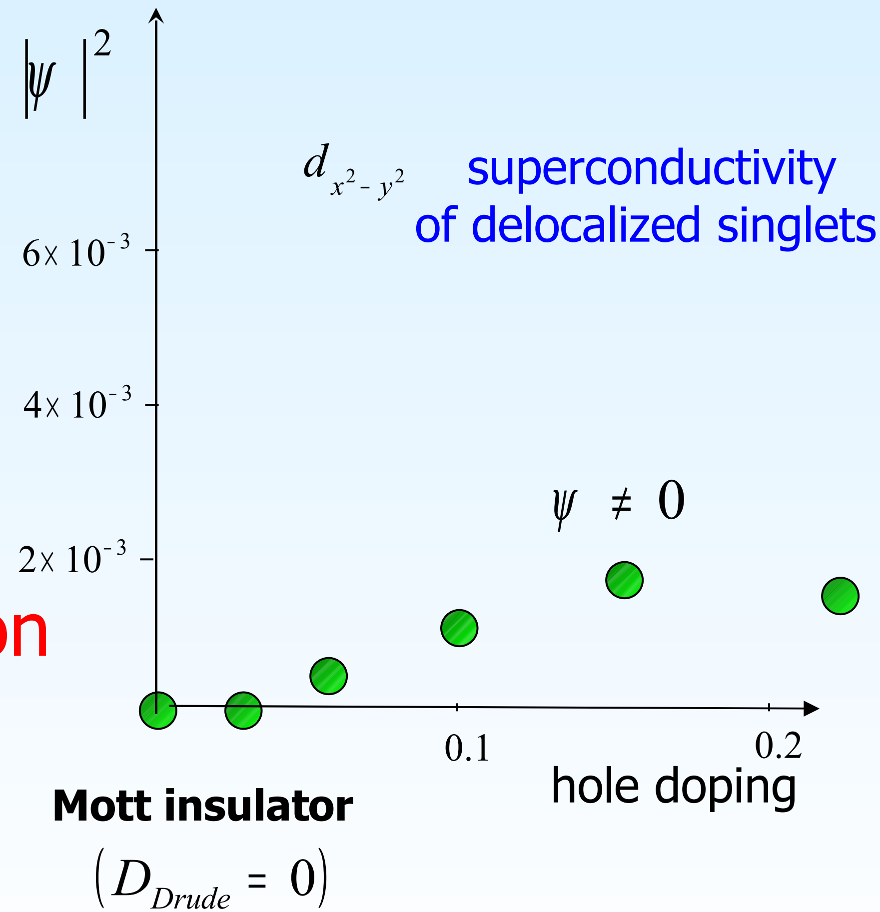
Mott insulator

$(D_{Drude} = 0)$

hole doping

hole doping

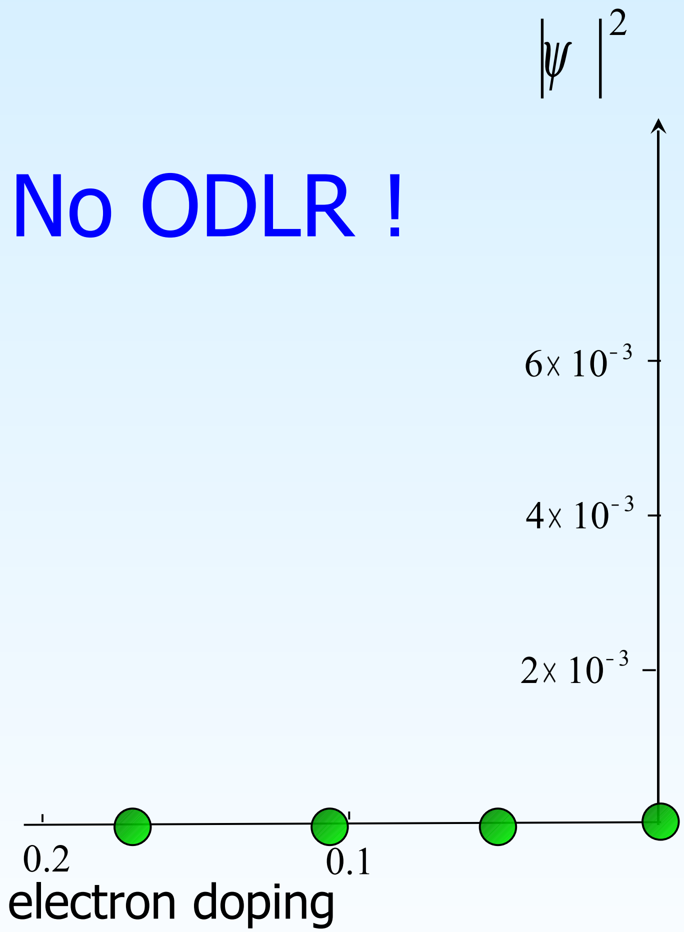




s.c. in not a delocalization
of preformed singlets !

electron doping

No ODLR !



$\Delta_{ij} \neq 0!$

$$|\Psi\rangle = \prod_i \left(1 - n_{i\uparrow} n_{i\downarrow}\right) \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} f^{+}_{\mathbf{k}\uparrow} f^{+}_{-\mathbf{k}\downarrow}\right)|0\rangle$$

broken U(1) symmetry

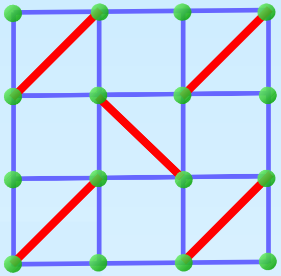
no ODLR → U(1) symmetry not broken

<u>full projection changes the the symmetry breaking</u>

- known at half filling:

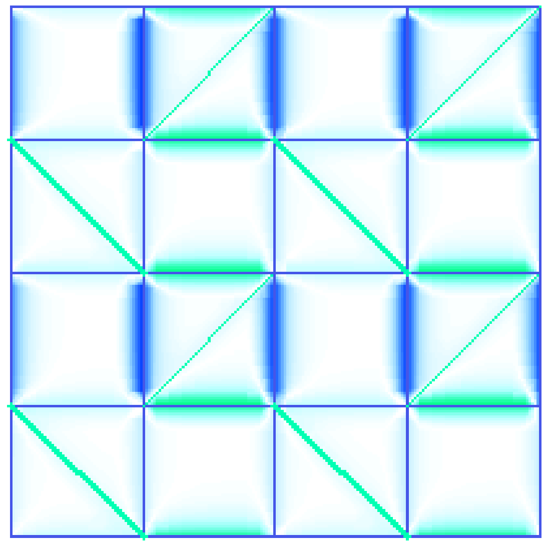
  Affleck, Zou, Hsu,Anderson PRB **38**, 745 (1988)
- new for doped systems

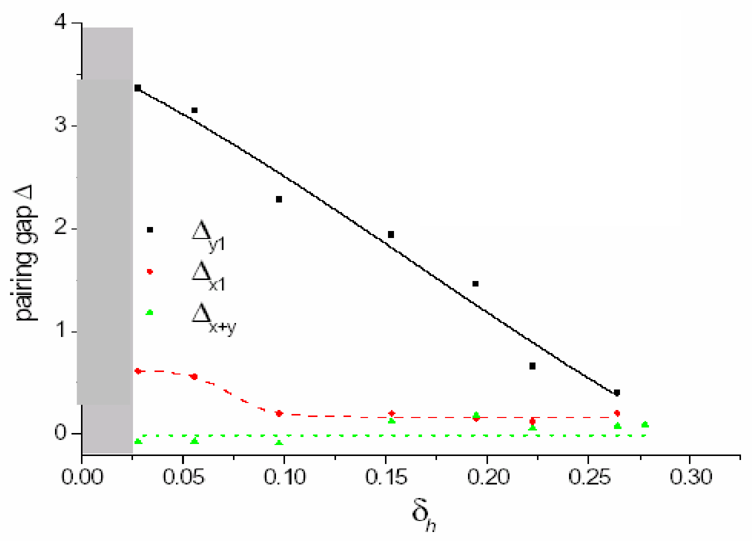
Are there other symmetries broken in the doped system?



hole doping: singlet pairing gap forms a plaquette state

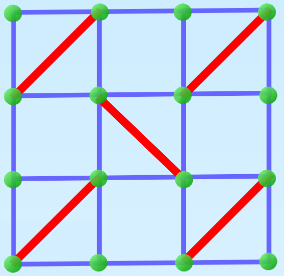
Δ_{ij}



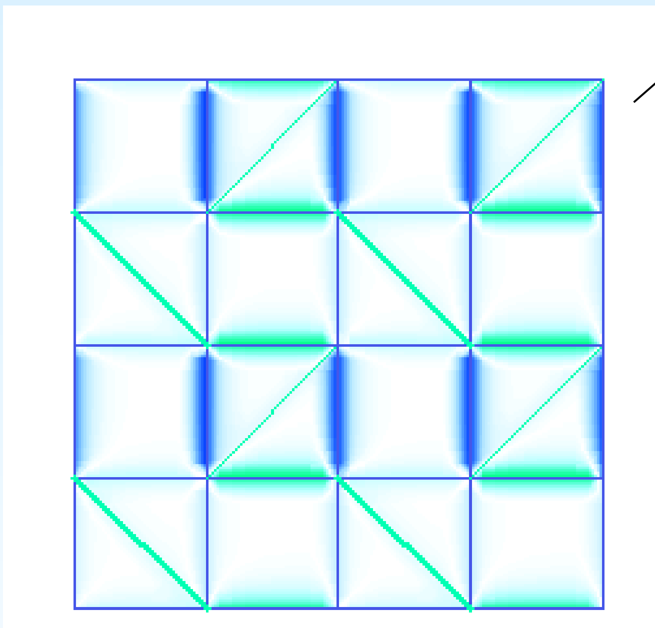


Are there other symmetries broken in the doped system?

hole doping: singlet pairing gap forms a plaquette state



Δ_{ij}



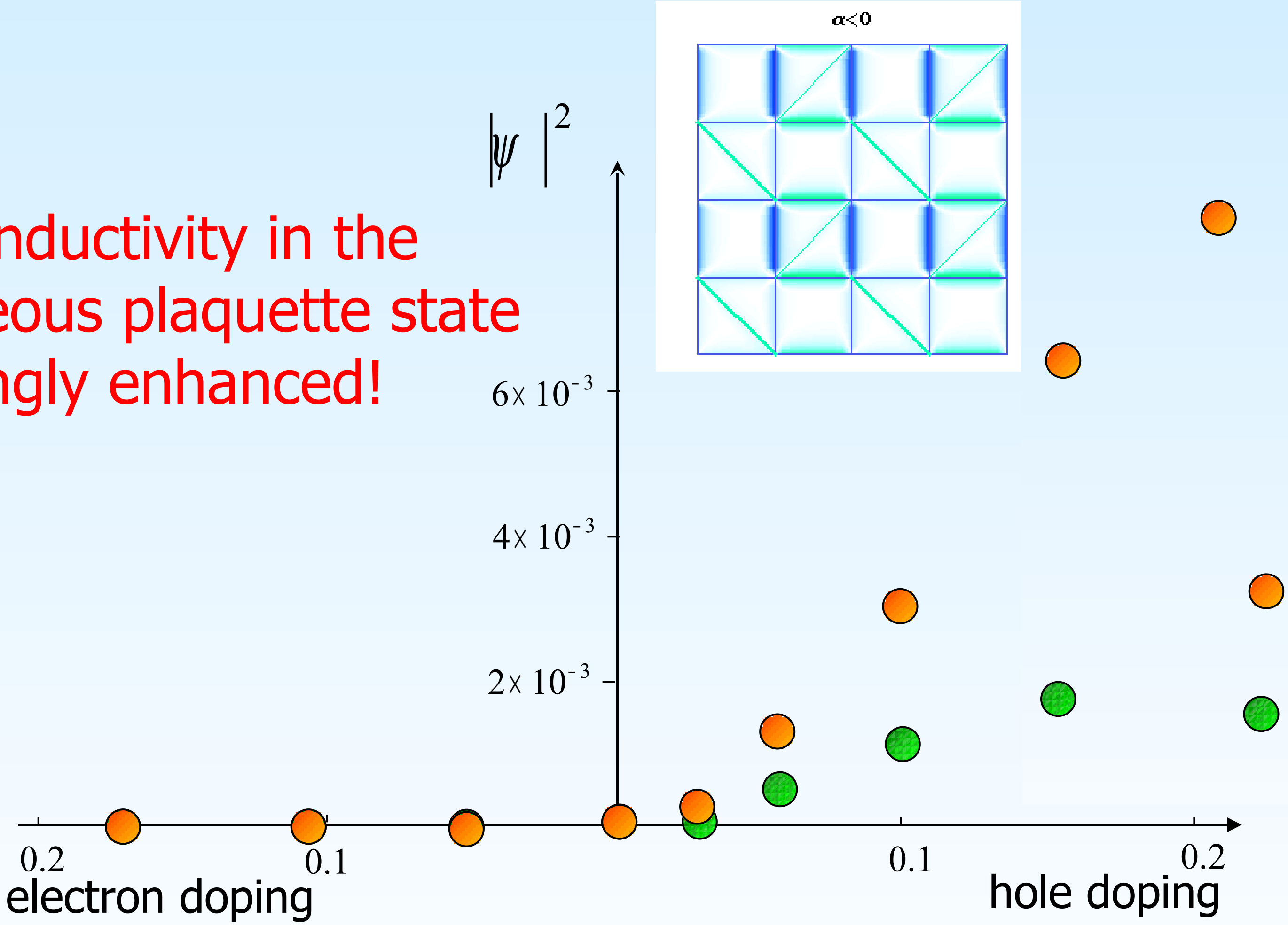
$$|\Psi\rangle = \frac{1}{\sqrt{3}}\left(|\,\shortparallel\,\rangle - |=\rangle\right)$$

- inhomogeneous bond order
- due to kinetic energy gain of doped holes
- no charge order

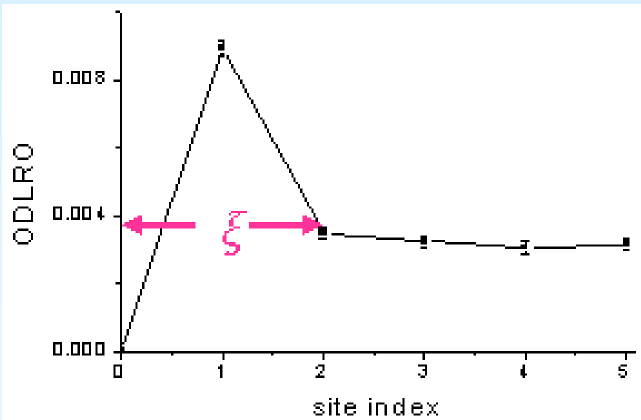
Is bond order helping or hurting superconductivity?

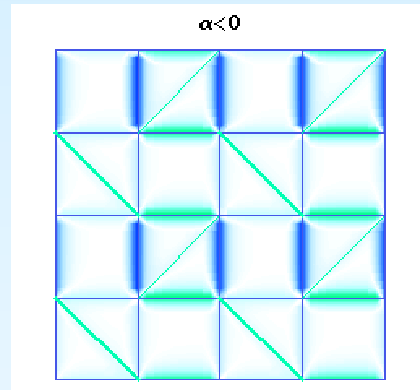
Results: superconductivity in the plaquette state

superconductivity in the inhomogeneous plaquette state is strongly enhanced!

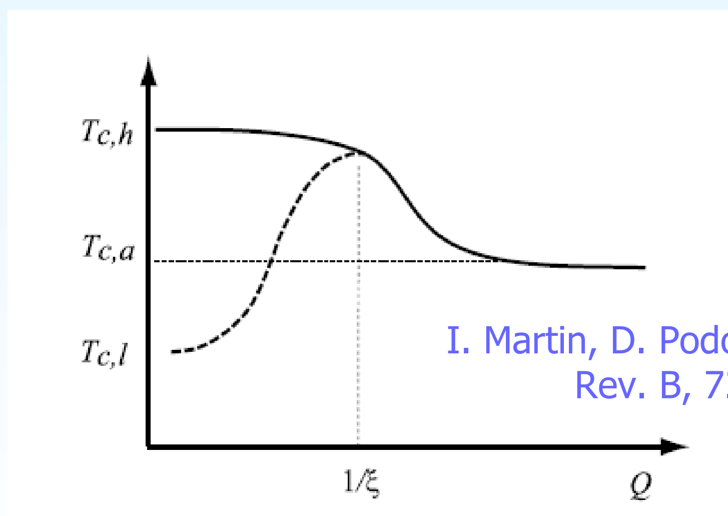


enhancement of superconductivity by inhomogeneities





$$Q_{\text{inh}} \approx \pi / a_0 \approx \xi^{-1}$$



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comparison with mean field theory

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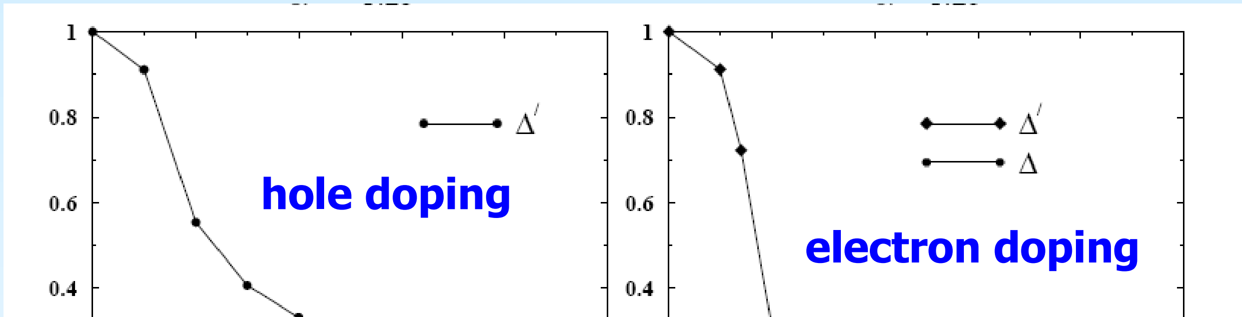
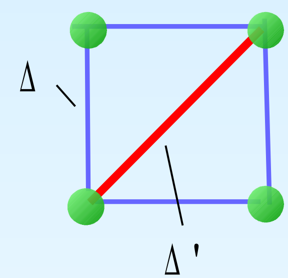




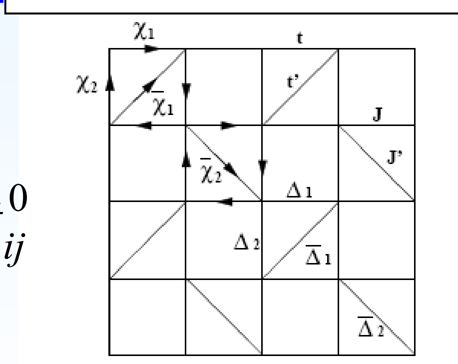
Proper projection is crucial

$$\left|\Psi\right\rangle = \prod_i \left(1 - n_{i\uparrow} n_{i\downarrow}\right)\left|\Phi_{\mathrm{BCS}}\right\rangle$$

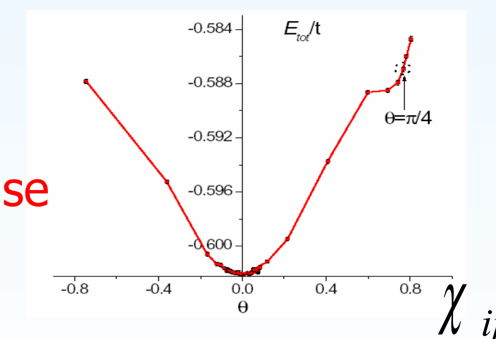
C.-I

flux phase

$$t_{ij} \rightarrow e^{i\chi_{ij}} t^0_{ij}$$



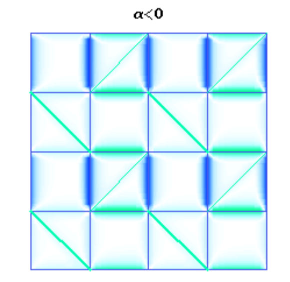
no flux phase



χ_{ij}

Conclusions

- $SrCu_2(BO_3)_2$: strong asymmetry between hole and electron doping
- hole doped $SrCu_2(BO_3)_2$
  d-wave RVB state with inhomogeneous bond order and enhanced superconductivity (T_c ~2 K)



- electron doped $SrCu_2(BO_3)_2$
  new metallic state
- the vicinity of the Mott state is full of surprises!