Orbital currents in strongly correlated systems

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SWISS NATIONAL SCIENCE FOUNDATION

MaNEP
SWITZERLAND

E. Orignac (ENS Lyon)

P. Chudzinski (Geneva U.)

M. Gabay (LPS, Orsay)

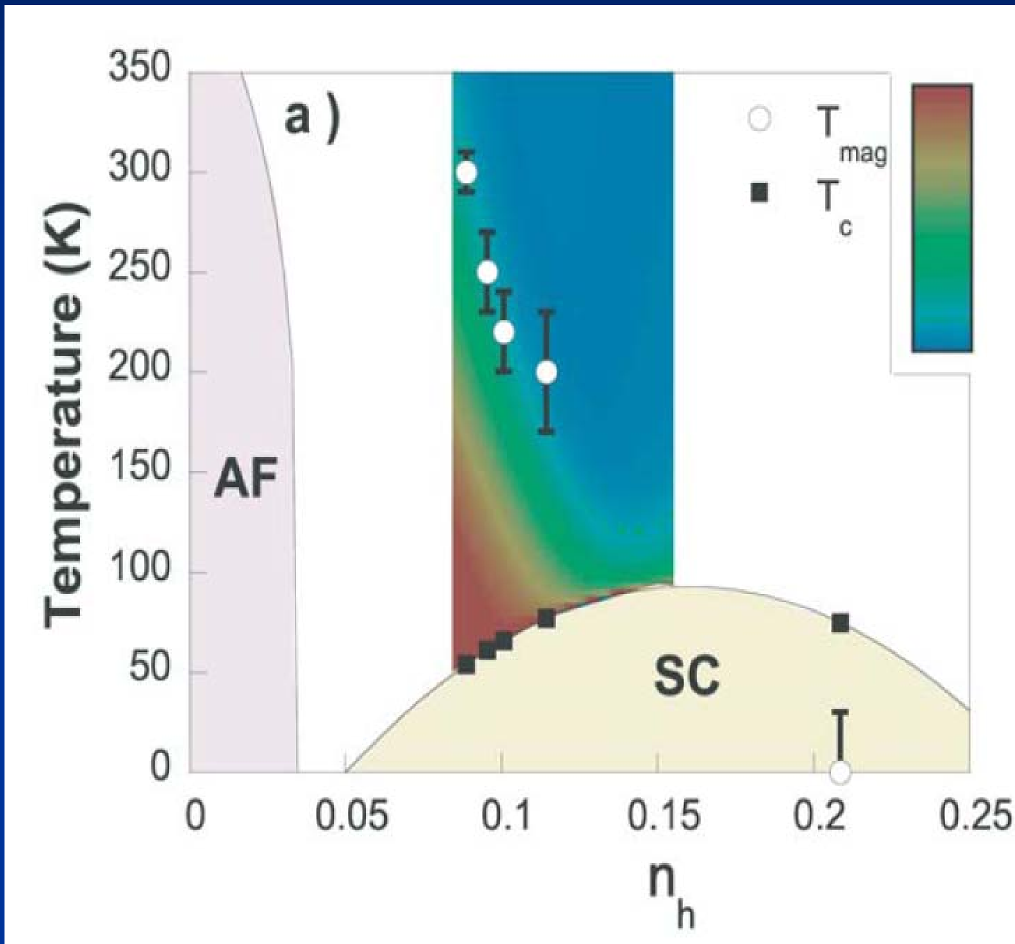
C. Weber (Rutgers U.)

A.Laüchli (IRRMA)

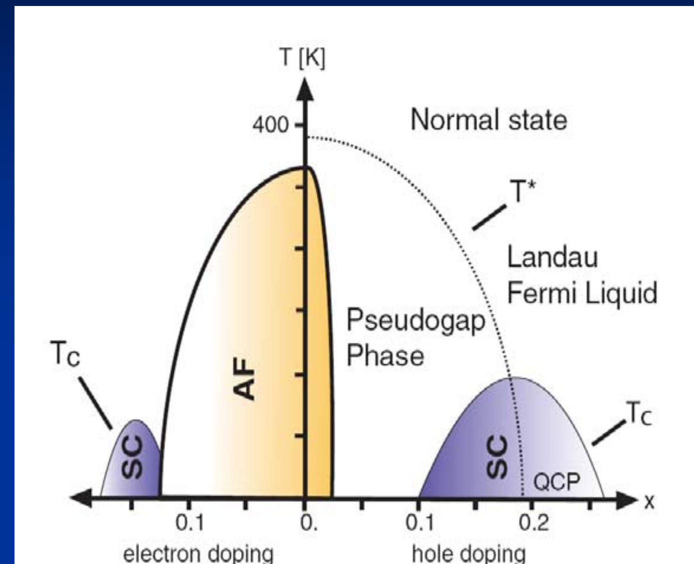
F. Mila (EPFL)

Discussions: C.M. Varma

Pseudogap phase: cuprates

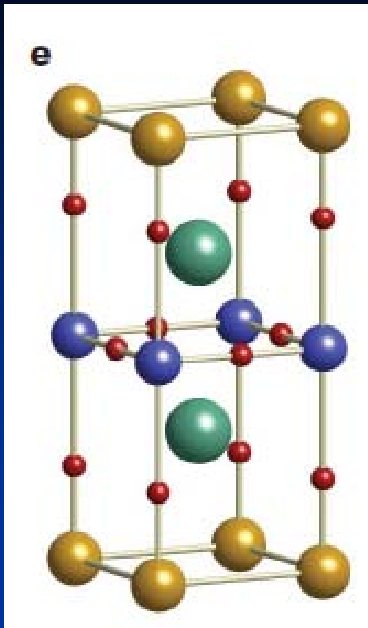


B. Fauque *et al.* PRL 96 197001 (2006)

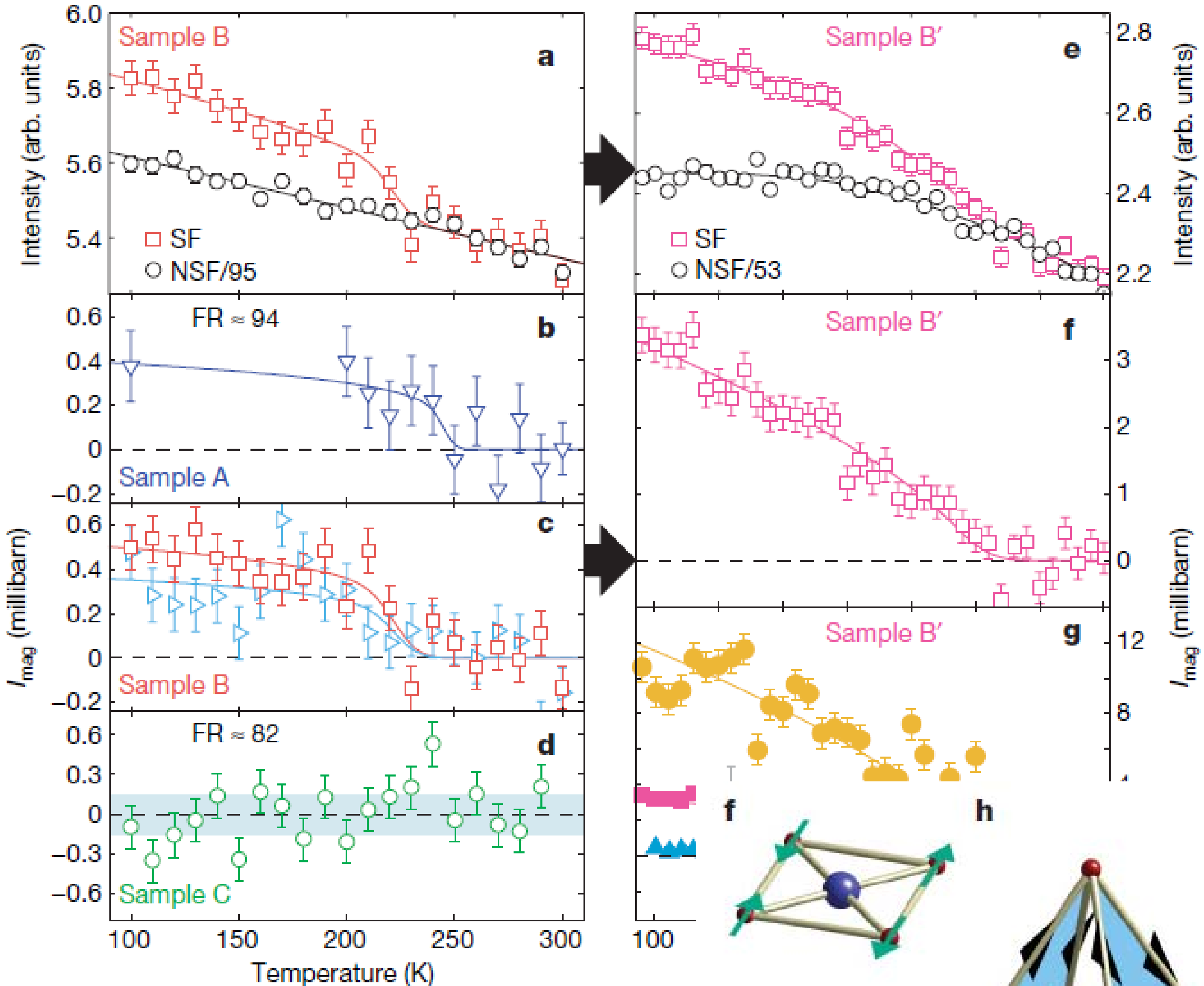


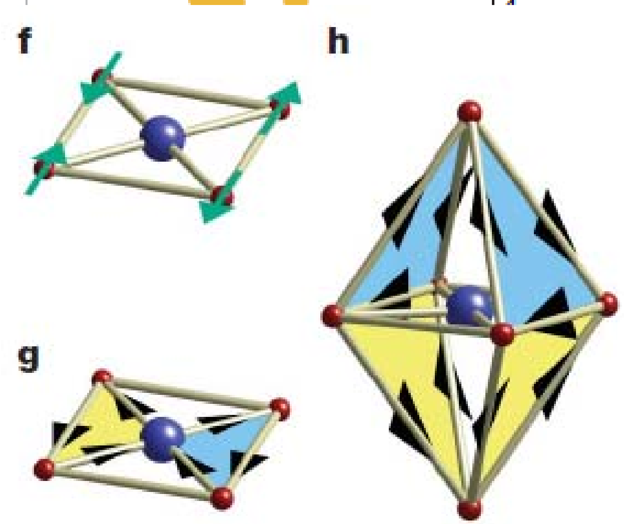
- Magnetic moments q=0

- Broken time reversal symmetry



$HgBa_2CuO_{4+\delta}$



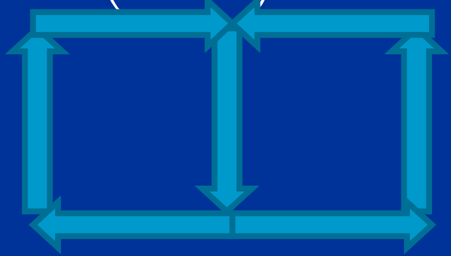


Y. Li *et al.* Nature 455 372 (2008)

Proposals for pseudo-gap with T-sym broken

- DDW phase

S. Chakravarty *et al.* PRB 63 094503 (2001)

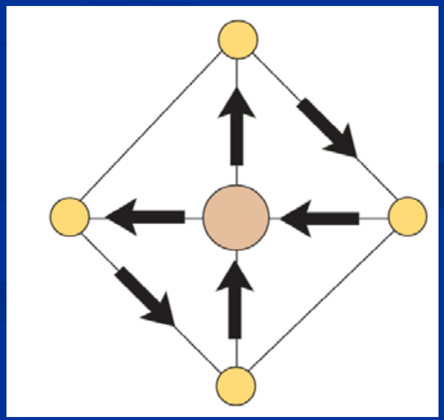


single band model

- CU-O currents phase

C. M. Varma PRB 73 155113 (2006)

three band model



Questions

- Do current phase exist ?
  [Mean field ? Other instabilities ?]

- One band or three bands ?

- Need an unbiased/controled method

  - Ladders
  - Variational Monte Carlo calculations

Single band

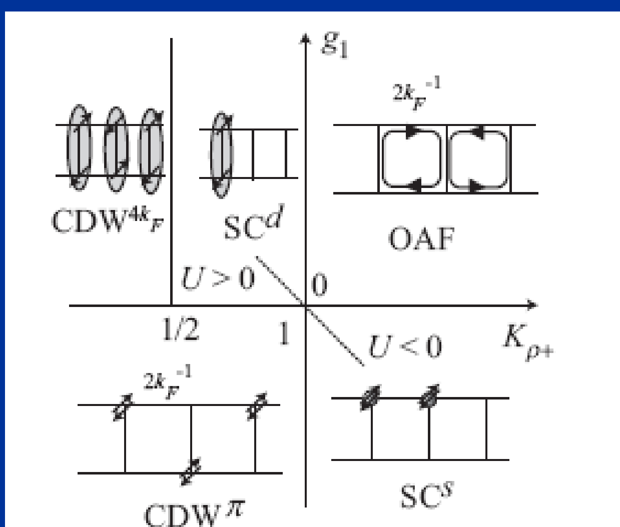
- 2D Flux phases ?

  proposed for Hubbard (Affleck+Marston (88))

  But unstable compared to d-wave

- Ladders:

E. Orignac+TG PRB 56 7167 (1997); U. Schollwöck et al. PRL 90 186401 (2003)



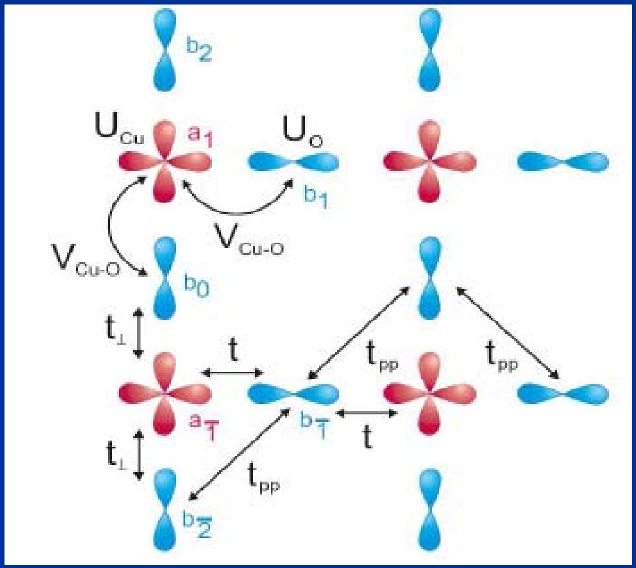
but weird interactions !

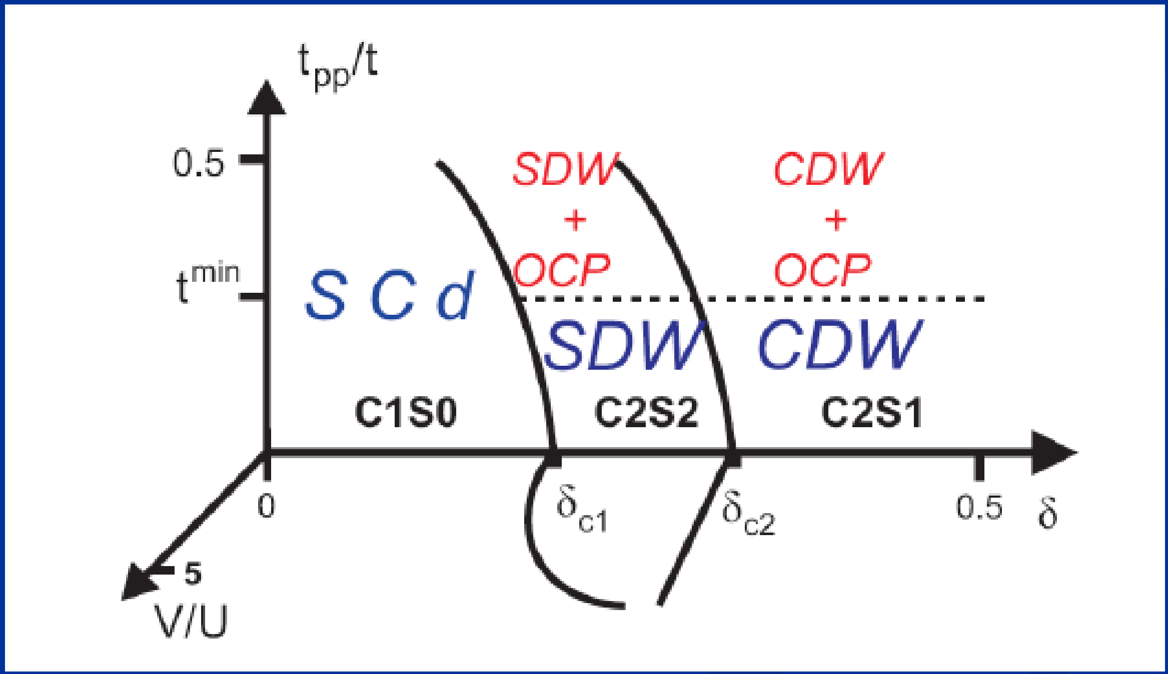
$$g_1 = Ua + 2Va\cos(2k_F a),$$

$$g_1 - 2g_2 = -[Ua + 2Va(2 - \cos(2k_F a))],$$

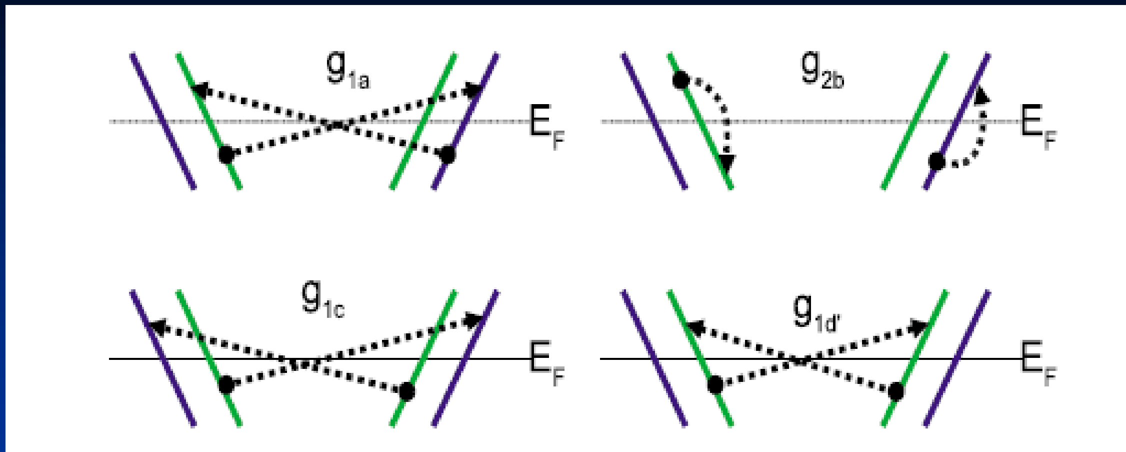
3 band ladders

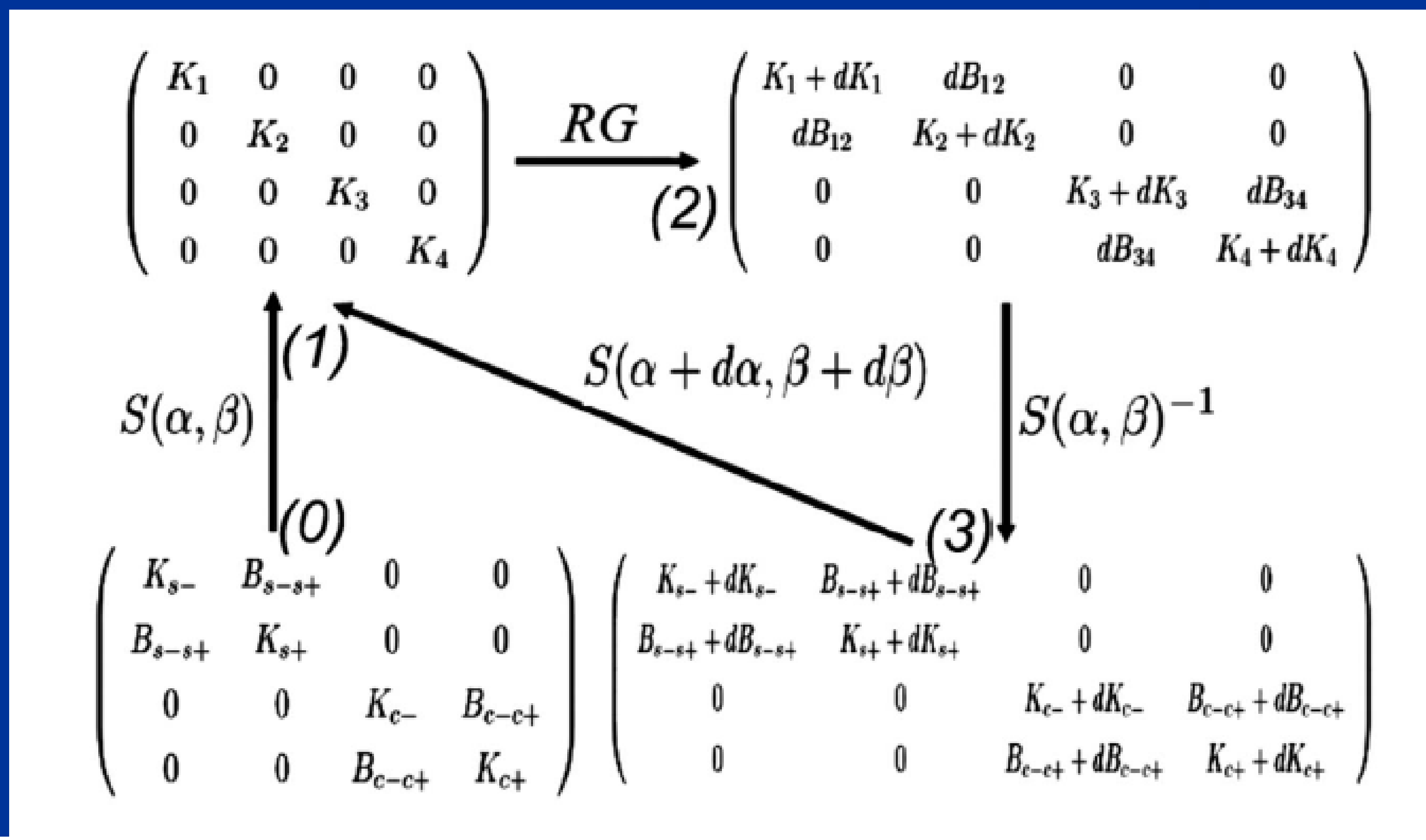
P. Chudzinski, M. Gabay, TG PRB 76 161101(R) (2007); PRB 78 075124 (2008)





Flux phase with ``reasonable” interactions!


g1a
E_F
g2b
E_F
g1c
E_F
g1d'
E_F


RG
(2)
(1)
(0)
(3)
S(α, β)
S(α + dα, β + dβ)
S(α, β)^{-1}

$$\frac{dK_1}{dl} = \frac{1}{2}\left\{ P_1^2(g_{1a}^2 + g_{ic}^2 + G_i^2) - K_1^2\left[Q_1^2 g_{1a}^2 + Q_1^2 g_{1c}^2 + P_1^2 G_p^2 + P_1^2 g_{2c}^2 + \frac{1}{2}(g_1^2 + g_2^2) + f(P_1)(g_1 g_2) \right]\right\}, \quad (17)$$

$$\frac{dK_2}{dl} = \frac{1}{2}\left\{ Q_1^2(g_{1a}^2 + g_{ic}^2 + G_i^2) - K_2^2\left[P_1^2 g_{1a}^2 + P_1^2 g_{1c}^2 + Q_1^2 G_p^2 + Q_1^2 g_{2c}^2 + \frac{1}{2}(g_1^2 + g_2^2) - f(P_1)(g_1 g_2) \right]\right\}, \quad (18)$$

$$\frac{dK_3}{dl} = \frac{1}{2} P_2^2 [g_{1c}^2 + g_{2c}^2 + g_{ic}^2], \quad (19)$$

$$\frac{dK_4}{dl} = \frac{1}{2} Q_2^2 [g_{1c}^2 + g_{2c}^2 + g_{ic}^2], \quad (20)$$

$$\frac{dg_{1c}}{dl} = g_{1c}[2 - (P_1^2 K_2 + P_2^2 K_3^{-1} + Q_1^2 K_1 + Q_2^2 K_4^{-1})] - (g_1 g_{2c} + g_{1a} g_{ic}), \quad (21)$$

$$\frac{dg_{1a}}{dl} = g_{1a}\{2 - [P_1^2(K_2 + K_1^{-1}) + Q_1^2(K_1 + K_2^{-1})]\} - g_{1c} g_{ic}, \quad (22)$$

$$\frac{dg_{2c}}{dl} = g_{2c}[2 - (P_2^2 K_3^{-1} + P_1^2 K_1 + Q_2^2 K_4^{-1} + Q_1^2 K_2)] - g_{1c} g_1, \quad (23)$$

$$\frac{dg_{ic}}{dl} = g_{ic}[2 - (P_1^2 K_1^{-1} + Q_1^2 K_2^{-1} + P_2^2 K_3^{-1} + Q_2^2 K_4^{-1})] - g_{1a} g_{1c}, \quad (24)$$

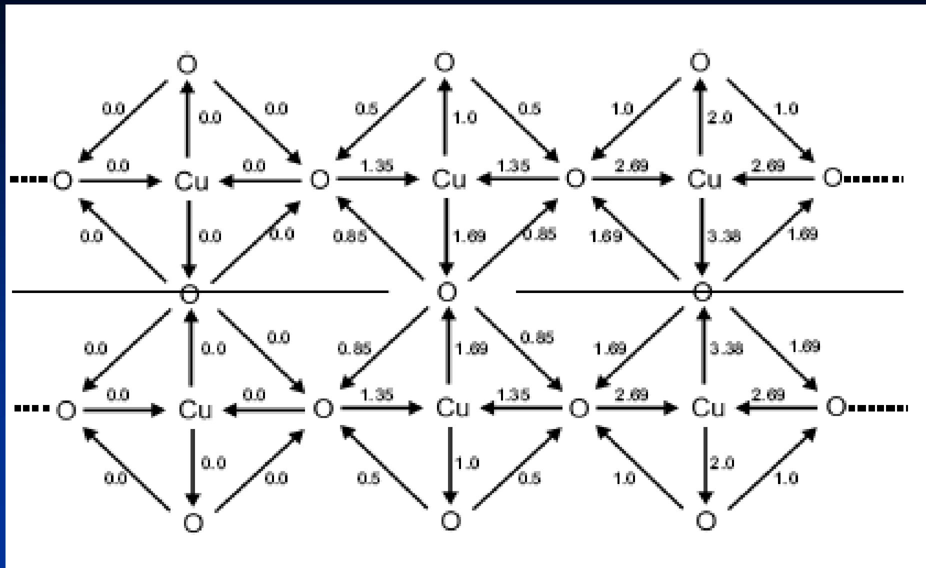
$$\frac{dg_{4a}}{dl} = g_{4a}\left\{ 2 - \frac{1}{2}[P_1^2(K_1 + K_1^{-1}) + Q_1^2(K_2 + K_2^{-1})] \right\}, \quad (25)$$

$$\frac{dg_1}{dl} = g_1[2 - (K_2 + K_1)] + P_1 Q_1 (K_2 - K_1) g_2 - \gamma g_{1c} g_{2c}, \quad (26)$$

$$\frac{dg_2}{dl} = -g_2[2 - (K_2 + K_1)] + P_1 Q_1 (K_2 - K_1) g_1, \quad (27)$$

$$\frac{dG_p}{dl} = G_p[1 - (P_1^2 K_1 + Q_1^2 K_2)] + g_{4a}^2[P_1^2(K_1 - K_1^{-1}) + Q_1^2(K_2 - K_2^{-1})], \quad (28)$$

$$\frac{dG_i}{dl} = G_i[1 - (P_1^2 K_1^{-1} + Q_1^2 K_2^{-1})] + g_{4a}^2[P_1^2(-K_1 + K_1^{-1}) + Q_1^2(-K_2 + K_2^{-1})]. \quad (29)$$



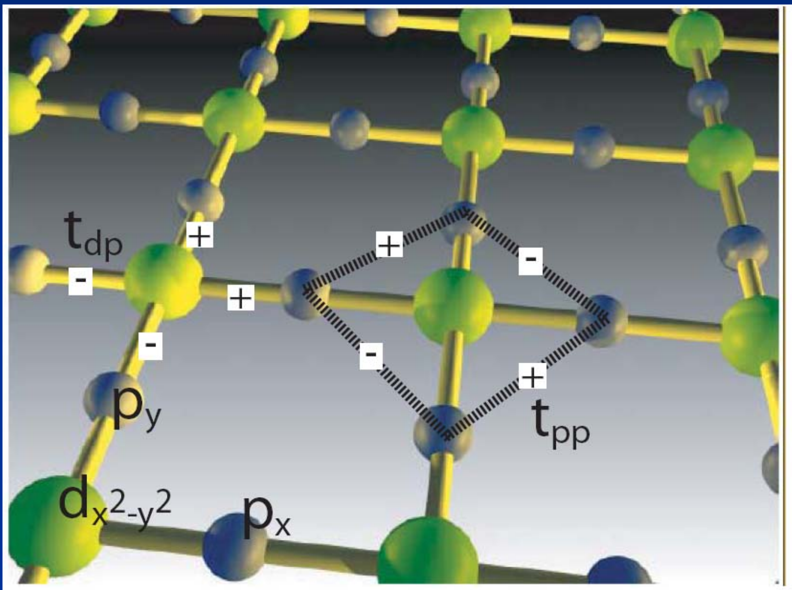
need three band model: θ_1 symmetry

staggered ($2k_F$) phase [weak interactions]

- Differences between 1 band and 3 band
- Circulating currents between Cu-O
- Strong coupling ?

S. Nishimoto et al. PRB 79 205115 (2009)

2D - 3 band system



- Hole notations
- LDA:

  $U_d=10$, $U_p=4$, $V_{dp}=1.2$ e

$$H=\sum_{\langle i,j\rangle\sigma}\left(t_{i,j}d^{\dagger}_{i\sigma}p_{j\sigma}+c.c.\right)+\sum_{\langle i,j\rangle\sigma}\left(t_{i,j}p^{\dagger}_{i\sigma}p_{j\sigma}+c.c.\right)+$$

$$U_p\sum_{p}\hat{n}_{p\uparrow}\hat{n}_{p\downarrow}+U_d\sum_{d}\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}+$$

$$\Delta_p\sum_{p,\sigma}\hat{n}_{p\sigma}+V_{dp}\sum_{d,p}\hat{n}_d\hat{n}_p \qquad (1)$$

How to treat ?

- Mean field method

$$H = \sum_{\langle i,j\rangle \sigma} \left(\left(t_{i,j} + V_{dp} \langle p^\dagger_{j\sigma} d_{i\sigma} \rangle \right) d^\dagger_{i\sigma} p_{j\sigma} + c.c. \right) + \sum_{\langle i,j\rangle \sigma} \left(t_{i,j} p^\dagger_{i\sigma} p_{j\sigma} + c.c. \right) + \Delta_p \sum_{p,\sigma} \hat{n}_{p\sigma}$$

- Exact diagonalizations:

  [M. Greiter and R. Thomale PRL 99 027005 (2007)]

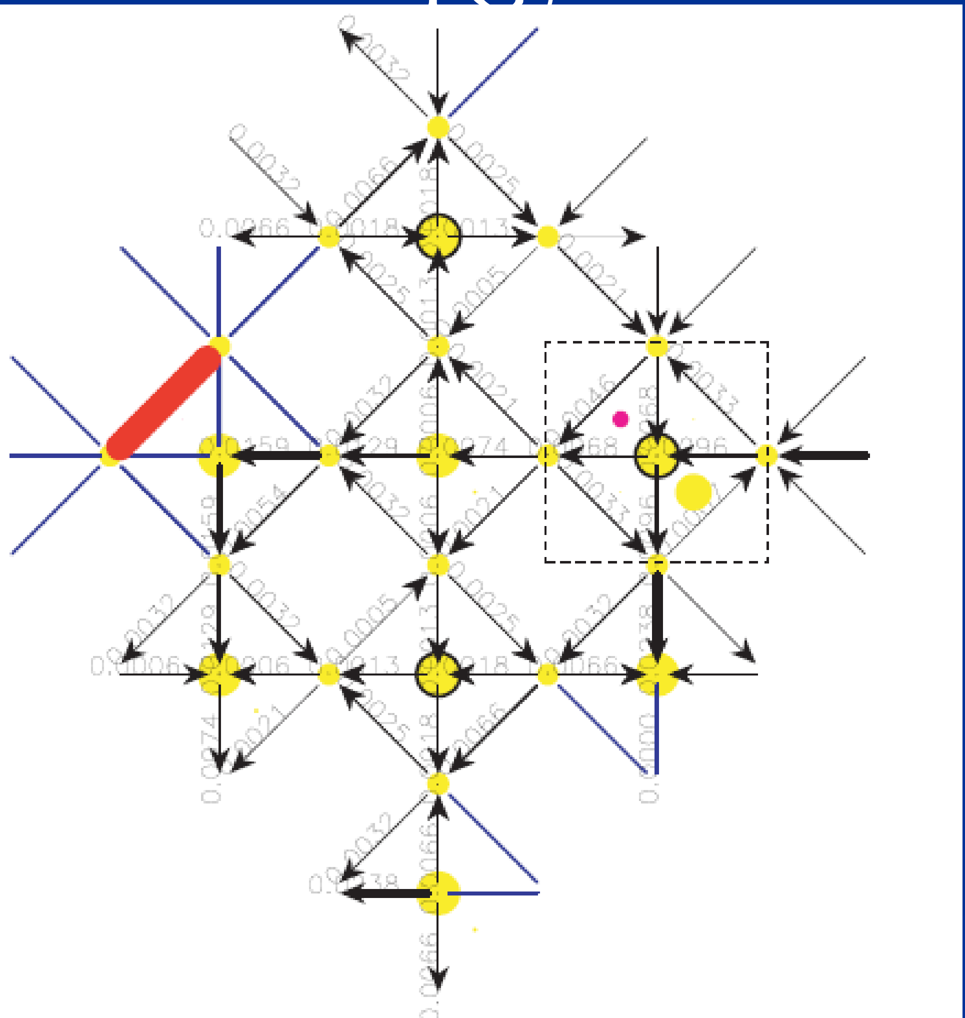
No orbital currents

But: t-J model ($\epsilon_p \gg t_{pd}$)

small clusters (8 Co)

Exact diagonalization

(C. Weber, A. Laüchli, F. Mila, TG)



8 copper sites
10 hole (± = 25 %)
small correlations 0.006
θ_2 symmetry

Variational Monte-Carlo

Give $|\psi\rangle$

$|\psi\rangle = \mathrm{P}\,|\psi_0\rangle$

$\langle\,\psi\,|\mathrm{H}\,|\,\psi\rangle = ?$

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \sum_{\alpha} \underbrace{\frac{|\langle\alpha|\psi\rangle|^2}{\langle\psi|\psi\rangle}}_{P(\alpha)} \left(\underbrace{\sum_{\beta} \langle\alpha|H|\beta\rangle \frac{\langle\beta|\psi\rangle}{\langle\alpha|\psi\rangle}}_{e(\alpha)} \right)$$

- Advantages
- No numerical problems (``exact method”)
- ``Equal” footing for the various instabilities
- Drawbacks
- Depends on choice of wavefunction
- Mostly ground state properties

VMC for orbital currents

C. Weber, A. Laüchli, F. Mila, TG
PRL 102 017005 (2008)

Trial wavefunction: ground state of

$$H_{MF} = \sum_{<i,j>} \left(t_{ij} e^{i\theta_{i,j}} c_{i\sigma}^{+} c_{j\sigma} + h.c. \right) + \left(\Delta_{i,j} c_{i\uparrow}^{+} c_{j\downarrow}^{+} + h.c. \right) + \sum_{i} \underline{h}_i \cdot \underline{S}_i$$

Antiferromagnetic, superconducting, current instabilities

$$< O > = \left\langle \psi_{MF} \,|\, \hat{P} \cdot O \cdot \hat{P} \,|\, \psi_{MF} \right\rangle / \left\langle \psi_{MF} \,|\, \psi_{MF} \right\rangle$$

Jastrow factors

$$\mathcal{J} = \exp\left(\sum_{i,j=1,N} v^c_{ij} n_i n_j\right) \exp\left(\sum_{i,j=1,N} v^S_{ij} S^z_i S^z_j\right)$$

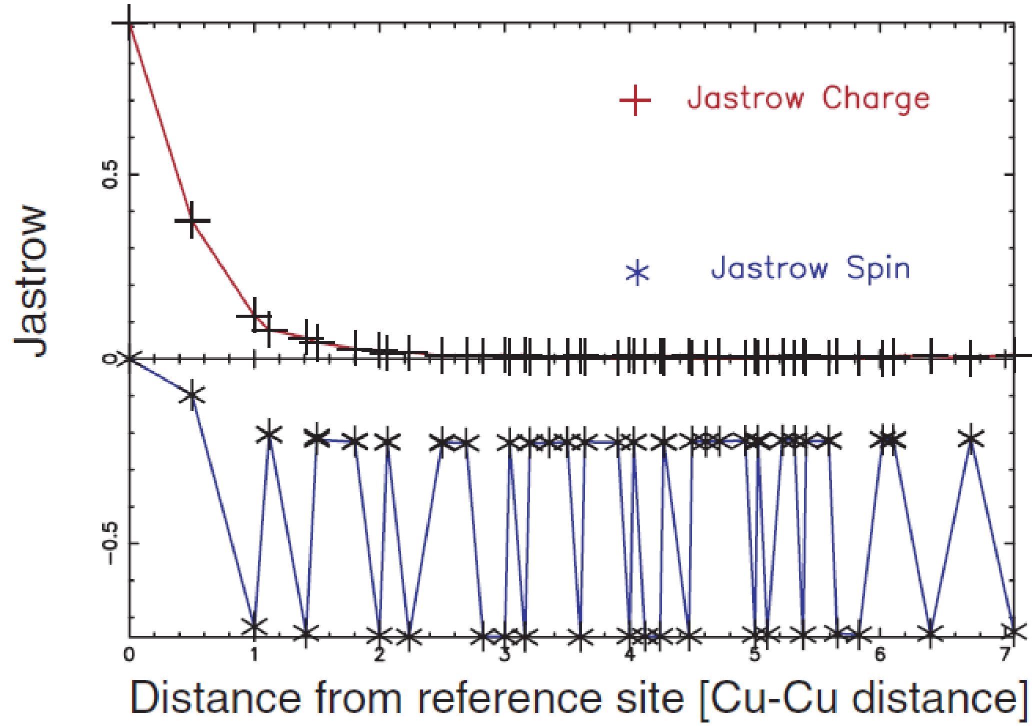
Need to ensure current conservation:

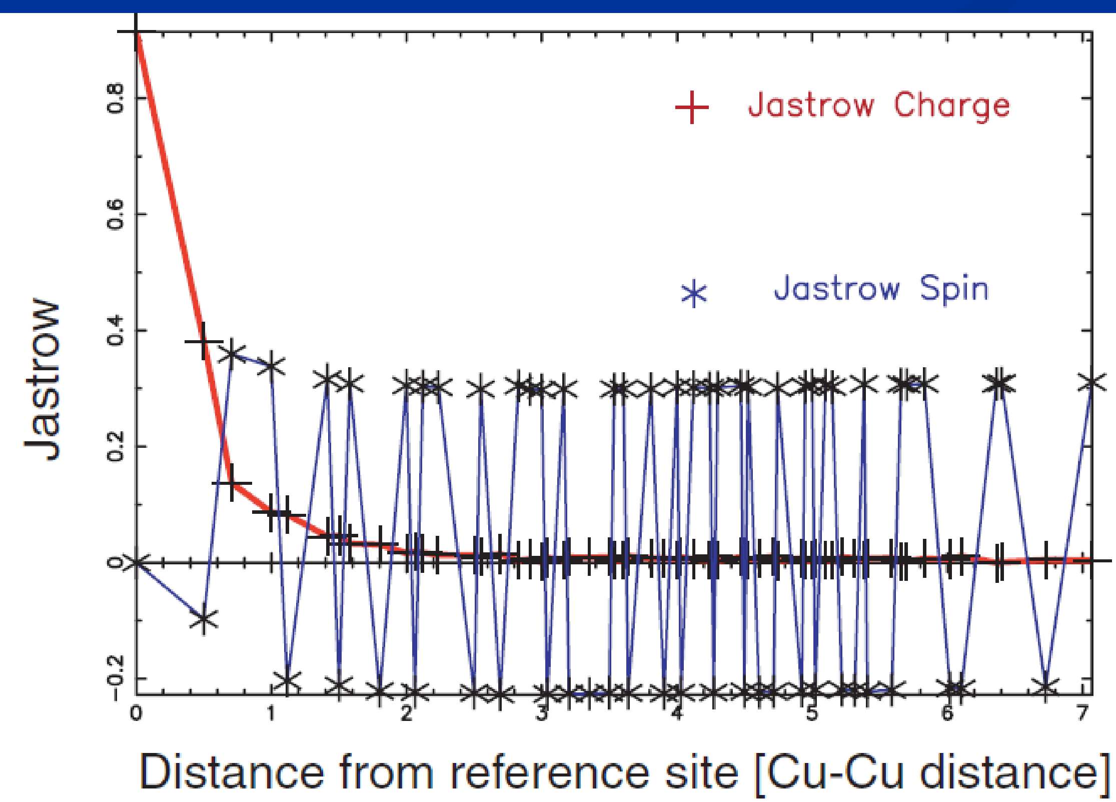
$$\mathcal{J}_c = \exp\left(\sum_{i=1,N} i\alpha_i n_i\right)$$

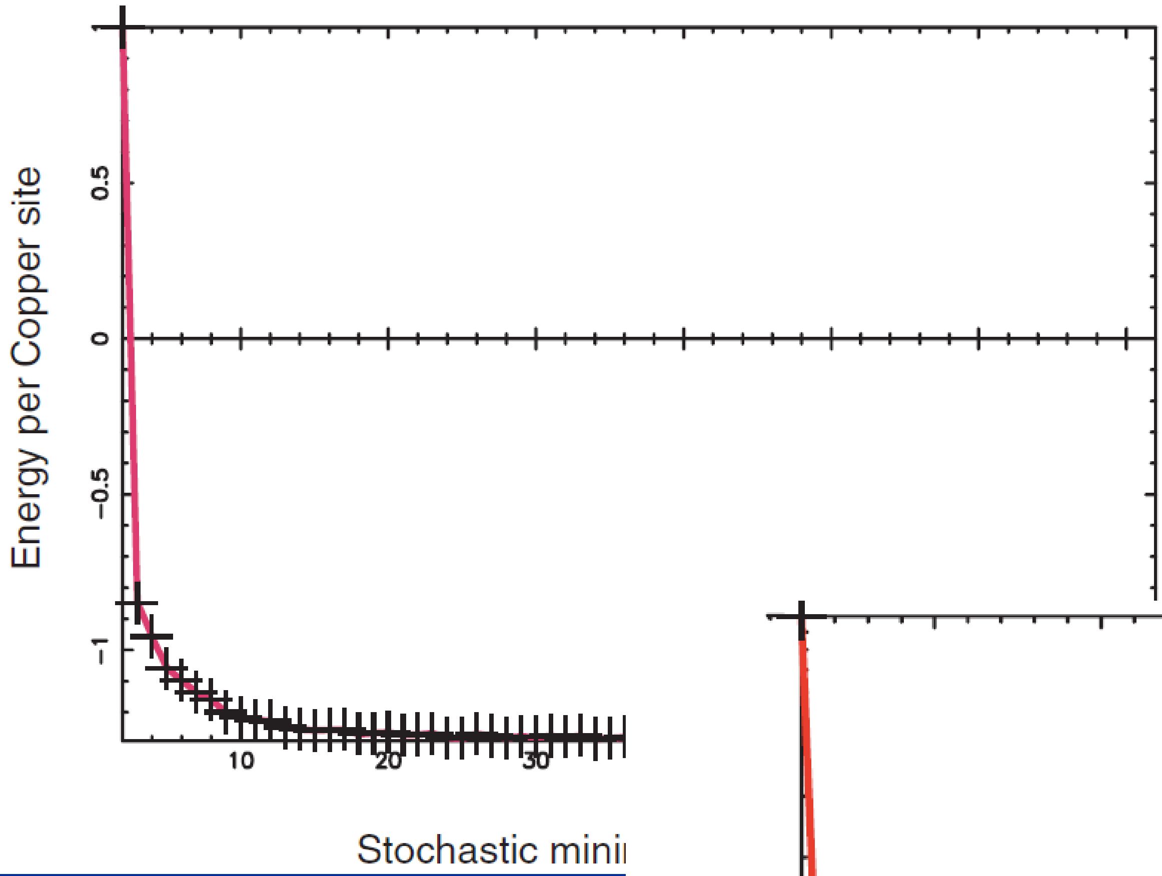
v^c, v^S, α variational parameters

Several tricks

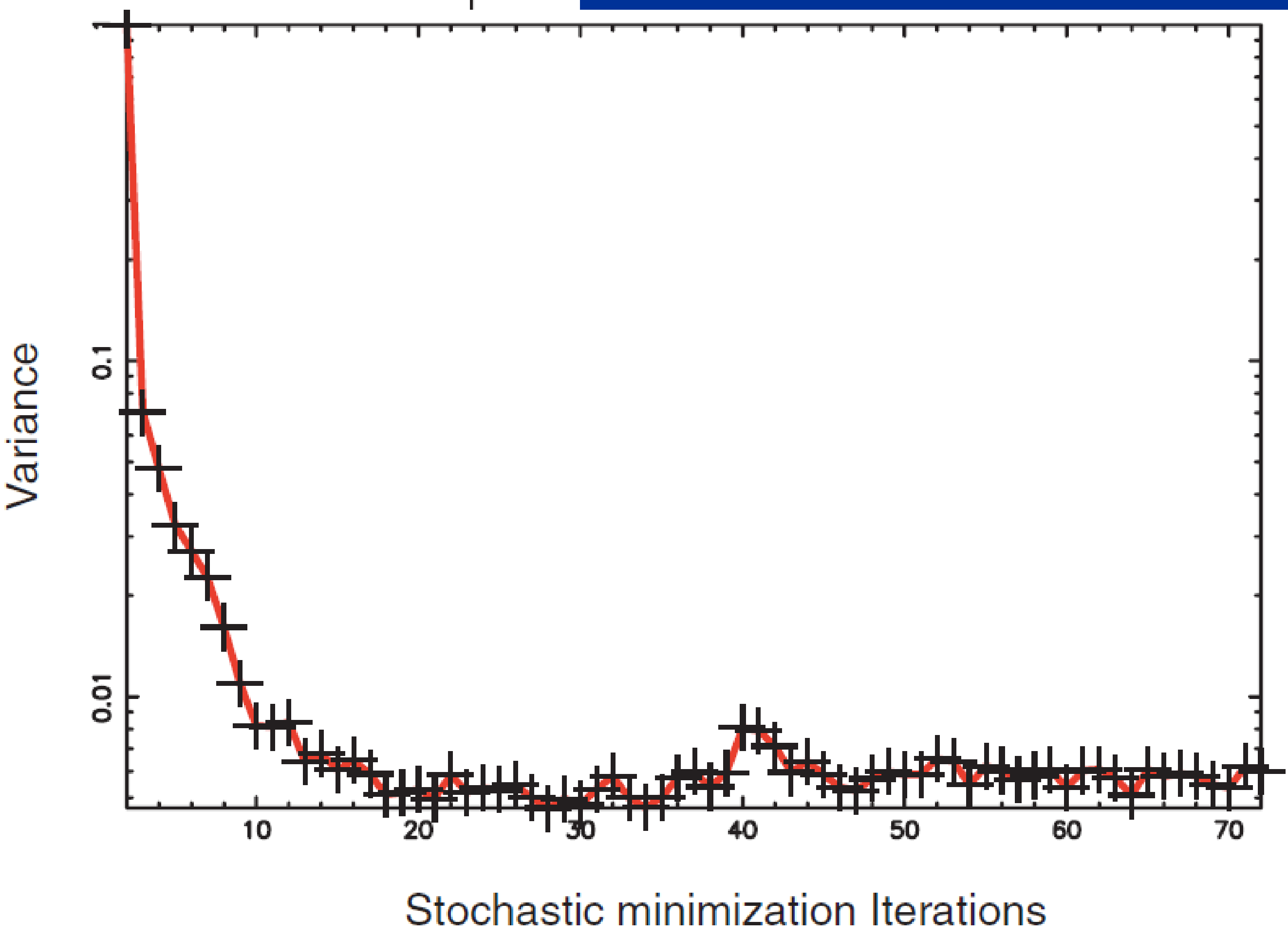
- Correlated minimization (Umrigar+Wilson)
- Stochastic minimizaton (Jastrow)
- Lanczos step(s)


Jastrow Charge
Jastrow Spin
Jastrow
0.5
0
-0.5
0
1
2
3
4
5
6
7
Distance from reference site [Cu-Cu distance]


Jastrow Charge
Jastrow Spin
Jastrow
0.8
0.6
0.4
0.2
0
-0.2
0
1
2
3
4
5
6
7
Distance from reference site [Cu-Cu distance]



Energy per Copper site
0.5
0
−0.5
−1
10
20
30
Stochastic mini



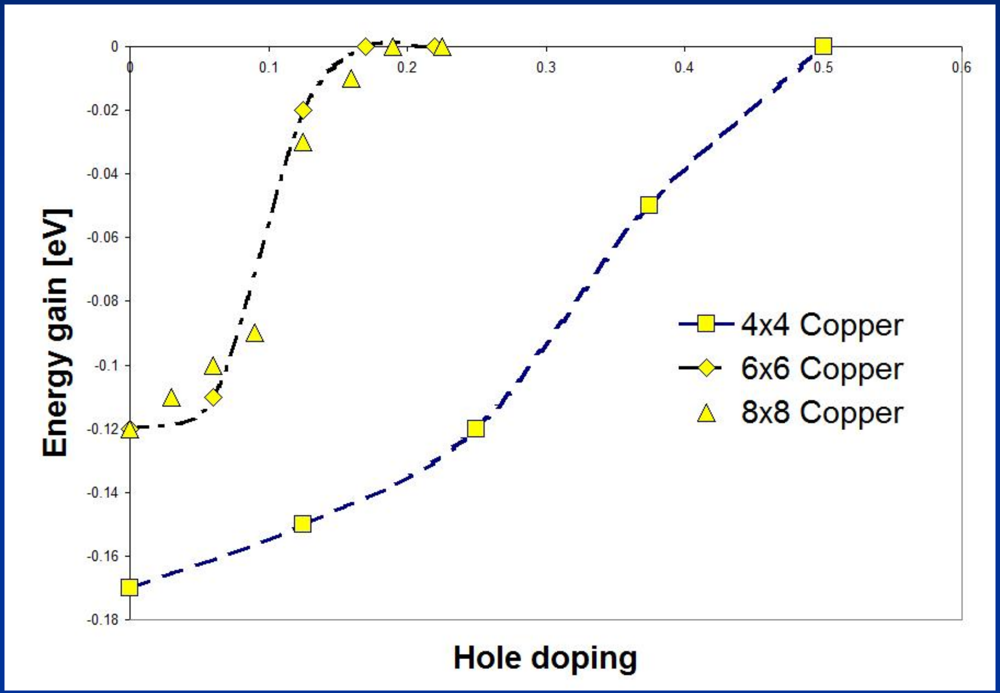
Variance
0.1
0.01
10
20
30
40
50
60
70
Stochastic minimization Iterations

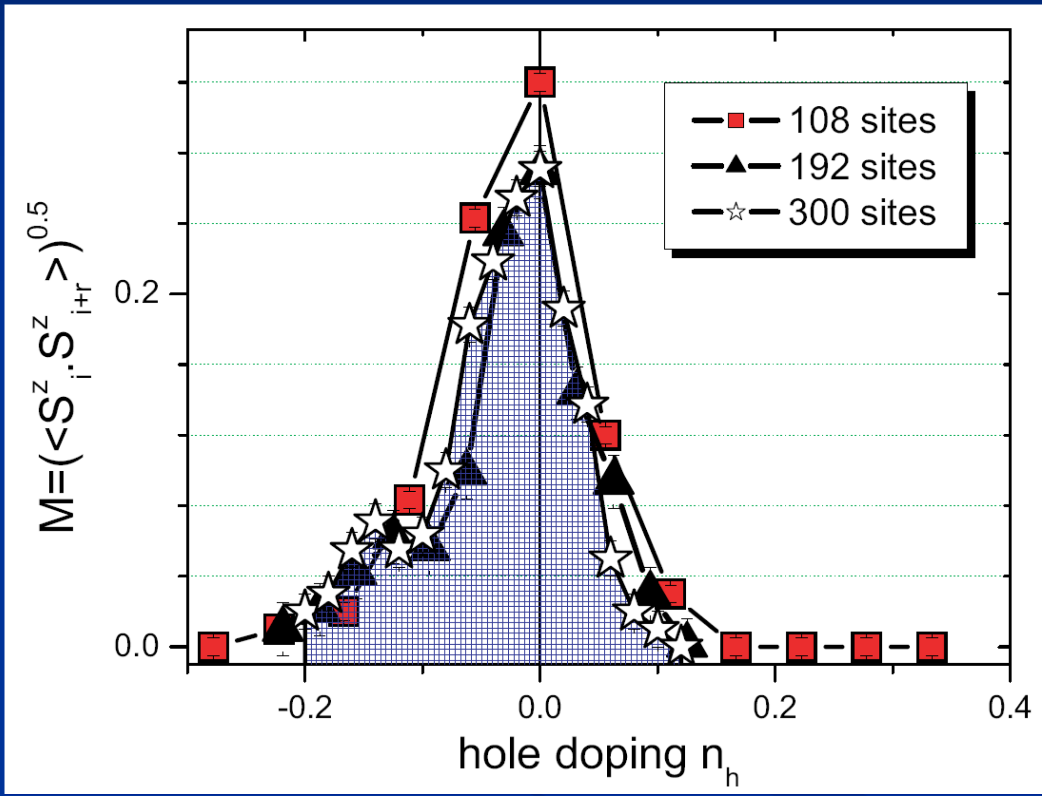
Benchmark with exact diag.

w.f.	E_{tot}	T_{dp}	T_{pp}	U_d	U_p	Δ_p	V_{dp}	variance
Lanczos	−1.13821	−3.10036	−0.79666	0.26737	0.08398	1.77545	0.63201	0
Jastrow wf	−1.0775(1)	−3.06068	−0.83073	0.26176	0.08197	1.83466	0.64076	0.018
1 Lanczos step	−1.1153(1)	−3.14070	−0.83715	0.26559	0.08736	1.86495	0.64469	0.018
Fixe node/ Jastrow	−1.1112(5)			0.26966	0.08708	1.77314	0.63177	0.001

- Good description of low energy sector
- 62% magnetization at half filling (MC: 60%)

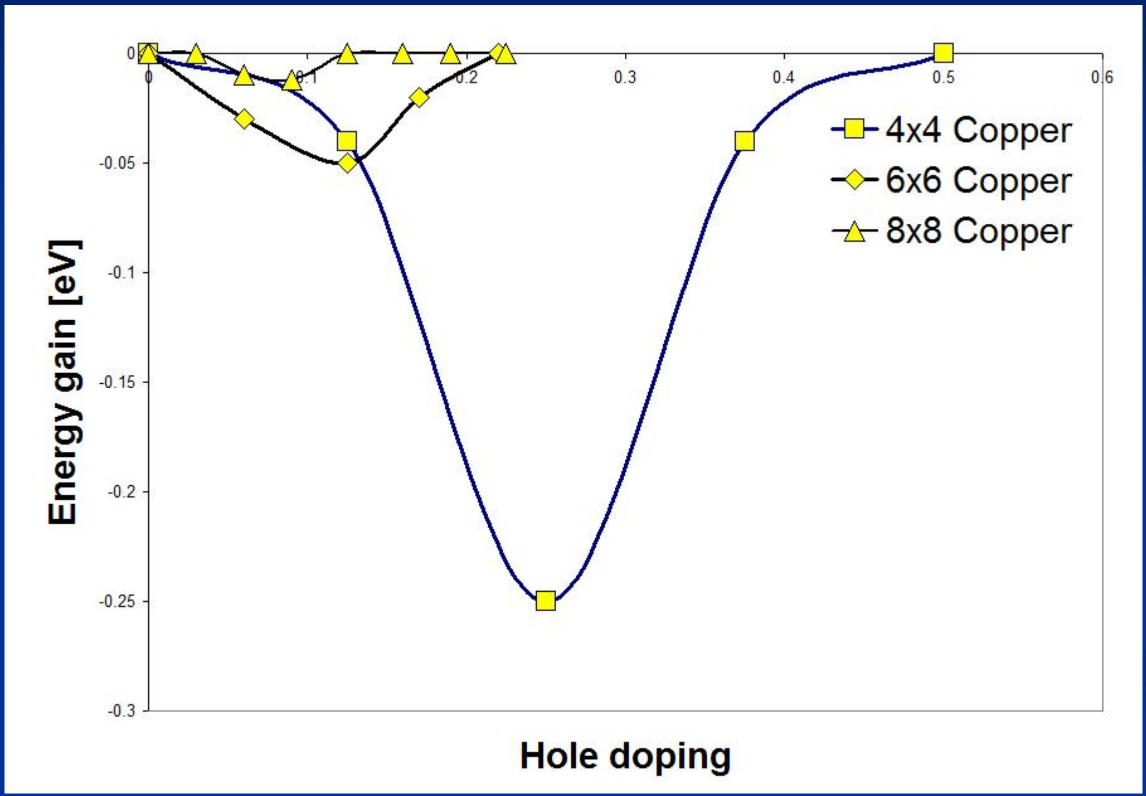
Antiferromagnetic instability

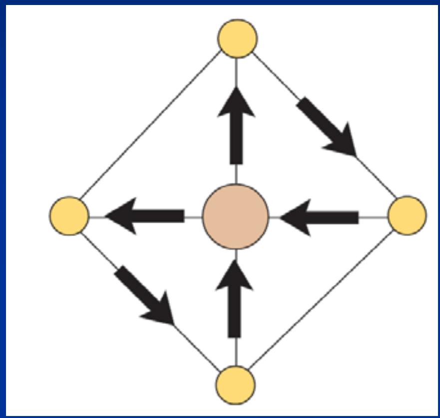




SDW : overestimated stability (usual)

Flux phases





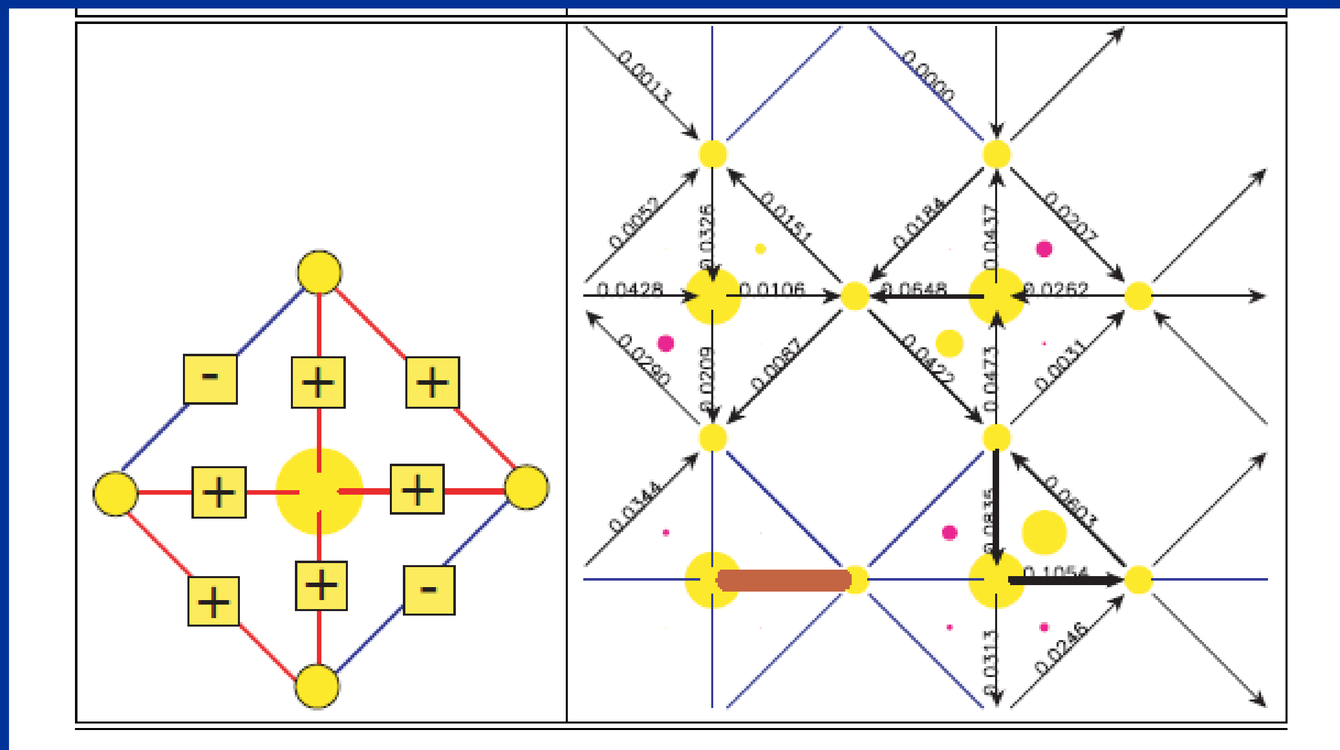
Only θ_2 stabilized

Energy gain decreases with size of the system

No flux phase in thermodynamic limit ?

How to stabilize ?

- Two particles, three site ring: $t<0$ no current
  $t>0$ currents
- Free cluster:



- Need to change the sign of t !!

Mean-Field

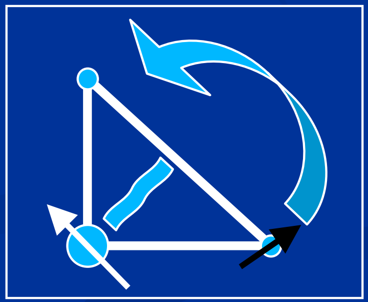
$$H = V_{pd} c^\dagger c d^\dagger d$$

$$H = V_{pd} c^\dagger \langle c d^\dagger \rangle d \rightarrow t_{pd}^* c^\dagger d$$

Different with full variational calculation
($\Delta_p \in [1,8]$, $U_d \in [4,20]$)

Possible candidates

- Two potential candidates
  - Correlated hopping
  - Apical oygens



Apical oxygens

$$H=\sum_{m,\alpha\sigma}\epsilon_\alpha n_{m,\alpha\sigma}+\epsilon_p+\sum_{k,\sigma}n_{k,a\sigma}+\sum_{\langle m,i\rangle,\alpha\sigma}t_{\alpha p}\left(d^\dagger_{m,\alpha\sigma}p_{i\sigma}+c.c.\right)+$$
$$t_{za}\sum_{\langle m,k\rangle,\sigma}\left(d^\dagger_{m,z\sigma}a_{k\sigma}+c.c\right)+t_{pp}\sum_{\langle i,j\rangle,\sigma}\left(p^\dagger_{i\sigma}p_{j\sigma}+c.c.\right)+t_{pa}\sum_{\langle i,k\rangle,\sigma}\left(p^\dagger_{i\sigma}a_{k\sigma}+c.c.\right)+$$
$$U_d\sum_{m\alpha}n_{m,\alpha\uparrow}n_{m,\alpha\downarrow}+U_p\sum_i n_{i,p\uparrow}n_{i,p\downarrow}+U_a\sum_k n_{k,a\uparrow}n_{k,a\downarrow}+\left(U_{xz}-\tfrac{1}{2}J_{xz}\right)\sum_m n_{mx}n_{mz}+$$
$$J_{xz}\sum_m\left(d^\dagger_{m,x\uparrow}d^\dagger_{m,x\downarrow}d_{m,z\downarrow}d_{m,z\uparrow}+c.c.\right)-2J_{xz}\sum_m s_{mx}\cdot s_{mz}+\sum_{\langle m,i\rangle}U_{\alpha p}n_{m\alpha}n_{ip}+$$
$$\sum_{\langle m,k\rangle,\alpha}U_{\alpha a}n_{m\alpha}n_{ka} \qquad (6.22)$$

$$d_{mx\sigma}=d_{x^2-y^2}$$

$$d_{mz\sigma}=d_{3z^2-r^2}$$

$a_{i\sigma}$ = apical oxygen

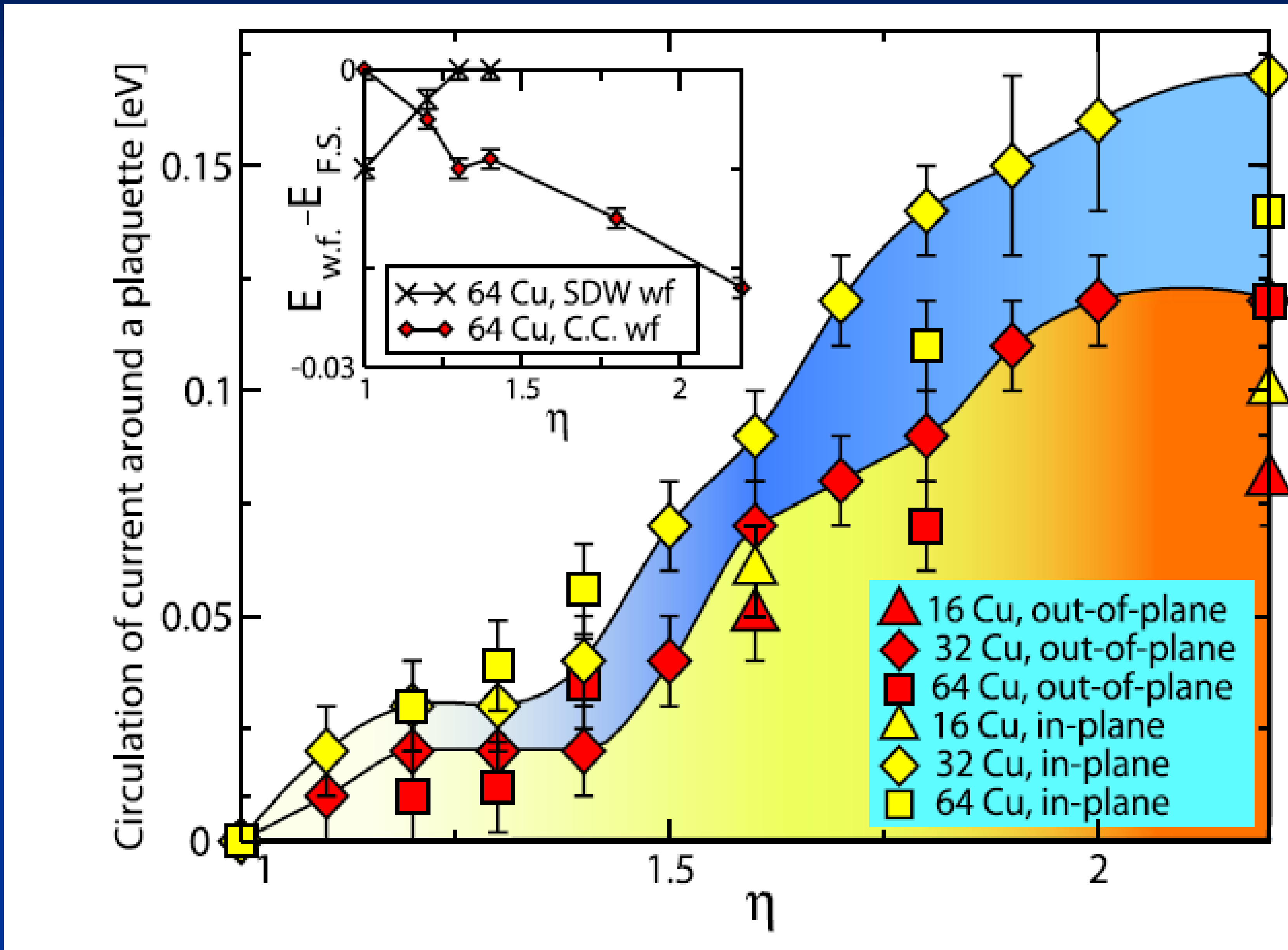
- Canonical parameters:

$\epsilon\left(d_{x^2-y^2}\right)$	0	$\epsilon\left(d_{3z^2-r^2}\right)$	0.64
$\epsilon\left(p_\sigma\right)$	3.51	$\epsilon\left(a_z\right)$	2.05
$t\left(d_{x^2-y^2}, p_\sigma\right)$	1.30	$t\left(d_{3z^2-r^2}, p_\sigma\right)$	0.95
$t\left(d_{3z^2-r^2}, a_z\right)$	0.82	$t\left(p_\sigma, p_\sigma\right)$	0.61
$t\left(p_\sigma, a_z\right)$	0.33		
$J_{xz}\left(d_{x^2-y^2}, d_{3z^2-r^2}\right)$	1.19		
$U\left(p_\sigma\right)$	4.19	$U\left(a_z\right)$	3.67
$U\left(a, d\right)$	0.18	$U\left(p, d\right)$	0.60
$U\left(d_{x^2-y^2}\right) = U\left(d_{3z^2-r^2}\right)$	8.96	$U\left(d_{x^2-y^2}, d_{3z^2-r^2}\right)$	6.58

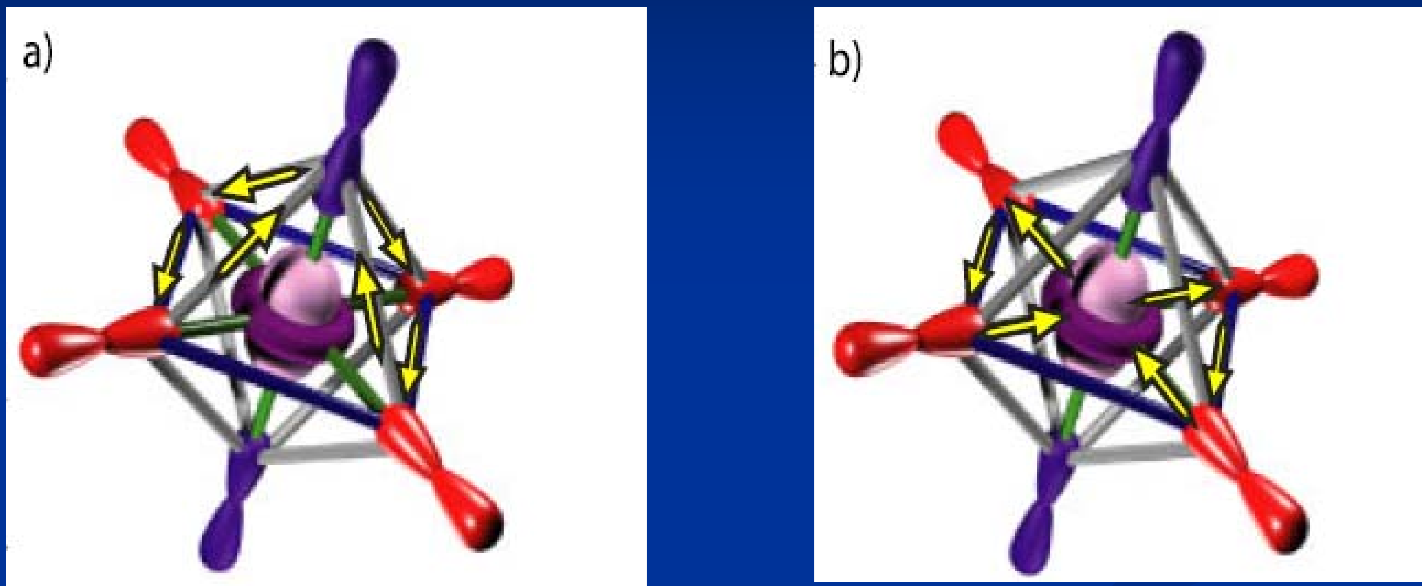
- Fudging factor ´

´ t_{za}, ´ t_{pa}

Variational results



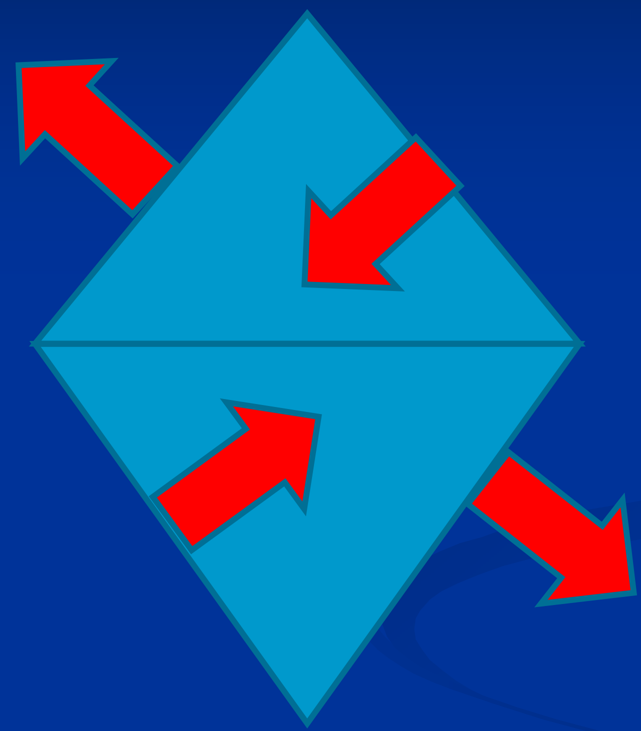
Current patterns



Θ_2 symmetry

Moments out of plane

- Structure:



- Reasonably compatible with experiments

Conclusions

- Differences between 1 band and 3 band model
- Ladders: orbital currents stabilized for 3band
- 2D: variational calculation points at θ_2 symmetry, but energy decreases; Currents ?
- Potentially strong stabilization of currents with apical oxygens
- Compatibility with experiments