Spectra of intertwined-order states in the strongly correlated model

Ting-Kuo Lee

Institute of Physics, Academia Sinica

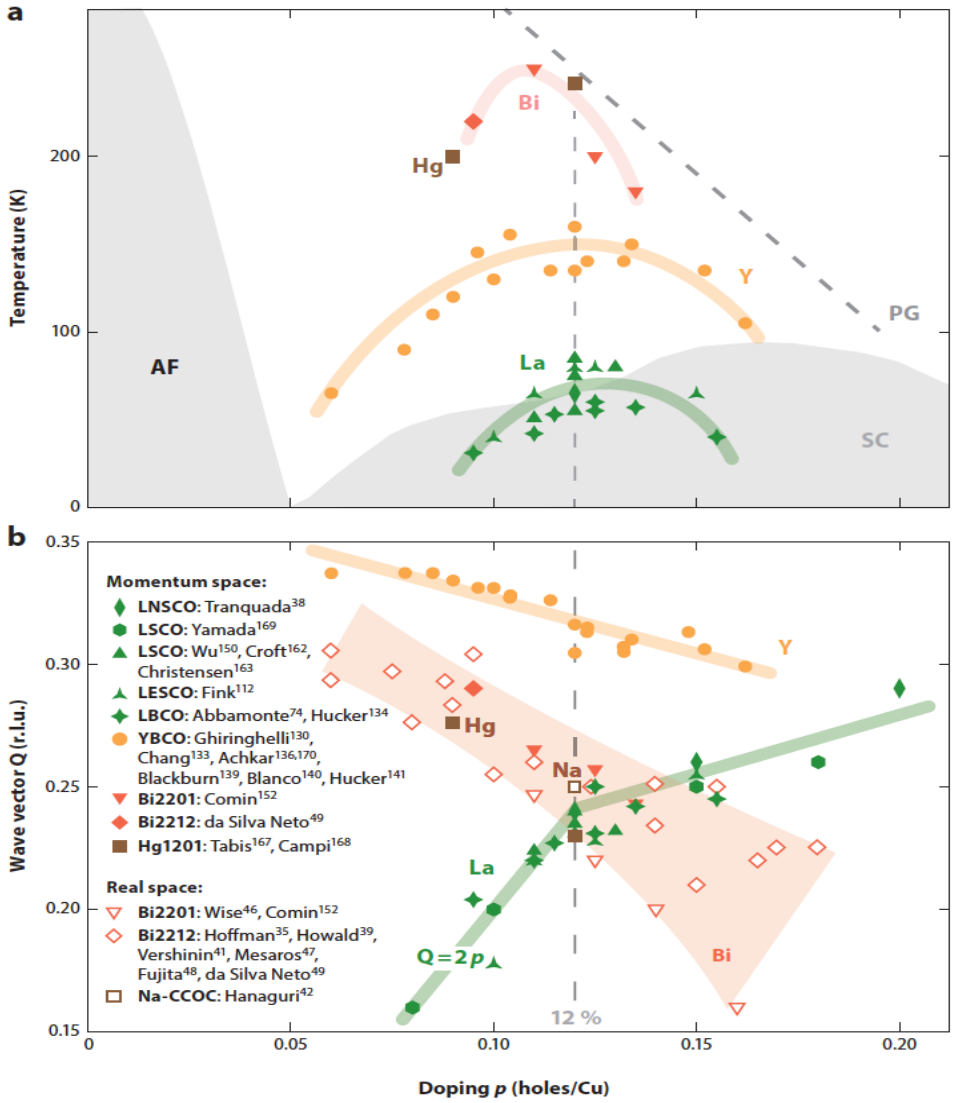
Wei-Lin Tu, Institute of Physics, Academia Sinica
Peayush Choubey and P. J. Hirschfeld, Univ. of Florida

KIST Forum, March. 28, 2017

Congratulations to KITS!
-- they got Fuchun and Jiang Pin

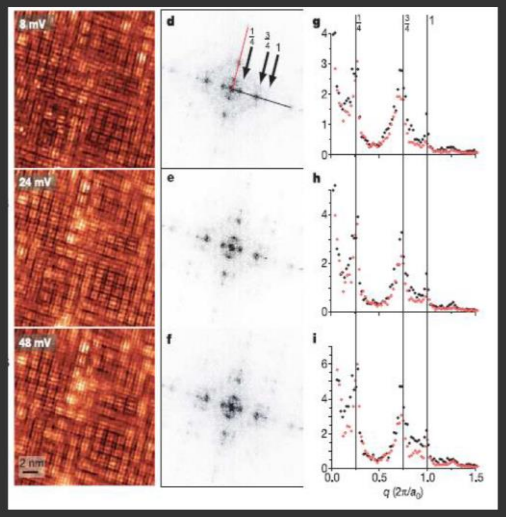
人生七十才開始!
(Life start at 70 years old!)
Have a great new life!-- Fuchun

Comin & Damascelli, Ann, Rev. Cond. Mat. Phys., 2016



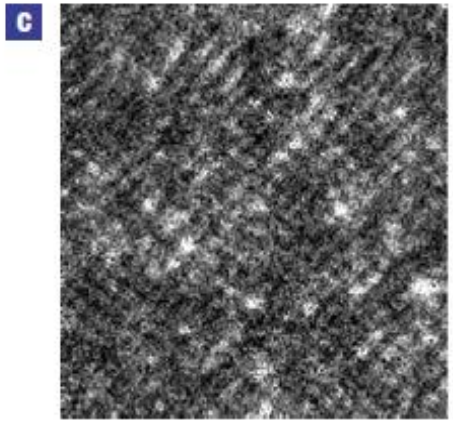
electron-doped NCCO is similar with LSCO

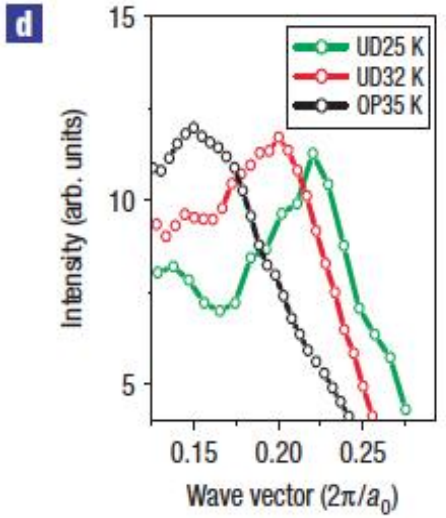
Checkerboard in CaNaCuOCl



- x(Tc) = 0.08 (0K), 0.10 (15K) and 0.12 (20K), checkerboard at all energies < 100 meV
- Non-dispersive, commensurate checkerboard, $\lambda = 4a_0$ independent of doping

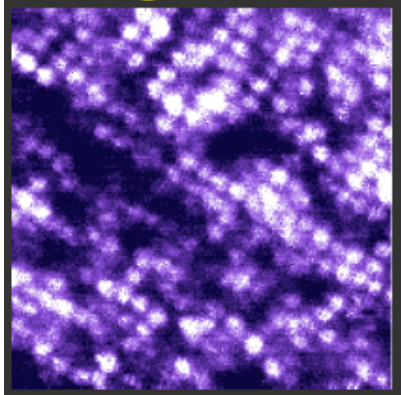
Hanaguri et al, Nature 1001, 430 (2004)



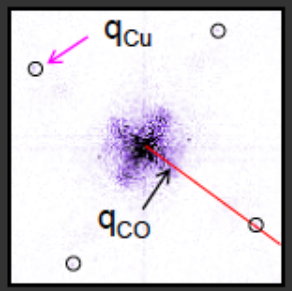


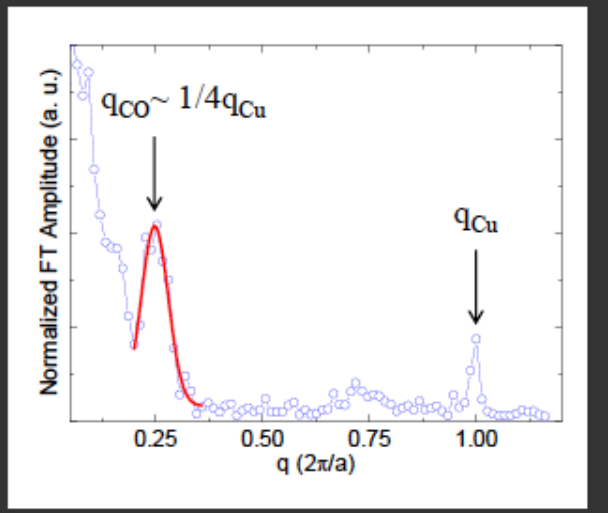
Checkerboard in Bi-2201
Wise et al, Nature Phys. 4, 696, 2008

I@ +100 mV



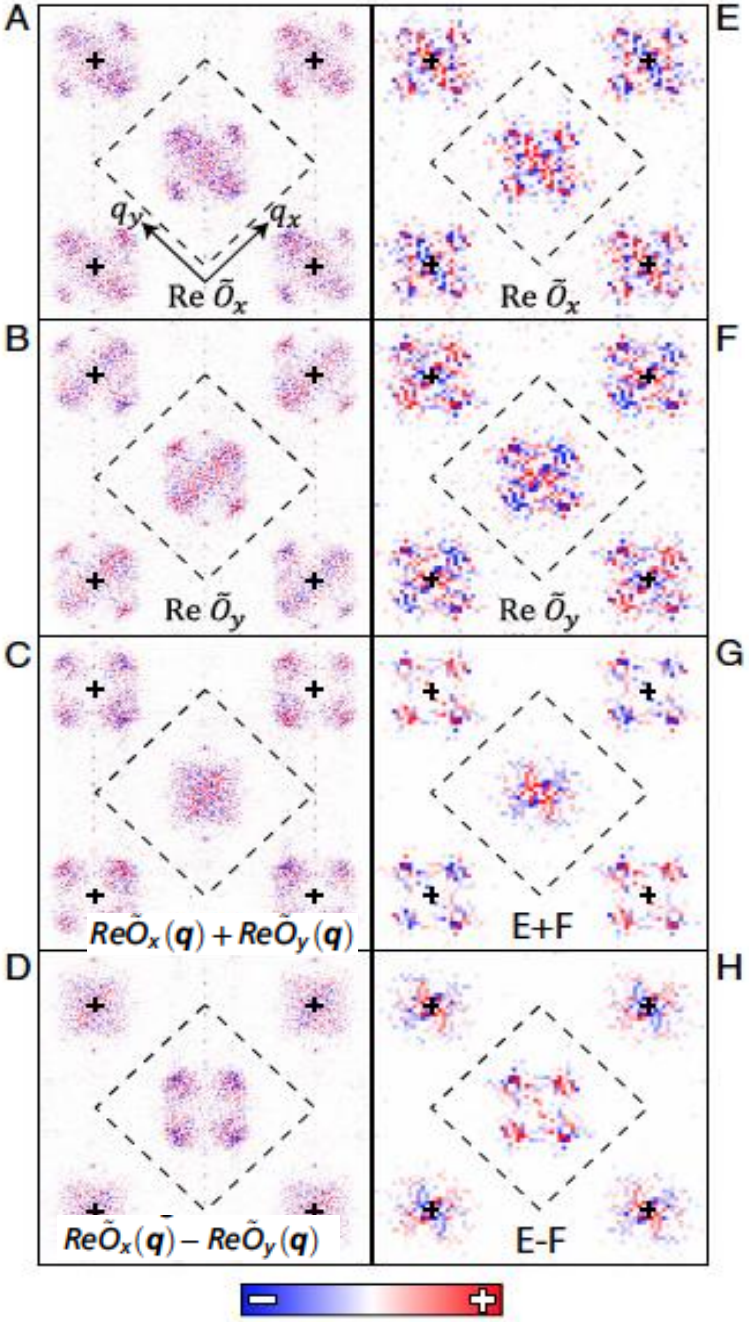
low High





Checkerboard in La-doped Bi-2201
By P. Cai et al. Nat. Phys. 3840 (2016)

BSCCO-2212, 8% NaCCOC, 12%



Symmetry of charge order

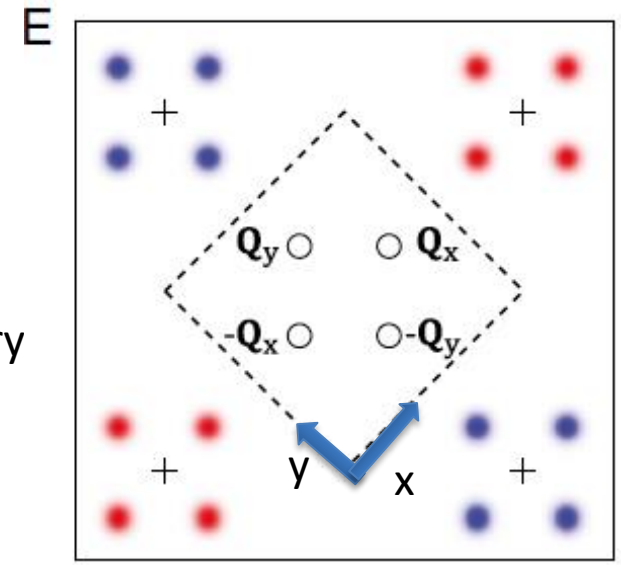
Fujita et al, PNAS 111, E3026 (2014).

The R- map

$$R(q,E) = FFT\{\frac{\int_0^E dw LDOS(r,w)}{\int_E^0 dw LDOS(r,w)}\}$$ Take the real part

Energy E is 150 meV, r either Ox or Oy

D-symmetry



Red: positive
Blue: negative

S'-symmetry

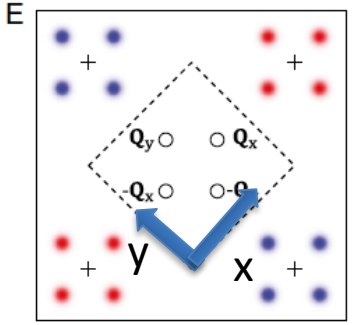
Fujita et al, PNAS 111, E3026 (2014).

$$\langle c^{\dagger}_{i\alpha} c_{j\alpha} \rangle = \sum_{\boldsymbol{Q}} \left[\sum_{\boldsymbol{k}} P(\boldsymbol{k}, \boldsymbol{Q}) e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)} \right] e^{i\boldsymbol{Q}\cdot(\boldsymbol{r}_i + \boldsymbol{r}_j)/2}.$$

P(k,Q) is intra-unit-cell form factor

This is named bond order by Metlitski and Sachdev, PRB &NJP 2010
and Sachdev and La Placa, PRL 2013.

$$\left\langle c^{\dagger}_{i\alpha} c_{j\alpha} + c^{\dagger}_{j\alpha} c_{i\alpha} \right\rangle = \begin{cases} \frac{1}{K} \rho(\boldsymbol{r}_{\mathrm{Cu}}) \text{ for } i = j \\ \frac{1}{K'} \rho(\boldsymbol{r}_{\mathrm{O}_x}) \text{ for } i,j \text{ n.n along } x \text{ direction} \\ \frac{1}{K'} \rho(\boldsymbol{r}_{\mathrm{O}_y}) \text{ for } i,j \text{ n.n along } y \text{ direction.} \end{cases}$$



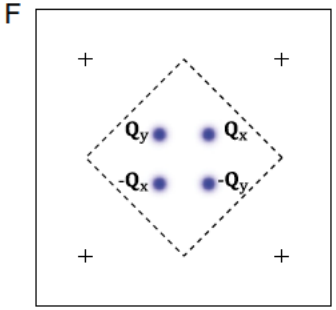
d-form factor

$$P_d(k,Q) \sim \cos(k_x) - \cos(k_y)$$

$$Q = (\pm 3\pi/2, 0) \quad Q = (0, \pm 3\pi/2)$$

Li et al, PRB 74, 184515 (2006)

$$\left\langle C^{+}_{k+Q/2,\alpha} C_{k-Q/2} \right\rangle \sim \cos(k_x) - \cos(k_y)$$



S'-form factor

$$P_s(k,Q) \sim \cos(k_x) + \cos(k_y)$$

$$Q = (\pm \pi/2, 0) \quad Q = (0, \pm \pi/2)$$

Different from D-density wave (DDW)

$$P(k,Q) \sim \sin(k_x) - \sin(k_y)$$ at Q=(π, π)

Hamidian et al. Nat. Phys 12, 150 (2016), Bi-2212

Davis STS, z-map

$$z(q,E) = FFT\{\frac{LDOS(r,E)}{LDOS(r,-E)}\}$$

$$\tilde{O}_x(\boldsymbol{q}) = Re\tilde{O}_x(\boldsymbol{q}) + iIm\tilde{O}_x(\boldsymbol{q})$$

$$\tilde{O}_y(\boldsymbol{q}) = Re\tilde{O}_y(\boldsymbol{q}) + iIm\tilde{O}_y(\boldsymbol{q})$$

Next we can define different form factors

$$\tilde{D}^z(\boldsymbol{q}) = (\tilde{O}_x(\boldsymbol{q}) - \tilde{O}_y(\boldsymbol{q}))/2$$

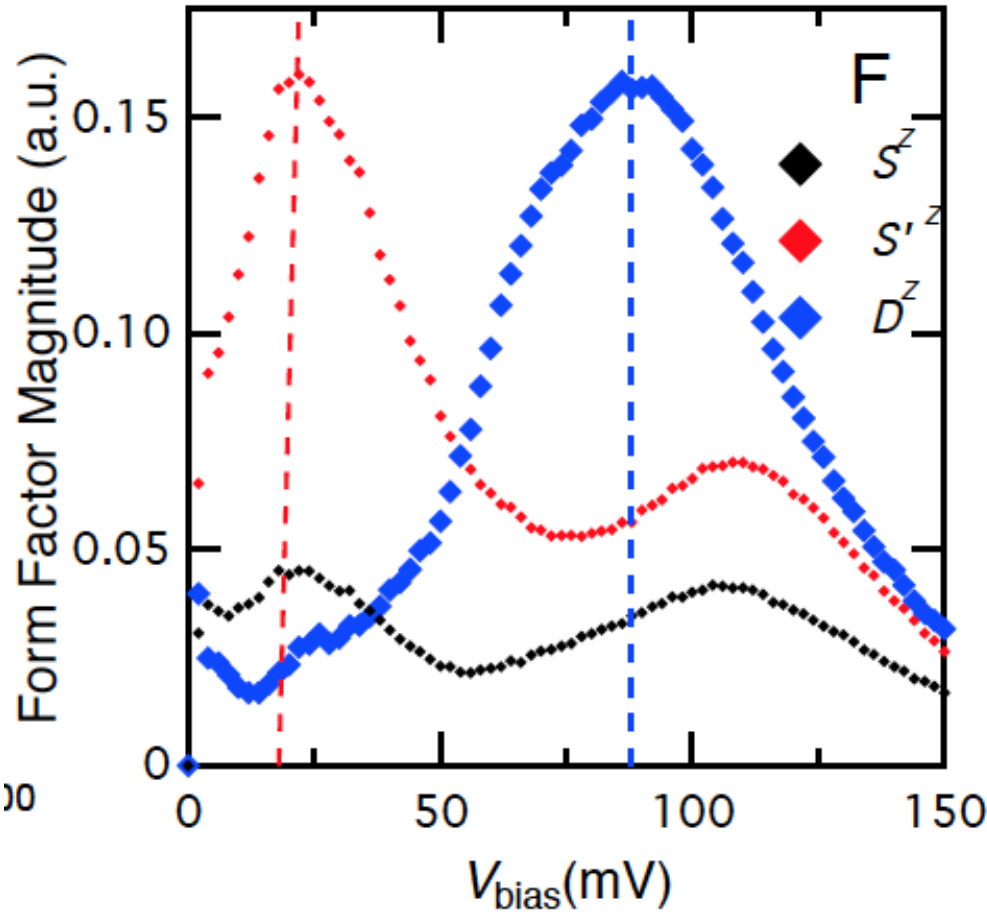
$$\tilde{S}'^z(\boldsymbol{q}) = (\tilde{O}_x(\boldsymbol{q}) + \tilde{O}_y(\boldsymbol{q}))/2$$

$$\tilde{S}^z(\boldsymbol{q}) = \widetilde{Cu}(\boldsymbol{q})$$

Look at the magnitude only

The form factor has an energy dependence

q near (π/2,0) and (0, π/2)



From REXS or RIXS,

For YBCO and Bi-2201, R. Comin et al., Nature Materials 4295, (2015), -- **d-**wave bond order dominates

For $La_{1.875}Ba_{0.125}CuO_4$ (LBCO) A. J. Achkar et al, arXiv 1409.6787, Nature material 15,616 (2016).
- **s'**-wave dominates over d

Detection of Cooper Pair Density Wave of 4a in Bi-2212 , Hamidian et al, nature 17411

Why are there so many different kinds of low- energy "competing" states in cuprates , like stripes, charge-density wave (CDW), checkerboard (CB) states, etc.?
They seem to be scattered around in the phase diagram.

Besides information about wave vector or period vs. doping, there are more details of the properties like
symmetry of intra-unit cell form factor, its energy dependence, pair density wave (PDW)? Intertwined orders? etc..

Theory????

Answer from a minimal model!

The minimal t-J Hamiltonian

$$-\sum_{i,j,s} t_{ij}\left(\tilde{c}^{\dagger}_{i,s}\tilde{c}_{j,s} + h.c.\right) + J\sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j$$

With the projection operator

$$P_d = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})$$

t_{ij} = n.n.(t), 2nd n.n.(t')

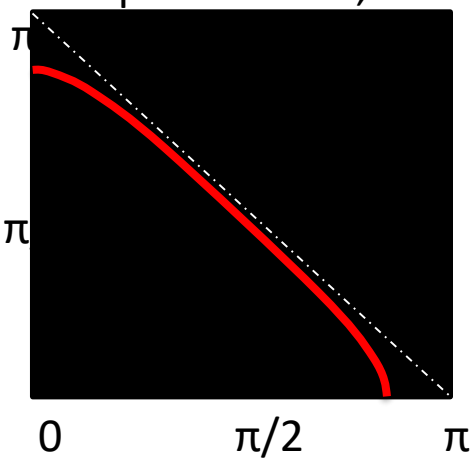
J = n.n. AF spin-spin interaction, t'=0. & -0.3t

J=0.3t

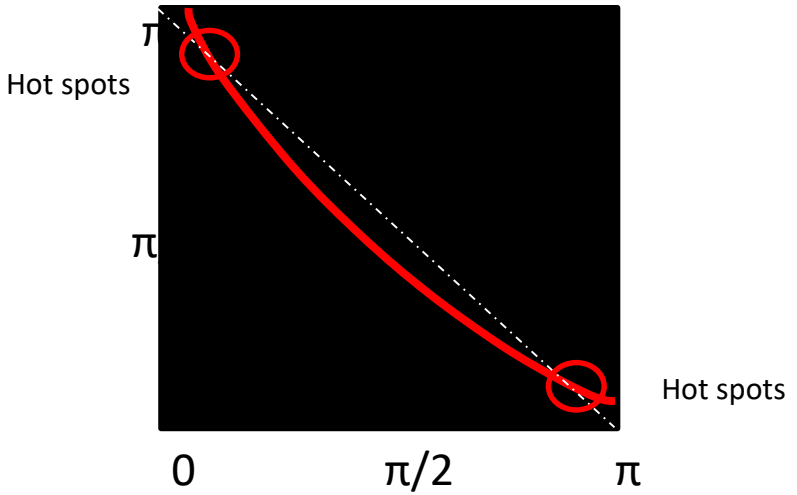
Strong constraint -- no two electrons on the same site

Fermi surface has no nesting, Van Hove singularity and hot spots if t'=0!

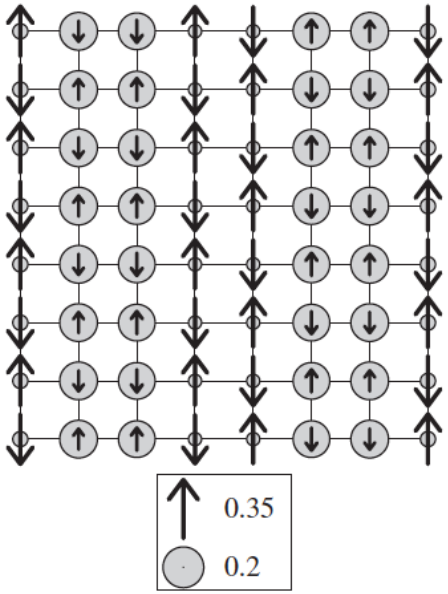
Fermi liquid x=0.125, t'=0

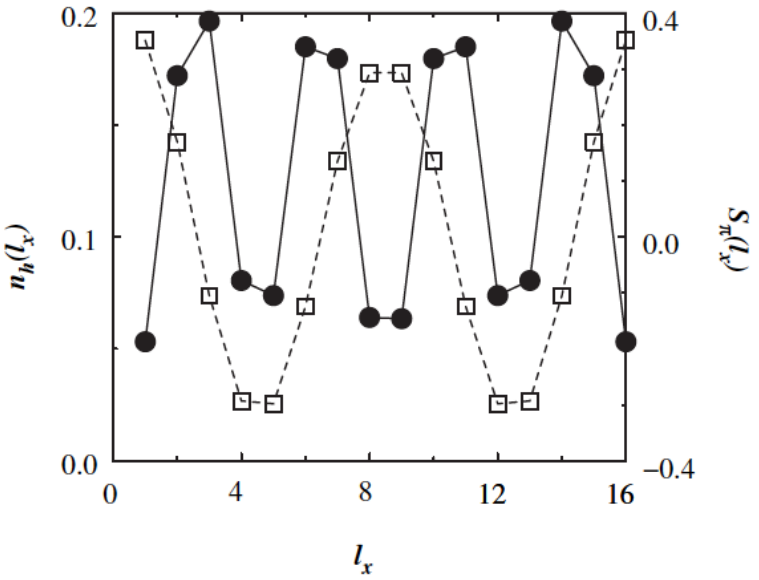


FS for Fermi liquid x=0.125, t'=-0.3



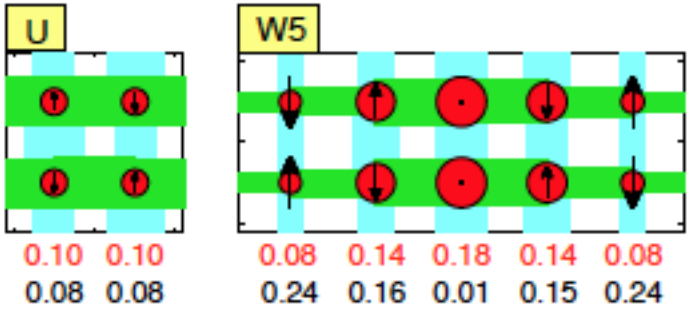
DMRG by White and Scalapino, PRL 1998, J/t=0.35, d =1/8, 4a wave
y-PBC, x-OBC for 16x8, bond-centered





Bond- and site-centered states are degenerate, sensitive to BC

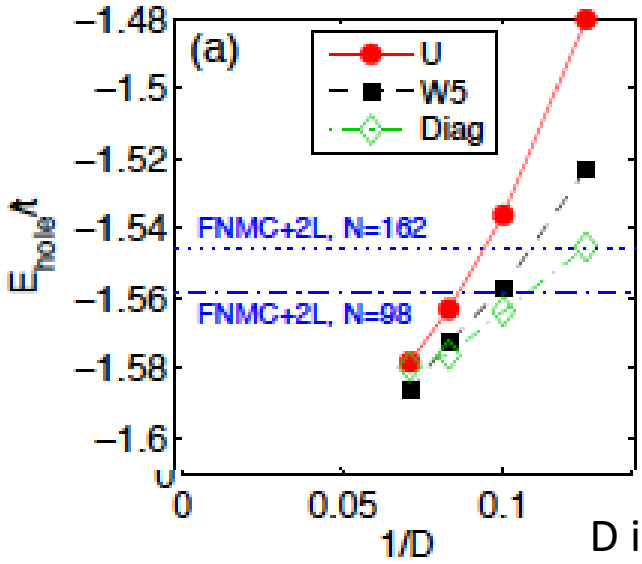
iPEPS (infinite projected-entangled pair state
results by P. Corboz et al., PRL113,046402 (2014)



δ=0.1, D=14

δ=0.125, J/t=0.4,
D=14

The uniform AF-dSC state has about same energy as the IP-CDW-SDW(AF-RVB) stripe state



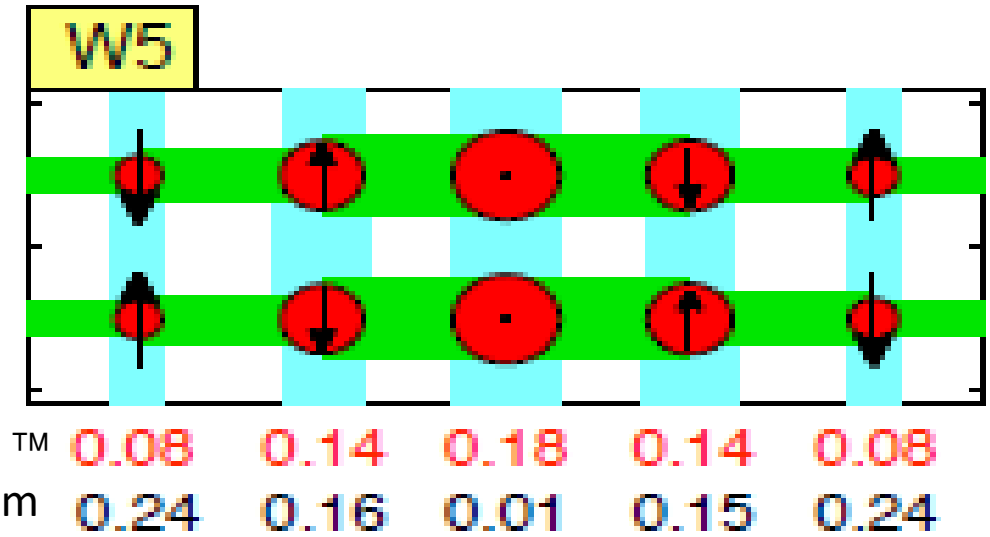
The antiphase stripe (not shown) has energy 0.001t higher than In-phase-CDW-SDW (W5) stripe at 1/D=0.1

The value of pairing order parameter Is about the same as VMC and GWA.

D is the bond dimension

FNMC+2L– fix node MC + 2 steps of Lanczos, Hu et al, PRB85,081110 (2012)

Corboz et al : the IP-CDW-SDW 5a pattern with IPEPS method(™=0.125)



Our result of IP-CDW-SDW 5a pattern(for J=0.4 & ™=0.125)

site number	1	2	3	4	5
δ	0.0751	0.1435	0.1871	0.1435	0.0751
$\|m\|$	0.3242	0.2192	0	0.2192	0.3242
Δ	0.0222	0.027	0.0318	0.027	0.0222

The moment is overestimated about 4/3 by our result, same at half filling

Renormalized mean-field theory

F. C. Zhang *et al*., Supercond. Sci. Technol. 1, 36 (1988).

Gutzwiller approximation (GWA) – to replace the projection operator by a renormalization factor

$$\hat{P}_d = \tilde{\prod}_i \left(1 - \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\right) \qquad |\Psi\rangle = \hat{P}_d |\Psi_0\rangle$$

$$\langle\Phi|\hat{A}|\Phi\rangle \approx g(\hat{A})\langle\Phi_0|\hat{A}|\Phi_0\rangle$$

g(A) is the Gutzwiller renormalization factor for the operator A.

$$H = -\sum_{i,j,\sigma} g^t_{ij\sigma} t (c^\dagger_{i\sigma} c_{j\sigma} + H.C.)$$

$$+ \sum_{\langle i,j\rangle} J \left[g^{s,z}_{ij} S^{s,z}_i S^{s,z}_j + g^{s,xy}_{ij} \left(\frac{S^+_i S^-_j + S^-_i S^+_j}{2} \right) \right]$$

$$g^t_{ij\sigma} = g^t_{i\sigma} g^t_{j\sigma} \qquad g^{s,xy}_{ij} = g^{s,xy}_i g^{s,xy}_j$$

$$g^t_{i\sigma} = \sqrt{\frac{2\delta_i(1-\delta_i)}{1-\delta_i^2+4(m^v_i)^2}} \frac{1+\delta_i+\sigma 2m^v_i}{1+\delta_i-\sigma 2m^v_i} \qquad g^{s,xy}_i = \frac{2(1-\delta_i)}{1-\delta_i^2+4(m^v_i)^2}$$

Ogata and Himeda JPSJ, 72, 374 (2003); Yang, Rice, Fuchun *et al*. N. J. of Phys., 11, 055053 (2009)

Mean field treatment

$$g_i^t = \sqrt{\frac{2\delta_i}{1+\delta_i}}$$ If no moment

$$E_t = \langle \Psi_0 | H | \Psi_0 \rangle$$

$$= -\sum_{\langle i,j\rangle,\sigma} g^t_{\langle i,j\rangle,\sigma} t_{\langle i,j\rangle} [\chi_{\langle i,j\rangle,\sigma} + \text{h.c.}] - \sum_{\langle i,j\rangle,\sigma} J_{\langle i,j\rangle} \left(\frac{g^{s,z}_{\langle i,j\rangle}}{4} + \frac{g^{s,xy}_{\langle i,j\rangle}}{2} \frac{\Delta^*_{\langle i,j\rangle,\bar{\sigma}}}{\Delta^*_{\langle i,j\rangle,\sigma}} \right) \Delta^*_{\langle i,j\rangle,\sigma} \Delta_{\langle i,j\rangle,\sigma}$$

$$- \sum_{\langle i,j\rangle,\sigma} J_{\langle i,j\rangle} \left(\frac{g^{s,z}_{\langle i,j\rangle}}{4} + \frac{g^{s,xy}_{\langle i,j\rangle}}{2} \frac{\chi^*_{\langle i,j\rangle,\bar{\sigma}}}{\chi^*_{\langle i,j\rangle,\sigma}} \right) \chi^*_{\langle i,j\rangle,\sigma} \chi_{\langle i,} + \sum_{\langle i,j\rangle} g^{s,z}_{\langle i,j\rangle} J_{\langle i,j\rangle} m_i m_j .$$

Intertwined orders: charge density, bond order, pair field and spin moment

$n_{i,s}$, $c_{(i,j)s}$, $D_{<i,j>,s}$, m

$$m_i = \langle \Psi_0 | \hat{S}^z_i | \Psi_0 \rangle ,$$

$$\Delta_{\langle i,j\rangle,\sigma} = \sigma \langle \Psi_0 | \hat{c}_{i,\sigma} \hat{c}_{j,-\sigma} | \Psi_0 \rangle ,$$

$$\chi_{\langle i,j\rangle,\sigma} = \langle \Psi_0 | \hat{c}^\dagger_{i,\sigma} \hat{c}_{j,\sigma} | \Psi_0 \rangle ,$$

$$\delta_i = 1 - \langle \Psi_0 | \hat{n}_i | \Psi_0 \rangle ,$$

In-phase(IP) domains or anti-phase (AP) domains

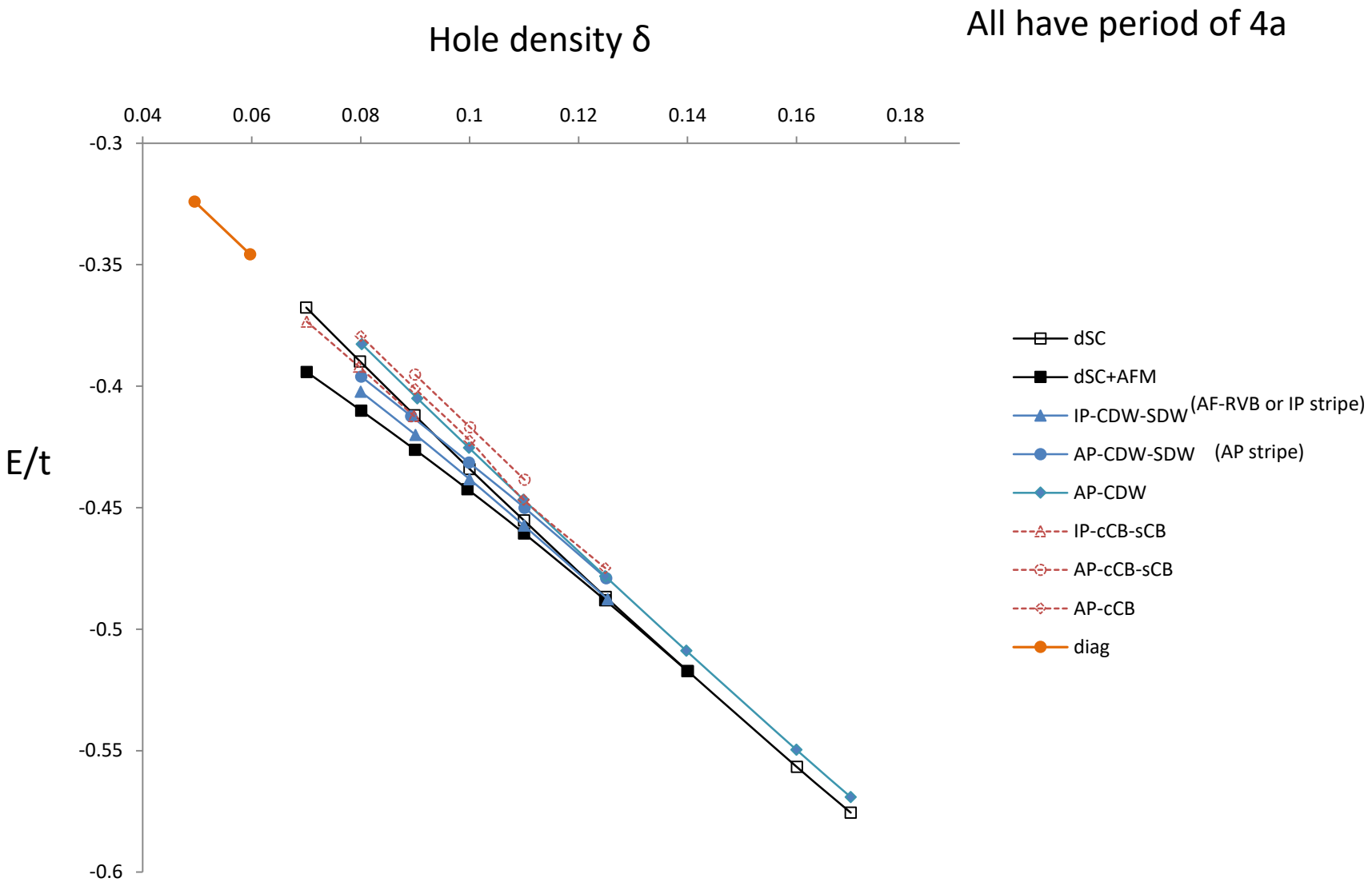
x-bond and y-bond could have a π phase shift in the density wave

Find the wave function with optimal parameters that minimizes W

$$W = \langle \Psi_0 | H | \Psi_0 \rangle - \lambda \left(\langle \Psi_0 | \Psi_0 \rangle - 1 \right) - \mu \left(\sum_i \hat{n}_i - N_e \right)$$

Solve self-consistent BdG equations for 16x16 cell with 16x16 supercell methods

Including the CB (checkerboard) patterns, diagonal stripes, CDW..



Antiphase CDW

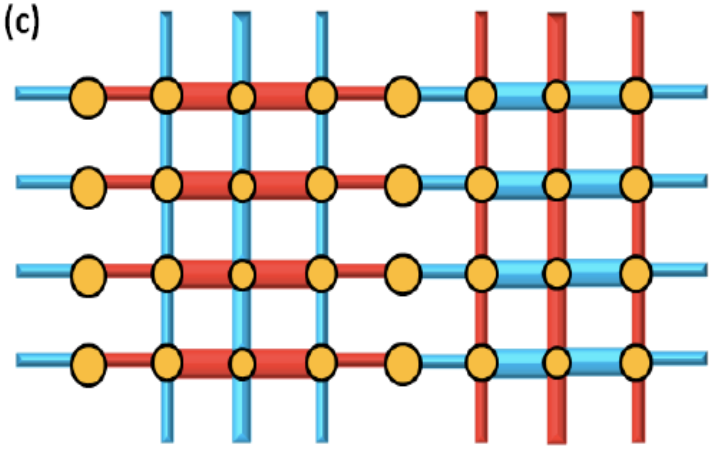
AP-CDW(δ=0.125 J/t=0.3)

Two pairing domains of size 4a

site number	1	2	3	4
δ	0.1315	0.1256	0.1168	0.1256
$\|m\|$	0	0	0	0
Δ	0	0.0194	0.0247	0.0194
$K_{i,i+\hat{y}}$	0.1151	0.0901	0.0625	0.0901
$K_{i,i+\hat{x}}$	0.0688	0.0972	0.0972	0.0688

Red bond for +ve pairing

Blue -ve

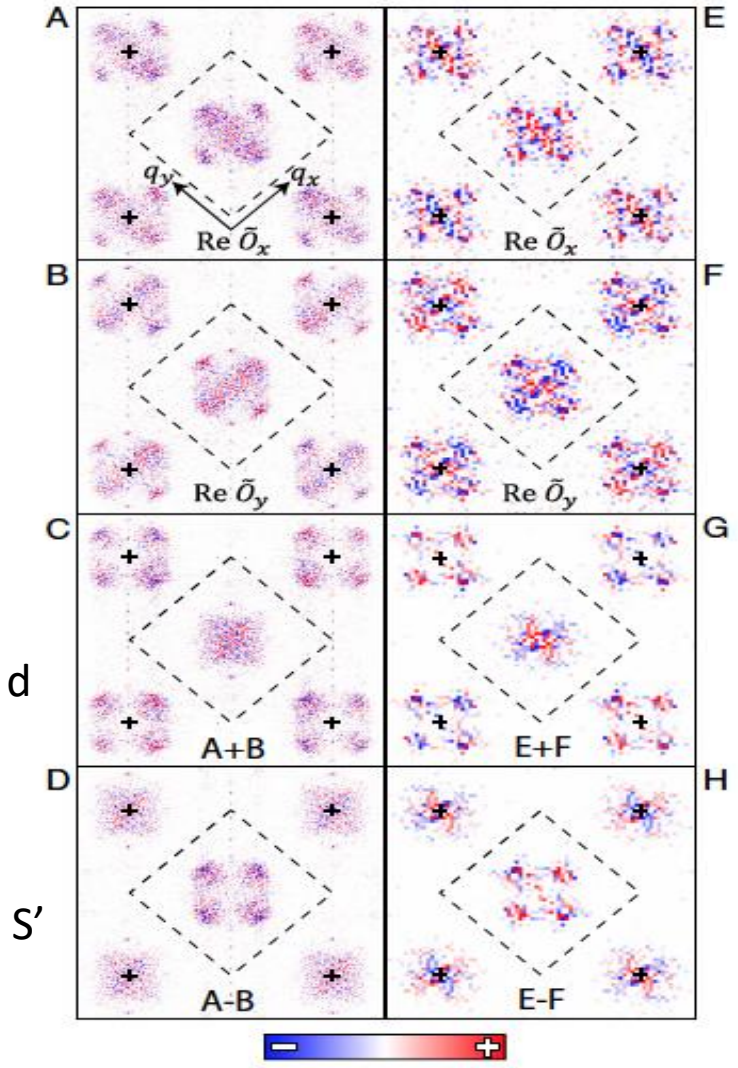


Yellow circle: hole density

$$\Delta_i = \sum_{\sigma} (g^t_{i,i+\hat{x},\sigma}\Delta^v_{i,i+\hat{x},\sigma} + g^t_{i,i-\hat{x},\sigma}\Delta^v_{i,i-\hat{x},\sigma} - g^t_{i,i+\hat{y},\sigma}\Delta^v_{i,i+\hat{y},\sigma} - g^t_{i,i-\hat{y},\sigma}\Delta^v_{i,i-\hat{y},\sigma})/8$$

Bond order $K_{\langle i,j\rangle} = \sum_s g^t_{\langle i,j\rangle,s}\, c^v_{\langle i,j\rangle,s} = \sum_s g^t_{\langle i,j\rangle,s} \langle \Psi_0 | c^+_{i,s} c_{j,s} | \Psi_0 \rangle$

Large d-form factor for bond order was seen in BSCCO-2212 and NaCCOC by Fujita et al , PNAS 111, E3026 (2014), Sachdev and La Placa, PRL 2013



$$\langle c_{i\alpha}^{\dagger} c_{j\alpha} \rangle = \sum_{\boldsymbol{Q}} \left[\sum_{\boldsymbol{k}} P(\boldsymbol{k},\boldsymbol{Q}) e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)} \right] e^{i\boldsymbol{Q}\cdot(\boldsymbol{r}_i+\boldsymbol{r}_j)/2},$$

P(k,Q) is intra-unit-cell form factor

For d-form factor

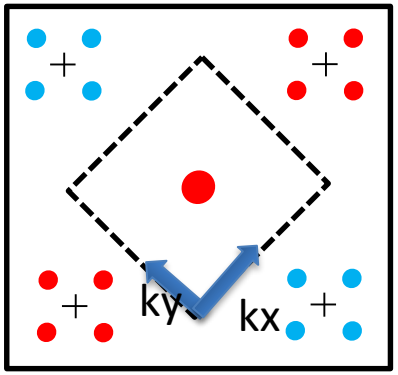
$$P_d(k,Q) \sim \cos(k_x) - \cos(k_y) \qquad Q = (\pm 3\pi/2, 0) \qquad Q = (0, \pm 3\pi/2)$$

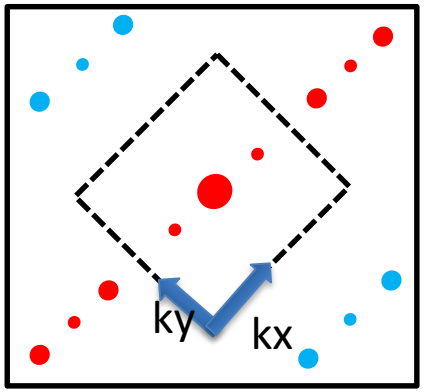
For s'-form factor

$$P_s(k,Q) \sim \cos(k_x) + \cos(k_y) \qquad Q = (\pm \pi/2, 0) \qquad Q = (0, \pm \pi/2)$$

Our calculated AP-CDW x- stripe

δ=0.125

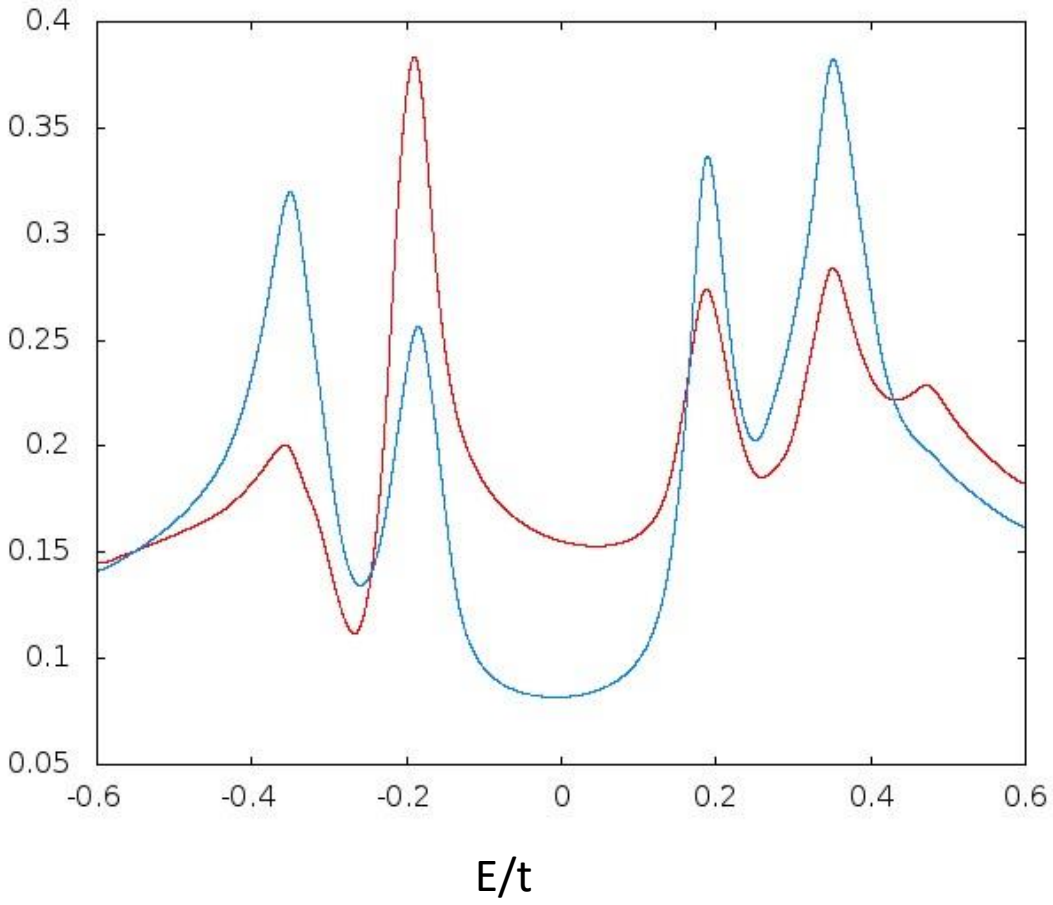


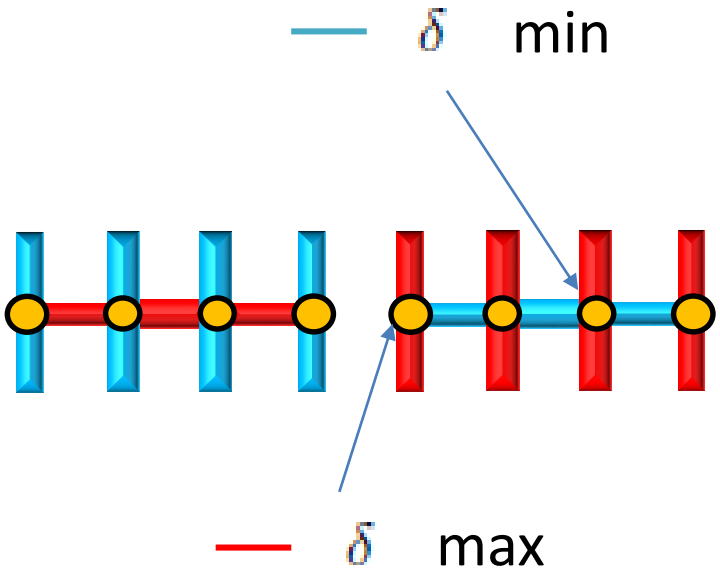


Red: positive
Blue: negative

1st BZ inside the dashed square

LDOS of AP-CDW (bond-centered) pattern(δ =0.125)



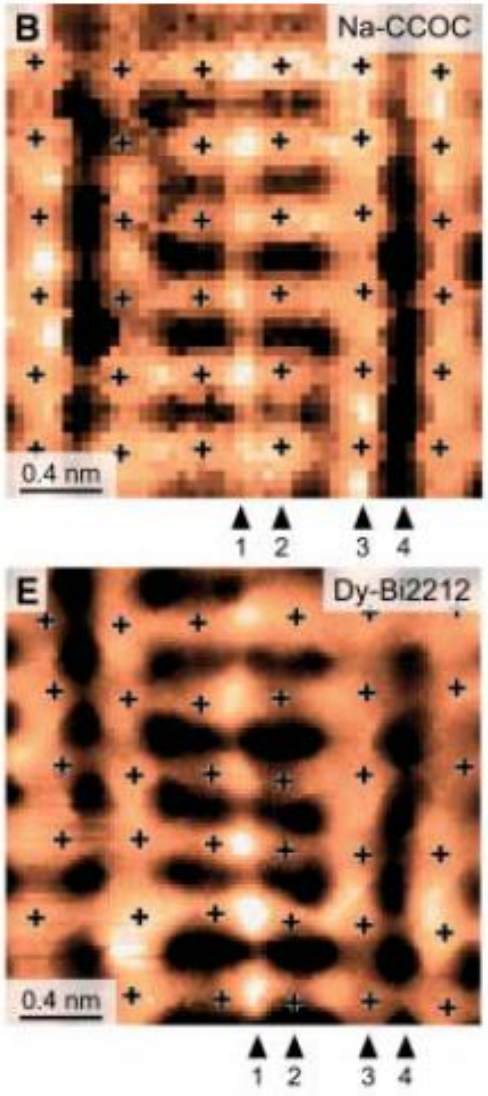


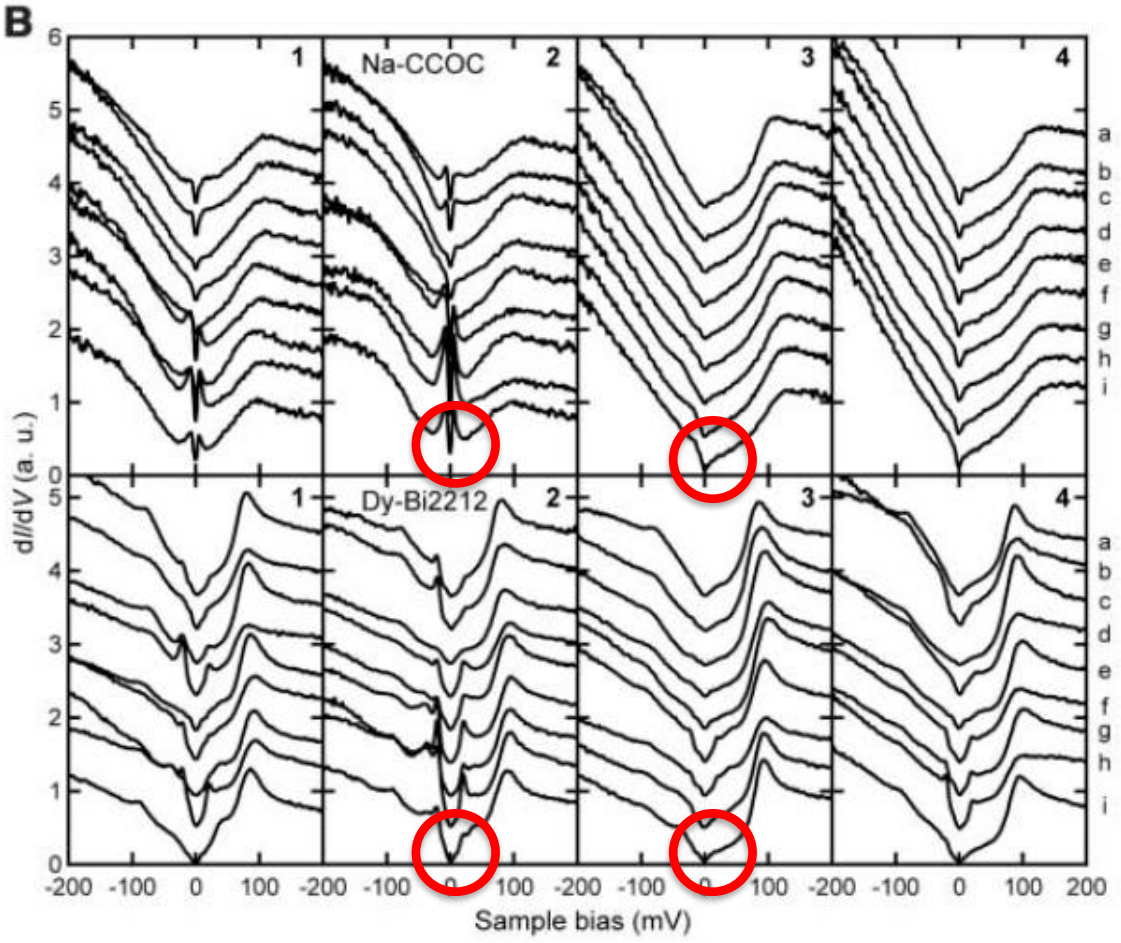
Finite DOS and No nodal DOS near zero energy -- A “normal” state!

Site-centered: Yang, Zhang,Rice *et al*. N. J. of Phys. 2009 ; Berg et al N.J. Phys.2009

In the SC state local density of states at low energy has nodes

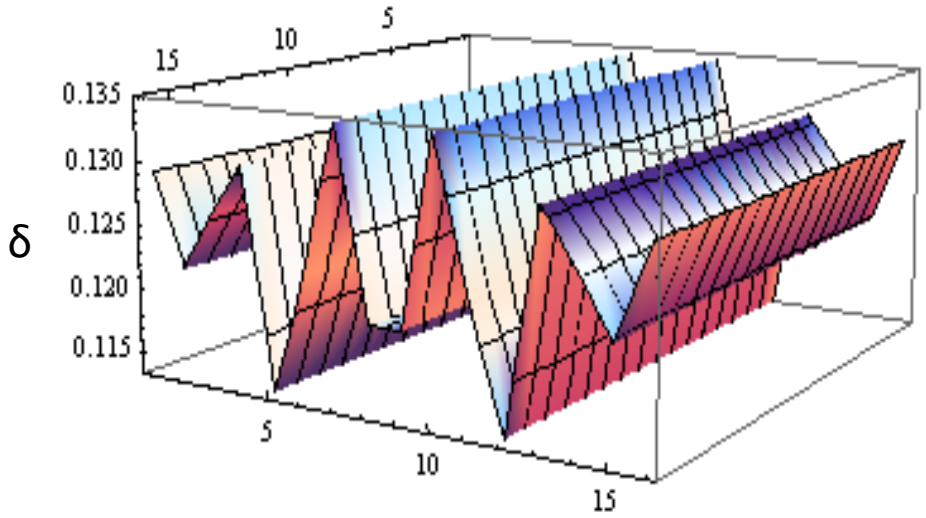
K. Kohsaka et al, Science 315, 1380 (2007)

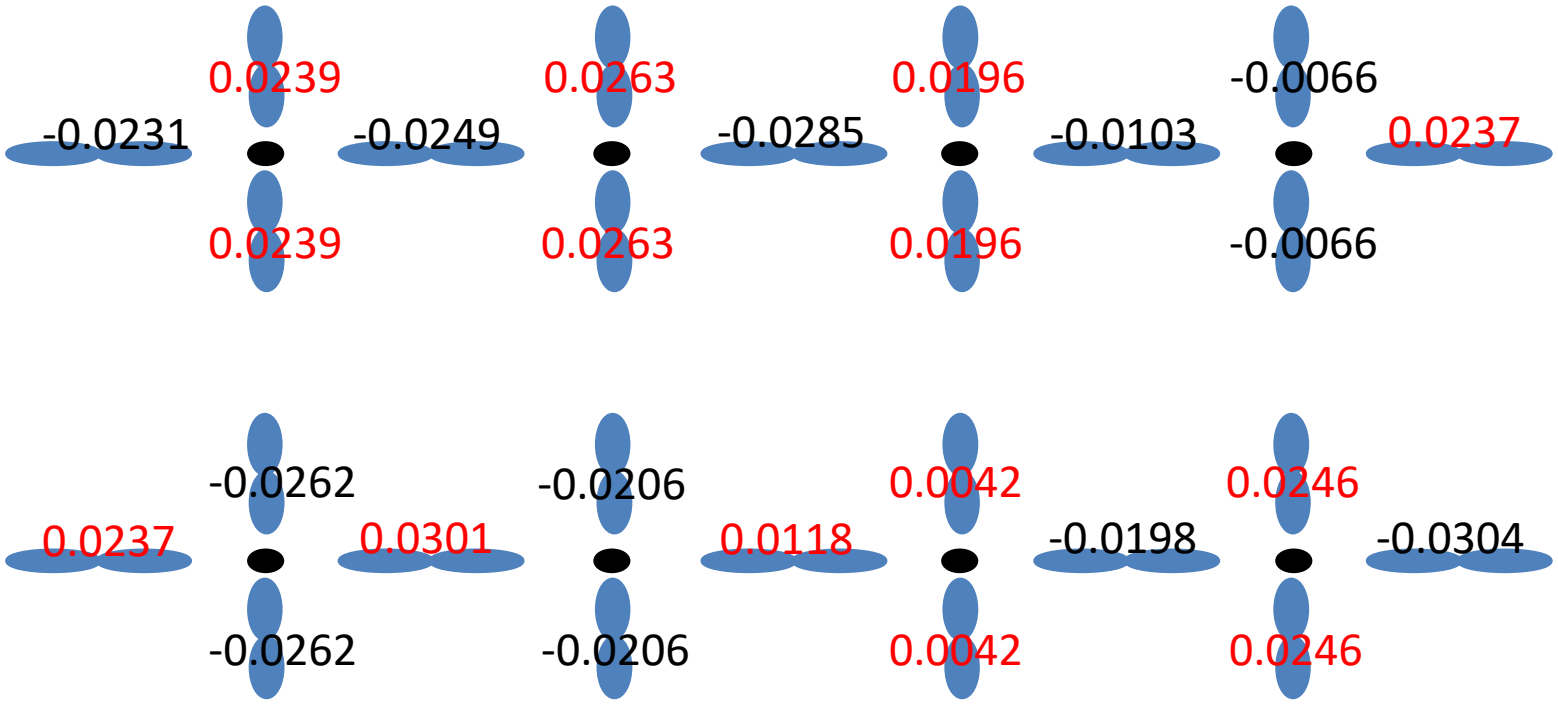




Nodal AP-CDW (**nPDW**) state,
APCDW+SC

Pairing order parameter, ™=0.125
t'=0

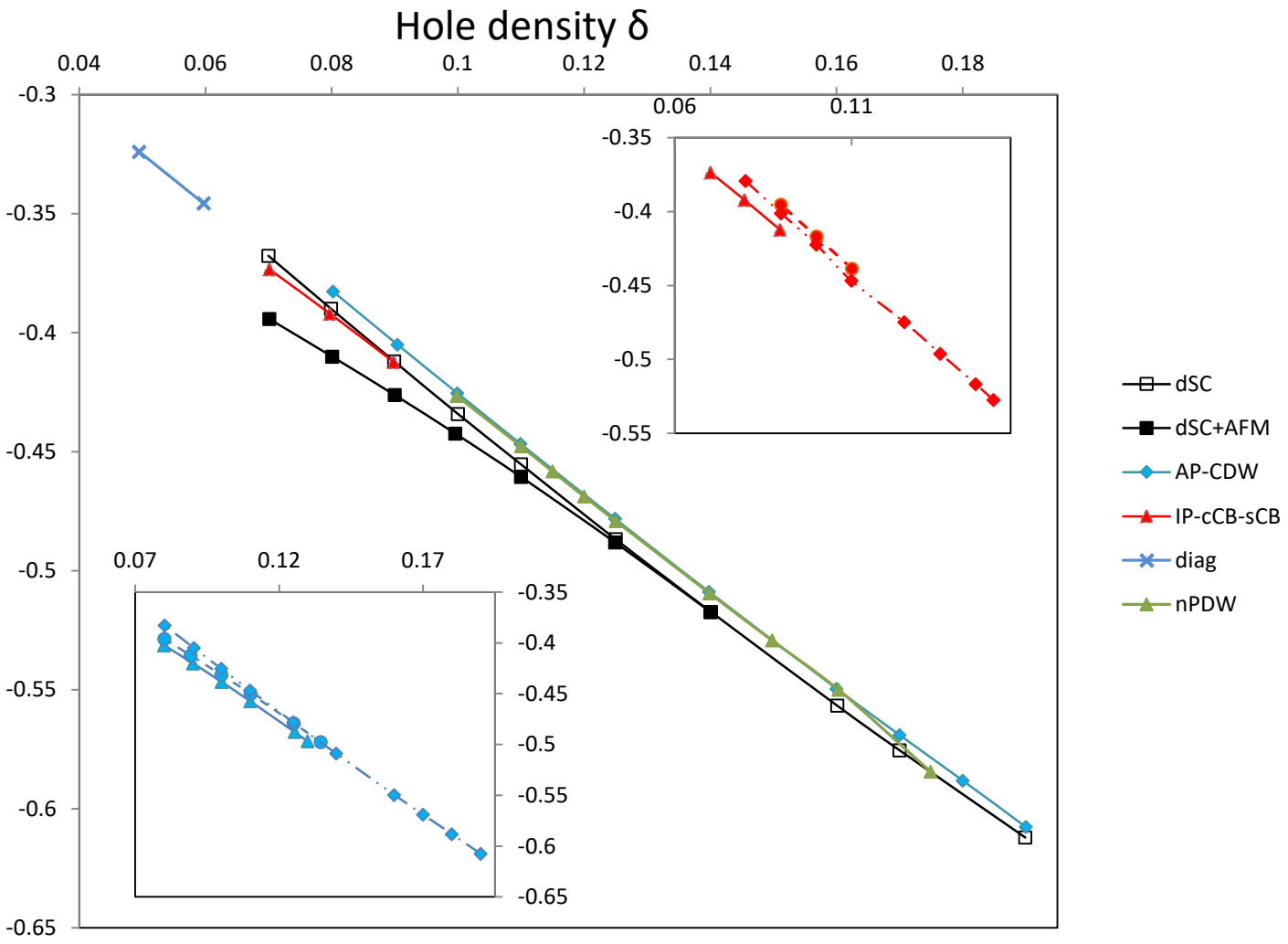




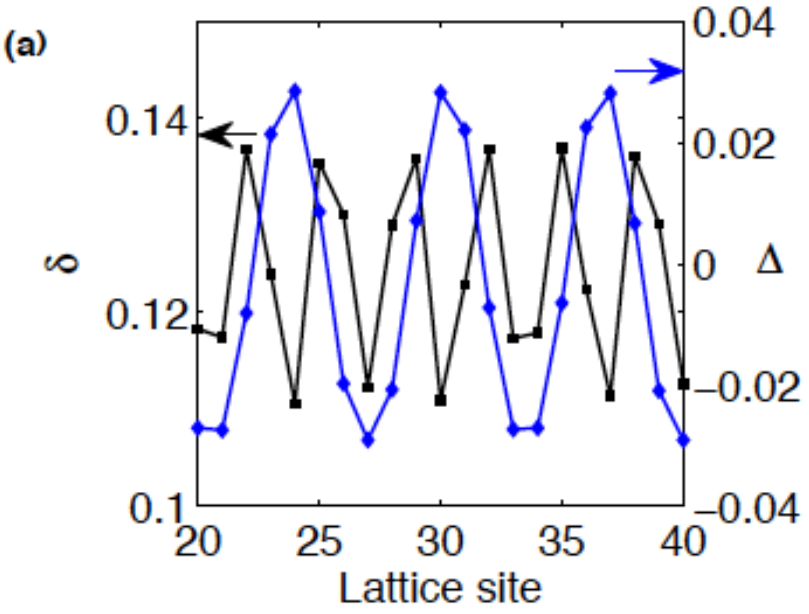
$\overline{\Delta_x} = -0.0056$
$\overline{\Delta_y} = 0.0057$

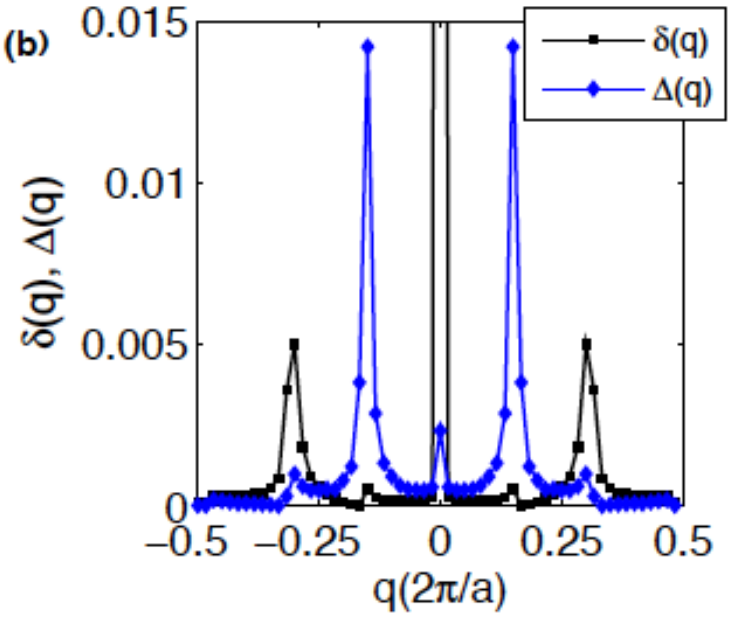
nPDW has same energy as AP-CDW

t'=0. J=0.3t

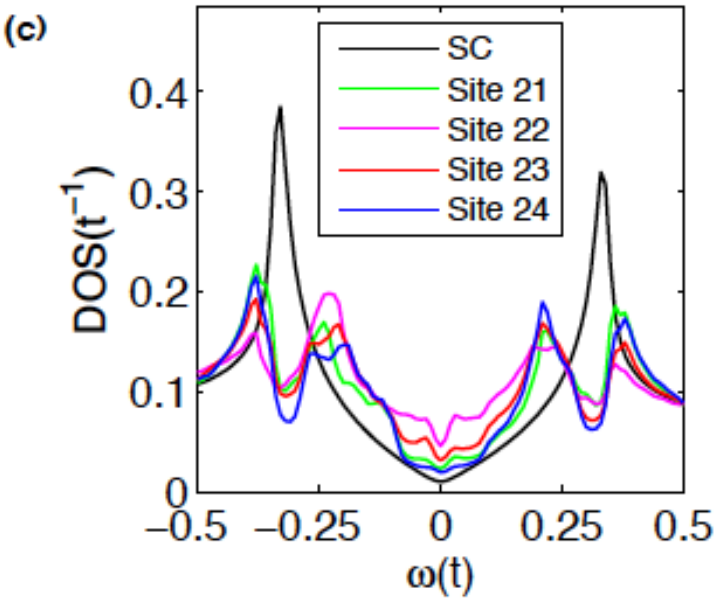


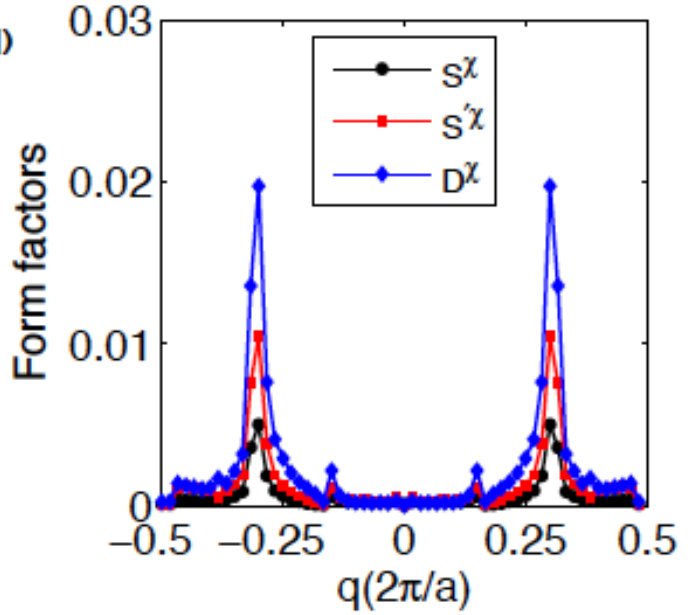
t'=-0.3t, for a 60x60 lattice, Q~0.15 for pairing, Q~0.3 for charge





Site 22 & 23 are near domain wall



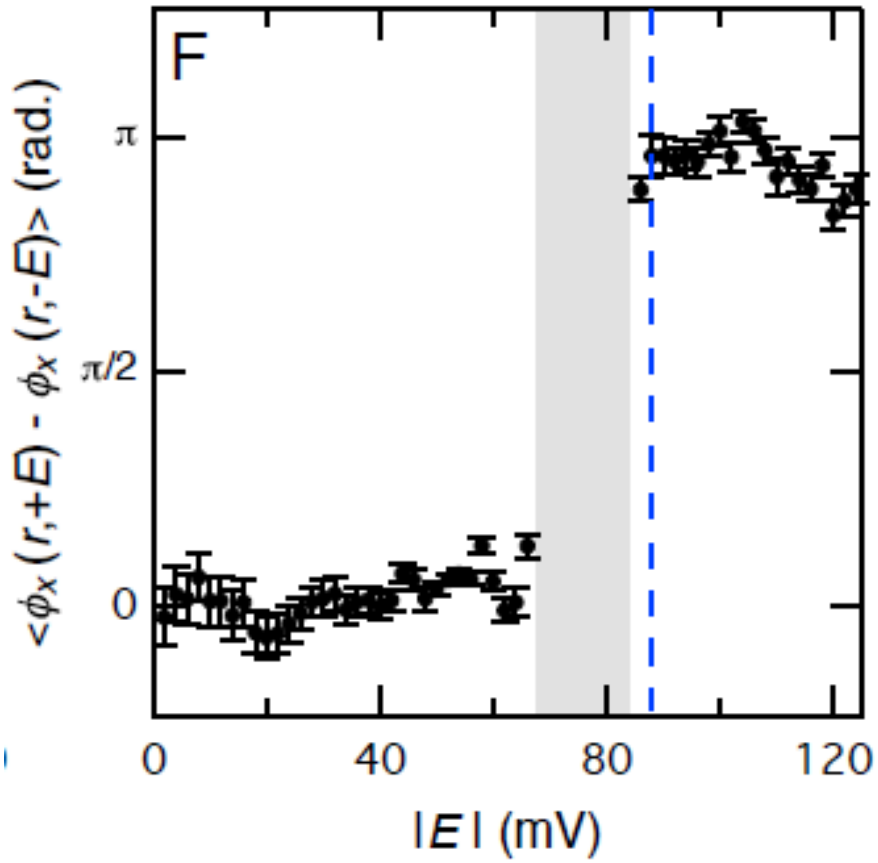


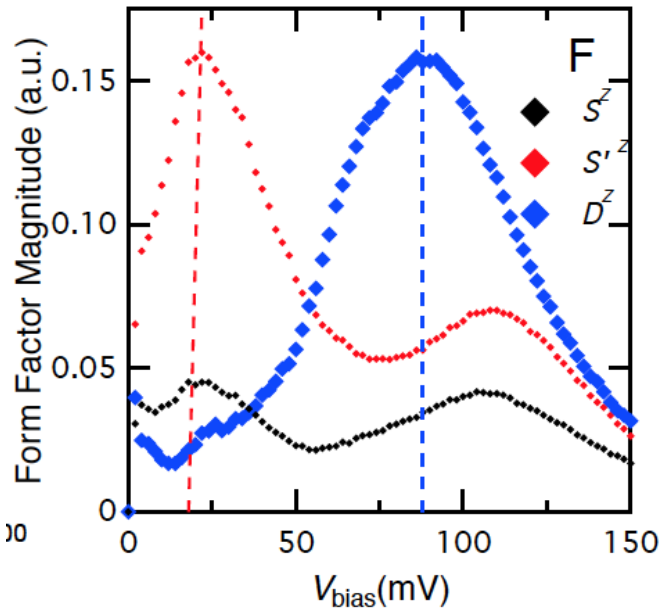
$$D^g(\mathbf{q},\omega) = (\tilde{O}^g_x(\mathbf{q},\omega) - \tilde{O}^g_y(\mathbf{q},\omega))/2$$

$$D(\mathbf{r},\omega) = \frac{2}{(2\pi)^2}\int d\mathbf{q} e^{i\mathbf{q}\mathbf{r}} D^g(\mathbf{q},\omega) e^{-\frac{(\mathbf{q}-\mathbf{Q}_d)^2}{2\Lambda^2}}$$

$$\phi(\mathbf{r},\omega) = \arctan\left(\mathrm{Im}[D(\mathbf{r},\omega)]/\mathrm{Re}[D(\mathbf{r},\omega)]\right)$$

$$\Delta\phi = \langle\phi(\mathbf{r},\omega) - \phi(\mathbf{r},-\omega)\rangle,$$





Hamidian et al. Nat. Phys 12, 150 (2016)
Bi-2212, 8% doping

We only have a Cu square lattice, how do we explain LDOS at O_x and O_y sites?

A. Kreisel, Peayush Choubey, T. Berlijn, W. Ku, B. M. Andersen, and P. J. Hirschfeld
Phys. Rev. Lett., 114,217002 (2015).

From a lattice Green function, for a super cell of 16x16,

$$G(\mathbf{R},\mathbf{R}';\omega)=\sum_n\left(\frac{g^t_{\mathbf{R}\mathbf{R}'\uparrow}u^n_{\mathbf{R}}u^{n*}_{\mathbf{R}'}}{\omega-E_n+i0}+\frac{g^t_{\mathbf{R}\mathbf{R}'\downarrow}v^{n*}_{\mathbf{R}}v^n_{\mathbf{R}'}}{\omega+E_n+i0}\right)$$

R- Cu site

Insert Wannier function calculated from LDA

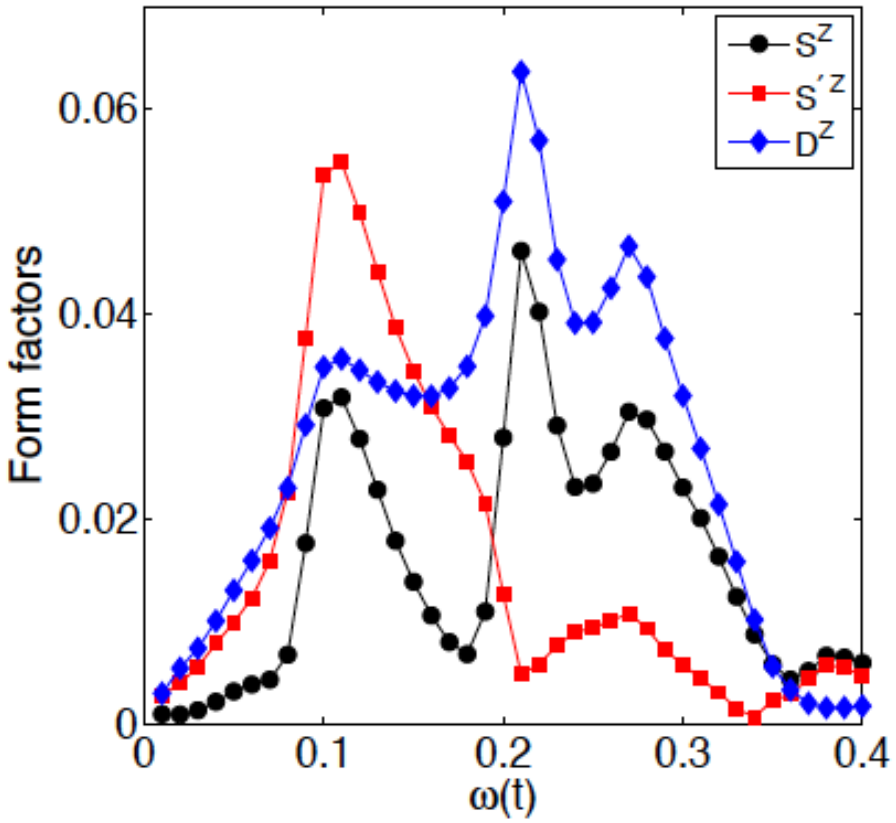
$$G_\sigma(\mathbf{r},\mathbf{r}';\omega)=\sum_{\mathbf{R},\mathbf{R}'}G_\sigma(\mathbf{R},\mathbf{R}';\omega)w_{\mathbf{R}}(\mathbf{r})w^*_{\mathbf{R}'}(\mathbf{r}')$$

r – continuum positions

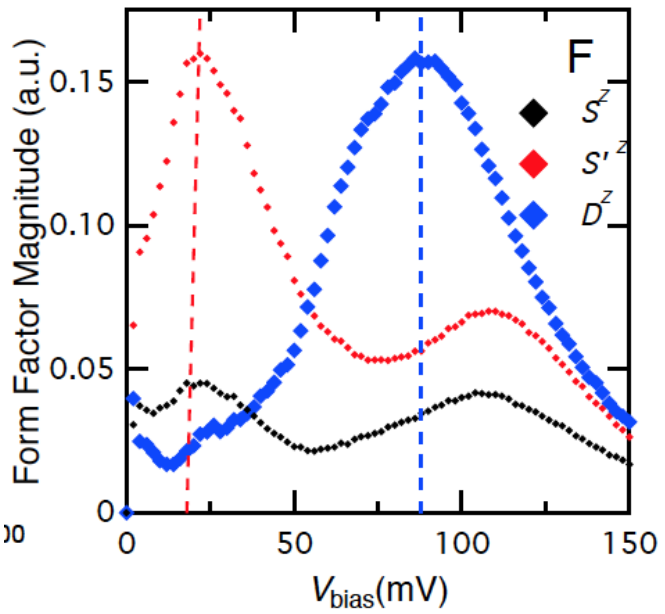
A continuus LDOS!
Now we can calculate LDOS at any position!

nPDW, CDW Q~0.3

At doping=0.125

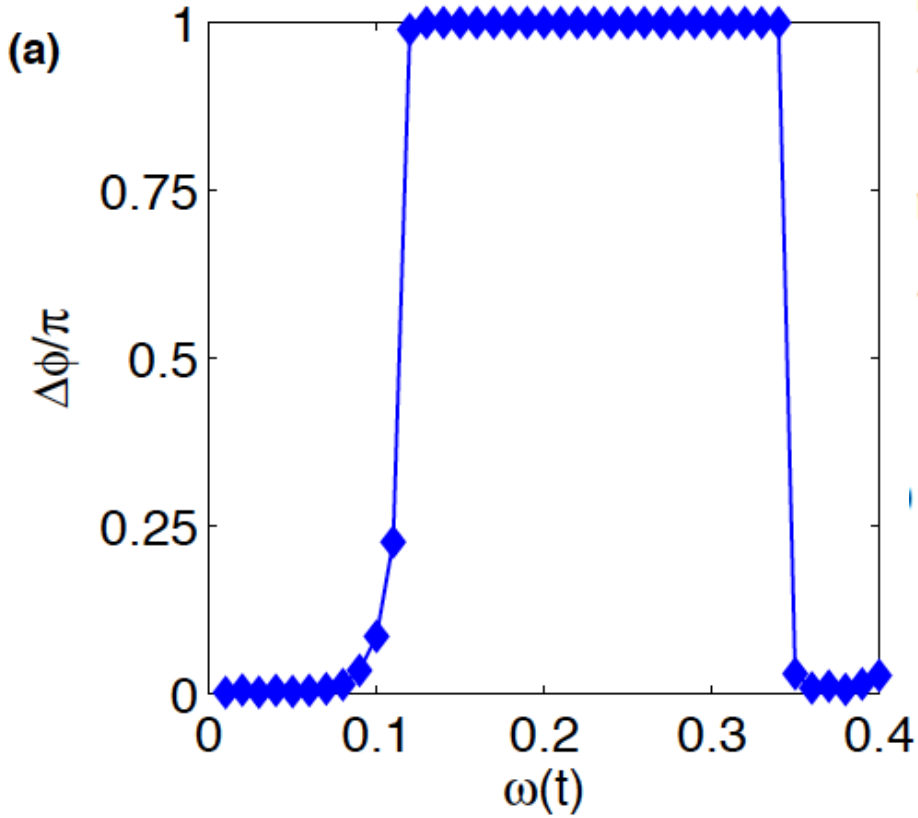


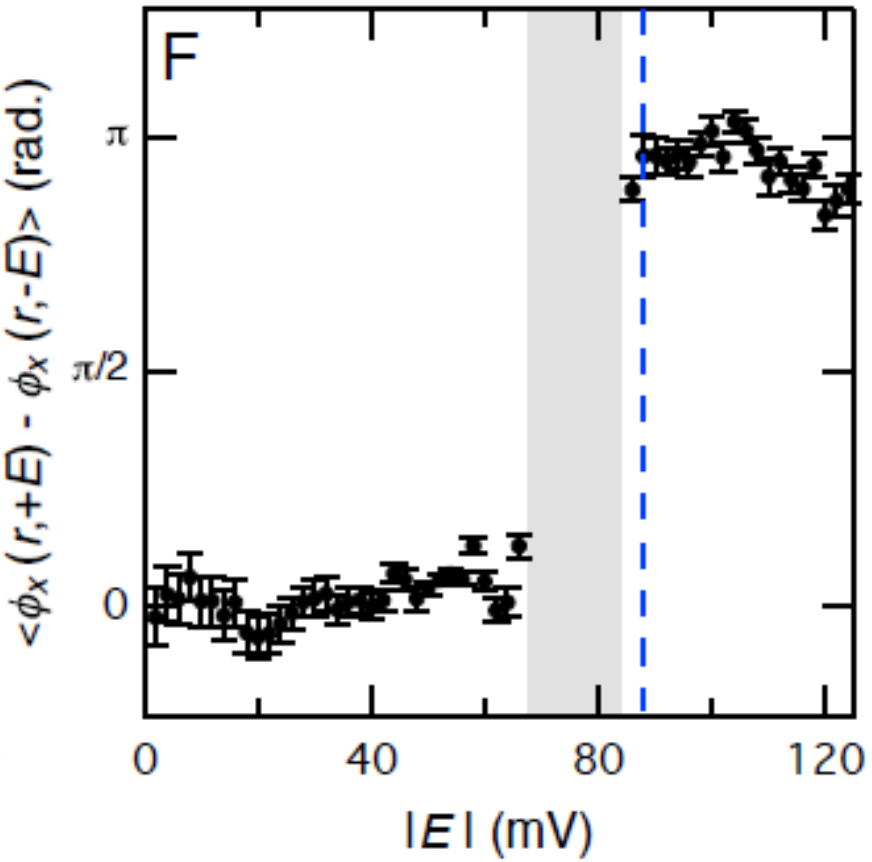
Hamidian et al. Nat. Phys 12, 150 (2016)
Bi-2212, 8% doping

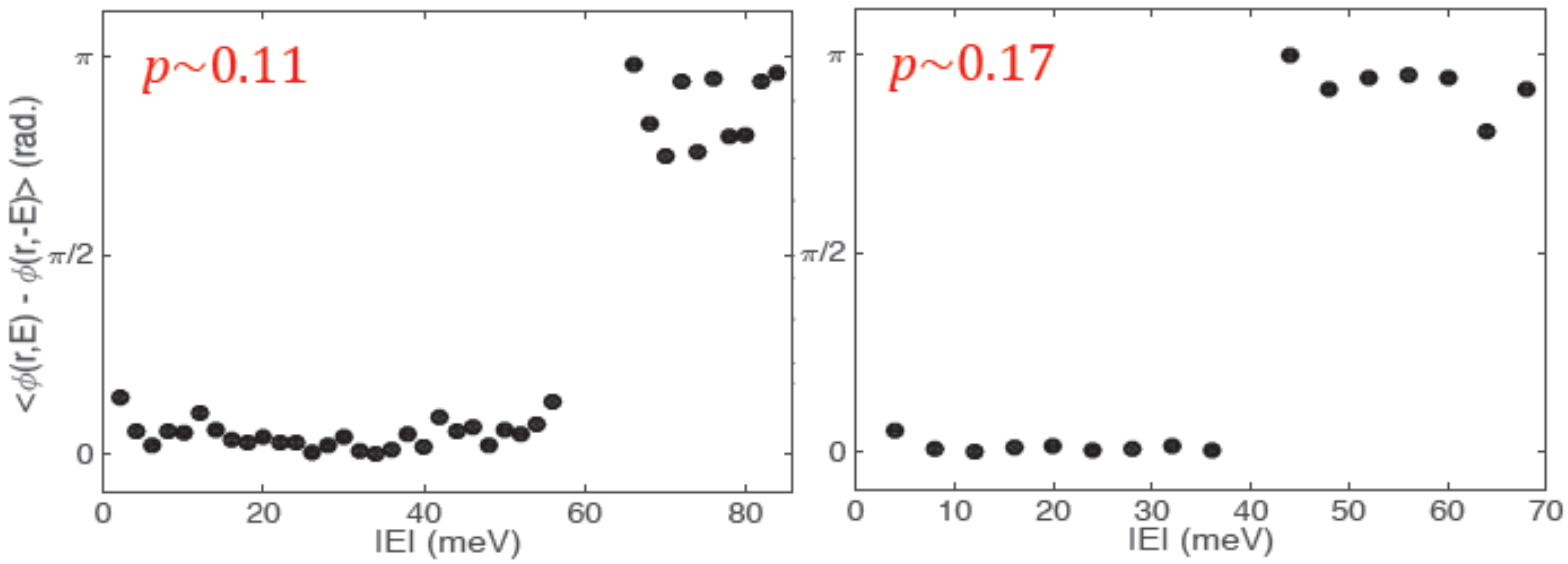


Hole density δ=8%

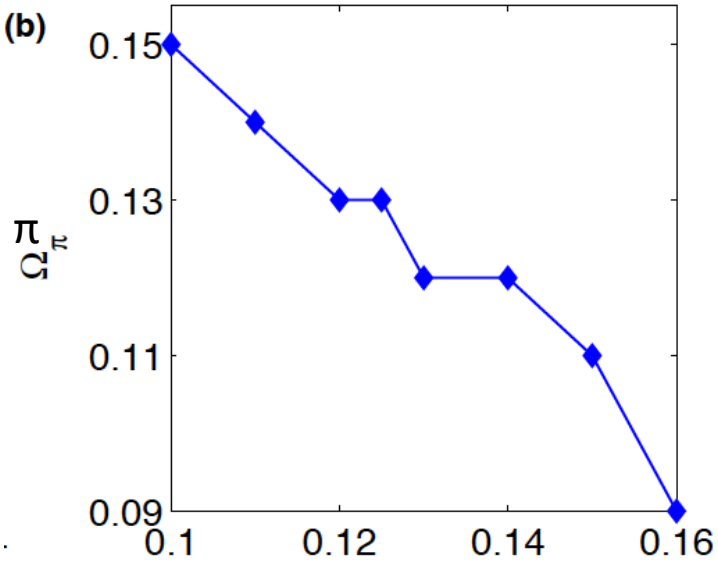
Hole density δ=0.125







Our calc.
Energy with a π jump



Summary:

Based on t-J lattice model, and well known approximations (GW) and renormalized meand field theory,

It is **generic** to have (w or wo Fermi surafce nesting and hot spots)

1. pair-density-wave (PDW) intertwined with CDW and/or spin density wave. Commensurate and incomm. DW with different periods are also likely, depending on many details not included in the t-J model.

2. These states may or may not have global superconductivity.

3. for these SC intertwined–order states -- continuous LDOS and energy dependent intra-unit cell form factors have very good agreement with STS experiments

Thank you for your attention!