

Kinetic energy driven high- T_c superconductivity

Shiping Feng (冯世平)

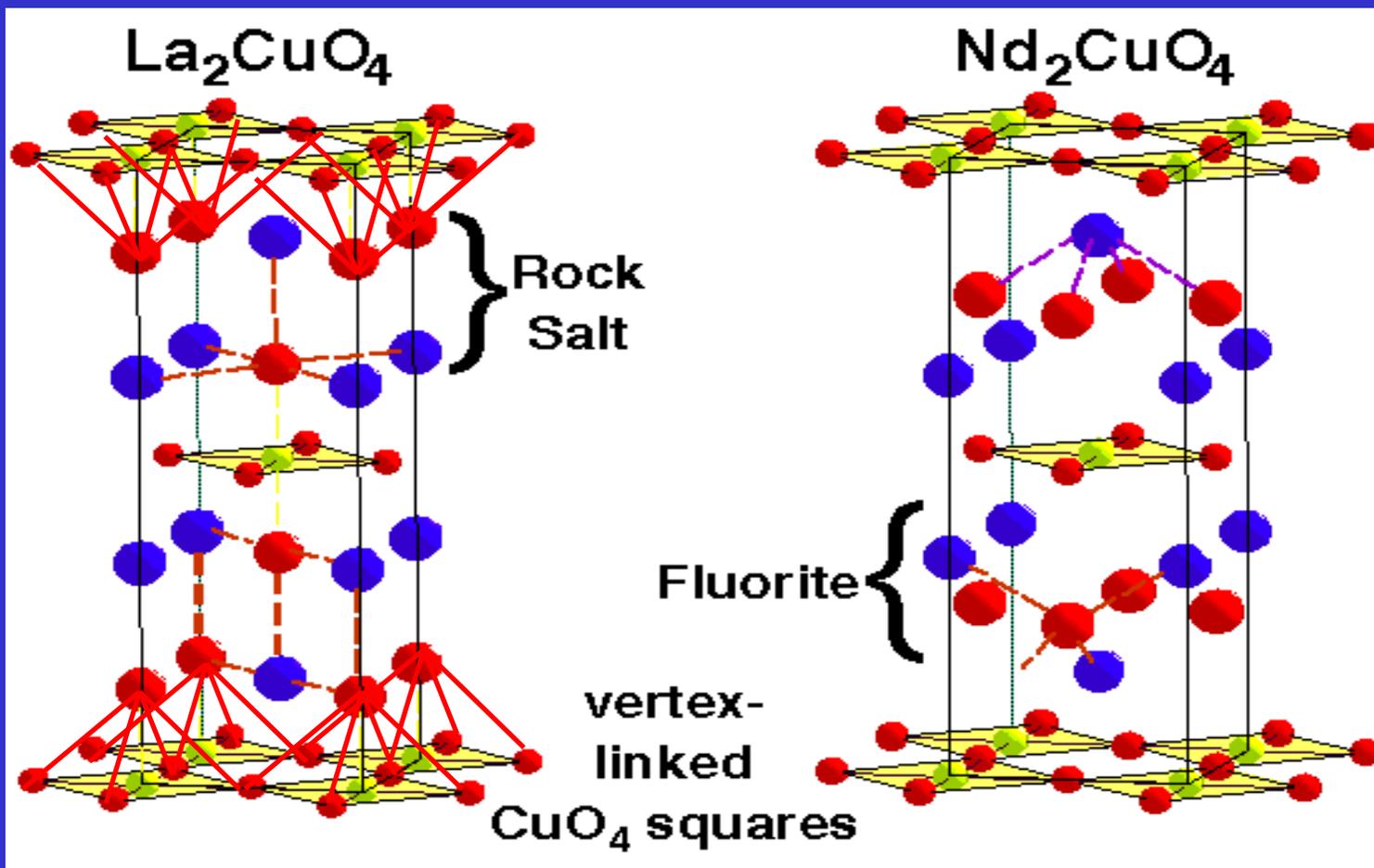
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1. Unconventional superconducting mechanism: evidences from experiments
2. Kinetic energy driven high- T_c superconductivity
3. Doping and temperature dependent electronic structure
4. The impurity effect on the electronic structure
5. Doping and energy dependent incommensurate magnetic scattering and commensurate resonance
6. Conclusion

* Collaborators: Tianxing Ma (马天星), Huaiming Guo (郭还明), Yu Lan (蓝郁), Li Cheng (程力), Zhi Wang (王志), and Jingge Zhang (张景阁)

1. The unconventional superconducting mechanism: evidences from experiments

A. The layered electronic structure of the square lattice of CuO_2 plane



hole-doped case,

electron-doped case

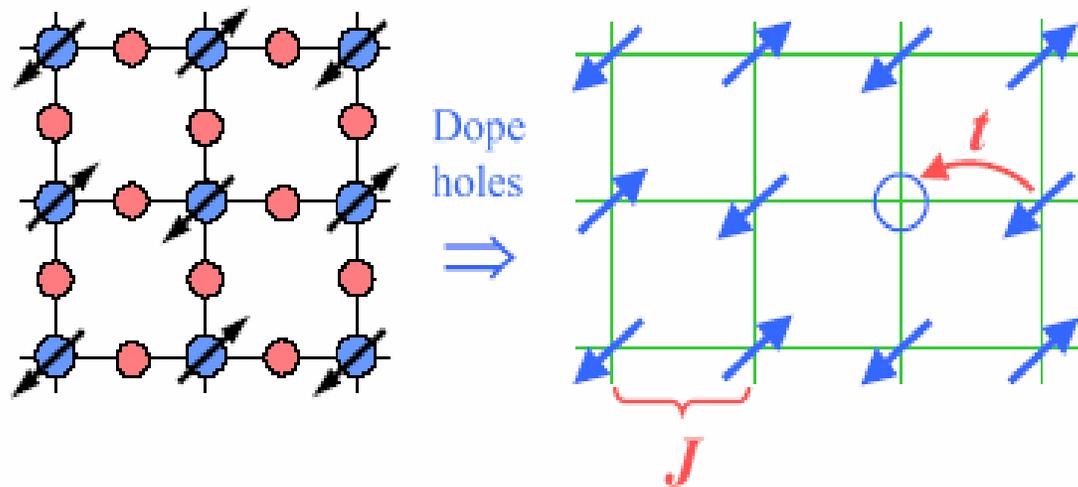
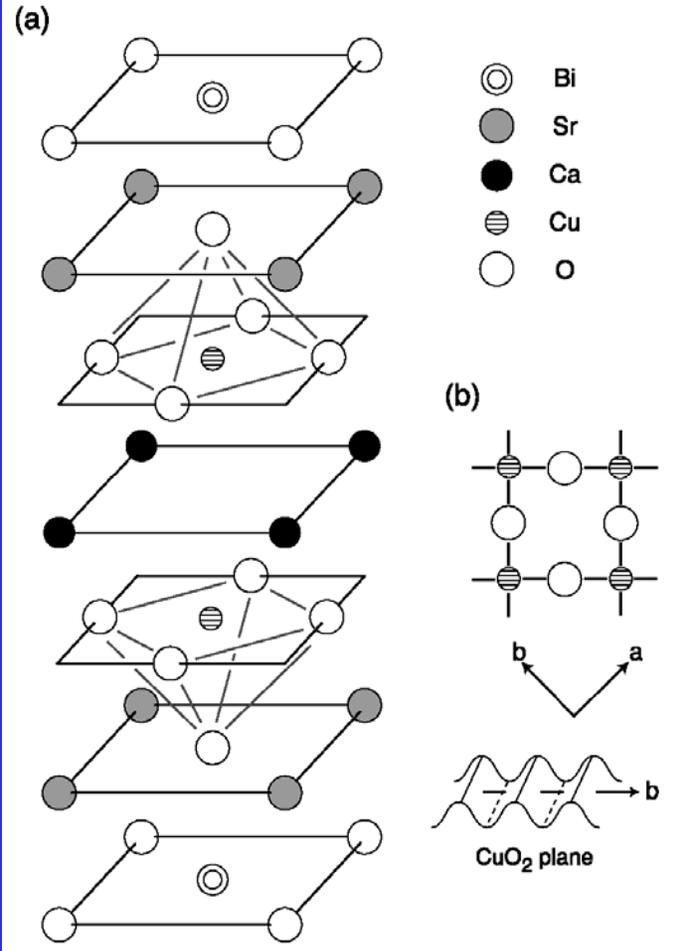
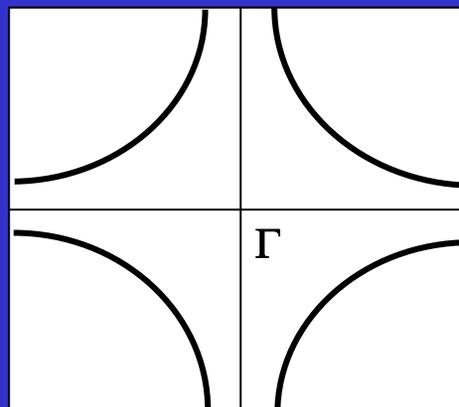


FIG. 1: Structure of the Cu-O layer in high T_c materials. Copper atoms sit on a square lattice with oxygen atoms in between. The electronic structure is simplified to a one band model shown on the right, with electrons hopping with matrix element t . There is an antiferromagnetic exchange J between spins on neighboring sites.

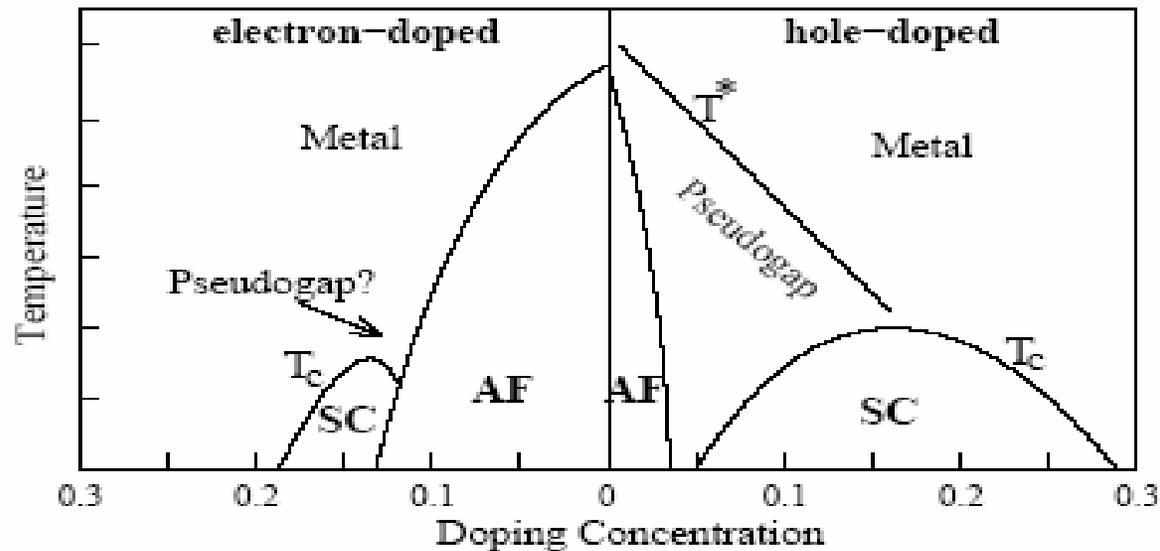
Crystal structure of Bi-2212

- Layered structure
- Strong transport anisotropy



Anderson, 1987

2D Fermi Surface
of cuprates

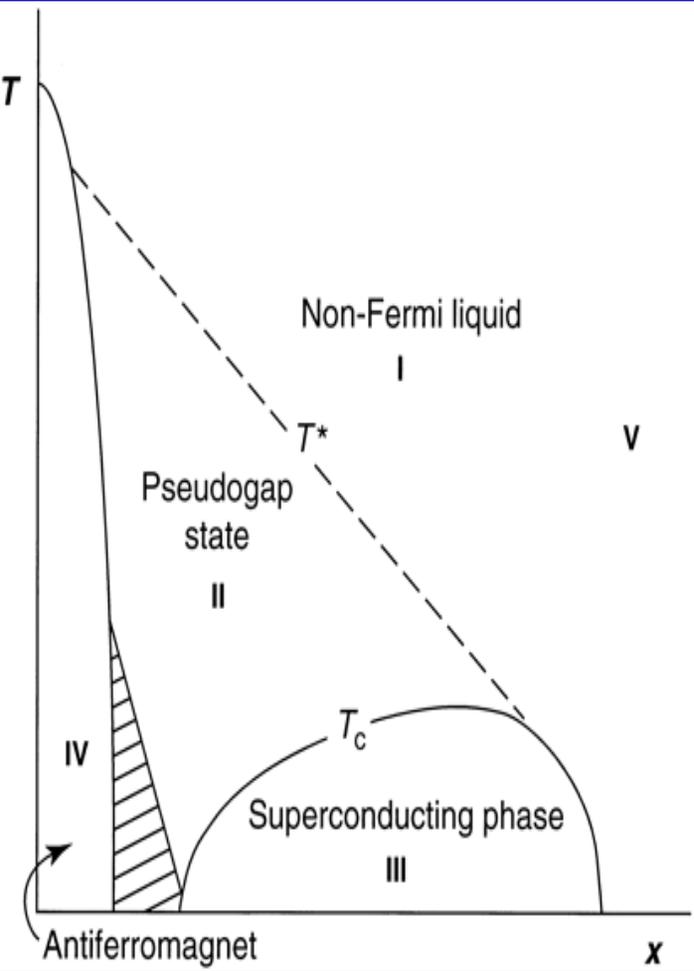


Generic phase diagram for the high temperature superconductors (antiferromagnetic region AF, superconducting phase SC). The temperature below which superconductivity (a pseudogap) is observed is denoted by T_c (T^*). T^* is possibly a crossover temperature, though some experiments (compare

The parent compounds of cuprate superconductors are believed to belong to a class of materials known as Mott insulators with an antiferromagnetic long-range order, then superconductivity emerges when charge carriers, holes or electrons, are doped into these Mott insulators. It has been found that only an approximate symmetry in the phase diagram exists about the zero doping line between the hole doped and electron doped cuprate superconductors, and the significantly different behavior of the hole doped and electron doped cases is observed, reflecting the electron-hole asymmetry.

Phase diagram

Phase diagram ($\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$)



Reflects a competition between kinetic energy and magnetic energy!

II. Lightly doped ($0.02 \leq x \leq 0.06$)

Unusual physics?

I+II. Underdoped regimes ($0.06 \leq x \leq 0.15$) -----

Strange metal (non-Fermi liquid):

Unusual properties { Pseudogap effects
Anomalous spin dynamics
Anomalous charge dynamics
.....

III. Superconducting state: d-wave symmetry

IV. Undoped and very small doped regimes

($0 \leq x \leq 0.02$) --- Mott insulators:

antiferromagnetic long-range order

V. Overdoped regime ($0.15 \leq x \leq 0.25$) ---

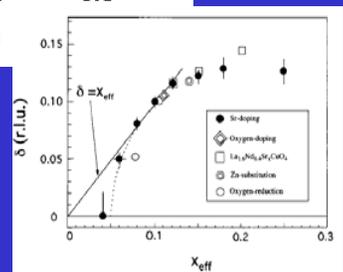
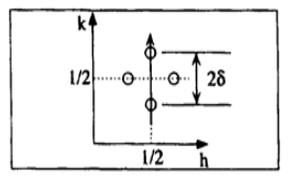
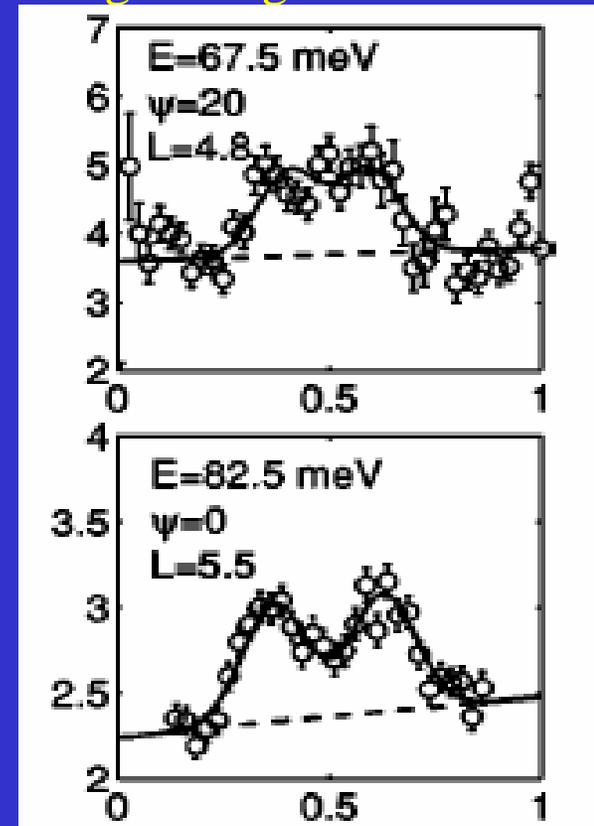
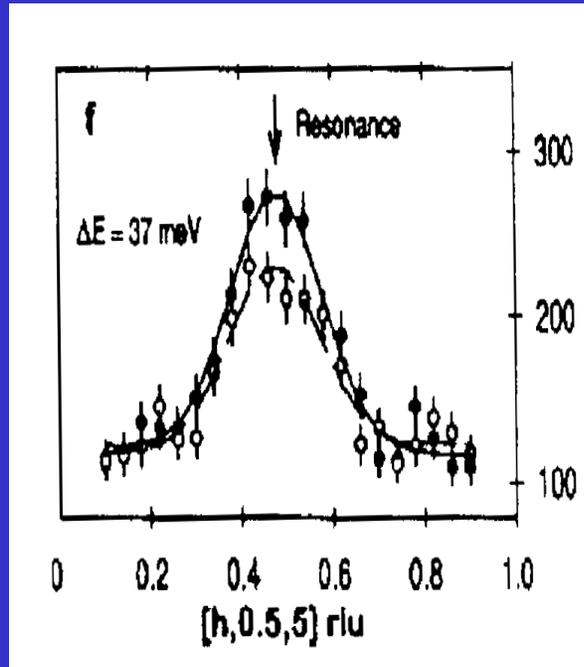
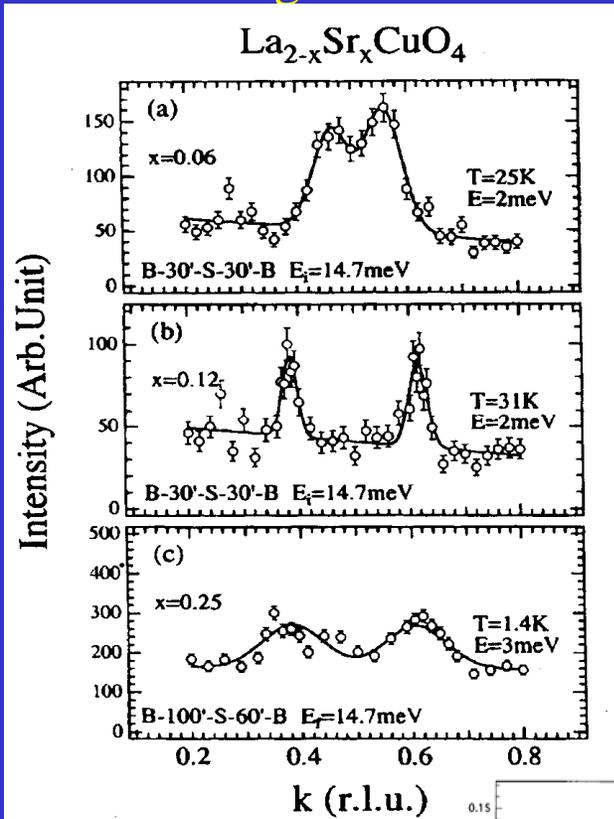
strange metal (non-Fermi liquid)

B. The neutron scattering measurements at superconducting-state

Incommensurate scattering at low energies

Commensurate resonance at intermediate energies

Incommensurate scattering at high energies

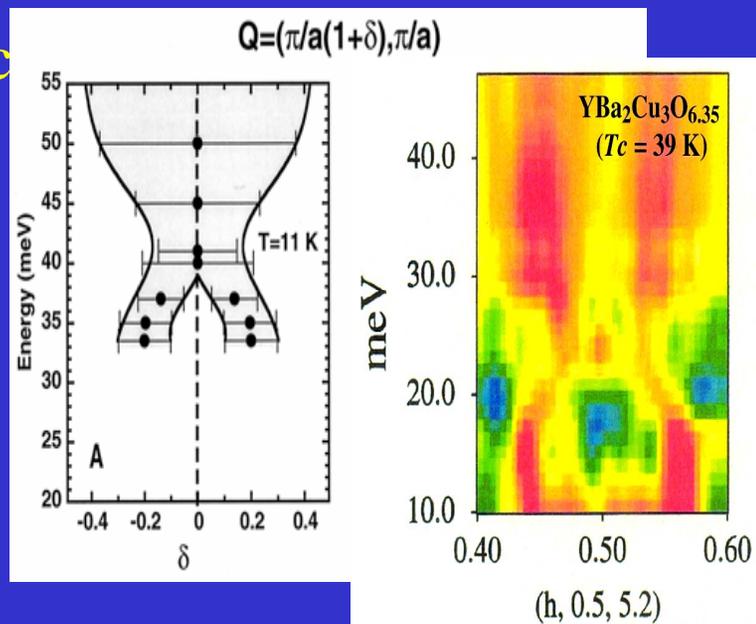
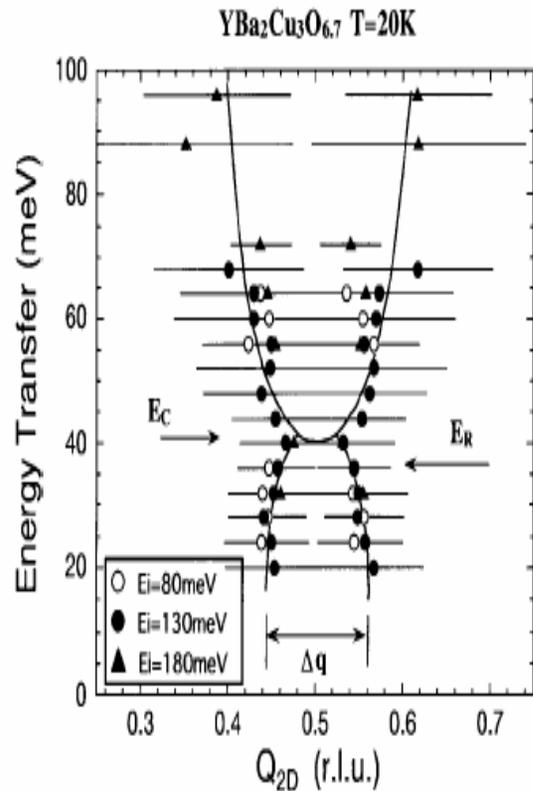


K. Yamada *et al.*, PRB 57, 6165(1998).

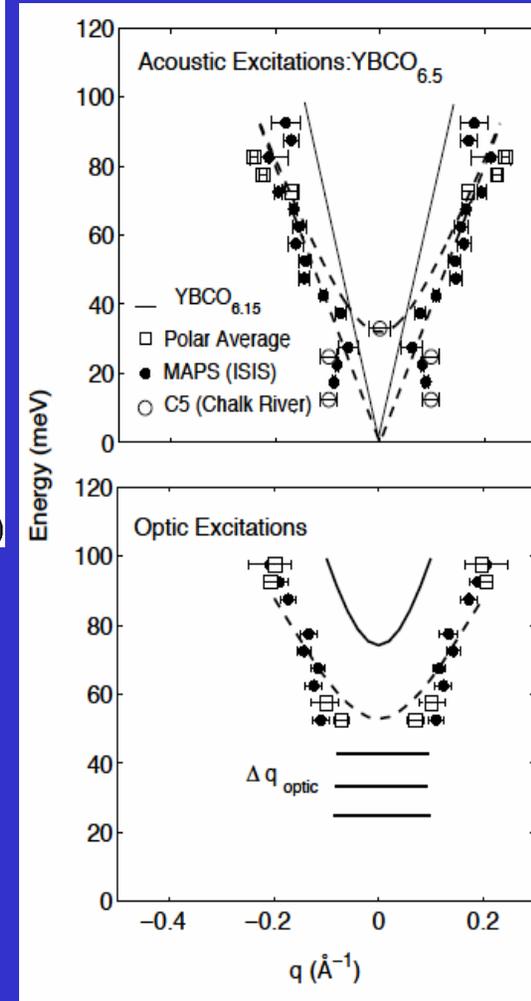
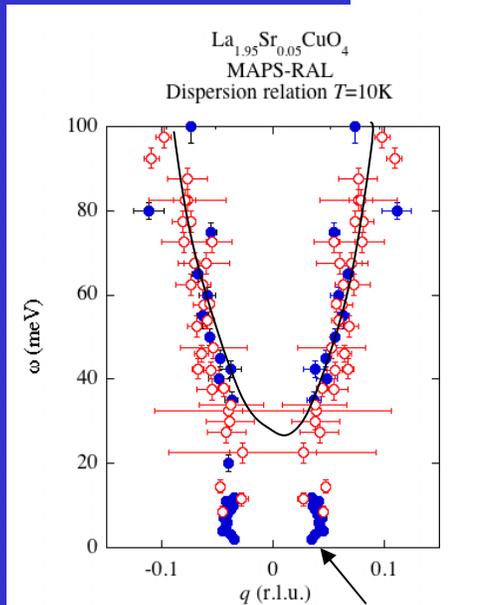
P. Dai *et al.*, PRB 63, 54525 (2001); P. Bourges *et al.*, Science 288, 1234 (2000)

C. Stock *et al.*, PRB 71, 24522 (2005); S.M. Haden *et al.*, Science 429, 531 (2004).

Dispersion of magnetic scattering peaks

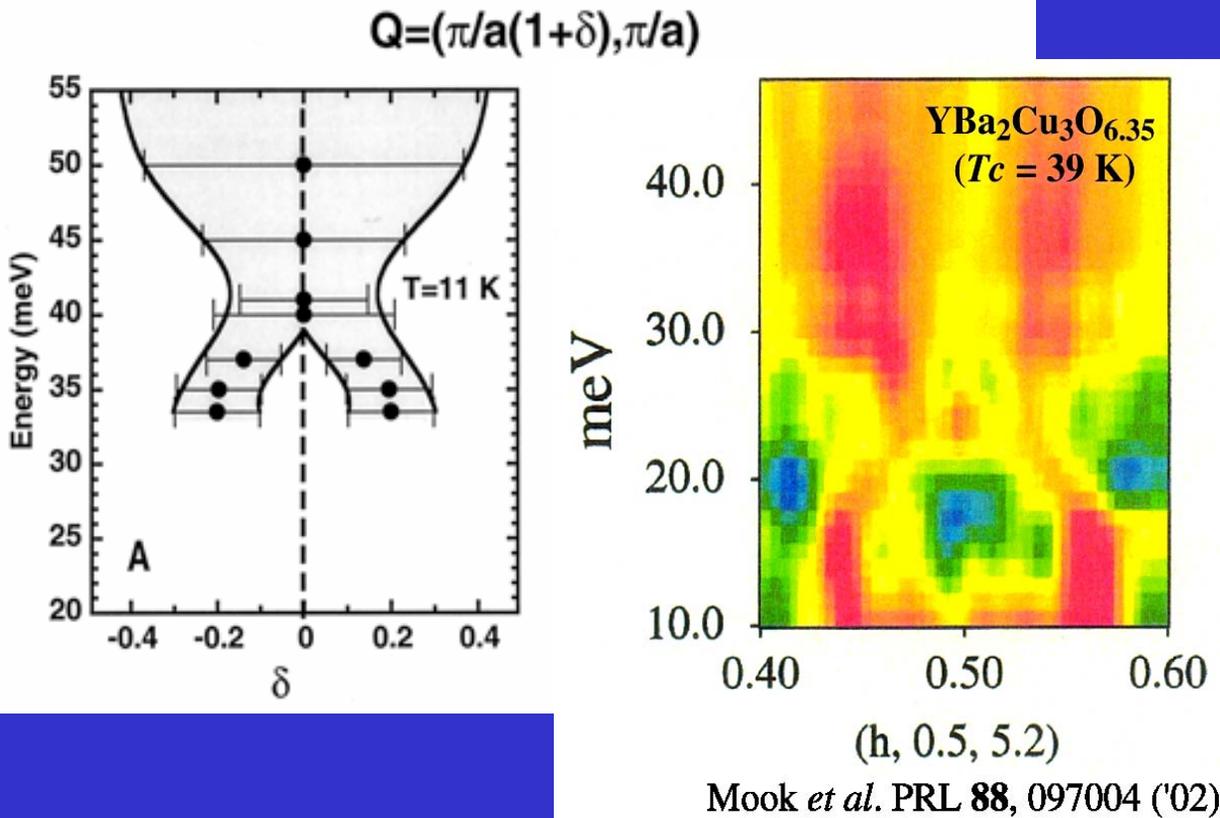


et al. PRL 88, 097004 ('02)

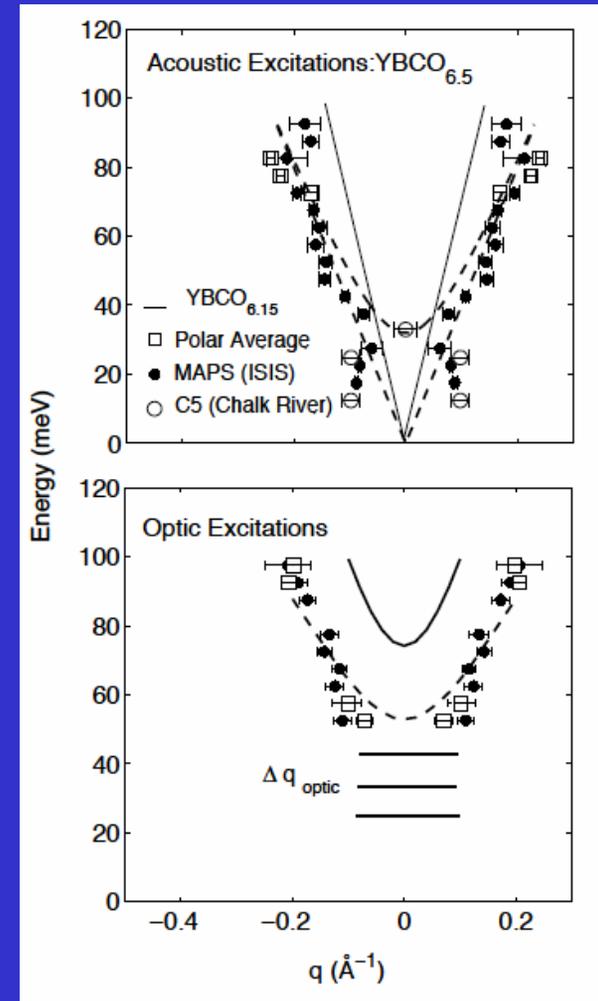


M. Arai *et al.*, PRL 83, 608 (1999); C. Stock *et al.*, PRB 71, 24522 (2005); S.M. Haden *et al.*, Science 429, 531 (2004).

sand glass-type dispersion is commonly observed in YBCO



P. Bourdges *et al.* Science
also M. Arai *et al.* PRL

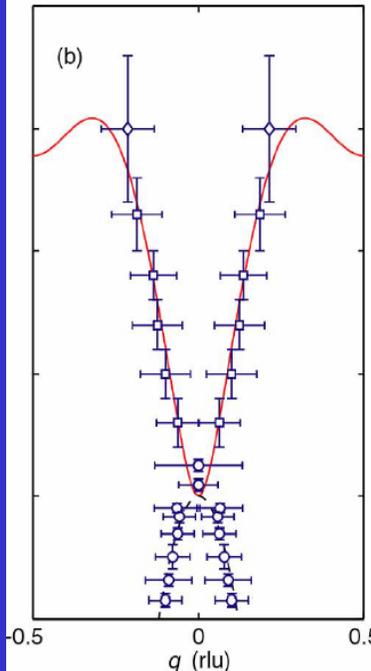
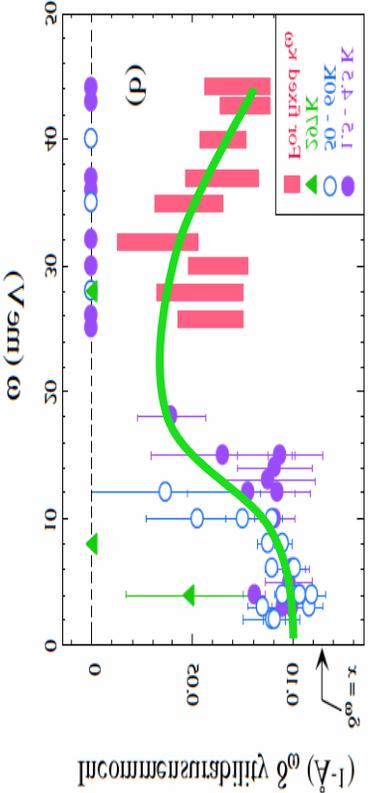
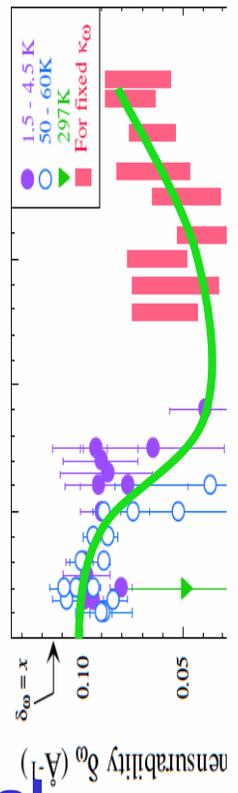
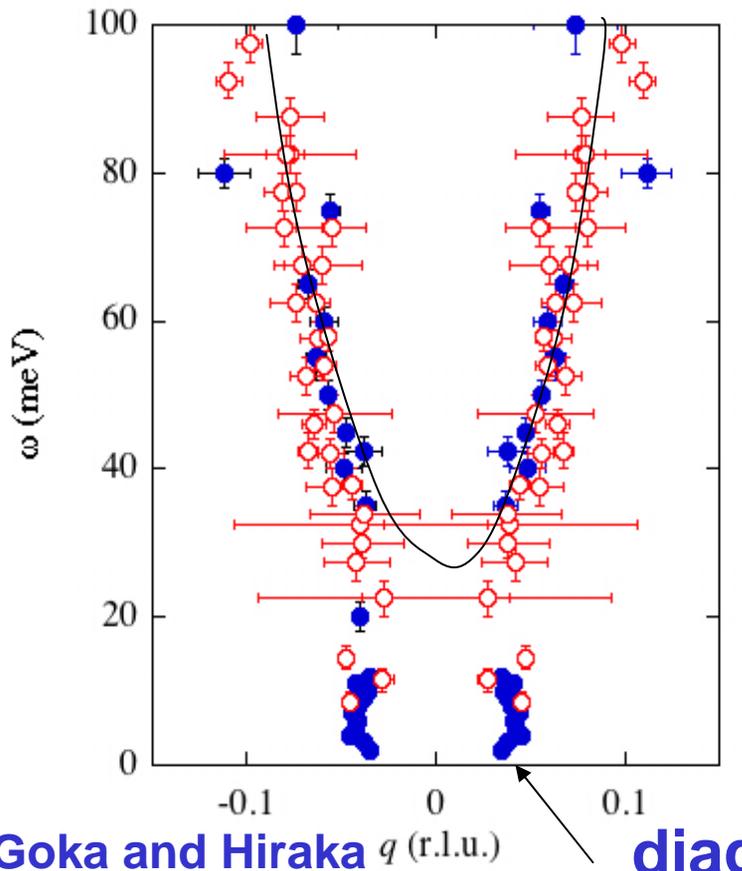


C. Stock *et al.*, PRB **71**,
24522 (2005)

sand glass-type magnetic dispersion is also suggested in LSCO

LSCO(x=0.07)

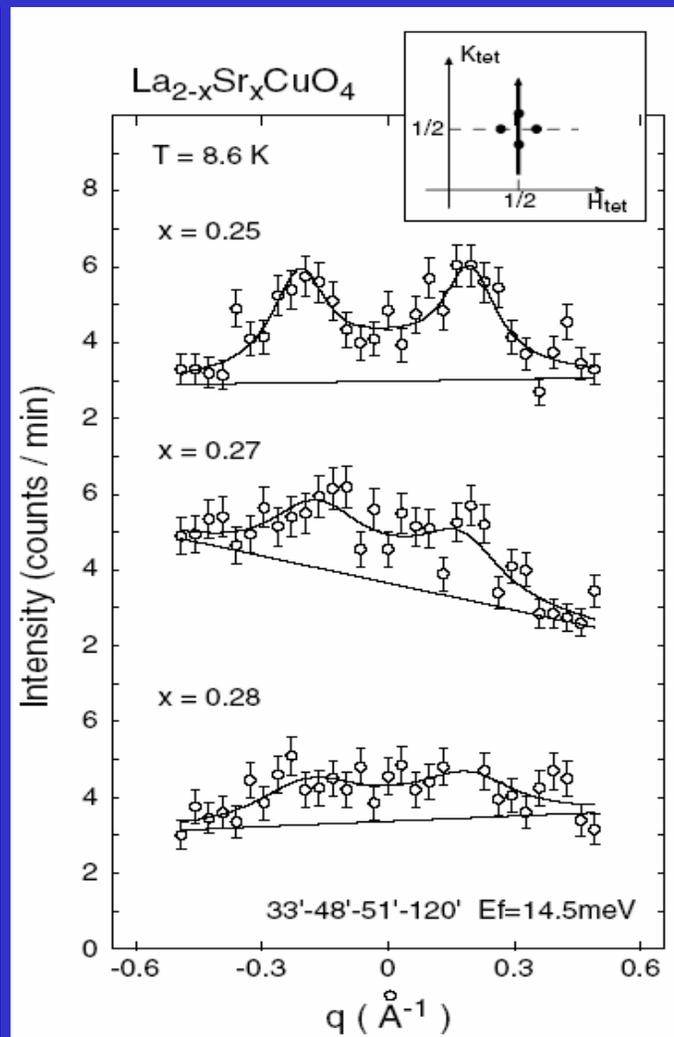
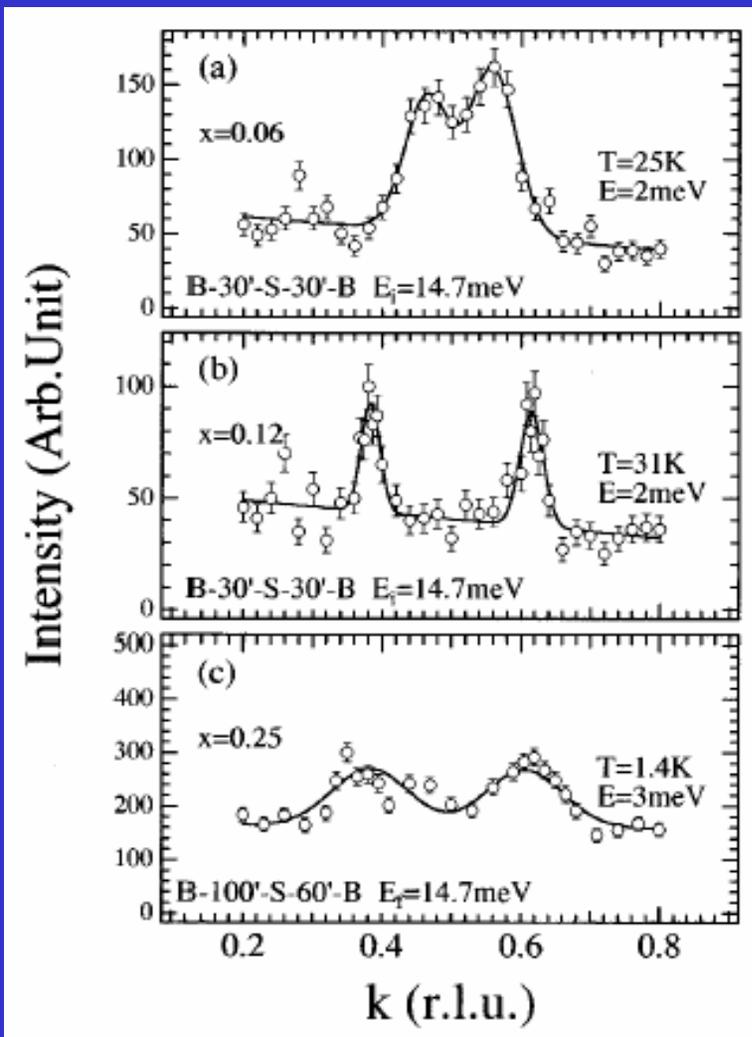
La_{1.95}Sr_{0.05}CuO₄
 MAPS-RAL
 Dispersion relation T=10K



Goka and Hiraka *q* (r.l.u.) diagonal

Hiraka *et al.*

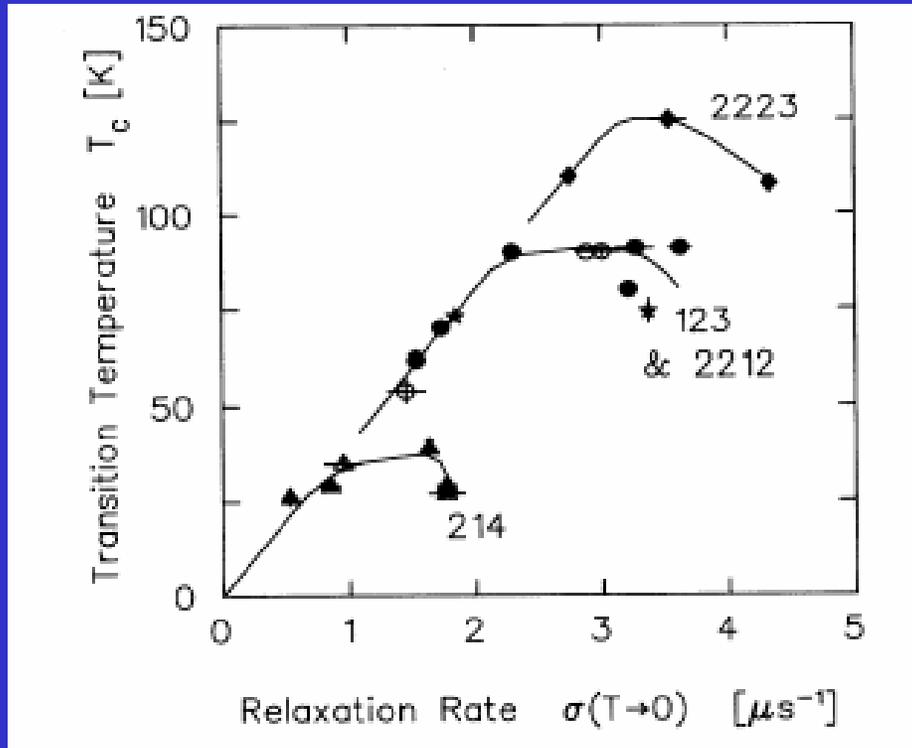
The spin fluctuations always in the superconducting phase



K. Yamada *et al.*,
PRB 57, 6165
(1998);
S. Wakimoto *et al.*,
PRL 92, 217004
(2004)

- (1) interplay between magnetic fluctuations and high- T_c superconductivity, i.e., a clear link between the superconducting mechanism and magnetic excitations
- (2) universal magnetic framework of high- T_c superconducting cuprates

C. Gossamer superconductors

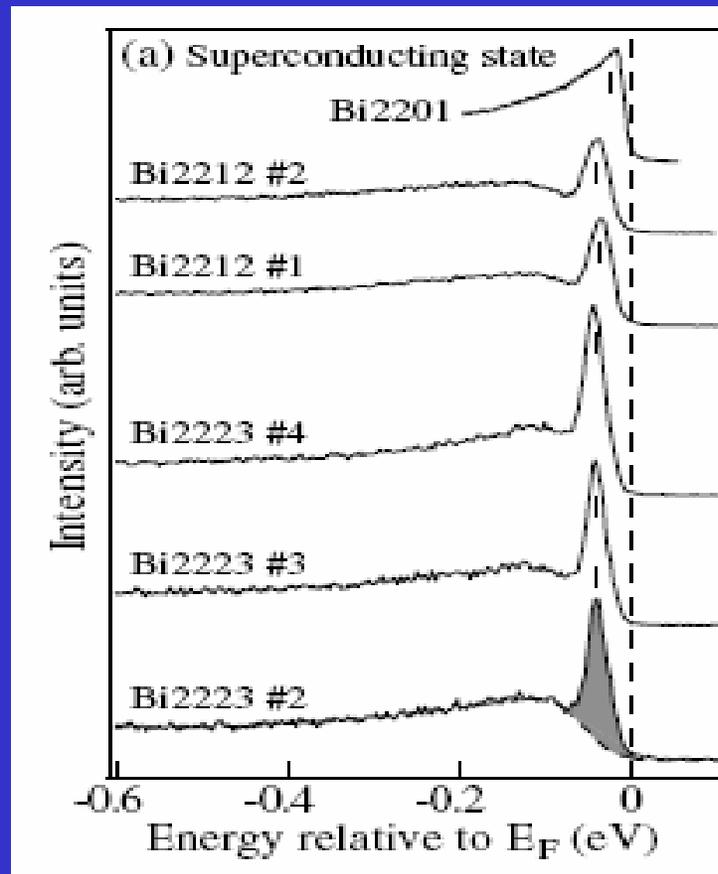
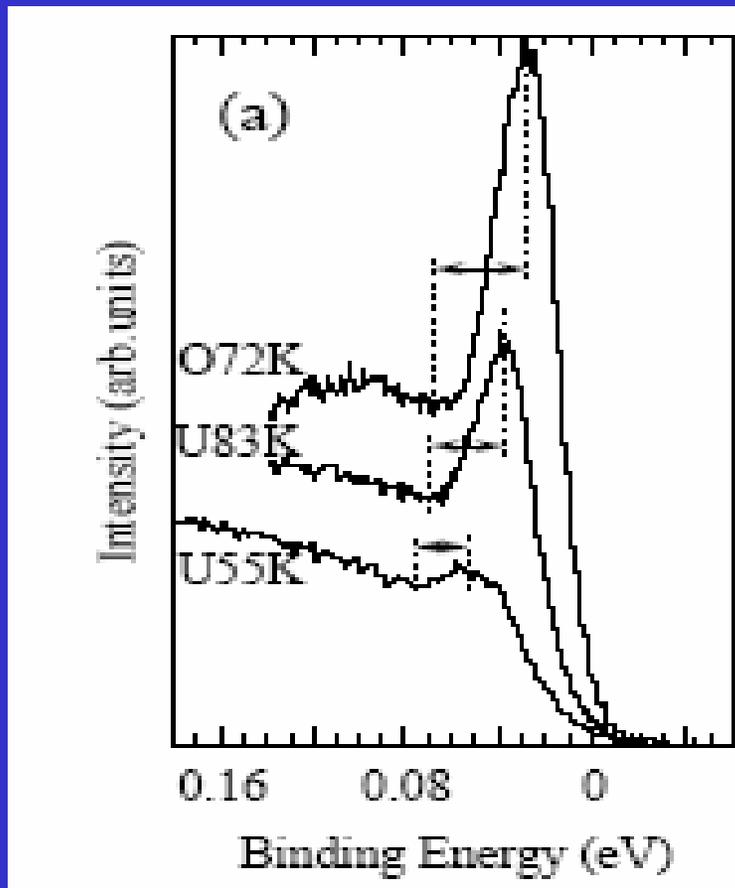


Y.J. Uemura *et al.*, PRL62, 2317 (1989).

i.e., T_c is proportional to the doping concentration in the underdoped regime (Uemura relation), $T_c \propto x$

This is also an evidence that superconductivity is driven by the kinetic energy, since in the doped Mott insulator, the kinetic energy is proportional to the doping concentration.

D. The angle-resolved photoemission spectroscopy measurements



J. Campuzano *et al.*, PRL83, 3709 (1999)

D.L. Feng *et al.*, PRL 88, 107001 (2002)

- There is tendency towards to the Fermi energy with increasing doping for the position of the sharp quasiparticle peak;
- Bogoliubov-quasiparticle nature of the sharp superconducting quasiparticle peak;
- The charge carriers doped into the parent Mott insulators first enter into around the $[\pi,0]$ point.

Temperature dependence of the electron spectrum

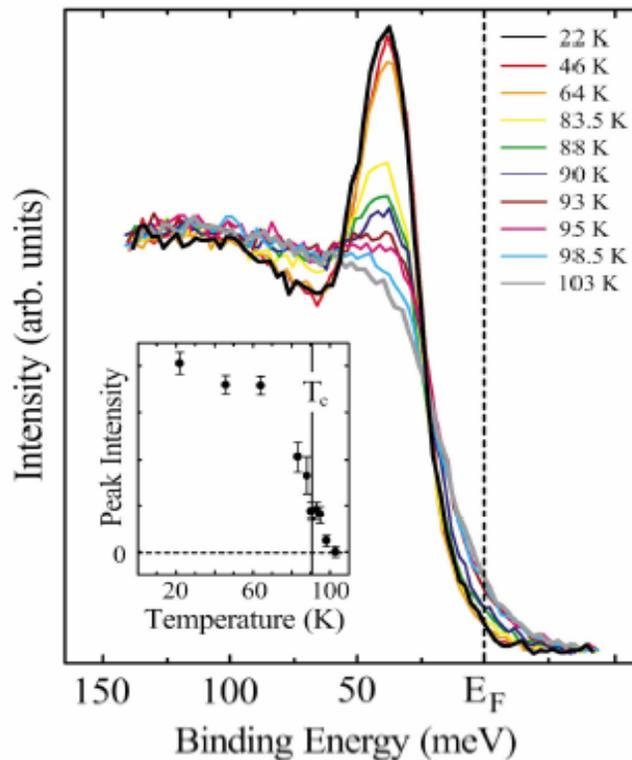
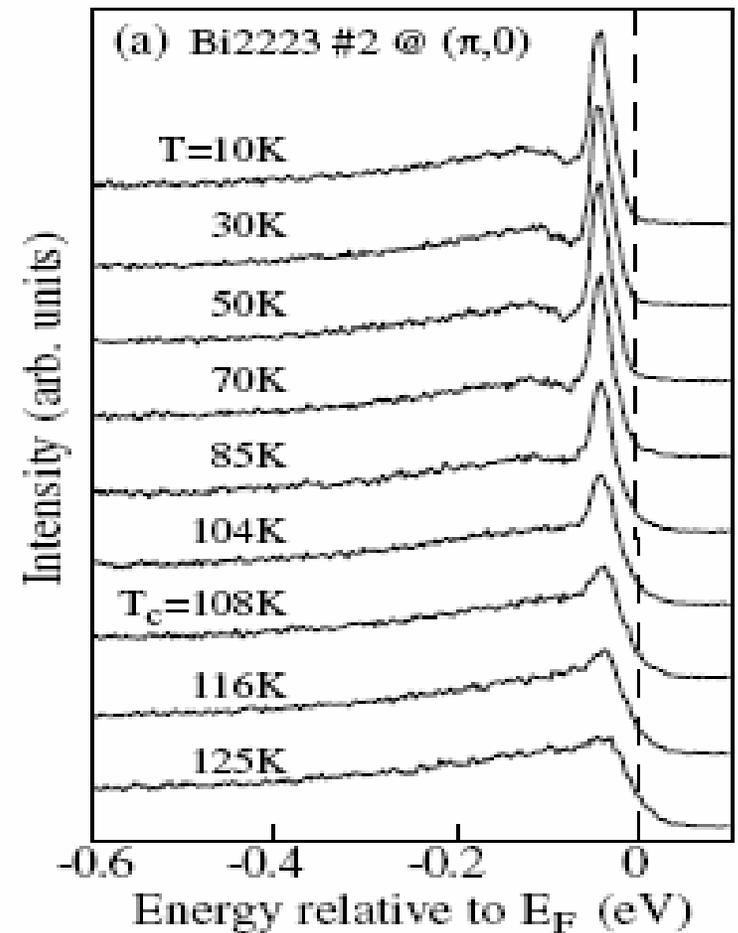


FIG. 51. Temperature-dependent photoemission spectra from optimally doped Bi2212 ($T_c=91$ K), angle integrated over a narrow cut at $(\pi,0)$. Inset: superconducting-peak intensity vs temperature. After Fedorov *et al.*, 1999 (Color).

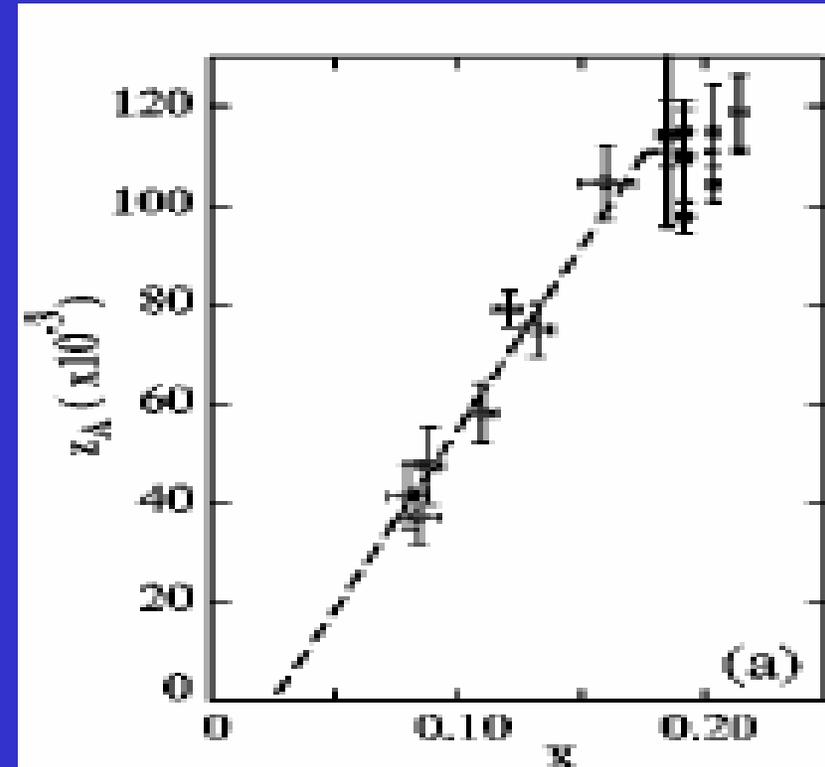
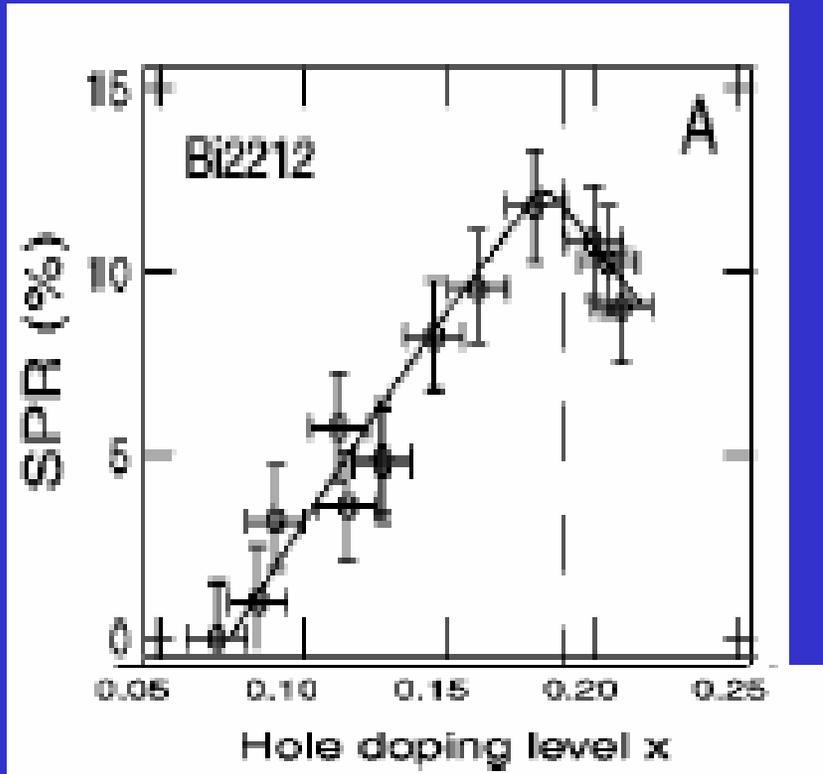


Fedorov *et al.*, PRL 82, 2179 (1999)

D.L. Feng *et al.*, PRL 88, 107001 (2002)

The weight of the peak is decreases with increasing temperature.

The doping dependent superconducting quasiparticle coherent weight



D. Feng *et al.*, *Science* 289, 277 (2000);
He *et al.*, *PRB* 69, 220502 (2004)

Ding *et al.*, *PRL* 87, 227001 (2001)

The superconducting state is controlled by both superconducting gap function and quasiparticle coherent weight.

The peak-dip-hump structure

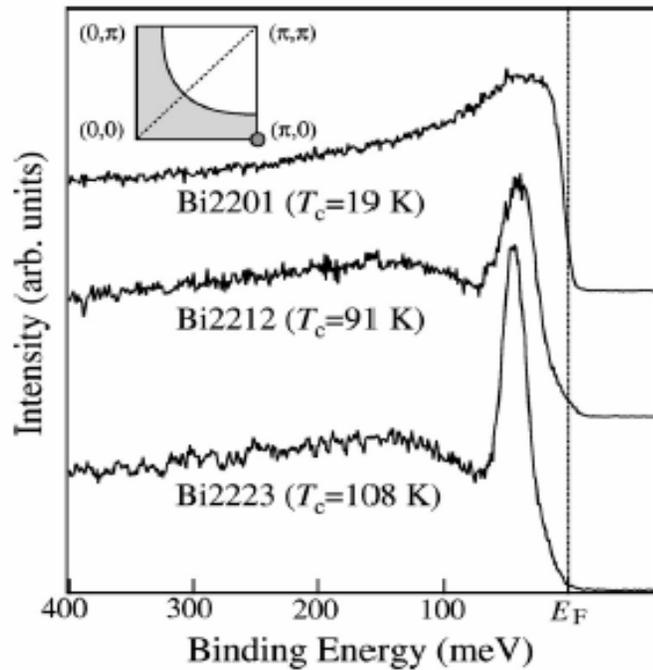


FIG. 57. Superconducting state $(\pi,0)$ ARPES spectra from Bi2201 ($T_c=19$ K), Bi2212 ($T_c=91$ K), and Bi2223 ($T_c=108$ K). The data were taken with 21.2-eV photons at 13.5 K for Bi2201, and 40 K for both Bi2212 and Bi2223. From Sato, Matsui, *et al.*, 2002.

This peak-dip-hump structure was only observed from ARPES on the bilayer and trilayer cuprate superconductors, and may be related to the bilayer band splitting effects [see, e.g., Kordyuk *et al.*, PRB 67, 64504 (2003); PRL89, 77003 (2002)].

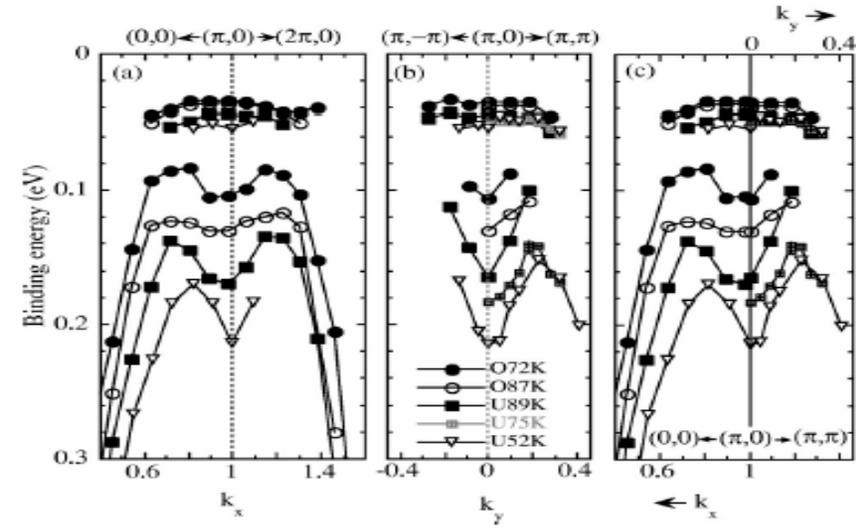
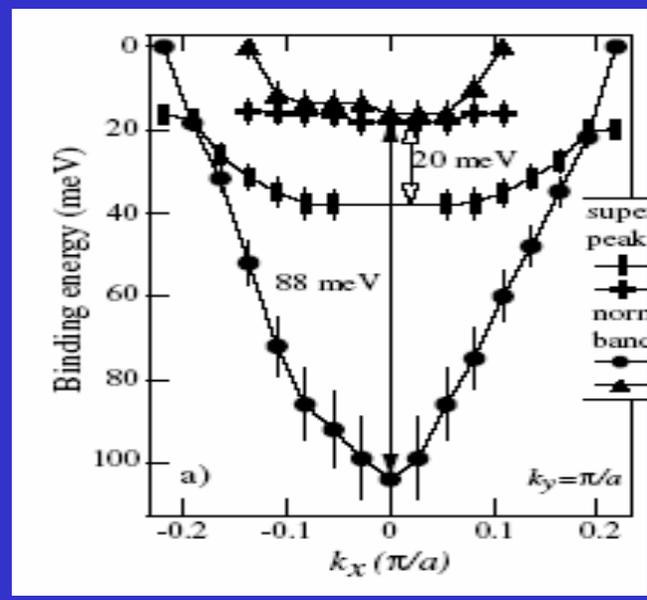


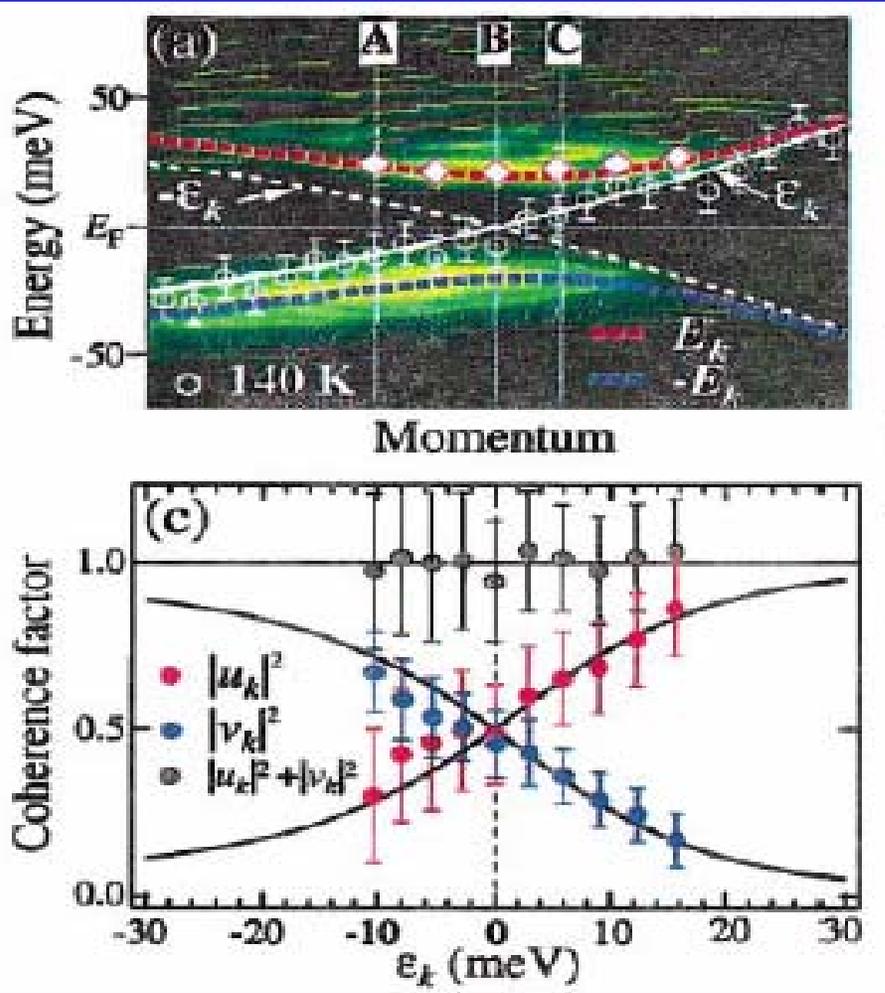
FIG. 54. Peak and hump dispersion in the superconducting state of Bi2212, for several dopings from underdoped to overdoped (bottom to top). From Campuzano *et al.*, 1999.

Campuzano *et al.* (1999)



D.L. Feng *et al.* (2001)

BCS-Bogoliubov quasiparticles



BCS coherent factors

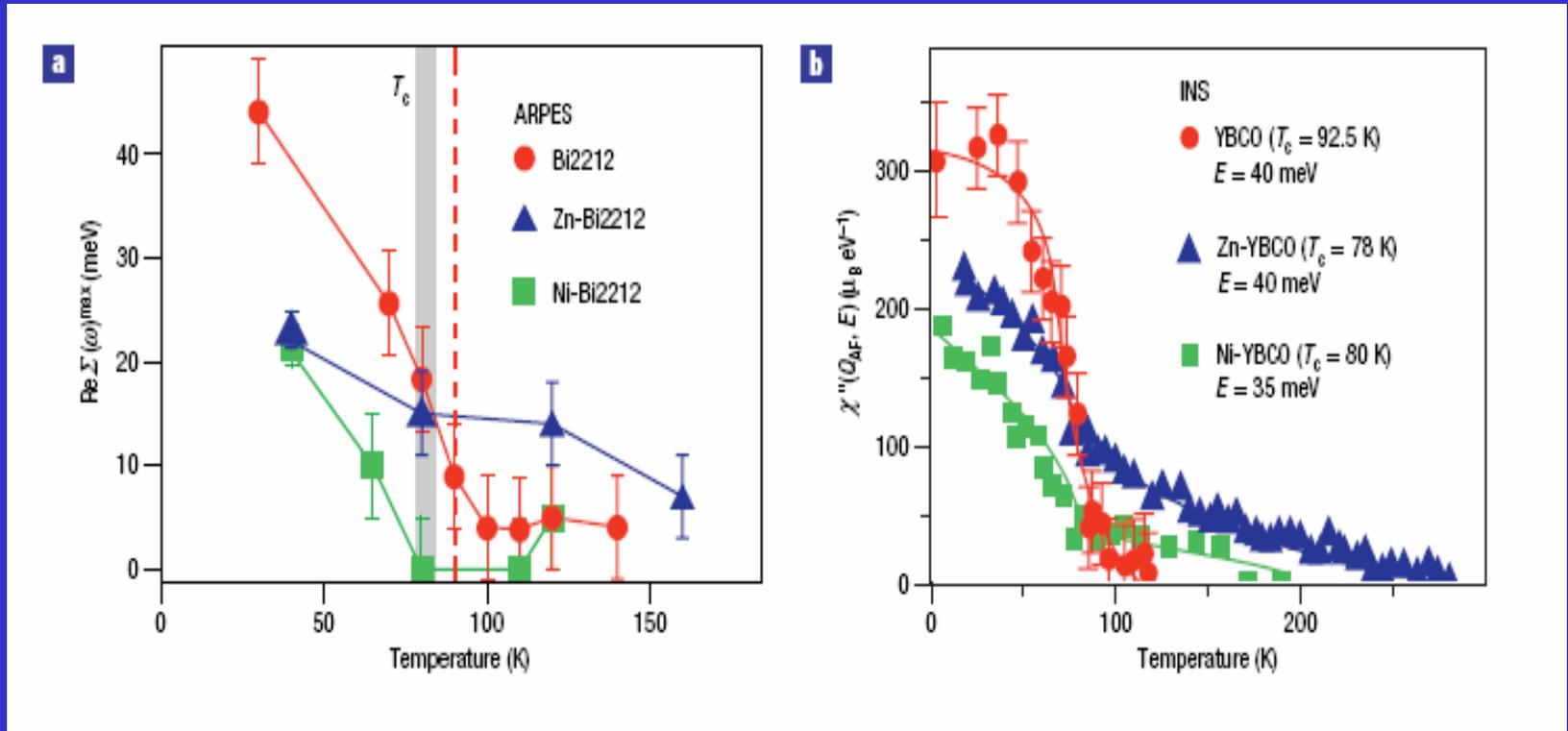
$$U_k^2 = \frac{1}{2} \left(1 + \frac{\epsilon_k}{E_k} \right),$$

$$V_k^2 = \frac{1}{2} \left(1 - \frac{\epsilon_k}{E_k} \right),$$

Although the superconducting pairing mechanism is beyond the conventional electron-phonon mechanism, the superconducting state is the conventional BCS-like.

H. Matsui *et al.*, Phys. Rev. Lett. 90, 217002 (2003).

The 'isotope' effect for magnetically mediated superconductors



Terashima *et al.*, Nature Phys. 2, 27 (2006)

This remarkable similarity between the angle-resolved photoemission spectroscopy and neutron scattering measurements demonstrates that the kink in the antinodal region is produced by coupling between electrons and spin fluctuations

A comparison of some physical properties between the cuprate superconductors and conventional superconductors

The cuprate superconductors

A. Symmetry of the Cooper pair d-wave

$$\Delta_k = \Delta[\cos k_x - \cos k_y]$$

See, e.g., C.C. Tsuei *et al.*,
Rev. Mod. Phys. 72, 969
(2000); P. Chaudhari *et al.*,
PRL72, 1084 (1994).

The conventional superconductors

A. Symmetry of the Cooper pair uniform s-wave

$$\Delta_k = \Delta$$

J. Bardeen, L.N. Cooper, and
J.R. Schrieffer, Phys. Rev. 108,
1175 (1957); J.R. Schrieffer,
Theory of Superconductivity
(Addison-Wesley, 1988).

The cuprate superconductors

B. Short-range pairing force, i.e., the gap function and pairing force have a range of one or few lattice spacings.

Z.X. Shen *et al.*, PRL70, 1553 (1993); H. Ding *et al.*, PRB54, R9678 (1996).

C. Coexistence of the superconducting state and antiferromagnetic short-range correlation

See, e.g., M.A. Kastner *et al.*, Rev. Mod. Phys. 70, 897 (1998)

The conventional superconductors

B. Long-range pairing force

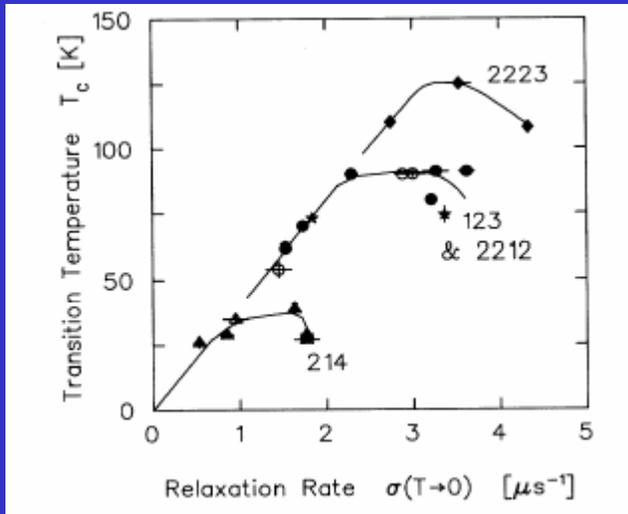
J. Bardeen, L.N. Cooper, and J.R. Schrieffer, Phys. Rev. 108, 1175 (1957).

C. Without antiferromagnetic fluctuation in the superconducting state

J.R. Schrieffer, Theory of Superconductivity (Addison-Wesley, 1988).

The cuprate superconductors

D. The gossamer superconductors



Y.J. Uemura *et al.*, PRL62, 2317 (1989).

i.e., T_c is proportional to doping concentration in the underdoped regime (Uemura relation)

$$T_c \propto x$$

The conventional superconductors

D. T_c is independence of doping

J. Bardeen, L.N. Cooper, and J.R. Schrieffer, Phys. Rev. 108, 1175 (1957).

The cuprate superconductors

E. Normal-state: Non-Fermi liquid

Almost all normal-state properties are unusual!

See, e.g., M.A. Kastner *et al.*, *Rev. Mod. Phys.* 70, 897 (1998); P.W. Anderson, *The Theory of Superconductivity in the High T_c Cuprates* (Princeton, New Jersey, 1997)

The conventional superconductors

E. Normal-state: Fermi liquid

The normal-state properties show Fermi liquid behaviors

J.R. Schrieffer, *Theory of Superconductivity* (Addison-Wesley, 1988).

The cuprate superconductors

F. The superconducting mechanism is based on non-Fermi liquid

Charge carriers interaction via the magnetic medium?

The kinetic energy term in the higher powers of doping causes superconductivity?

P.W. Anderson,
PRL67, 2092 (1991);
Science 288,480 (2000);
cond-mat/0108522

The conventional superconductors

F. The superconducting mechanism is based on Fermi liquid

Conventional electron-phonons mechanism: charge carriers interact by exchanging phonons, this interaction lead to a net attractive force between charge carriers, then the system can lower its potential energy by forming electron Cooper pairs!

J. Bardeen, L.N. Cooper, and J.R. Schrieffer,
Phys. Rev. 108, 1175 (1957); G. Chester,
Phys. Rev. 103, 1693 (1965)

The cuprate superconductors

G. The superconducting state is controlled by both gap parameter and quasiparticle coherence

$$\Delta_k = \Delta(\cos k_x - \cos k_y)$$

$$\frac{1}{Z_F(k, \omega)} = 1 - \Sigma_{10}(k, \omega)$$

H. Ding *et al.*, PRL 87, 227001 (2001); R.H. He *et al.*, PRB 69, 220502 (2004).

The conventional superconductors

G. The superconducting state only is controlled by gap parameter

$$\Delta_k = \Delta$$

J. Bardeen, L.N. Cooper, and J.R. Schrieffer, Phys. Rev. 108, 1175 (1957).

2. Kinetic energy driven high- T_c superconductivity

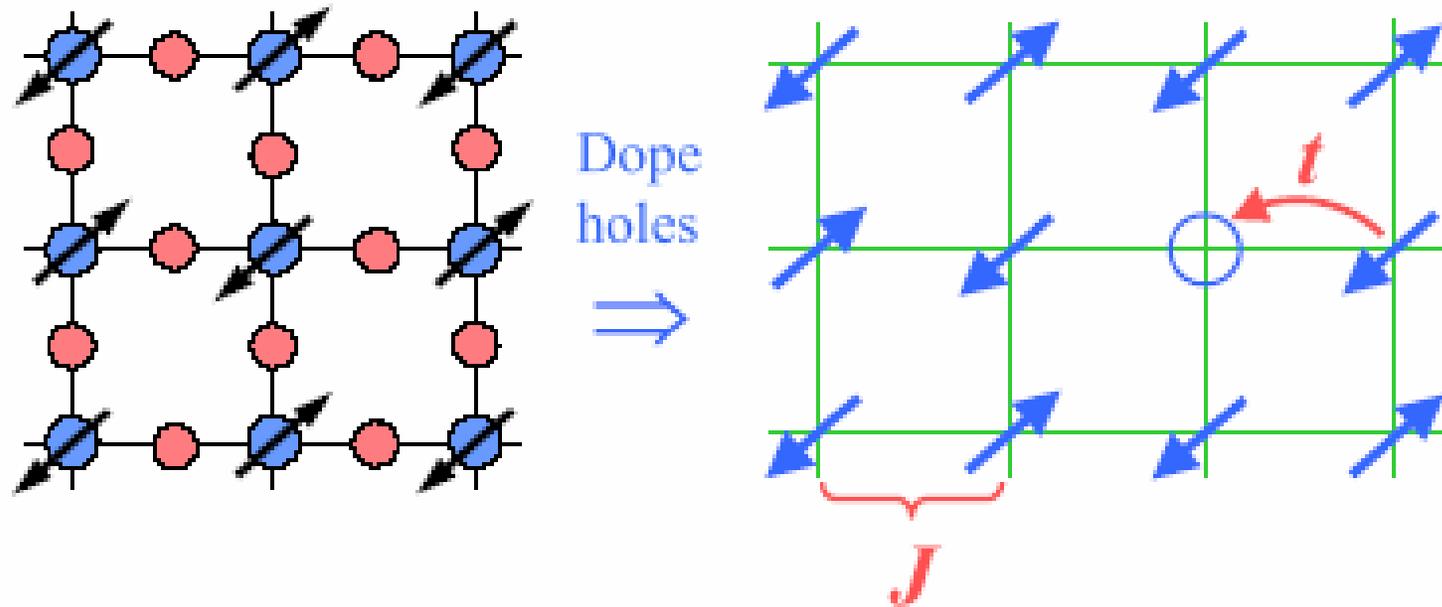


FIG. 1: Structure of the Cu-O layer in high T_c materials. Copper atoms sit on a square lattice with oxygen atoms in between. The electronic structure is simplified to a one band model shown on the right, with electrons hopping with matrix element t . There is an antiferromagnetic exchange J between spins on neighboring sites.

A. t-J model: since cuprate superconductors are doped antiferromagnetic systems, the antiferromagnetic correlation may dominate physical property of systems. It has been argued that the most helpful for discussions of physical properties of doped cuprates is large-U Hubbard model [Anderson, 1987],

$$H = -t \sum_{i\eta\sigma} C_{i\sigma}^+ C_{i+\eta\sigma} + \mu \sum_{i\sigma} C_{i\sigma}^+ C_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad n_{i\sigma} = C_{i\sigma}^+ C_{i\sigma}$$

↓
↓

kinetic energy on-site Coulomb interaction

with $\hat{\eta} = \pm\hat{x}, \pm\hat{y}$. The strong electron correlation in Hubbard model manifests itself by the strong on-site interaction ($U \rightarrow \infty$). In the large-U limit, this Hubbard model is transferred as the t-J model (Gros *et al.*, 1987):

$$H = -t \sum_{i\eta\sigma} \tilde{C}_{i\sigma}^+ \tilde{C}_{i+\eta\sigma} + \mu \sum_{i\sigma} \tilde{C}_{i\sigma}^+ \tilde{C}_{i\sigma} + J \sum_{i\eta} \vec{S}_i \cdot \vec{S}_{i+\eta}$$

↓
↓
↓

kinetic energy competition magnetic energy

\Leftrightarrow

with $\vec{S}_i = (S_i^x, S_i^y, S_i^z)$, and the constrained electron operators $\tilde{C}_{i\sigma} = (1 - n_{i-\sigma}) C_{i\sigma}$

The constrained electron operator:

$$\tilde{C}_{i\sigma} = (1 - n_{i-\sigma})C_{i\sigma}$$



strongly correlated effects



large U

1. $\tilde{C}_{i\sigma}$ does not destroy any doubly occupied sites, and therefore represents physical annihilation operator acting in the restricted Hilbert space without double electron occupancy;

Restricted Hilbert space (Hilbert subspace):

$$|0\rangle, |\uparrow\rangle, |\downarrow\rangle$$

2. $C_{i\sigma}$ is to be thought of as operating within the full Hilbert space;

Full Hilbert space:

$$|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$$

3. The sum rules for the constrained electrons:

$$(1). \left\langle \sum_{\sigma} \tilde{C}_{i\sigma}^{\dagger} \tilde{C}_{i\sigma} \right\rangle = 1 - x$$

$$(2). \left\langle \sum_{\sigma} \left\{ \tilde{C}_{i\sigma}^{\dagger}, \tilde{C}_{i\sigma} \right\} \right\rangle = 1 + x, \quad \sum_{\sigma} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_{\sigma}(k, \omega) = 1 + x$$

where x is the charge carrier doping concentration.

Remarks :

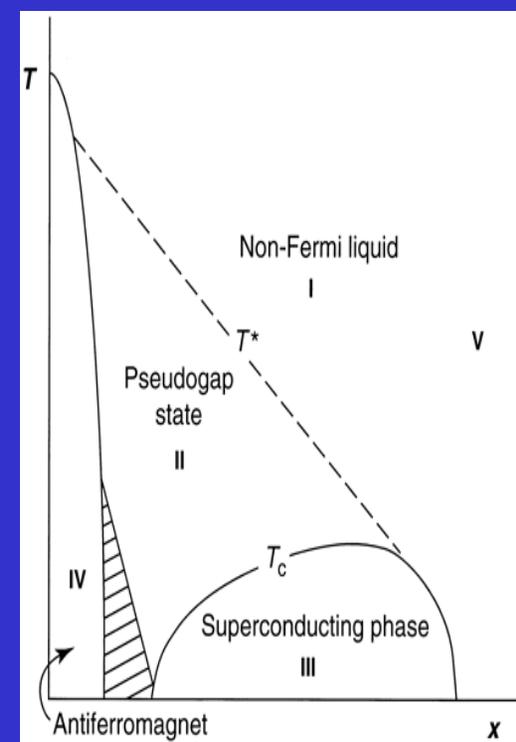
1. This t-J model,

$$H = -t \sum_{i\eta\sigma} \tilde{C}_{i\sigma}^+ \tilde{C}_{i+\eta\sigma} + \mu \sum_{i\sigma} \tilde{C}_{i\sigma}^+ \tilde{C}_{i\sigma} + J \sum_{i\eta} \vec{S}_i \cdot \vec{S}_{i+\eta}$$

can describe the antiferromagnetic correlation, and reflect a competition between the kinetic energy (xt) and magnetic energy (J). At the half-filling, this t-J model is reduced as antiferromagnetic Heisenberg model, and in this case, only the spin degree of freedom is available, then the ground state is the quantum antiferromagnetic state!

2. These constrained electron operators do not obey anticommutation at the same site, i.e., $\tilde{C}_{i\sigma} \tilde{C}_{i\sigma}^+ + \tilde{C}_{i\sigma}^+ \tilde{C}_{i\sigma} = ?$ then it is difficult to apply usual many-particle technique (Wick theorem) to treat this strongly correlated system, since the Wick theorem is based on fermion and boson statistics in the full Hilbert space.

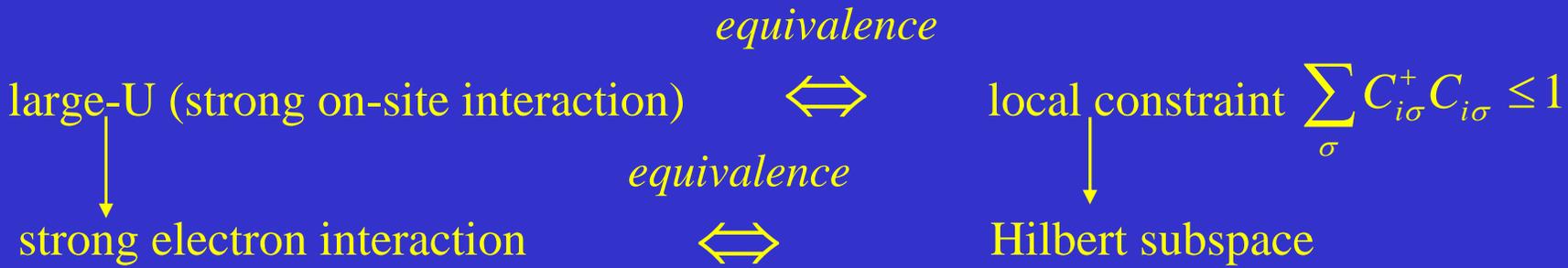
3. Alternatively, this t-J model also can be expressed as,



$$\left\{ \begin{array}{l}
 H = -t \sum_{i\eta\sigma} C_{i\sigma}^+ C_{i+\eta\sigma} + \mu \sum_{i\sigma} C_{i\sigma}^+ C_{i\sigma} + J \sum_{i\eta} \vec{S}_i \cdot \vec{S}_{i+\eta} \\
 \downarrow \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \downarrow \\
 \textit{kinetic energy} \qquad \qquad \qquad \xleftrightarrow{\textit{competition}} \qquad \qquad \qquad \textit{magnetic energy}
 \end{array} \right.$$

with the additional nonholonomic on-site local constraint: $\sum_{\sigma} C_{i\sigma}^+ C_{i\sigma} \leq 1$.

In this t-J model, the strong electron correlation manifests itself by this electron on-site local constraint. This local constraint leads to that electrons move in the Hilbert sub-space, i.e.,



and therefore this local constraint should be treated properly [Zhang+Jain+Emery, Phys. Rev. B47, 3368 (1993); Feng *et al.*, Phys. Rev. B47, 15192 (1993)].

B. The charge-spin separation fermion-spin theory implemented the gauge invariant charge carriers and spins [Feng *et al.*, J. Phys. Condens. Matter 16, 343 (2004); Feng *et al.* Mod. Phys. Lett. B17, 361 (2003); Feng *et al.*, Phys. Rev. B49, 2368 (1994)].

In the following discussions, we will use both representations for the t-J model. Firstly, we start from:

$$H = -t \sum_{i\eta\sigma} C_{i\sigma}^+ C_{i+\eta\sigma} + \mu \sum_{i\sigma} C_{i\sigma}^+ C_{i\sigma} + J \sum_{i\eta} \vec{S}_i \cdot \vec{S}_{i+\eta}$$

$$\sum_{i\sigma} C_{i\sigma}^+ C_{i\sigma} \leq 1$$



The single occupancy on-site local constraint

The crucial requirement for the t-J model is to impose the single occupancy constraint.

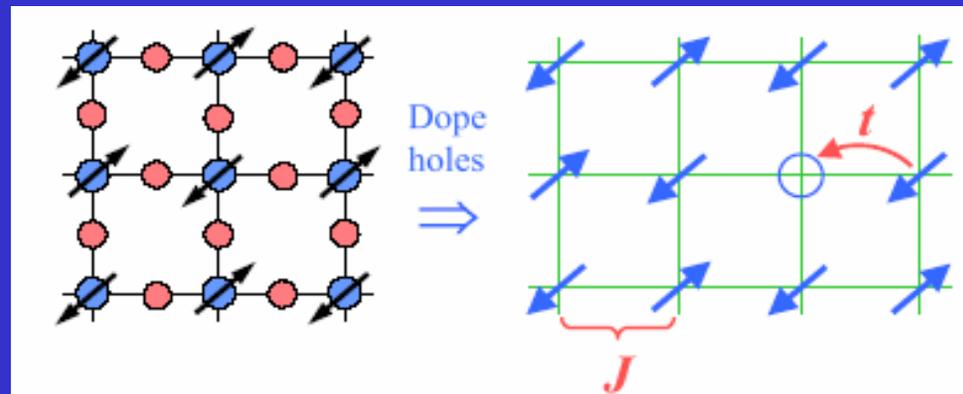


FIG. 1: Structure of the Cu-O layer in high T_c materials. Copper atoms sit on a square lattice with oxygen atoms in between. The electronic structure is simplified to a one band model shown on the right, with electrons hopping with matrix element t . There is an antiferromagnetic exchange J between spins on neighboring sites.

An intuitively appealing approach to implement this on-site local constraint is the slave-particle formalism. In this case, we developed a charge-spin separation fermion-spin theory implemented the real charge carrier and spin [Feng *et al.*, J. Phys. Condens. Matter 16, 343 (2004); Phys. Rev. B **49**, 2368 (1994)]:

1. We start from the electron's CP^1 representation,

$$C_{i\sigma} = h_i^+ a_{i\sigma}$$

charge degree of freedom
spin degree of freedom

with the on-site local constraint,

$$\sum_{\sigma} a_{i\sigma}^+ a_{i\sigma} = 1 \quad \rightarrow \quad \sum_{\sigma} C_{i\sigma}^+ C_{i\sigma} = \sum_{\sigma} h_i h_i^+ a_{i\sigma}^+ a_{i\sigma} = 1 - h_i^+ h_i \leq 1$$

and the local U(1) gauge transformation,

$$h_i \rightarrow h_i e^{i\theta_i}, \quad a_{i\sigma} \rightarrow a_{i\sigma} e^{i\theta_i}$$

then the t-J model can be rewritten as,

$$H = -t \sum_{i\eta\sigma} h_i h_{i+\eta}^+ a_{i\sigma}^+ a_{i+\eta\sigma} + J \sum_{i\eta} (h_i h_i^+) S_i \cdot S_{i+\eta} (h_{i+\eta} h_{i+\eta}^+)$$

2. Now we concentrate on the CP^1 bosons $a_{i\sigma}$ and related constraint $\sum_{\sigma} a_{i\sigma}^+ a_{i\sigma} = 1$

(1). For a free spinless boson d_i^+ :

$$d_i^+ = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \dots \\ 0 & 0 & 2 & 0 & 0 & \dots \\ 0 & 0 & 0 & 3 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix} \quad (\text{infinite Fock space})$$

if the occupied number of spinless bosons is restricted as 0 or 1, i.e., $d_i^+ d_i \leq 1$, then the infinite Fock space is reduced immediately as the two dimensional space, namely,

$$d_i^+ = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \dots \\ 0 & 0 & 2 & 0 & 0 & \dots \\ 0 & 0 & 0 & 3 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix} \quad \text{constraint } d_i^+ d_i \leq 1$$

$$\Rightarrow d_i^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = s_i^+ \quad (\text{hard-core boson})$$

\downarrow
 spin operator

infinite-Fock space \longleftrightarrow two-dimensional space

while these constrained bosons are the hard-core bosons.

Since $\sum_{\sigma} a_{i\sigma}^+ a_{i\sigma} = 1$, then,

for spin-up $|occupancy\rangle_{\uparrow} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{\uparrow(occupancy)}$ $|empty\rangle_{\uparrow} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_{\uparrow(empty)}$

for spin-down $|occupancy\rangle_{\downarrow} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_{\downarrow(occupancy)}$ $|empty\rangle_{\downarrow} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{\downarrow(empty)}$

because of single occupancy constraint and the symmetry of spin-up and spin-down, *i.e.*,

$$|occupancy\rangle_{\uparrow} = |empty\rangle_{\downarrow} \quad |occupancy\rangle_{\downarrow} = |empty\rangle_{\uparrow}$$

therefore we have

$$a_{\uparrow} = e^{i\Phi_{\uparrow}} |occupancy\rangle_{\downarrow\uparrow} \langle occupancy| = e^{i\Phi_{\uparrow}} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = e^{i\Phi_{\uparrow}} S^{-}$$

$$a_{\downarrow} = e^{i\Phi_{\downarrow}} |occupancy\rangle_{\uparrow\downarrow} \langle occupancy| = e^{i\Phi_{\downarrow}} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = e^{i\Phi_{\downarrow}} S^{+}$$

then the electron operators can be expressed as,

$$C_{i\uparrow} = h_i^+ e^{i\Phi_{\uparrow}} S^{-}, \quad C_{i\downarrow} = h_i^+ e^{i\Phi_{\downarrow}} S^{+}$$

with the local U(1) gauge transformation is,

$$h_i \rightarrow h_i e^{i\theta_i}, \quad \Phi_{i\sigma} \rightarrow \Phi_{i\sigma} + \theta_i$$

Furthermore, the phase factor $\Phi_{i\sigma}$ can be incorporated into the charge carrier operator, and the new transformation then is obtained as,

$$C_{i\uparrow} = h_{i1}^+ S_i^- = h_{i\uparrow}^+ S_i^-, \quad C_{i\downarrow} = h_{i2}^+ S_i^+ = h_{i\downarrow}^+ S_i^+$$

charge carrier

spin



charge-spin separation

$h_{i\sigma} = e^{-i\Phi_{i\sigma}} h_i$, \longrightarrow charge degree of freedom together with some effects of the spin configuration rearrangements due to the presence of the doped hole itself

S_i , \longrightarrow spin degree of freedom

then the on-site local constraint,

$$\begin{aligned} \sum_{\sigma} C_{i\sigma}^+ C_{i\sigma} &= S_i^+ h_{i\uparrow}^+ h_{i\uparrow}^+ S_i^- + S_i^- h_{i\downarrow}^+ h_{i\downarrow}^+ S_i^+ \\ &= h_i h_i^+ (S_i^+ S_i^- + S_i^- S_i^+) = 1 - h_i^+ h_i \leq 1 \end{aligned}$$

is exactly satisfied, and the double spinful fermion occupancy,

$$h_{i\sigma}^+ h_{i-\sigma}^+ = e^{i\Phi_{i\sigma}} h_i^+ h_i^+ e^{-i\Phi_{i\sigma}} = 0,$$

is ruled out automatically. These charge carrier and spin are invariant under the local U(1) gauge transformation, and therefore the charge carrier and spin are real.

In particular, this is a natural representation for the constrained electrons.

See, e.g., the review, Feng *et al.*, Int. J. Mod. Phys. B22, 3757-3811 (2008).

$$H = -t \sum_{i\eta\sigma} \tilde{C}_{i\sigma}^+ \tilde{C}_{i+\eta\sigma} + t' \sum_{i\tau\sigma} \tilde{C}_{i\sigma}^+ \tilde{C}_{i+\tau\sigma} + \mu \sum_{i\sigma} \tilde{C}_{i\sigma}^+ \tilde{C}_{i\sigma} + J \sum_{i\eta} \vec{S}_i \cdot \vec{S}_{i+\eta}$$

$$\tilde{C}_{i\uparrow} = C_{i\uparrow} (1 - C_{i\downarrow}^+ C_{i\downarrow}) = C_{i\downarrow} C_{i\downarrow}^+ C_{i\uparrow} = C_{i\downarrow} S^- = C_{ia} S^-$$

$$\tilde{C}_{i\downarrow} = C_{i\downarrow} (1 - C_{i\uparrow}^+ C_{i\uparrow}) = C_{i\uparrow} C_{i\uparrow}^+ C_{i\downarrow} = C_{i\uparrow} S^+ = C_{ib} S^+$$

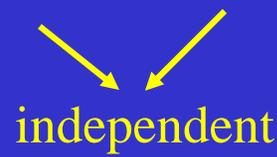
$\tilde{C}_{i\sigma}^+$ ($\tilde{C}_{i\sigma}$) is the constrained electron operator, and it does not create (destroy) any doubly occupied sites, therefore represents physical creation (annihilation) operator acting in the restricted Hilbert space without double electron occupancy;

$C_{i\sigma}^+$ ($C_{i\sigma}$) is to be thought of as operating within the full Hilbert space, therefore represents the charge degree of freedom;

S_i^+ (S_i^-) is spin operator, and therefore represent spin degree of freedom.

In the decouple scheme,

$$\tilde{C}_{i\downarrow} = C_{i2} \quad S_i^+ = C_{i\uparrow} \quad S_i^+$$

$$\tilde{C}_{i\uparrow} = C_{i1} \quad S_i^- = C_{i\downarrow} \quad S_i^-,$$


then $C_{i\sigma}$ and S_i^\pm are independent!

The particle-hole transformation: $C_{i\sigma} = h_{i-\sigma}^+$

$$\tilde{C}_{i\uparrow} = h_{i\uparrow}^+ S_i^-, \quad \tilde{C}_{i\downarrow} = h_{i\downarrow}^+ S_i^+.$$

see, e.g., the review, Feng *et al.*, Int. J. Mod. Phys. B22, 3757-3811 (2008)

In this representation, t-J model is expressed as,

$$H = t \sum_{i\eta} (h_{i+\eta\uparrow}^+ h_{i\uparrow} S_i^+ S_{i+\eta}^- + h_{i+\eta\downarrow}^+ h_{i\downarrow} S_i^- S_{i+\eta}^+) - \mu \sum_{i\sigma} h_{i\sigma}^+ h_{i\sigma} + J_{eff} \sum_{i\eta} \vec{S}_i \cdot \vec{S}_{i+\eta}$$

$$J_{eff} = J(1-x)^2 \text{ with the doping concentration } x$$

The advantages:

- (1). The strong correlation effect has been treated properly since the on-site local constraint has been treated properly.
- (2). The charge carriers and spins are gauge invariant, and in this sense, they are real, and can be explained as the physical excitations.

Although the present theory is a natural representation for constrained electrons under the decoupling scheme, so long as $h_i^+ h_i = 1$, $\sum_{i\sigma} C_{i\sigma}^+ C_{i\sigma} = 0$, no matter what the values of $S_i^+ S_i^-$ and $S_i^- S_i^+$ are, therefore it means that a 'spin' even to an empty site has been assigned. Obviously, this insignificant defect is originated from the decoupling approximation. We have shown that this defect can be cured by introducing a projection operator P_i . However, this projection operator is cumbersome to handle in the many cases, and it has been dropped in the actual calculations. We have also shown that such treatment leads to errors of the order x in counting the number of spin states, which is negligible for small doping.

$$H = t \sum_{i\eta} (h_{i+\eta\uparrow}^+ h_{i\uparrow} S_i^+ S_{i+\eta}^- + h_{i+\eta\downarrow}^+ h_{i\downarrow} S_i^- S_{i+\eta}^+) - \mu \sum_{i\sigma} h_{i\sigma}^+ h_{i\sigma} + J_{eff} \sum_{i\eta} \vec{S}_i \cdot \vec{S}_{i+\eta}$$

Remarks:

- (1). The kinetic energy term (xt) have been transferred as the charge carrier-spin interaction, while the magnetic energy (J) term is only to form an adequate spin configuration, which reflect that even kinetic energy terms in the t-J model has strong Coulombic contributions due to the restriction of single occupancy of a given site, and therefore dominate the essential physics of cuprate superconductors.
- (2). The kinetic energy terms in the higher powers of doping cause superconductivity.
- (3). The spirit of the present theory is very similar to that of the bosonization in one-dimensional interacting electron systems, where the electron operators are mapped onto the boson (electron density) representation, and then the recast Hamiltonian is exactly solvable.

C. The gauge invariant charge carrier spin description of the normal-state of cuprate superconductors (above T_c):

Charge transport:

Feng *et al.*, J. Phys. Condens. Matter 16, 343 (2004); Yuan *et al.*, Phys. Rev. B67, 134504 (2003); Qin *et al.*, Phys. Rev. B65, 155117 (2002); Feng *et al.*, Eur. Phys. J. B15, 607 (2000); Feng *et al.*, Phys. Rev. B60, 7565 (1999); Feng *et al.*, Phys. Lett. A232, 293 (1997).

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Heat transport:

Qin *et al.*, Phys. Lett. A335, 477 (2005); Ma *et al.*, Phys. Lett. A328, 212 (2004);

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Dynamical spin response:

Feng *et al.*, J. Phys. Condens. Matter 16, 343 (2004); He *et al.*, Phys. Rev. B67, 094402 (2003); Feng *et al.*, Phys. Rev. B66, 064503 (2002); Yuan *et al.*, Phys. Rev. B64, 224505 (2001); Feng *et al.*, Phys. Rev. B57, 10328 (1998).

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Electronic structure:

Lan *et al.*, Phys. Rev. B75, 134513 (2007); Guo *et al.*, Phys. Lett. A355, 473 (2006); Feng *et al.*, Phys. Rev. B55, 642 (1997).

D. Kinetic energy driven superconductivity [Feng, PRB 68, 184501 (2003); Feng *et al.*, Physica C 436, 14 (2006). See, e.g., the review, Feng *et al.*, in *Superconductivity Research Horizons*, edited by B. Peterson (Nova Science Publishers, New York, 2007) chapter 5, p129. See, e.g., the review, Feng *et al.*, Int. J. Mod. Phys. B22, 3757-3811

PHYSICAL REVIEW B 68, 184501 (2003)

Kinetic energy driven superconductivity in doped cuprates

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(Received 30 June 2003; published 3 November 2003)

Within the t - J model, the mechanism of superconductivity in doped cuprates is studied based on the partial charge-spin separation fermion-spin theory. It is shown that dressed holons interact, occurring directly through the kinetic energy by exchanging dressed spinon excitations, leading to a net attractive force between dressed holons; then the electron Cooper pairs originating from the dressed holon pairing state are due to the charge-spin recombination, and their condensation reveals the superconducting ground state. The electron superconducting transition temperature is determined by the dressed holon pair transition temperature and is proportional to the concentration of doped holes in the underdoped regime. With the common form of the electron Cooper pair, we also show that there is a coexistence of the electron Cooper pair and antiferromagnetic short-range correlation, and hence the antiferromagnetic short-range fluctuation can persist into the superconducting state. Our results are qualitatively consistent with experiments.

As in the conventional superconductors, the superconducting state in cuprate superconductors is also characterized by the electron Cooper pairs, forming superconducting quasiparticle. Since the gap function and pairing force have a range of one lattice spacing [Z.X. Shen *et al.*, PRL70, 1553 (1993); H. Ding *et al.*, PRB54, R9678 (1996)], then the order parameter for the electron Copper pair can be expressed as,

$$\Delta = \left\langle C_{i\uparrow}^+ C_{i+\eta\downarrow}^+ - C_{i\downarrow}^+ C_{i+\eta\uparrow}^+ \right\rangle = \left\langle h_{i\uparrow} h_{i+\eta\downarrow} S_i^+ S_{i+\eta}^- - h_{i\downarrow} h_{i+\eta\uparrow} S_i^- S_{i+\eta}^+ \right\rangle$$

In the spin liquid state without long-range-order, $\langle S_i^+ S_{i+\eta}^- \rangle = \langle S_i^- S_{i+\eta}^+ \rangle$ then this order parameter can be written as,

$$\Delta = -\langle S_i^+ S_{i+\eta}^- \rangle \Delta_h \quad \Delta_h = \left\langle h_{i\downarrow} h_{i+\eta\uparrow} - h_{i\uparrow} h_{i+\eta\downarrow} \right\rangle$$

which shows that the superconducting order parameter is closely related to the charge carrier pairing amplitude, and is proportional to the number of doped holes, and not to the number of electrons. Moreover, there is a coexistence of the electron Cooper pair and antiferromagnetic short-range correlation.

However, in the extreme low doped regime with the antiferromagnetic long-range order, where $\langle S_i^+ S_{i+\eta}^- \rangle \neq \langle S_i^- S_{i+\eta}^+ \rangle$, then the conduct is disrupted by the antiferromagnetic long-range order, i.e., there is no coexistence of the electron Cooper pair and antiferromagnetic long-range correlation. Therefore we only focus on the case without the antiferromagnetic long-range order. Now we define charge carrier diagonal and off-diagonal Green's functions as,

$$g(i-j, t-t') = \langle\langle h_{i\sigma}(t); h_{j\sigma}^+(t') \rangle\rangle,$$

$$J(i-j, t-t') = \langle\langle h_{i\downarrow}(t); h_{j\uparrow}(t') \rangle\rangle,$$

$$J^+(i-j, t-t') = \langle\langle h_{i\uparrow}^+(t); h_{j\downarrow}^+(t') \rangle\rangle,$$

and spin Green's functions as,

$$D(i-j, t-t') = \langle\langle S_i^+(t); S_j^-(t') \rangle\rangle,$$

$$D_z(i-j, t-t') = \langle\langle S_i^z(t); S_j^z(t') \rangle\rangle,$$

In the framework of equation of motion, the time-Fourier transform of the two-time Green's function satisfies the equation,

$$\omega \langle\langle A(t); A^+(t') \rangle\rangle_{\omega} = \langle[A, A^+] \rangle + \langle\langle [A, H]; A^+ \rangle\rangle_{\omega}.$$

If we define the orthogonal operator L as,

$$[A, H] = \zeta A - iL \quad \text{with} \quad \langle[L, A^+] \rangle = 0,$$

then the full Green's function can be expressed as,

$$G(\omega) = G^{(0)}(\omega) + \frac{1}{\zeta^2} G^{(0)}(\omega) \langle\langle L(t); L(t') \rangle\rangle_{\omega},$$

where $\zeta = \langle[A, A^+] \rangle$, and the mean-field Green's function,

$$G^{(0)}(\omega) = \frac{\zeta}{\omega - \xi}.$$

It has been shown that if the self-energy $\Sigma(\omega)$ is identified as the irreducible part of $\langle\langle L; L^+ \rangle\rangle$, then the full Green's function can be evaluated as,

$$G(\omega) = \frac{\zeta}{\omega - \xi - \Sigma(\omega)}, \quad \Sigma(\omega) = \frac{\langle\langle L; L^+ \rangle\rangle_{\omega}^{irr}}{\zeta}.$$

In the framework of the diagrammatic technique, $\Sigma(\omega)$ corresponds to the contribution of irreducible diagrams.

Zubarev, *Sov. Phys.—Usp*, 3, 201 (1960); Plakida, *Phys. Lett. A*43, 481 (1973); Feng *et al.*, *J. Phys.: Condens. Matter* 16, 343 (2004).

$$H = t \sum_{i\eta} (h_{i+\eta\uparrow}^+ h_{i\uparrow} S_i^+ S_{i+\eta}^- + h_{i+\eta\downarrow}^+ h_{i\downarrow} S_i^- S_{i+\eta}^+) - \mu \sum_{i\sigma} h_{i\sigma}^+ h_{i\sigma} + J_{eff} \sum_{i\eta} \vec{S}_i \cdot \vec{S}_{i+\eta}$$

Following Eliashberg's strong coupling theory, we obtain the equations that satisfied by the full dressed holon diagonal and off-diagonal Green's functions as [Eliashberg, Sov. Phys. JETP 11,696 (1960); Scalapino *et al.*, Phys. Rev. 148, 263 (1966)],

$$g(k, \omega) = g^{(0)}(k, \omega) + g^{(0)}(k, \omega) [\Sigma_1^{(h)}(k, \omega) g(k, \omega) - \Sigma_2^{(h)}(-k, -\omega) \Gamma(k, \omega)]$$

$$J(k, \omega) = g^{(0)}(-k, -\omega) [\Sigma_1^{(h)}(-k, -\omega) \Gamma(-k, -\omega) + \Sigma_2^{(h)}(-k, -\omega) g(k, \omega)]$$

respectively, where the charge carrier self-energies are obtained from the spin bubble as,

$$\Sigma_1^{(h)}(k, \omega) = \frac{1}{N^2} \sum_{p, p'} (Zt\gamma_{p+p'+k} - zt'\gamma'_{p+p'+k})^2 \frac{1}{\beta} \sum_{ip_m} g(ip_m + i\omega_n, p+k) \Pi(ip_m, p)$$

$$\Sigma_2^{(h)}(k, \omega) = \frac{1}{N^2} \sum_{p, p'} (Zt\gamma_{p+p'+k} - zt'\gamma'_{p+p'+k})^2 \frac{1}{\beta} \sum_{ip_m} J(-ip_m - i\omega_n, -p-k) \Pi(ip_m, p)$$

$$\Pi(ip_m, p) = \frac{1}{\beta} \sum_{ip'_m} D^{(0)}(ip'_m, p') D^{(0)}(ip'_m + ip_m, p'+p)$$

In this case, the effective charge carrier gap function $\bar{\Delta}_h(k, \omega) = \Sigma_2^{(h)}(k, \omega)$ and self-energy function $\Sigma_1^{(h)}(k, \omega)$ are momentum and energy dependent. Moreover, $\Sigma_2^{(h)}(k, \omega)$ is an even function of energy, while $\Sigma_1^{(h)}(k, \omega)$ is not. For the convenience, $\Sigma_1^{(h)}(k, \omega)$ can be broken up into its symmetric and antisymmetric parts as, $\Sigma_1^{(h)}(k, \omega) = \Sigma_{1e}^{(h)}(k, \omega) + \omega \Sigma_{1o}^{(h)}(k, \omega)$. Now we define the quasiparticle coherent weight as,

$$\frac{1}{Z_F^{(h)}(k, \omega)} = 1 - \Sigma_{1o}^{(h)}(k, \omega)$$

As in the conventional superconductors, $\Sigma_{1e}^{(h)}(k, \omega)$ is a constant, it just renormalizes the chemical potential, and can be dropped. Furthermore, we only study the case in the static limit, i.e., $\bar{\Delta}_h(k) = \Sigma_2^{(h)}(k)$, and $Z_F^{-1}(k) = 1 - \Sigma_{1o}^{(h)}(k)$, then we obtain the charge carrier diagonal and off-diagonal Green's functions (BCS-like) as,

$$g(k, \omega) = Z_F^{(h)} \left[\frac{U_{hk}^2}{\omega - E_{hk}} + \frac{V_{hk}^2}{\omega + E_{hk}} \right],$$

$$J^+(k, \omega) = -Z_F^{(h)} \frac{\bar{\Delta}_{hZ}(k)}{2E_{hk}} \left[\frac{1}{\omega - E_{hk}} - \frac{1}{\omega + E_{hk}} \right],$$

with $\bar{\xi}_k = Z_F^{(h)}(k)\xi_k$, $\bar{\Delta}_{hZ}(k) = Z_F^{(h)}(k)\bar{\Delta}_h(k)$, $E_{hk} = \sqrt{\xi_k^2 + \bar{\Delta}_{hZ}^2(k)}$

and BCS coherent factors,

$$U_{hk}^2 = \frac{1}{2} \left(1 + \frac{\xi_k}{E_{hk}} \right), \quad V_{hk}^2 = \frac{1}{2} \left(1 - \frac{\xi_k}{E_{hk}} \right),$$

therefore, this superconducting state is conventional BCS like.

Although $Z_F(k)$ still is a function of k , the wave vector dependence is unimportant, since from ARPES experiments, it has been shown that in the superconducting state the lowest energy states are located at the $[\pi,0]$ point, which indicates that the majority contributions comes from the $[\pi,0]$ point. In this case, the wave vector can be chosen as $Z_F^{(h)} = Z_F^{(h)}(k_0)$ with $k_0 = [\pi,0]$. Then the quasiparticle coherent weight and superconducting gap parameter must be solved simultaneously with other self-consistent equations, then all the order parameters and chemical potential are determined by the self-consistent calculation without using adjustable parameters.

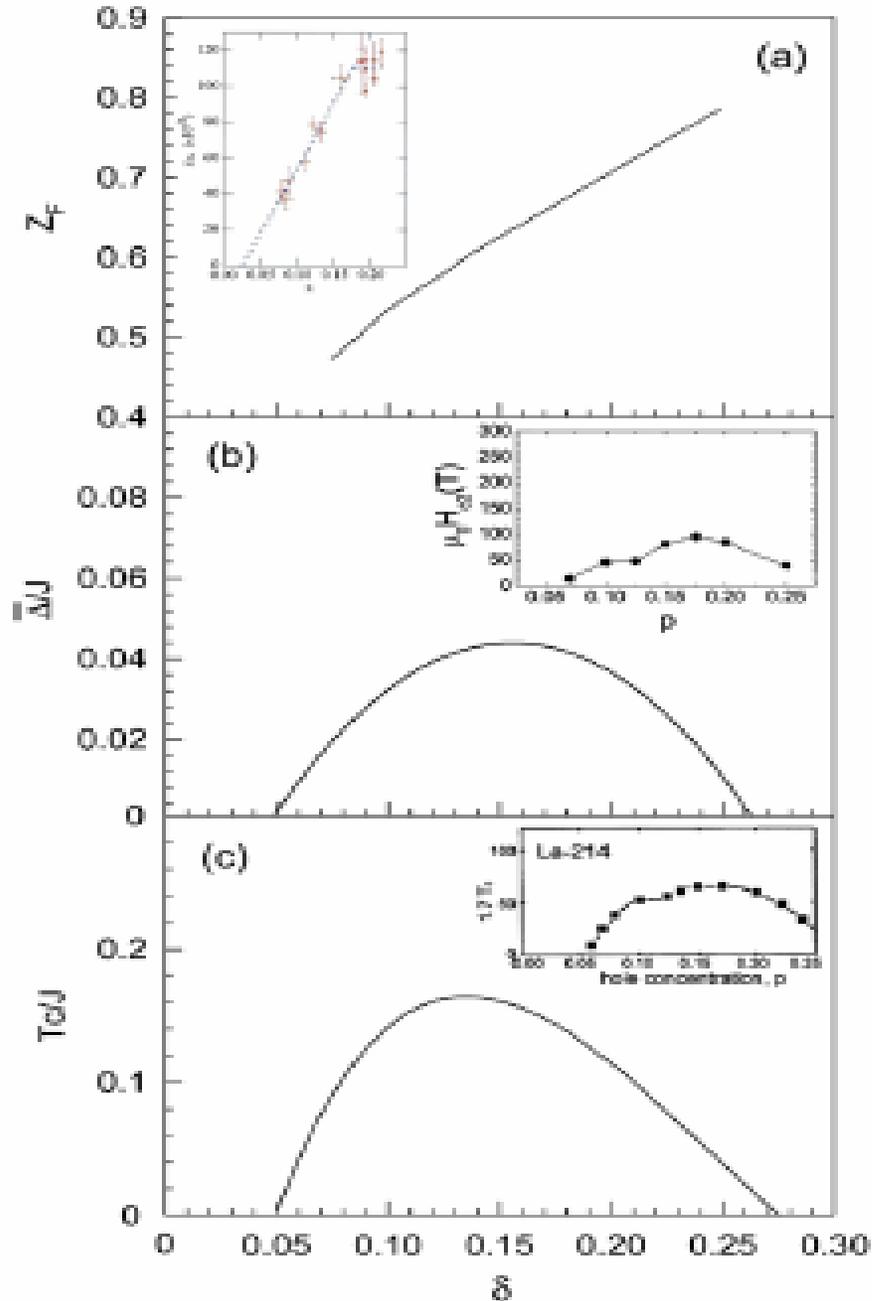
The charge carrier pairs condense with the d-symmetry in a wide range of doping, then the electron Cooper pairs originating from the charge carrier pairing state are due to the charge-spin recombination, and their condensation automatically gives the electron quasiparticle character.

the electron BCS type
Green's functions

$$G(k, \omega) \approx Z_F \left[\frac{U_k^2}{\omega - E_k} + \frac{V_k^2}{\omega + E_k} \right],$$

$$\Gamma^+(k, \omega) \approx -Z_F \frac{\overline{\Delta_Z(k)}}{2E_k} \left[\frac{1}{\omega - E_k} - \frac{1}{\omega + E_k} \right],$$

3. Doping and temperature dependent electronic structure



→ Doping dependent superconducting quasiparticle coherent weight

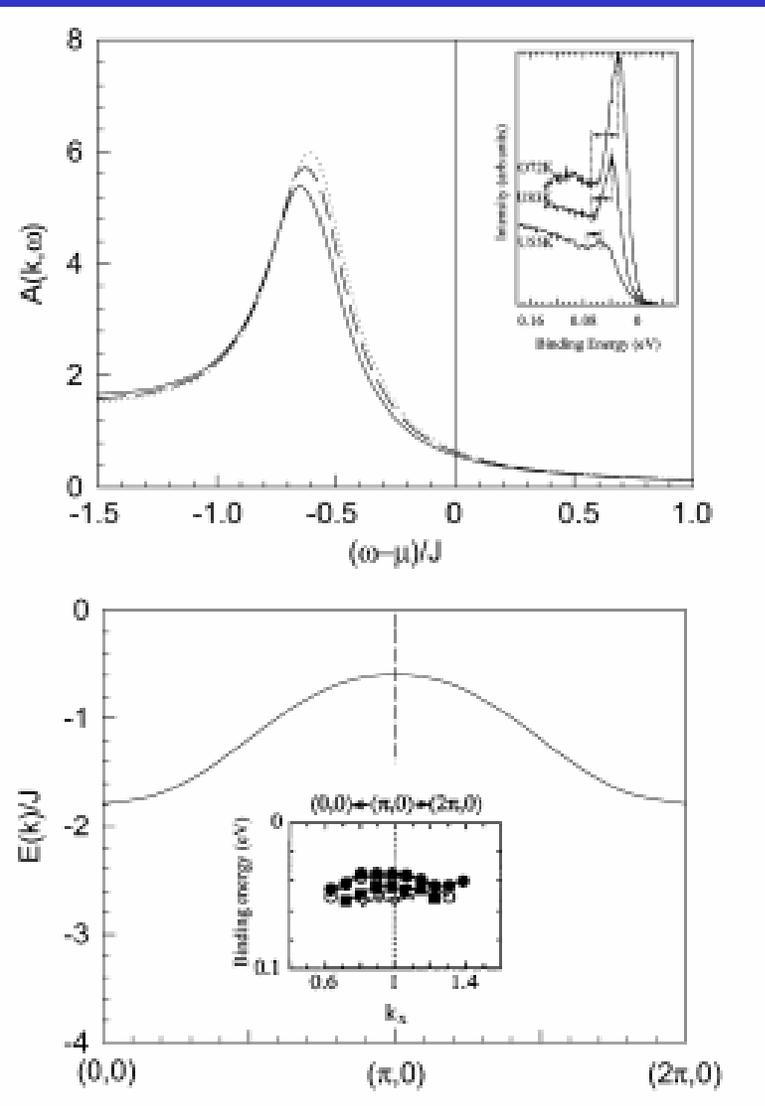
→ Doping dependent superconducting gap parameter

→ Doping dependent superconducting transition temperature

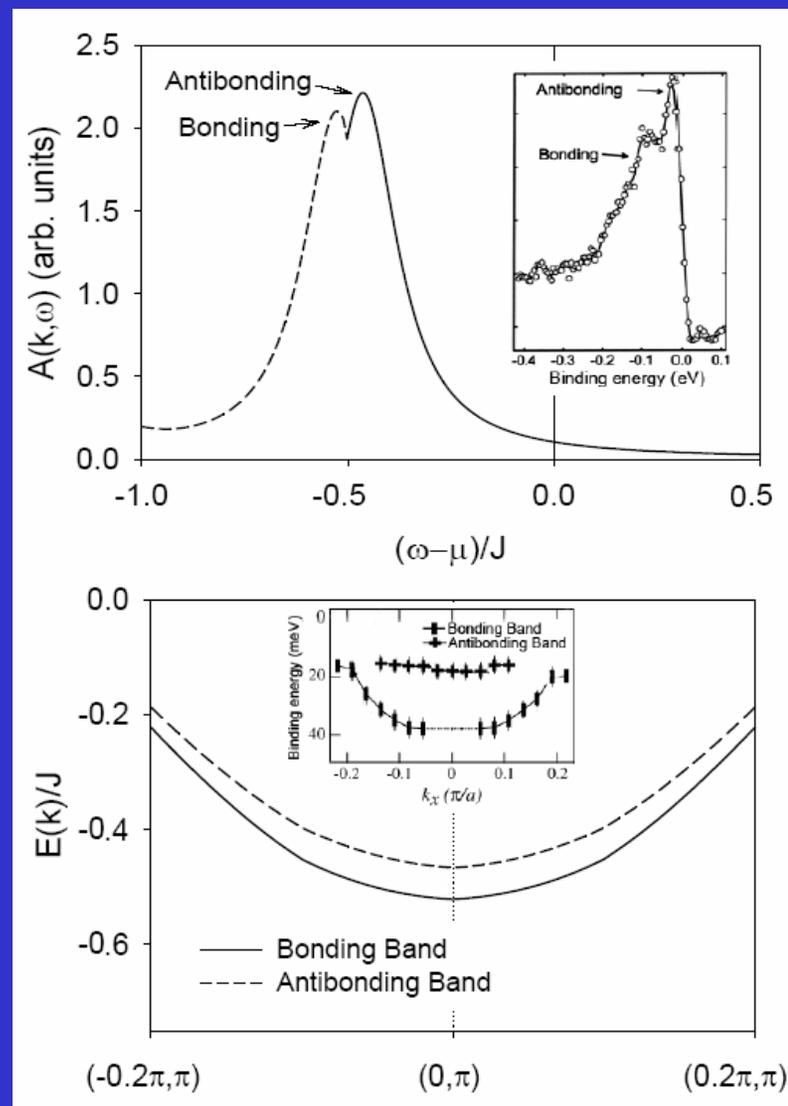
Feng, Phys. Rev. B68, 184501 (2003);
Feng *et al.*, Physica C436, 14 (2006);
Feng *et al.*, Phys. Lett. A350, 138 (2006);
Guo *et al.*, Phys. Lett. A 361, 382 (2007).

The electron spectral function in the superconducting state:

single layer case



bilayer case



Guo+Feng, Phys. Lett. A 361, 382 (2007);
Feng+Ma, Phys. Lett. A350, 138 (2006).

Lan+Qin+Feng, Phys. Rev. B76,
014533 (2007).

The doping dependence of the electron spectral function in the superconducting state:
 single layer case bilayer case

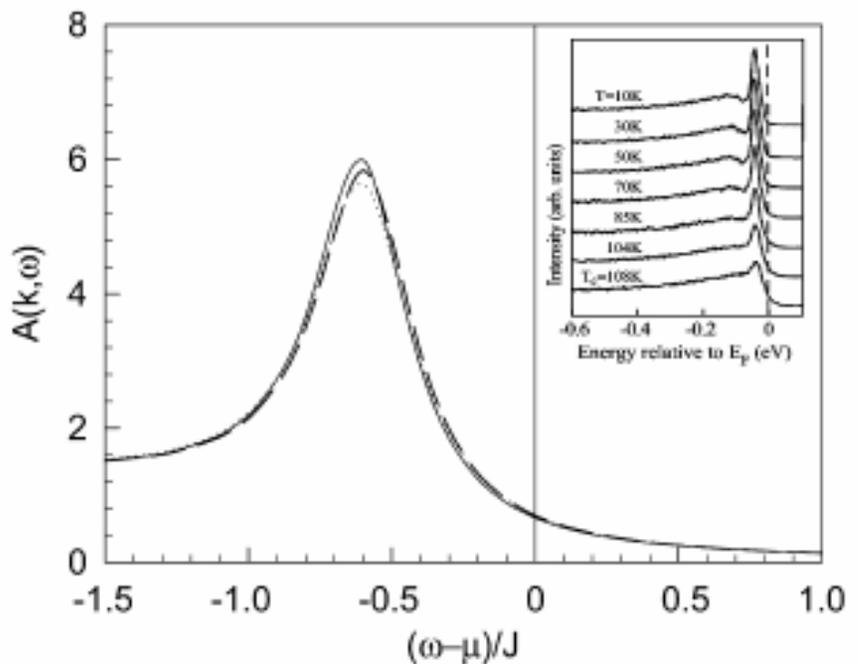


Fig. 3. The electron spectral function $A(k, \omega)$ in the $[\pi, 0]$ point with $\delta = 0.15$ at $T = 0.002J$ (solid line), $T = 0.10J$ (dashed line), and $T = 0.15J$ (dotted line) for $t/J = 2.5$ and $t'/J = 0.3$.

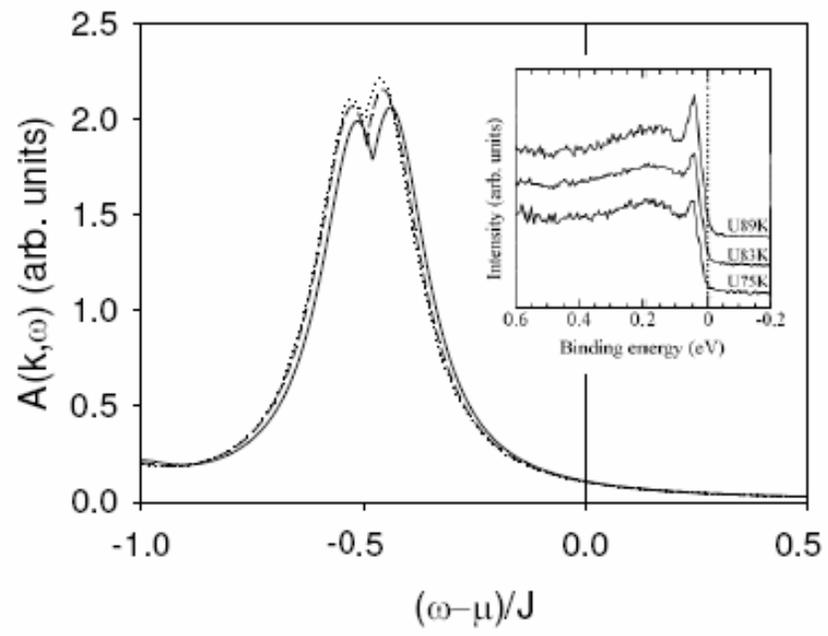
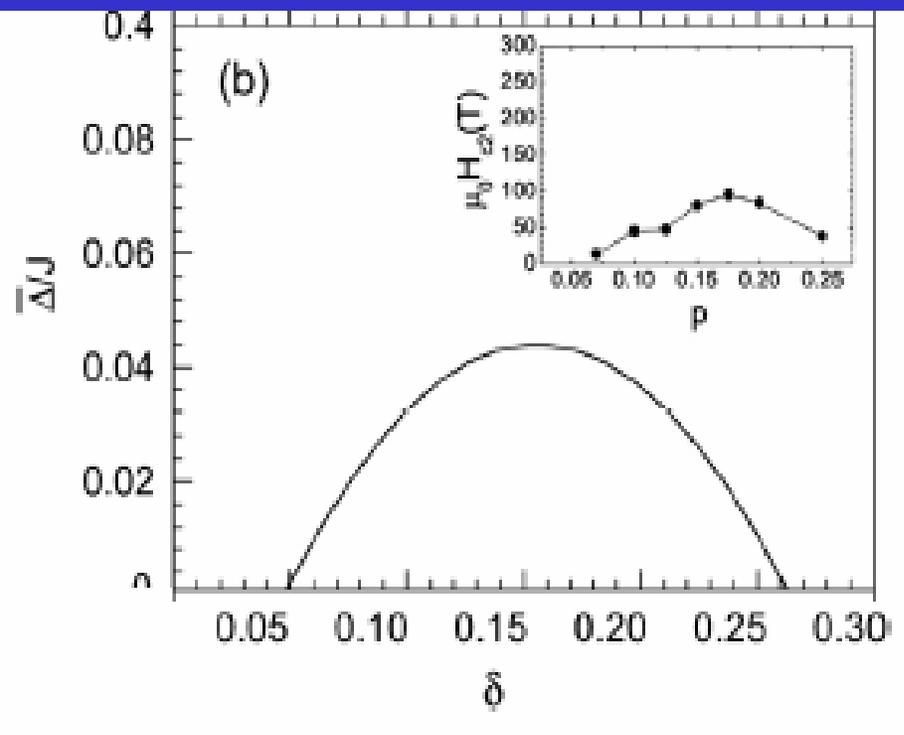


FIG. 2: The electron spectral functions at $[\pi, 0]$ point for $t/J = 2.5$, $t'/t = 0.3$, and $t_{\perp}/t = 0.35$ with $T = 0.002J$ at $\delta = 0.09$ (solid line), $\delta = 0.12$ (dashed line), and $\delta = 0.15$ (dotted line). Inset: the corresponding ARPES experimental results¹² of the bilayer cuprate superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$.

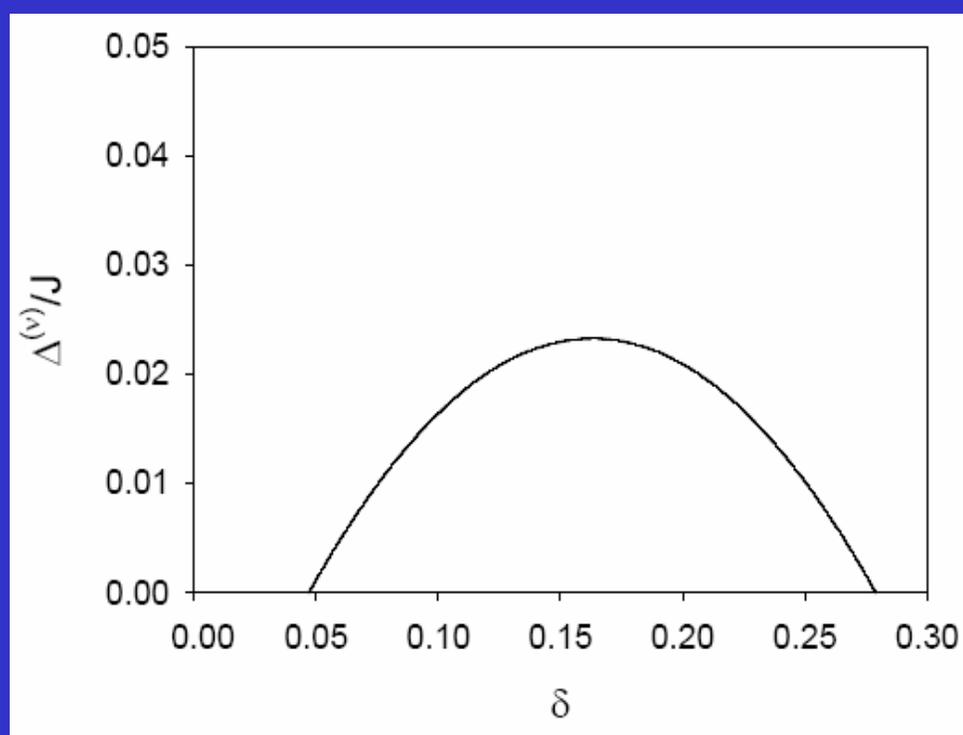
Guo+Feng, Phys. Lett. A 361, 382 (2007);
 Feng+Ma, Phys. Lett. A350, 138 (2006).

Lan+Qin+Feng, Phys. Rev. B76, 014533 (2007).

The superconducting gap parameter: single layer case



bilayer case



The peak-dip-hump structure is totally unrelated to superconductivity

$$\Delta^{(a)} = \Delta_{\parallel} - \Delta_{\perp}$$

$$\Delta^{(b)} = \Delta_{\parallel} + \Delta_{\perp}$$

$$\Delta_{\perp} \approx 0$$

Guo+Feng, Phys. Lett. A 361, 382 (2007);
Feng+Ma, Phys. Lett. A350, 138 (2006).

Lan+Qin+Feng, Phys. Rev. B76, 014533 (2007).

The typical features of the kinetic energy driven superconductivity

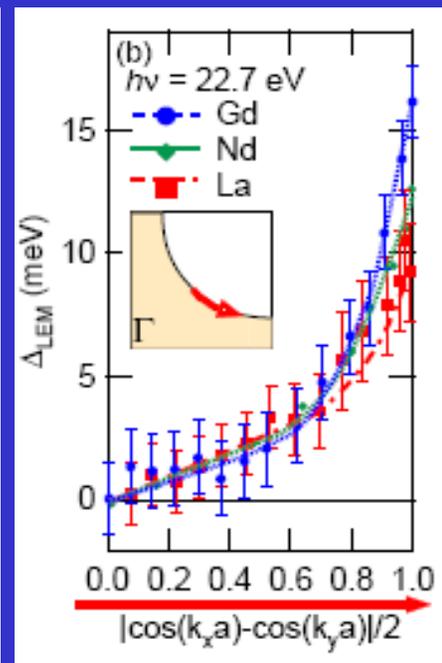
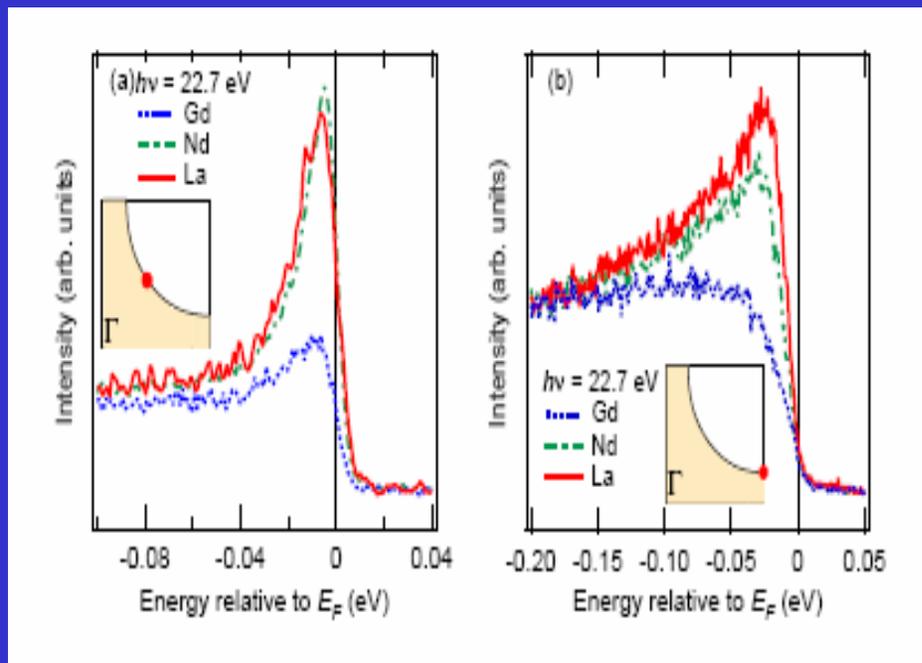
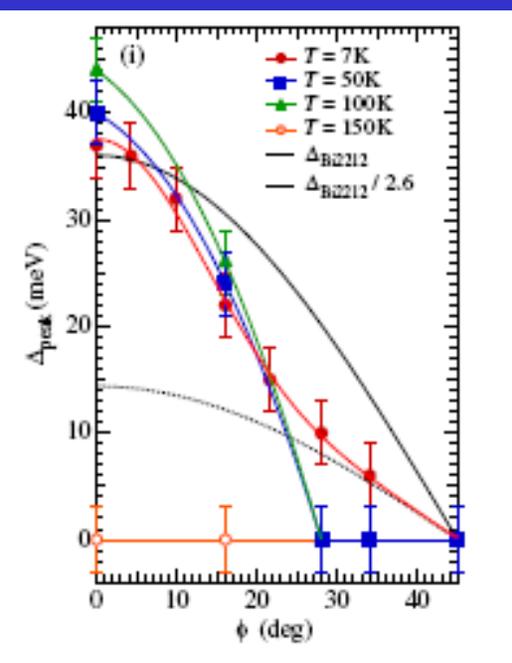
(a). In the kinetic energy driven superconducting mechanism, the charge carrier interact occurring directly through the kinetic energy by exchanging spin excitations (internal collective modes), leading to a net attractive force between charge carriers, then these Cooper pairs condensation reveals the superconducting ground-state. This is much different from the conventional electron-phonon superconducting mechanism, where the charge carrier interact occurring through the potential energy by exchanging phonons (external collective modes).

(b). In the kinetic energy driven superconducting mechanism, the superconducting state is controlled by both gap function and superconducting quasiparticle coherent weight, and then the maximal superconducting transition temperature occurs around the optimal doping, then decreases in both underdoped and overdoped regimes. This is also different from the conventional electron-phonon superconducting mechanism, where the superconducting state is only controlled by gap function.

(c). The superconducting state is the conventional BCS like with the d-wave symmetry, so that the basic BCS formalism is still valid in discussions of the superconducting gap parameter and superconducting transition temperature, and electronic structure, although the pairing mechanism is driven by the kinetic energy by exchanging spin excitations, and the exotic magnetic properties are beyond the BCS formalism.

4. The impurity effect on the electronic structure

In cuprate superconductors, since doped charge carriers are induced by the replacement of ions by those with different valences or the addition of excess oxygens in the block layer, therefore in principle, all cuprate superconductors have naturally impurities (or the disorder). However, the recent ARPES measurements on out-of-plane impurity-controlled cuprate superconductors $(\text{Bi,Pb})_2(\text{Sr,Ln})_2\text{CuO}_{6+x}$ and $\text{Bi}_2\text{Sr}_{1.6}\text{Ln}_{0.4}\text{CuO}_{6+x}$ with $\text{Ln}=\text{La, Nd, and Gd}$ observed the much stronger deviation from the monotonic d-wave gap form. In particular, the magnitude of this deviation increases with increasing the impurity concentration.



In the framework of the kinetic energy driven superconductivity, the charge carrier Green's function in the Nambu representation is obtained as,

$$\tilde{g}(k, \omega) = Z_{hF} \frac{\omega \tau_0 + \bar{\Delta}_{hz}(k) \tau_1 + \bar{\xi}_k \tau_3}{\omega^2 - E_{hk}^2}$$

In the presence of impurities, the unperturbed electron Green's function is dressed via the impurity as,

$$\begin{aligned} \tilde{g}_I(k, \omega) &= [\tilde{g}^{-1}(k, \omega) - \tilde{\Sigma}(k, \omega)]^{-1} \\ &= Z_F \frac{[\omega - \Sigma_0(k, \omega)] \tau_0 + [\bar{\Delta}_z(k) + \Sigma_1(k, \omega)] \tau_1 + [\bar{\xi}_k + \Sigma_3(k, \omega)] \tau_3}{[\omega - \Sigma_0(k, \omega)]^2 - E_{hk}^2} \end{aligned}$$

It has been shown experimentally that the superconducting transition temperature is considerably affected by the out-of-plane impurity scattering in spite of a relatively weak increase of the residual resistivity [Eisaki *et al.* PRB69,064512, (2004); Fujita *et al.*, PRL95, 097006 (2005)], this reflects that the superconducting pairing is very sensitive to this impurity scattering, and then the effect of this impurity scattering is always accompanied with a breaking of the superconducting pairing. In this case, the out-of-plane impurities can be described as the elastic off-diagonal scatterers or pairing impurity scatterers. In the framework of the kinetic energy driven superconductivity, we introduce following out-of-plane impurity scattering potential,

$$\tilde{V} = \sum_{kk'} V_{kk'} \tau_1 = V_0 \sum_{kk'} [\cos(k_x - k'_x) - \cos(k_y - k'_y)] \tau_1$$

In the charge-spin separation fermion-spin theory, the electron Green's function is a convolution of the spin Green's function and charge carrier Green's function. In this case, we can obtain the electron diagonal Green's function and the electron spectral function in the presence of this out-of-plane impurity scattering potential as,

$$A(k, \omega) = \frac{1}{N} \sum_p \frac{B_p}{2\omega_p} \left\{ [n_B(\omega_p) + n_F(\omega_p - \omega)] A_h(p - k, \omega_p - \omega) - [n_B(-\omega_p) + n_F(-\omega_p - \omega)] A_h(p - k, -\omega_p - \omega) \right\}$$

where ω_p is the spin excitation spectrum, and $A_h(k, \omega) = -2 \text{Im} \tilde{g}_{I0}(k, \omega)$ is the charge carrier spectral function.

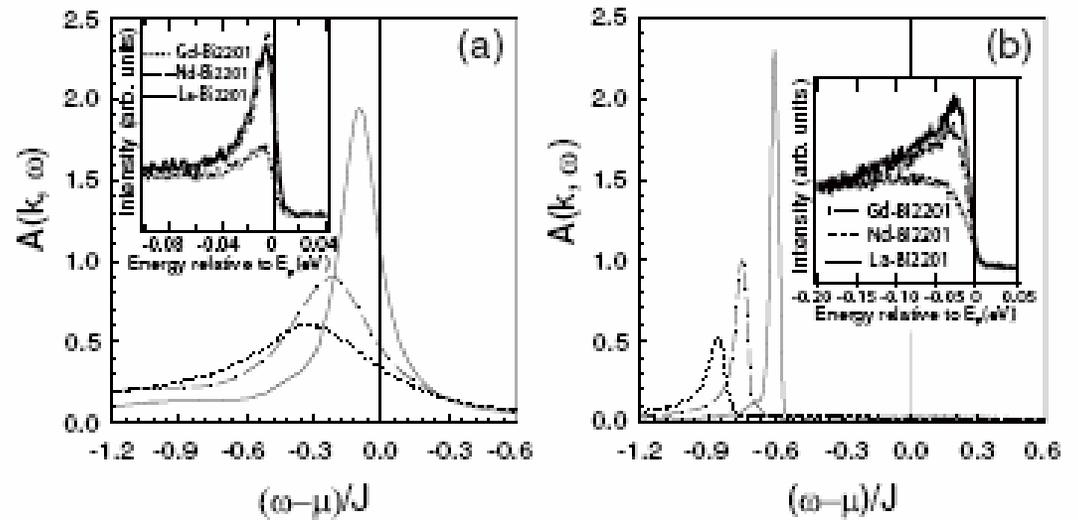
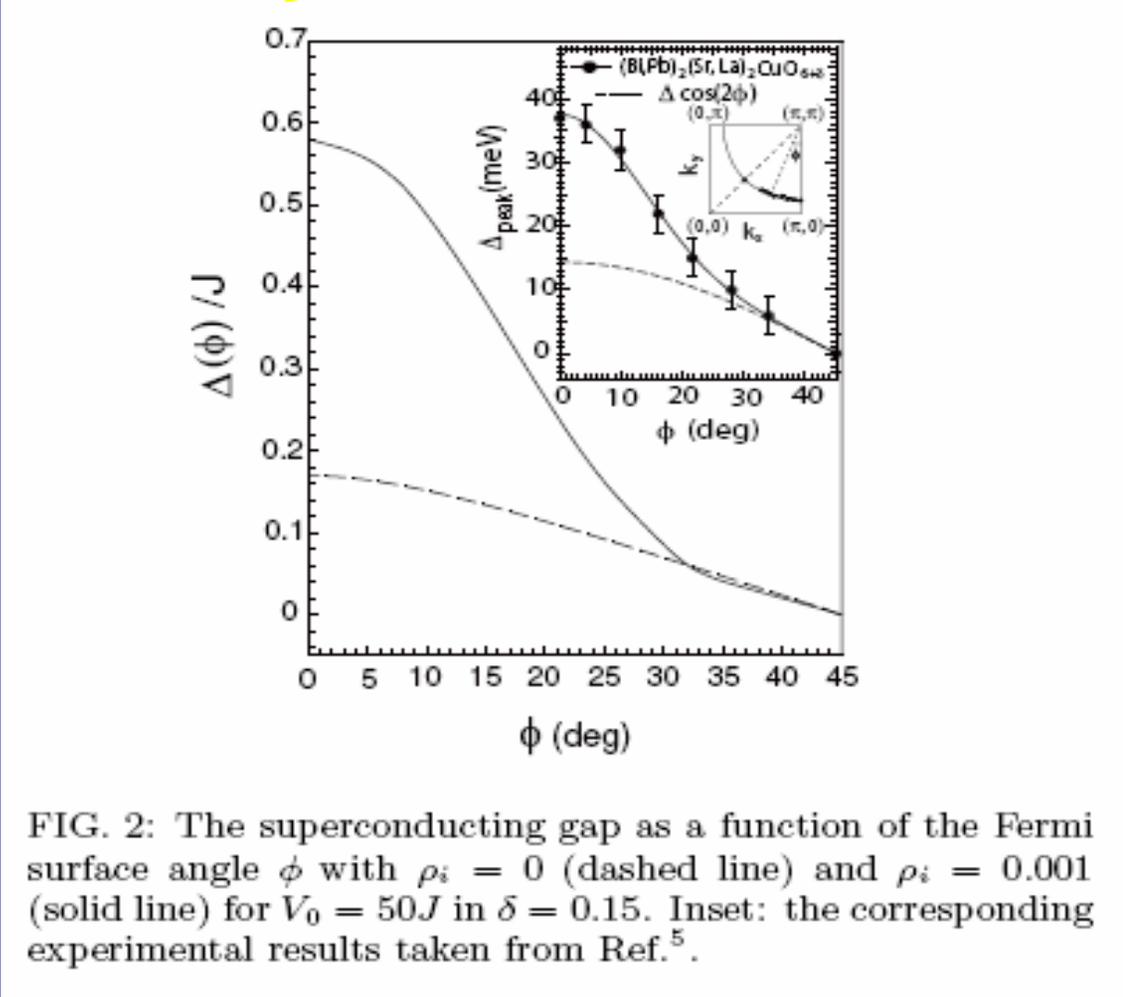


FIG. 1: The electron spectral function at (a) the nodal point and (b) the antinodal point with $\rho_i = 0.001$ (solid line), $\rho_i = 0.002$ (dashed line), and $\rho_i = 0.003$ (dotted line) for $V_0 = 50J$ in $\delta = 0.15$. Inset: the corresponding experimental results taken from Ref.⁶.

At the node ($[\pi/2, \pi/2]$), there is a quasiparticle peak near Fermi energy, however, the position of the leading-edge mid-point of the electron spectral function remains at the almost same position. In particular, the position of the leading-edge mid-point of the electron spectral function reaches the Fermi level, indicating there is no superconducting gap. On the other hand, the position of the leading-edge mid-point of the electron spectral function at the antinode ($[\pi, 0]$) is shifted towards higher binding energies with increasing the impurity concentration, this is in contrast with the case at the node, and indicates the presence of the superconducting gap.

We employ the shift of the leading-edge mid-point as a measure of the magnitude of the superconducting gap at each momentum as in experiments.

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The superconducting gap increases as decreasing the Fermi surface angle from 45° (node) to 0° (antinode). Although the superconducting gap in the presence of the impurity scattering is basically consistent with the d-wave symmetry, it is obvious that there is a strong deviation from the monotonic d-waveform around the antinodal region.

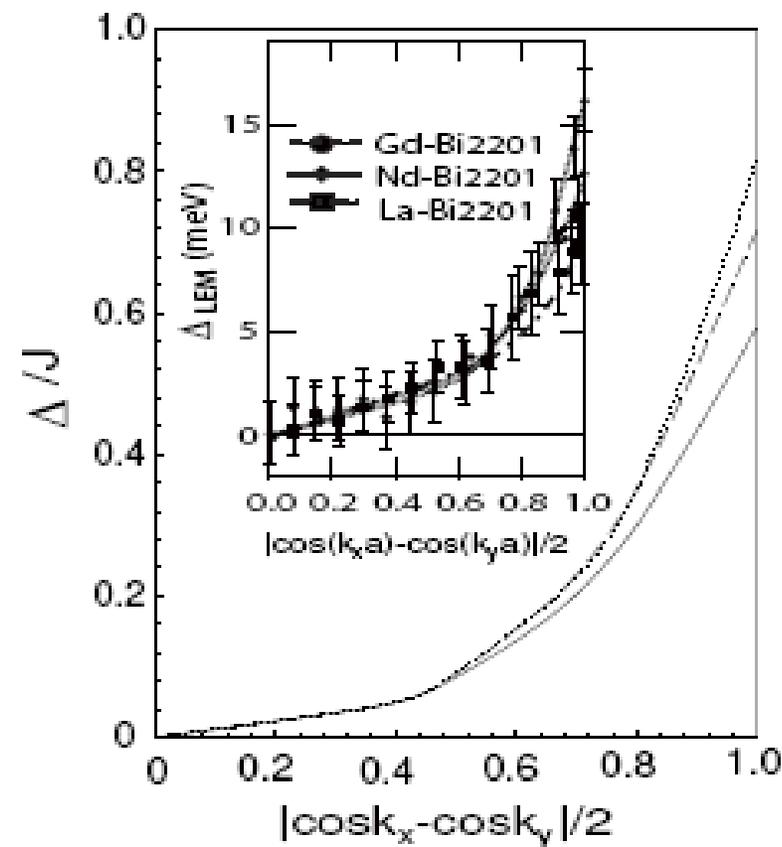


FIG. 3: The superconducting gap as a function of $[\cos k_x - \cos k_y]/2$ with $\rho_i = 0.001$ (solid line), $\rho_i = 0.002$ (dashed line), and $\rho_i = 0.003$ (dotted line) for $V_0 = 50J$ in $\delta = 0.15$. Inset: the corresponding experimental results taken from Ref.⁶.

The magnitude of the deviation from the monotonic-d-wave form around the antinodal region increases with increasing the impurity concentration.

We have shown very clearly in this paper that if the out-of-plane impurity scattering is taken into account within the kinetic energy driven superconducting mechanism, the quasiparticle spectrum of the t-J model calculated based on the off-diagonal impurity scattering potential per se can correctly reproduce some main features found in ARPES measurements on the out-of-plane impurity-controlled cuprate superconductors. In the presence of the out-of-plane impurities, although both sharp superconducting coherence peaks around nodal and antinodal regions are suppressed, the effect of this impurity scattering is stronger in the antinodal region than that in the nodal region, this leads to a strong deviation from the monotonic d-wave gap form in the out-of-plane impurity-controlled cuprate superconductors.

5. Doping and energy dependent incommensurate magnetic scattering and commensurate $[\pi, \pi]$ resonance in the superconducting state

In the charge-spin separation fermion-spin theory, the magnetic fluctuation is dominated by the scattering of spins. In the kinetic energy driven superconducting mechanism, this magnetic fluctuation has been incorporated into the electron off-diagonal Green's function (hence the electron Cooper pair) due to the charge-spin recombination in the superconducting state, therefore there is a coexistence of the electron Cooper pair and magnetic short-range correlation, and then the magnetic short-range correlation is persist into superconducting state [Feng, PRB 68, 184501 (2003); Phys. Lett. A257, 325 (1999)].

In the normal state, spins moves in the charge carrier background, then the spin response in the normal state has been discussed in terms of the collective mode in the charge carrier particle-hole channel [Feng *et al.*, J. Phys. Condens. Matter 16, 343 (2004); Yuan *et al.*, PRB64, 224505 (2001); Feng *et al.*, PRB66, 064503 (2002); He *et al.*, PRB67, 094402 (2003); Ma *et al.*, PLA337, 61 (2005)].

In the superconducting state, spins moves in the charge carrier pair background, in this case, the spin response in the superconducting state should be discussed in terms of the collective mode in the charge carrier particle-particle channel [Feng *et al.*, Physica C436, 14 (2006); Feng *et al.*, Phys. Lett. A352, 438 (2006); Cheng *et al.*, PRB77, 054518 (2008)].

Within the kinetic energy driven superconductivity, the dynamical spin structure factor in the superconducting state with the d-wave symmetry is obtained as,

$$S(k, \omega) = - \frac{2[1 + n_B(\omega)] B_k^2 \text{Im} \Sigma_s(k, \omega)}{\left[\omega^2 - \omega_k^2 - B_k \text{Re} \Sigma_s(k, \omega) \right]^2 + \left[B_k \text{Im} \Sigma_s(k, \omega) \right]^2},$$

with $\text{Im} \Sigma_s(k, \omega)$ and $\text{Re} \Sigma_s(k, \omega)$ are the corresponding imaginary and real parts of the second order dressed spin self-energy,

$$\begin{aligned} \Sigma_s(k, \omega) = & (Zt)^2 \frac{1}{N^2} \sum_{pp'} \left(\gamma_{p'+p+k}^2 + \gamma_{p-k}^2 \right) \frac{B_{q+k}}{\omega_{q+k}} \frac{Z_{hF}^2}{4} \frac{\bar{\Delta}_{hz}^{(d)}(p) \bar{\Delta}_{hz}^{(d)}(p+q)}{E_{hp} E_{hp+q}} \\ & \times \left(\frac{F_s^{(1)}(k, p, q)}{\omega^2 - (E_{hp} - E_{hp+q} + \omega_{q+k})^2} + \frac{F_s^{(2)}(k, p, q)}{\omega^2 - (E_{hp} - E_{hp+q} - \omega_{q+k})^2} \right. \\ & \left. + \frac{F_s^{(3)}(k, p, q)}{\omega^2 - (E_{hp} + E_{hp+q} + \omega_{q+k})^2} + \frac{F_s^{(4)}(k, p, q)}{\omega^2 - (E_{hp} + E_{hp+q} - \omega_{q+k})^2} \right) \end{aligned}$$

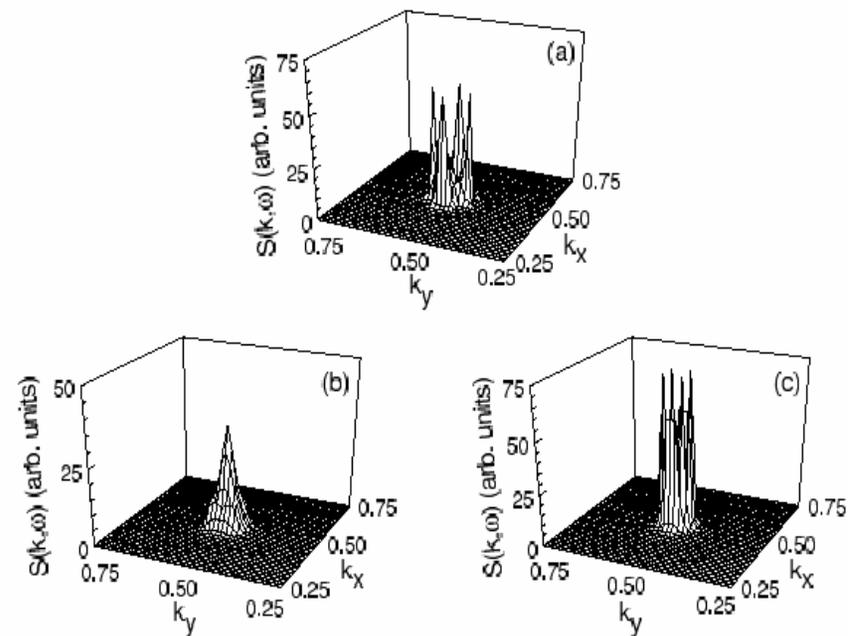
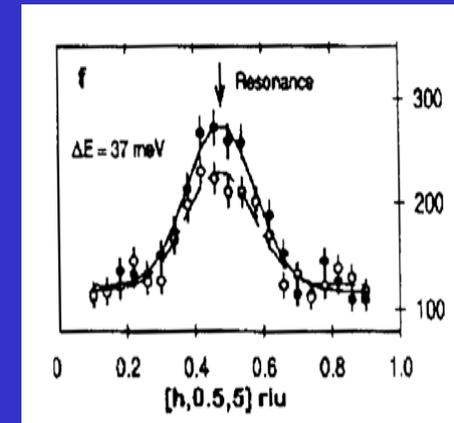
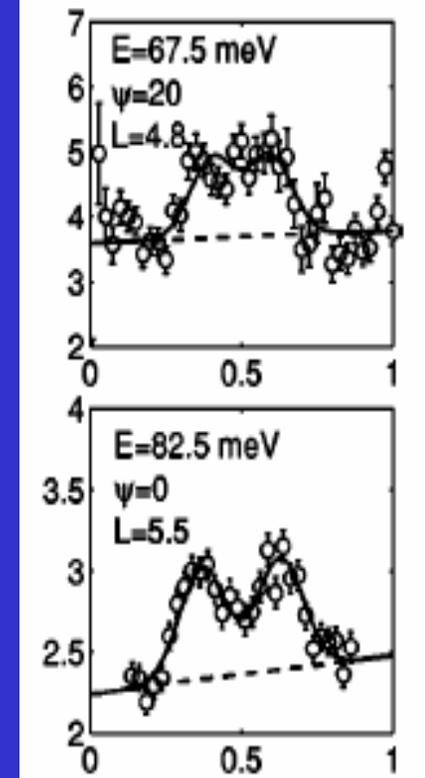
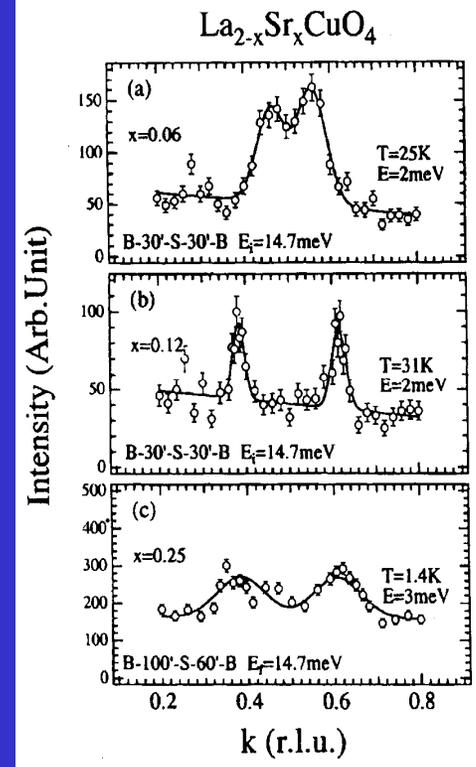


Figure 1.5: The dynamical spin structure factor $S(\mathbf{k}, \omega)$ in the (k_x, k_y) plane at $x_{\text{opt}} = 0.15$ with $T = 0.002J$ for $t/J = 2.5$ and $t'/t = 0.3$ at (a) $\omega = 0.12J$, (b) $\omega = 0.4J$, and (c) $\omega = 0.82J$.



- a. Incommensurate scattering at low energies;
- b. Commensurate resonance at intermediate energies;
- c. Incommensurate scattering at high energies.

Feng *et al.*, Lett. A352, 438 (2006); Feng *et al.*, Physica C436, 14 (2006); Feng+Ma, in *Superconductivity Research Horizons* (Nova Science Publishers, New York, 2007) Chapter 5, pp129-158; Cheng *et al.*, PRB77, 054518 (2008).

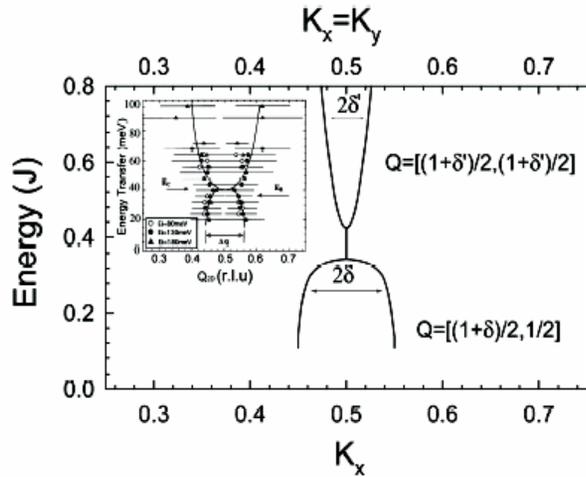
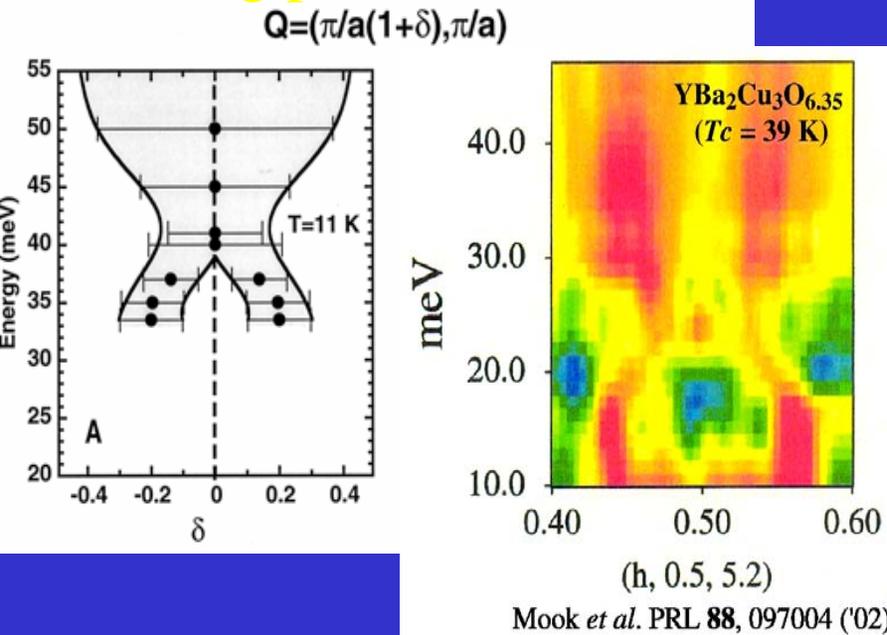
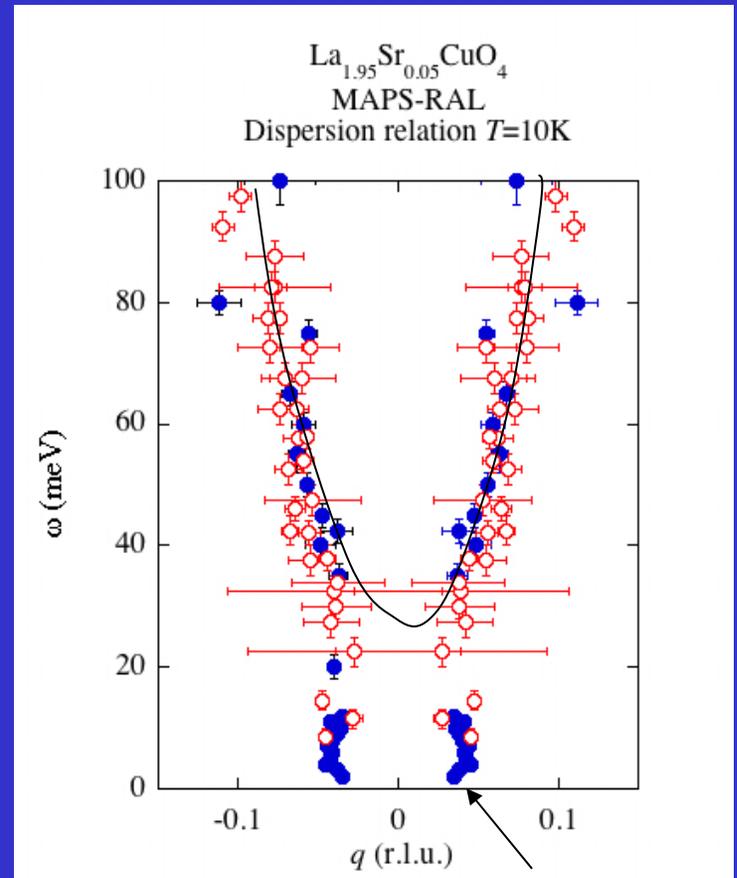


Figure 1.6: The energy dependence of the position of the magnetic scattering peaks at $x_{\text{opt}} = 0.15$ and $T = 0.002J$ for $t/J = 2.5$ and $t'/t = 0.3$. Inset: the experimental result on $\text{YBa}_2\text{Cu}_3\text{O}_{6.85}$ in the superconducting-state taken from Ref. [24].

The dispersion of magnetic scattering peaks



Feng *et al.*, Phys. Lett. A352, 438 (2006);
 Feng *et al.*, Physica C436, 14 (2006);
 Feng+Ma, in *Superconductivity Research Horizons* (Nova Science Publishers, New York, 2007) Chapter 5, pp129-158; Cheng *et al.*, PRB77, 054518 (2008).

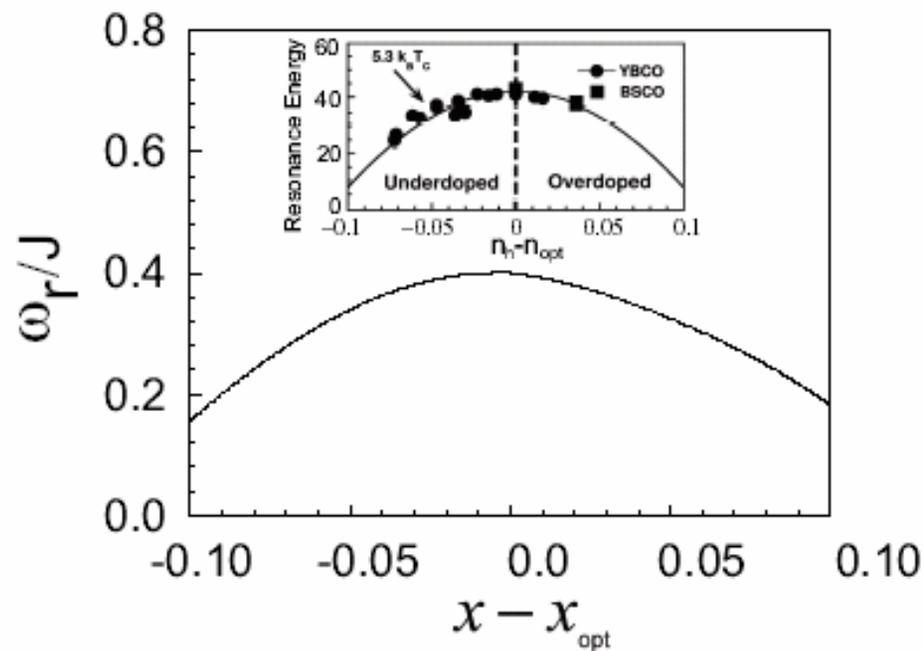


Figure 1.7: The resonance energy ω_r as a function of $x - x_{\text{opt}}$ with $T = 0.002J$ for $t/J = 2.5$ and $t'/t = 0.3$. Inset: the experimental result taken from Ref. *Physica C* 424, 45 (2005)

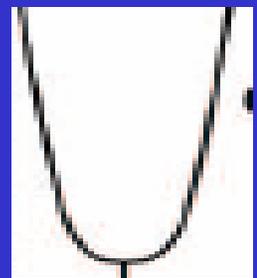
The doping dependent commensurate resonance energy

Feng *et al.*, *Phys. Lett. A* 352, 438 (2006); Feng *et al.*, *Physica C* 436, 14 (2006);
 Feng+Ma, in *Superconductivity Research Horizons* (Nova Science Publishers, New York, 2007) Chapter 5, pp129-158; Cheng *et al.*, *PRB* 77, 054518 (2008).

Physical picture:

Since in the superconducting state, the spins moves in the charge carrier pair background, where charge carrier quasiparticle spectrum has two branches, upper band $+E_k$ and lower band $-E_k$, in this case,

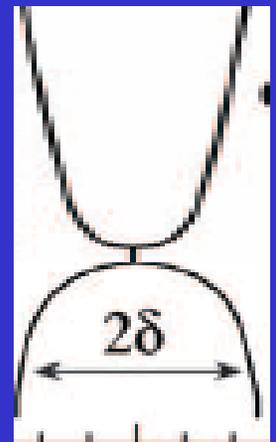
(a). The mode which opens upward is mainly determined by spins scattering in terms of the upper band of the charge carrier quasiparticle spectrum $+E_k$



(b). The mode which opens downward is mainly determined by spins scattering in terms of the lower band of the charge carrier quasiparticle spectrum $-E_k$



(c). Then two modes meet at the commensurate resonance at intermediate energy.



6. Conclusion

(1). We have developed a charge-spin separation fermion-spin theory implemented the gauge invariant charge carrier and spin, where the charge carrier represents the charge degree of freedom together with some effects of the spin configuration rearrangements due to the presence of the doped hole itself, while the spin represents the spin degree of freedom, then the electron local constraint is satisfied.

(2). Based on the charge-spin separation fermion-spin theory, we have developed the kinetic energy driven superconducting mechanism for cuprate superconductors, where the charge carriers interact occurring directly through the kinetic energy by exchanging spin excitations, leading to a net attractive force between charge carriers, then the electron Cooper pairs originating from the charge carrier pairing state are due to the charge-spin recombination, and their condensation reveals the superconducting ground-state.

(3). The superconducting state is controlled by both gap function and superconducting quasiparticle coherent weight, which leads to that the maximal superconducting transition temperature T_c occurs around the optimal doping, and then decreases in both underdoped and overdoped regimes. In other words, the strong electron correlation favors superconductivity because the main ingredient was identified into a pairing mechanism involving the internal spin degree of freedom.

(4). The charge carrier pairs condense with the d-symmetry in a wide range of doping, then the electron Cooper pairs originating from the charge carrier pairing state are due to the charge-spin recombination, and their condensation automatically gives the electron quasiparticle character. Moreover, the superconducting state is conventional BCS like, so that some of the basic BCS formalism is still valid in discussions of the doping dependence of the superconducting gap parameter and superconducting transition temperature, and electron structure, although the pairing mechanism is driven by the kinetic energy by exchanging spin excitations, and other exotic magnetic properties are beyond the BCS theory.

(5). Within this kinetic energy driven superconducting mechanism, we have discussed the effect of the impurity off-diagonal scatterers on the electronic structure of cuprate superconductors in the superconducting state. We show that the strong deviation from the monotonic d-wave superconducting gap form occurs due to the presence of the out-of-plane impurity scattering.

(6). Based on the this kinetic energy driven superconducting mechanism, we have calculated the dynamical spin structure factor in the superconducting state, and reproduce all main features of inelastic neutron scattering experiments, including the doping and energy dependence of the incommensurate magnetic scattering at both low and high energies and commensurate resonance at intermediate energy.

Thanks