Multiband effects on T_c

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New ingredient: orbital weights

Multiorbital/multiband problem

$$H_I = U \sum_{i,o} n_{i,o,\uparrow} n_{i,o,\downarrow} + \frac{U'}{2} \sum_{\substack{i,o\neq o' \\ s,s'}} n_{i,o,s} n_{i,o',s'}$$

$$= \frac{1}{2} \sum_{\substack{i,o1\ldots o4 \\ s,s'}} V_{o1\ldots o4} c^{\dagger}_{i,o3,s} c^{\dagger}_{i,o4,s'} c_{i,o2,s'} c_{i,o1,s}$$

Transform into band representation $\gamma_{n,\vec{k},s} = \sum_{o} u_{no}(\vec{k}) c_{o,\vec{k},s}$

$$V_{n1n2n3n4}(\vec{k}_1, \vec{k}_2; \vec{k}_3, \vec{k}_4) = \sum_{o1,o2,o3,o4} u_{n1o1}(\vec{k}_1) u_{n2o2}(\vec{k}_2) u^*_{n3o3}(\vec{k}_3) u^*_{n4o4}(\vec{k}_4) V_{o1\ldots o4}$$

the ‚orbital makeup‘

For multi-orbital case, bare interactions in band language are much richer!

Besides Fermi surface shape/density of states, orbital makeup is important!

Can one find simple principles that determine T_c?

T_c trends in pnictides

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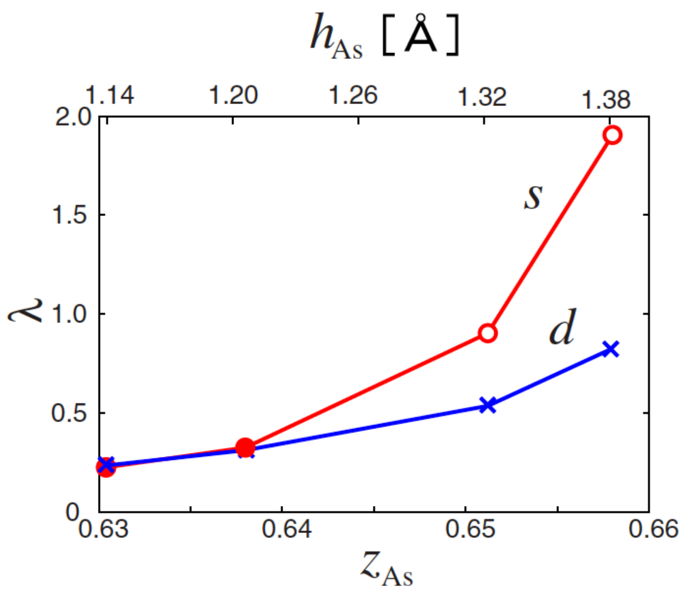
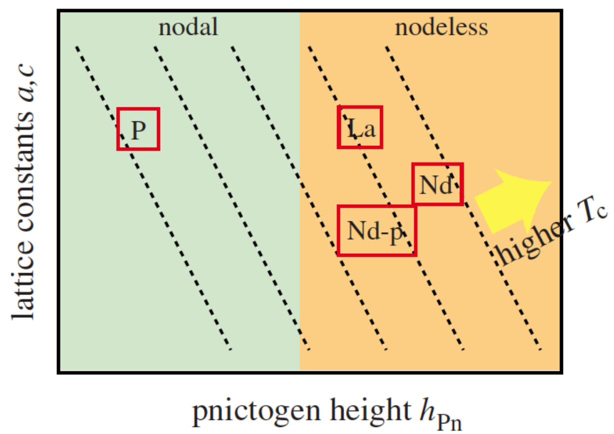
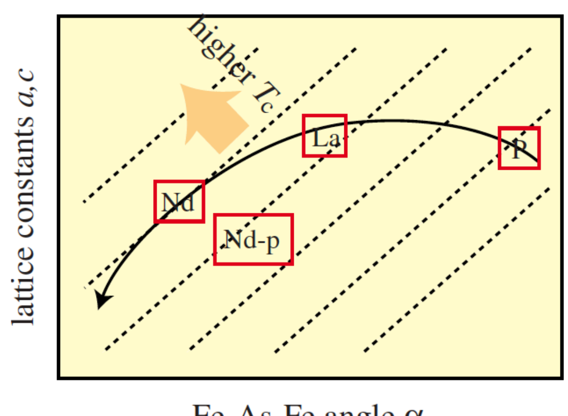
Pnictogen height as a possible switch between high-T_c nodeless and low-T_c nodal pairings in the iron-based superconductors

Kazuhiko Kuroki,[1,2] Hidetomo Usui,[1] Seiichiro Onari,[2,3] Ryotaro Arita,[2,4,5] and Hideo Aoki[2,6]







Electronic structure trends in cuprates

Band-Structure Trend in Hole-Doped Cuprates and Correlation with $T_{c\,\max}$

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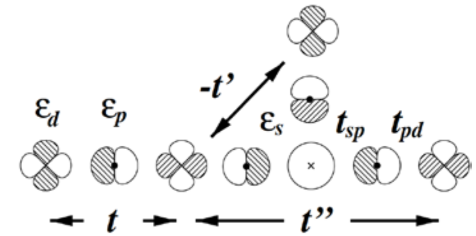
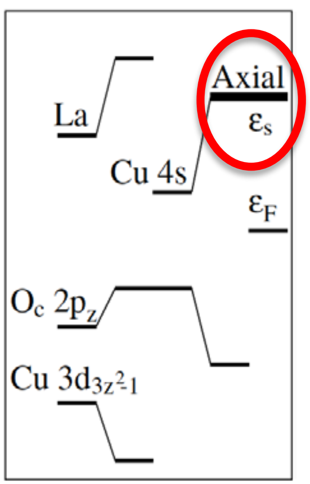
(Received 4 December 2000; published 10 July 2001)

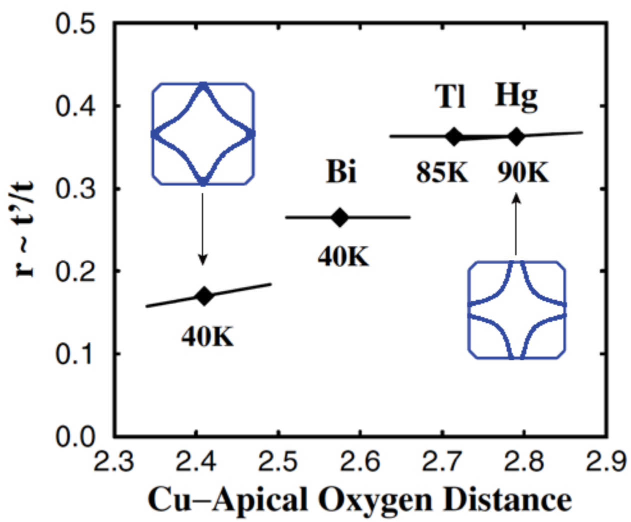
By calculation and analysis of the bare conduction bands in a large number of hole-doped high-temperature superconductors, we have identified the range of the intralayer hopping as the essential, material-dependent parameter. It is controlled by the energy of the axial orbital, a hybrid between Cu 4*s*, apical-oxygen $2p_z$, and farther orbitals. Materials with higher $T_{c\,\max}$ have larger hopping ranges and axial orbitals more localized in the CuO_2 layers.

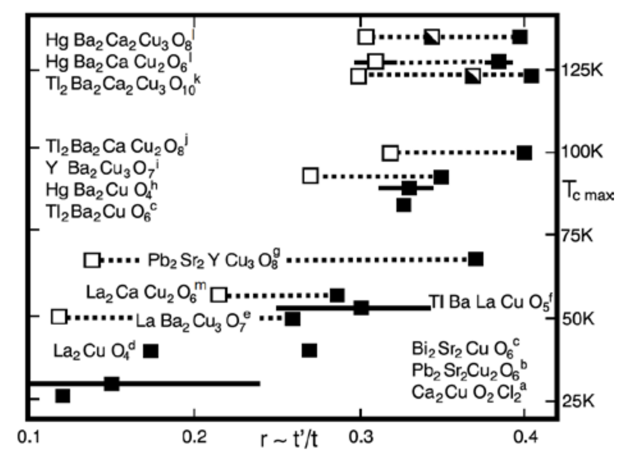


Nearest-neighbor hopping *t'* through 'axial orbital' (Cu 4*s* hybridized with apical O p_z)

Energy of axial orbital decreases with apical O distance, *t'* grows, T_c grows







Trend: T_c rises with *t'/t*, although Fermi surface more curved

Trend in cuprates

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Two-Orbital Model Explains the Higher Transition Temperature of the Single-Layer Hg-Cuprate Superconductor Compared to That of the La-Cuprate Superconductor

Hirofumi Sakakibara,[1] Hidetomo Usui,[1] Kazuhiko Kuroki,[1,4] Ryotaro Arita,[2,4,5] and Hideo Aoki[3,4]

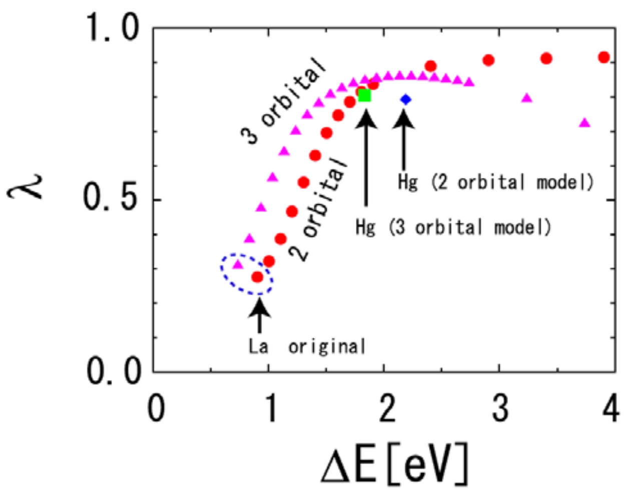
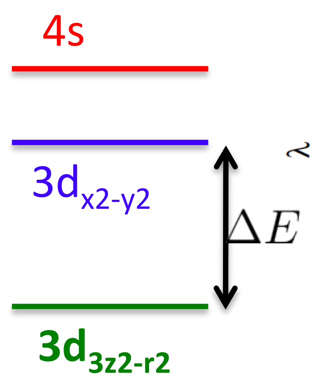


FIG. 3 (color online). The eigenvalue λ of the Eliashberg equation for d-wave superconductivity is plotted against $\Delta E = E_{x^2-y^2} - E_{z^2}$ for the two-orbital (circles) or three-orbital (triangles) models for La_2CuO_4. Corresponding eigenvalues for $HgBa_2CuO_4$ are also indicated.



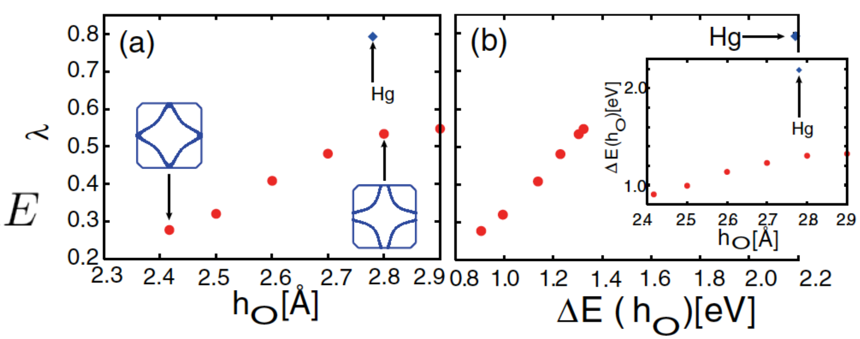


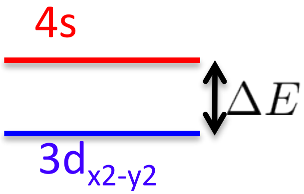
FIG. 4 (color online). The eigenvalue of the Eliashberg equation λ (circles) when h_O (a) or ΔE (b) is varied hypothetically in the lattice structure of La_2CuO_4. The diamond indicates the eigenvalue of $HgBa_2CuO_4$. The inset in (b) shows the relation between h_O and ΔE.

$$\Delta E_{4s-3dz^2} = const.$$

Qualitative & simple understanding?

@ weak coupling (fRG)

What are the tuning parameters besides density of states and Fermi surface shape?



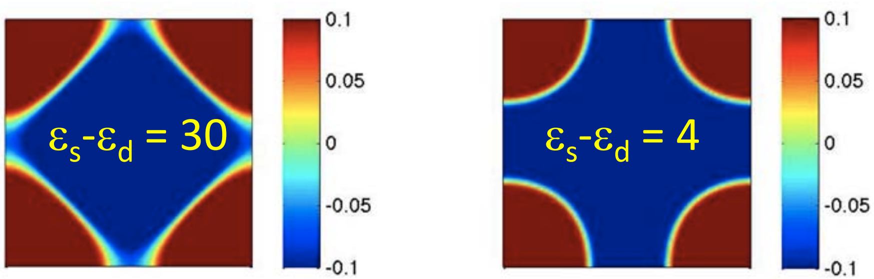
Two-orbital scenario

$$H = \begin{pmatrix} \epsilon_d + W_d(1-u) & -v\sqrt{W_d W_s} \\ -v\sqrt{W_d W_s} & \epsilon_s + W_s(1-u) \end{pmatrix}$$

$$u = \frac{1}{2}(\cos k_y + \cos k_x)$$
$$v = \frac{1}{2}(\cos k_y - \cos k_x)$$

Hybridization between $d_{x2\text{-}y2}$ orbital and s-like orbital

- changes sign upon 90deg rotation
- increases Fermi surface curvature, causes *t'*



W_d=1, W_s=2

Simplest approximation:

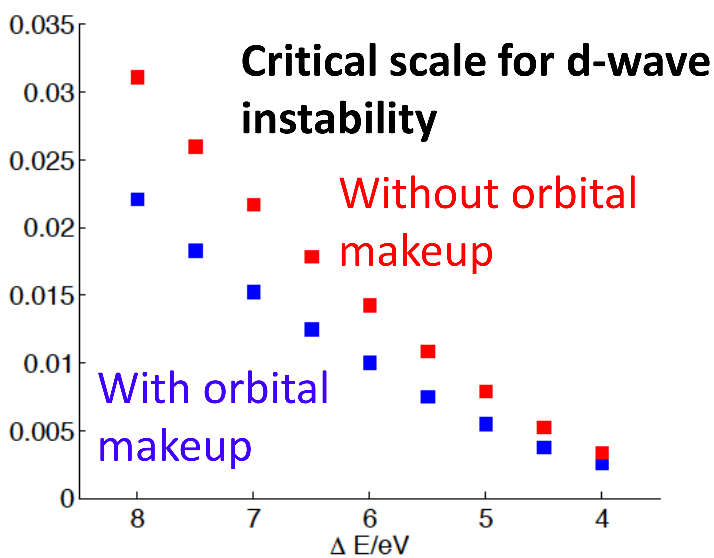
Keep only interaction on *d*-dominated band at Fermi level

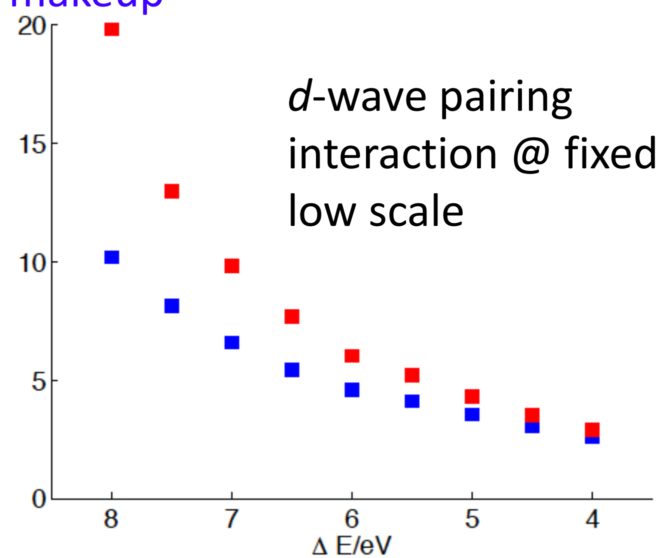
Two-orbital scenario, RG flow to strong coupling

Keep only interaction on band at Fermi surface
Run RG flow with/without orbital makeup

$$V_{n1n2n3n4}(\vec{k}_1, \vec{k}_2; \vec{k}_3, \vec{k}_4) = \sum_{o1,o2,o3,o4} u_{n1o1}(\vec{k}_1) u_{n2o2}(\vec{k}_2) u^*_{n3o3}(\vec{k}_3) u^*_{n4o4}(\vec{k}_4) V_{o1\ldots o4}$$

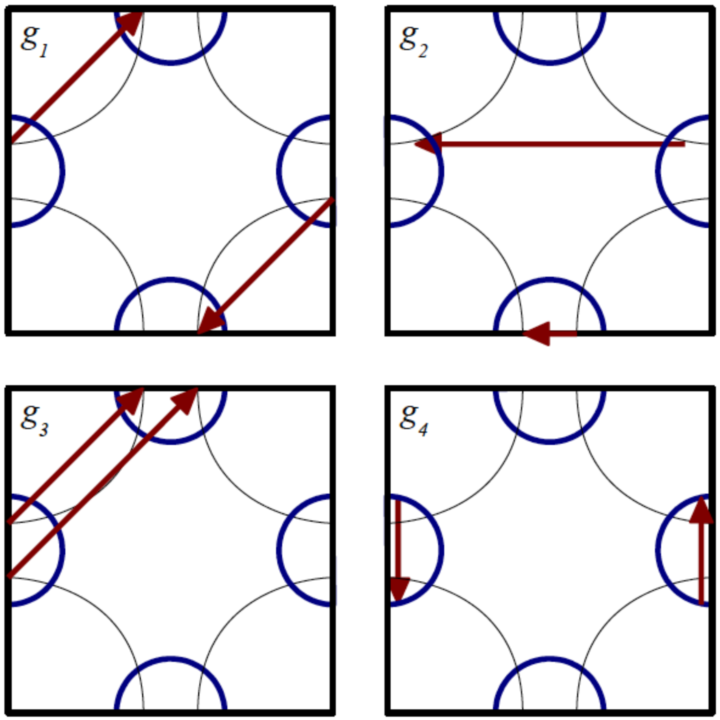
the ‚orbital makeup‘

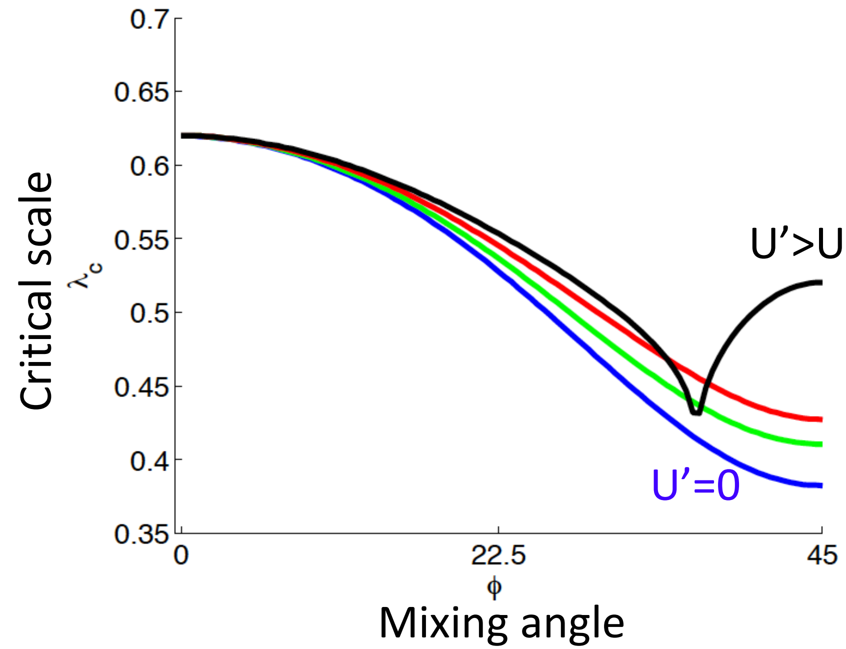




Orbital make-up reduces T_c, reduces *d*-wave pairing strength

Make-up hurts: Two-patch analysis





Local interactions U, U' lead to

$$g_{1,3} = (c^4 + s^4)U - 2c^2 s^2 U'$$
$$g_{2,4} = (c^4 + s^4)U + 2c^2 s^2 U'$$
$$c = \cos\phi \text{ and } s = \sin\phi$$

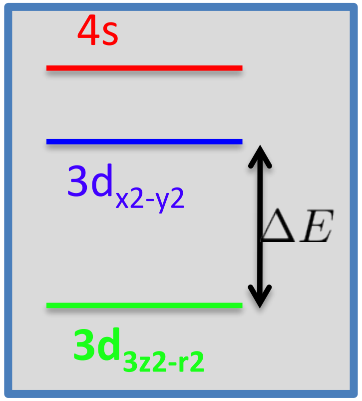
d-wave pairing wants large g_3-g_4!

At least for this system, orbital makeup does not help T_c!

Three-band case

Hybridizations between

- Central d_{x2-y2} orbital
- s-like orbital above
- d_{3z2-r2}-orbital below



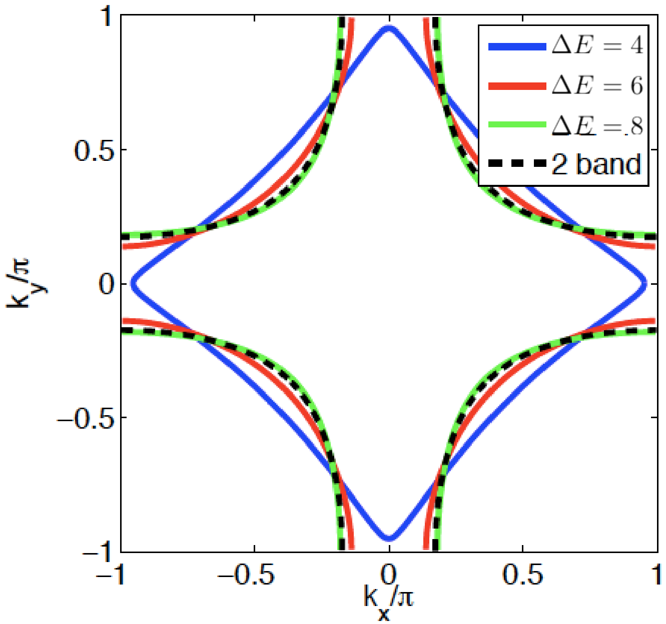
Vary

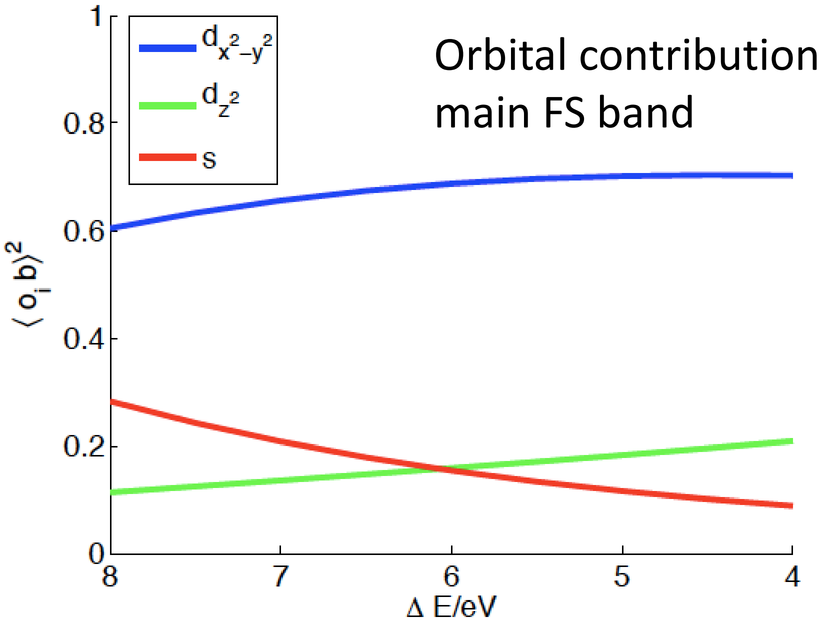
$$\Delta E = \epsilon_d - \epsilon_z$$

Keep constant

$$\Delta E_{4s-3dz^2} = 8eV, const.$$

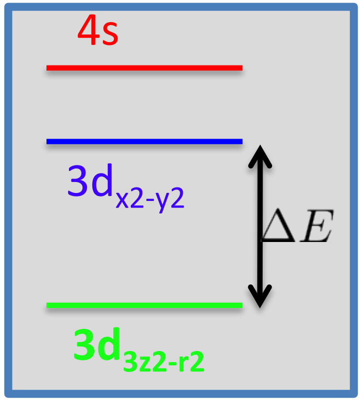
$$H = \begin{pmatrix} \epsilon_z + W_z(1-u) & -v\sqrt{W_d W_z} & u\sqrt{W_z W_s} \\ -v\sqrt{W_d W_z} & \epsilon_d + W_d(1-u) & -v\sqrt{W_d W_s} \\ u\sqrt{W_z W_s} & -v\sqrt{W_d W_s} & \epsilon_s + W_s(1-u) \end{pmatrix}$$





Orbital contributions to main FS band

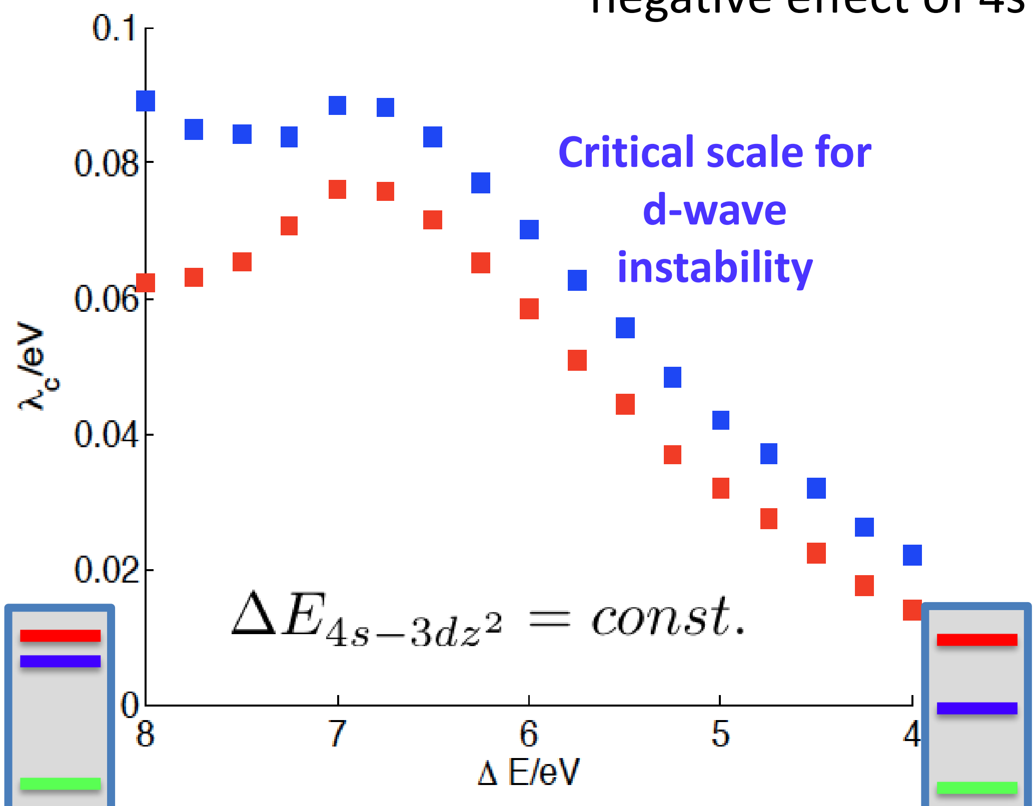
Trend for T_c



4s-like band should be wider than $3d_{z2}$-band!

Change of 4s admixture occurs on larger energy scale than change of $3d_{z2}$-admixture!

Negative effect of $3d_{z2}$ disappears more quickly than negative effect of 4s grows!

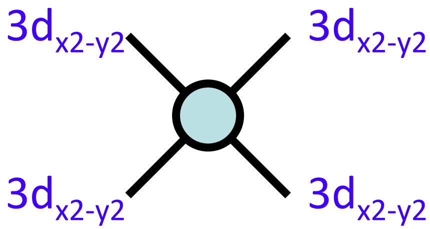


Marked increase of T_c when 4s, $3d_{z2}$ orbital are lowered with respect to $3d_{x2-y2}$!

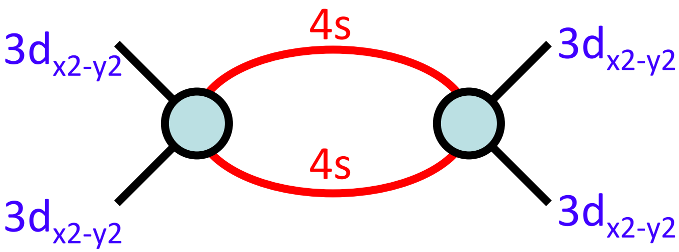
Relevance to be clarified …

Additional interaction contributions

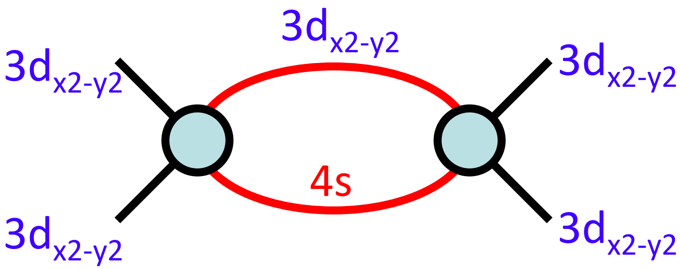
So far interactions are projected onto $3d_{x2-y2}$-dominated band near Fermi level



Corrections due to virtual excitations in occupied/empty bands



Could be captured by cRPA



Not captured by cRPA, but possibly largest, as only one intermediate particle gapped