IV. Renormalization of EPI by Strong Correlations in HTSC

↓

- Crystal structure of HTSC oxides

↓

- Electronic structure

↓

- Madelung (ionic) and covalent EPI

↓

- Strong correlations in HTSC

↓

- Self-energy due to EPI

↓

- Forward scattering peak in EPI

↓

- Resistivity of HTSC due to EPI

$\downarrow$

Ionic and Covalent EPI Coupling in HTSC Oxides

$\downarrow$

- Crystal structure (see **Fig**.**Struc**)

$\downarrow$

- Layered materials with CuO_2 conducting planes

$\downarrow$

- Tight binding model of conduction and valence bands

$\downarrow$

- There are 2(O-ions) $\times 3$(p-orbitals) $= 6$ p-orbitals $+ 5$ Cu d-orbitals

$=$ **11 orbitals** per CuO_2 ”unit” cell in the plane

$\Downarrow$

p-orbitals (see Fig. p-orbit)

$\downarrow$

$$\Psi_{p_x} = xR_{l=1}, \quad \Psi_{p_y} = yR_{l=1}, \quad \Psi_{p_z} = zR_{l=1} \tag{1}$$

$\downarrow$

d-orbitals (see Fig.d-orbit)

$\downarrow$

$$\Psi_{d_{x^2-y^2}} = (x^2 - y^2)R_{l=2}, \ \Psi_{d_{z^2}} = (2z^2 - x^2 - y^2)R_{l=2}$$

$$\Psi_{d_{xy}} = (xy)R_{l=2}, \ \Psi_{d_{xz}} = (xz)R_{l=2}, \Psi_{d_{yz}} = (yz)R_{l=2} \tag{2}$$

$\Downarrow$

7 π-bands and **4 σ-bands** = **11 bands** (see Fig. Orbit.)

$\downarrow$

Basic Hamiltonian

$\downarrow$

$$H = H_0 + H_{int} \tag{3}$$

$\downarrow$

$$H_0 = \sum_{i,\sigma}(\epsilon_d^0 - \mu)d_{i\sigma}^\dagger d_{i\sigma} + \sum_{j,\alpha,\sigma.}(\epsilon_{p\alpha}^0 - \mu)p_{j\alpha\sigma}^\dagger p_{j\alpha\sigma}$$
$$+ \sum_{i,j,\alpha,\sigma} t_{ij\alpha}^{pd} d_{i\sigma}^\dagger p_{j\alpha\sigma} + \sum_{j,j',\alpha,\beta,\sigma} t_{jj',\alpha\beta}^{pp} p_{j\alpha\sigma}^\dagger p_{j'\beta\sigma} + h.c \tag{4}$$

$\downarrow$

$\alpha, \beta = x, y, z$

$\downarrow$

- Bands for $t^{pp}_{jj',\alpha\beta} << t^{pd}_{ij\alpha}$

$\downarrow$

$$H_0 = H^{d_{xz},p_z}_{0,\pi} + H^{d_{yz},p_z}_{0,\pi} + H^{d_{xy},p_x,p_y}_{0,\pi} + H^{d_{x^2-y^2},d_{z^2},p_x,p_y}_{0,\sigma} \quad (5)$$

$\downarrow$

$\pi - BONDS$

$\downarrow$

2π-bonds from $\Psi_{d_{xz}}$ and Ψ_{p_z} ($t_{d_{xz}p_z} = t_1$) along x-axis

$\downarrow$

$$H^{d_{xz},p_z}_{0,\pi} = t_1 \sum_{i\sigma} [p^\dagger_{i\sigma}(d_{i+x,\sigma} - d_{i-x,\sigma}) + c.c.] = -2it_1 \sum_{\mathbf{k}\sigma} \sin\theta_x [p^\dagger_{\mathbf{k}\sigma} d_{\mathbf{k}\sigma} - d^\dagger_{\mathbf{k}\sigma} p_{\mathbf{k}\sigma}] \quad (6)$$

$\downarrow$

Spectrum (2 $\pi - bands$) ($a = 1$)

$$E_{1,2,\mathbf{k}} = \frac{\epsilon_p^0 + \epsilon_d^0}{2} \pm \frac{1}{2}\sqrt{(\epsilon_p^0 - \epsilon_d^0)^2 + 16t_1^2 \sin^2 k_x} \tag{7}$$

↓

- Next two bands from $\Psi_{d_{yz}}$ and Ψ_{p_z} bonds (O along y-axis)

$$E_{3,4,\mathbf{k}} = E_{1,2,\mathbf{k}}(k_x \to k_y) \tag{8}$$

↓

Three $\pi - bands$ from bonding $\Psi_{d_{xy}}$ with Ψ_{p_y} (O along the x-axis) and $\Psi_{d_{xy}}$ with Ψ_{p_x} (O along the y-axis) ; $t_1 \lesssim 1\ eV$

↓

$$E_{5,\mathbf{k}} = \epsilon_p^0 \tag{9}$$

↓

$$E_{6,7,\mathbf{k}} = \frac{\epsilon_p^0 + \epsilon_d^0}{2} \pm \frac{1}{2}\sqrt{(\epsilon_p^0 - \epsilon_d^0)^2 + 16t_1^2[\sin^2 k_x + \sin^2 k_y]} \tag{10}$$

↓

$\sigma - BONDS$

$\downarrow$

- Made from $\Psi_{d_{x^2-y^2}}$, $\Psi_{d_{z^2}}$ and Ψ_{p_x} (O along the x-axis) and Ψ_{p_y} (O along the y-axis)

$\Downarrow$

4 $\sigma - bands$

$$E_{8,9,\mathbf{k}} = \epsilon_p^0,\ \epsilon_d^0 \tag{11}$$

$\downarrow$

$$E_{10,11,\mathbf{k}} = \frac{\epsilon_p^0 + \epsilon_d^0}{2} \pm \frac{1}{2}\sqrt{(\epsilon_p^0 - \epsilon_d^0)^2 + 4t_{pd\sigma}^2[\sin^2 k_x + \sin^2 k_y]} \tag{12}$$

$$t_{pd\sigma}^2 = t_{pd_{x^2-y^2}}^2 + t_{pd_{z^2}\sigma}^2$$

$\downarrow$

- Band width W

$$W = 4\sqrt{2}\ \mid\ t_{pd\sigma}\ \mid \approx 9\ eV \tag{13}$$

- Top (antibonding) band $E_{11,\mathbf{k}} = E_{a,\mathbf{k}} \Rightarrow$ conduction band (see Fig. AB)

HALF-FILLING CASE

- **One hole** on Cu-site (9 electrons in d-state)

- **No holes** on O-site (6 electrons in p-state)

$\Downarrow$

- One hole per unit cell $\Rightarrow$ system (La_2CuO_4) should be metallic!

- Experiment: La_2CuO_4 is AF isolator !

$\Downarrow$

Strong correlations are important

$\Downarrow$

INTERACTION

$\downarrow$

$$H_{int} = U_d \sum_i n^d_{i\uparrow} n^d_{i\downarrow} + U_p \sum_{j,\alpha} n^p_{j\alpha\uparrow} n^p_{j\alpha\downarrow} + V_c + H_{ep}. \tag{14}$$

$$U_d \sim 10\ eV,\ U_d \sim 5\ eV$$

$\downarrow$

- What happens when one hole is added $\Rightarrow$ it goes to O into$\Rightarrow$p-state $\Rightarrow$makes (Zhang-Rice) singlet with d-hole

$\Downarrow$

- The **p-d singlet** behaves as a hole in the singlet Hubbard model

$\downarrow$

- Effective single-band Hubbard model

$\downarrow$

$$H_{int} = -t \sum_{i,j,\alpha,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} - t' \sum_{i,i',\alpha,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma}$$

$$+ U_{ZR} \sum_{i} n_{i\uparrow} n_{i\downarrow} + V_c + H_{ep} \qquad (15)$$

$$U_{ZR} \approx \epsilon^0_p - \epsilon^0_d$$

$\downarrow$

For $\epsilon^0_p - \epsilon^0_d >> t \Rightarrow$ **large U limit**

$\downarrow$

$$H_{tJ} = -\sum_{i,j,\sigma} t_{ij} X^{\sigma 0}_i X^{0\sigma}_j + \sum_{i,j,} J_{ij} (\mathbf{S}_i \bullet \mathbf{S}_j - \frac{1}{4} n_i n_j)$$

$$+ V_c + H_{ph} + H_{ep} \qquad (16)$$

$\downarrow$

$\downarrow$

EPI INTERACTION

↓

$$H_{ep} = H_{ep}^{ion} + H_{ep}^{cov}$$

↓

- Ionic EPI

↓

$$H_{ep}^{ion} = \sum_{i,\sigma} \Phi_i(\hat{X}_i^{\sigma\sigma} - \langle \hat{X}_i^{\sigma\sigma} \rangle) \qquad (17)$$

↓

Φ_i - nonlinear lattice distortion operator

↓

Due to Eq.(17) $\Rightarrow < \Phi_i >= 0$

↓

$$\Phi_i = -\sum_{L\kappa} e^2 Z_{L\kappa} [V_{el}(\mathbf{R}_i^0 - \mathbf{R}_{L\kappa}^0 + \hat{\mathbf{u}}_i - \hat{\mathbf{u}}_{L\kappa})$$

$$- V_{el}(\mathbf{R}_i^0 - \mathbf{R}_{L\kappa}^0)], \qquad (18)$$

↓

- Electron-lattixe potential V_{el}

↓

- **Covalent EPI**

↓

$$H_{ep}^{cov} = -\sum_{i,j,\sigma} \frac{\partial t_{ij}}{\partial(\mathbf{R}_i^0 - \mathbf{R}_j^0)} (\hat{\mathbf{u}}_i - \hat{\mathbf{u}}_j) X_i^{\sigma 0} X_j^{0\sigma} \; + $$

$$+ \sum_{i,j,} \frac{\partial J_{ij}}{\partial(\mathbf{R}_i^0 - \mathbf{R}_j^0)} (\hat{\mathbf{u}}_i - \hat{\mathbf{u}}_j) \mathbf{S}_i \bullet \mathbf{S}_j . \tag{19}$$

↓

- in HTSC for a number of phonons holds

↓

$$\frac{\partial V_{ion}}{\partial \mathbf{R}} >> \frac{\partial t_{ij}}{\partial \mathbf{R}} >> \frac{\partial J_{ij}}{\partial \mathbf{R}} \tag{20}$$

↓

IONIC EPI - DETAILS

- How to derive Σ_{ep}?

- To remain

$$g(1,2) = G(1,2) Q^{-1}(2) \tag{21}$$

↓

$$\gamma_c(1,2;3) = -\frac{\delta g^{-1}(1,2)}{\delta U^{\bar{\sigma}\bar{\sigma}}(3)}. \qquad (22)$$

↓

- **Migdal theorem**

$$\Sigma(1,2) = \Sigma_0(1,2) + \Sigma_{ep}^{(1)}(1,2) + .. \qquad (23)$$

↓

$\Sigma_0(1,2)$ picks up correlation effects

$\Sigma_{ep}^{(1)}(1,2)$ is linear w.r.t. V_{ep}

↓

Dyson equation

↓

$$(g_{00}^{-1} - \Sigma) \bullet g = 1 \qquad (24)$$

↓

- g_0 includes correlation effects

↓

$$(g_{00}^{-1} - \Sigma_0) \bullet g_0 = 1 \qquad (25)$$

⇓

$$(g_0^{-1} - \Sigma_{EP}) \bullet g = 1. \qquad (26)$$

$\Sigma_{ep} << \Sigma_0$

$\downarrow$

$$g^{-1} = g_0^{-1} + \delta g^{-1}$$

$$\delta g^{-1} = -\Sigma_{ep} \qquad (27)$$

$\downarrow$

From $g \bullet g^{-1} = 1$ and $\delta g^{-1} << g^{-1}$

$\Downarrow$

$$\delta g^{-1} = -g_0^{-1} \bullet \delta g \bullet g_0^{-1} \qquad (28)$$

$\Downarrow$

$$\Sigma_{ep}^{(1)} = g_0^{-1} \bullet \delta g \bullet g_0^{-1}. \qquad (29)$$

$\downarrow$

From Eq.(21)

$\downarrow$

$$\delta g = \delta G \bullet Q^{-1} - g_0 \bullet Q^{-1} \bullet \delta Q \qquad (30)$$

$\downarrow$

$\downarrow$

2-nd order perturbation

$\Downarrow$

O(1/N) terms in EPI

$\downarrow$

$$\delta G(1,2) = -\frac{1}{2!}\frac{\langle T_\tau S X^{0\sigma}(1) X^{\sigma 0}(2)\Phi(\bar{1})\Phi(\bar{2})\delta n(\bar{1})\delta n(\bar{2})\rangle}{\langle \bullet \rangle} \tag{31}$$

$$\delta n(1) = X^{\bar{\sigma}\bar{\sigma}}(1) - \langle X^{\bar{\sigma}\bar{\sigma}}(1)\rangle$$

$\Downarrow$

$$\delta G(1,2) = -\frac{1}{2}V_{ep}(\bar{1}-\bar{2})\frac{\delta^2 G(1,2)}{\delta U^{\bar{\sigma}_1\bar{\sigma}_1}(\bar{1})\delta U^{\bar{\sigma}_2\bar{\sigma}_2}(\bar{2})}. \tag{32}$$

$\downarrow$

$$\Sigma_{ep}^{(1)} = \Sigma_{ep}^{(dyn)} + \Sigma_{ep}^{(stat)} + \Sigma_{ep}^{(Q)} \tag{33}$$

$\downarrow$

- For SC is $\Sigma_{ep}^{(dyn)}$ important

$\downarrow$

$$\Sigma_{ep}^{(dyn)}(1-2) = -V_{ep}(\bar{1}-\bar{2})\gamma_c(1,\bar{3};\bar{1}) \times g_0(\bar{3}-\bar{4})\gamma_c(\bar{4},2;\bar{2}) \tag{34}$$

$$V_{ep}(1-2) = \varepsilon_e^{-1}(1-\bar{1})V_{ep}^0(\bar{1}-\bar{2})\varepsilon_e^{-1}(\bar{2}-2). \tag{35}$$

$$V_{ep}^{0}(1-2) = -\langle T\hat{\Phi}(1)\hat{\Phi}(2)\rangle \qquad (36)$$

$\downarrow$

- Harmonic EPI $\Rightarrow \hat{\Phi}(1) \sim \nabla V_{el}\mathbf{u}$

$\Downarrow$

$$V_{ep}(1,2) = \varepsilon_e^{-1}(1,\bar{1})\nabla V_{el}(\bar{1})D(\bar{1},\bar{2})\nabla V_{el}(\bar{2})\varepsilon_e^{-1}(\bar{2},2) \qquad (37)$$

$\downarrow$

SELF-ENERGY $\Sigma_{ep}(\mathbf{k},\omega)$

$\downarrow$

$$\Sigma_{ep}^{(dyn)}(\mathbf{k},\omega) = \int_0^\infty d\Omega \langle \alpha^2 F(\mathbf{k},\mathbf{k}',\Omega)\rangle_{\mathbf{k}'} R(\omega,\Omega) \qquad (38)$$

$\downarrow$

$\langle ... \rangle_{\mathbf{k}}$ - Fermi-surface average

$\downarrow$

$$R(\omega,\Omega) = -2\pi i (n_B(\Omega) + \frac{1}{2})$$

$$+\psi(\frac{1}{2} + i\frac{\Omega-\omega}{2\pi T}) - \psi(\frac{1}{2} - i\frac{\Omega+\omega}{2\pi T}) \qquad (39)$$

$$n_B(\Omega) = \frac{1}{e^{\beta\Omega} - 1}$$

$\downarrow$

ψ - di-gamma function

$\downarrow$

SPECTRAL FUNCTION $\alpha^2 F(\mathbf{k}, \mathbf{k}', \omega)$

$\downarrow$

$$\alpha^2 F(\mathbf{k}, \mathbf{k}', \omega) = N_{sc}(0) \sum_{\nu} \mid g_{eff}(\mathbf{k}, \mathbf{k} - \mathbf{k}', \nu) \mid^2$$
$$\times \delta(\omega - \omega_\nu(\mathbf{k} - \mathbf{k}'))\gamma_c^2(\mathbf{k}, \mathbf{k} - \mathbf{k}', \omega_\nu). \tag{40}$$

$\downarrow$

$g_{eff}(\mathbf{k}, \mathbf{p}, \nu)$ - EPI coupling in the ν-the mode

$\downarrow$

$$g_{eff}(\mathbf{k}, \mathbf{p}, \nu) = \frac{g(\mathbf{k}, \mathbf{p}, \nu)}{\varepsilon_e(\mathbf{p}, \omega_\nu)} \tag{41}$$

$\downarrow$

$\varepsilon_e(\mathbf{p}, \omega_\nu)$ - electronic dielectric function

$\downarrow$

$t - t'$ model ($J = 0$)

$\Rightarrow N_{sc}(0) = N_0(0)/q_0 \; q_0 = \delta/2$

↓

$t - J$ model

$\Rightarrow N_{sc}(0)(\sim 1/J_0) > N_0(0)$ (band density of states $N_0(0)$)

↓

CHARGE VERTEX γ_c IN O(1) ORDER

↓

Integral equation in O(1) order

↓

$$\gamma_{c0}(1,2;3) = -\frac{\delta g_0^{-1}(1,2)}{\delta U^{\bar{\sigma}\bar{\sigma}}(3)} \qquad (42)$$

↓

$$\begin{aligned}\gamma_{c0}(1,2;3) &= \delta(1-2)\delta(1-3)\\ &+ t_0(1-2)g_0(1,\bar{1})\gamma_{c0}(\bar{1},\bar{2};3)g_0(\bar{2},1^+)\\ &+ \delta(1-2)t_0(1-\bar{1})g_0(\bar{1},\bar{2})\gamma_{c0}(\bar{2},\bar{3};3)g_0(\bar{3},1) -\\ &- J_0(1-2)g_0(1-\bar{1})\gamma_{c0}(\bar{1},\bar{2};3)g_0(\bar{2},2)\ .\end{aligned} \qquad (43)$$

↓

- In $(\mathbf{k},\omega)$ space

$$\gamma_c(\mathbf{k},q) = 1 - \sum_{\alpha=1}^{6}\sum_{\beta=1}^{6} F_\alpha(\mathbf{k})[\hat{1} + \hat{\chi}(q)]^{-1}_{\alpha\beta}\chi_{\beta 2}(q), \tag{44}$$

↓

$$\chi_{\alpha\beta}(q) = \sum_p G_\alpha(p,q)F_\beta(\mathbf{p}), \tag{45}$$

↓

$$F_\alpha(\mathbf{k}) = [t(\mathbf{k}), 1, 2J_0\cos k_x, 2J_0\sin k_x, 2J_0\cos k_y, 2J_0\sin k_y], \tag{46}$$

↓

$$G_\alpha(p,q) = [1, t(\mathbf{p}+\mathbf{q}), \cos p_x, \sin p_x, \cos p_y, \sin p_y]\Pi(p,q), \tag{47}$$

$$\Pi(k,q) = -g(k)g(k+q) \tag{48}$$

↓

$q = (\mathbf{q}, iq_n)$, $q_n = 2\pi nT$

$p = (\mathbf{p}, ip_m)$, $p_m = \pi T(2m+1)$

$$\sum_{p_m}\Pi(p,q) = \frac{n_F(\xi_{\mathbf{q}+\mathbf{p}}) - n_F(\xi_{\mathbf{p}})}{\xi_{\mathbf{p}} - \xi_{\mathbf{q}+\mathbf{p}} - iq_n}. \tag{49}$$

$\Downarrow$

FORWARD SCATTERING PEAK IN $\gamma_c(\mathbf{k}_F, \mathbf{q})$

$\Rightarrow$ see Fig.FSP

$\Downarrow$

CONCLUSION

$\downarrow$

- Backward scattering $\mathbf{q} \sim \mathbf{k}_F$ is **strongly suppressed**!

$\downarrow$

RESISTIVITY

$\downarrow$

Transport spectral function

$\downarrow$

$$\alpha^2 F_{tr}(\omega) = \frac{\langle\langle \alpha^2 F(\mathbf{k}, \mathbf{k}', \omega)[\mathbf{v}(\mathbf{k}) - \mathbf{v}(\mathbf{k}')]^2 \rangle_{\mathbf{k}} \rangle_{\mathbf{k}'}}{2\langle\langle \mathbf{v}^2(\mathbf{k}) \rangle_{\mathbf{k}} \rangle_{\mathbf{k}'}}. \tag{50}$$

$\downarrow$

$\mathbf{v}(\mathbf{k}) = \partial\xi(\mathbf{k})/\mathbf{k}$ - quasiparticle velocity

Boltzmann equation $\Rightarrow \rho(T)$ (**Fig**.**Res**)

$\downarrow$

$$\rho(T) = \frac{4\pi}{\omega_p^2}\Gamma_{tr}(T) \quad (51)$$

$$\Gamma_{tr}(T) = \frac{\pi}{T}\int_0^\infty d\omega \frac{\omega}{\sin^2(\omega/2T)}\alpha_{tr}^2(\omega)F(\omega). \quad (52)$$

↓

- Transport EPI coupling λ_{tr}^{ep}

$$\lambda_{tr}^{ep} = 2\int d\omega \frac{\alpha_{tr}^2(\omega)F(\omega)}{\omega} \quad (53)$$

↓

- Pairing EPI coupling

$$\lambda^{ep} = 2\int d\omega \frac{\alpha^2(\omega)F(\omega)}{\omega} \quad (54)$$

↓

- For $T > \Theta_D/5$ (Debye spectrum)

↓

$$\rho(T) \simeq 8\pi^2\lambda_{tr}^{ep}\frac{k_B T}{\hbar\omega_{pl}^2}. \quad (55)$$

↓

- Plasma frequency ω_{pl}

⇓

- Due to **forward scattering peak** (**FSP**)

$\Downarrow$

$\lambda_{tr}^{ep} << \lambda^{ep}$!!

$\downarrow$

- **HTSC experiments**:

$\Downarrow$

$\lambda_{tr}^{ep} \sim 0.5 \qquad \lambda^{ep} \sim 1 - 2$