Why is the ARPES anti-nodal singularity at 40 meV shifted in superconducting state of HTSC, but the kink at 70 meV is not?

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The theoretical model for the quasiparticle self-energy $\Sigma(k, \omega)$ in HTSC is proposed, which is based on the forward scattering peak in the electron-phonon (EPI) interaction. By assuming that EPI dominates, the model explains qualitatively and in a consistent way the recent ARPES results. The latter show a kink in the normal state quasiparticle energy at 70 meV in the nodal direction, which is (surprisingly) not shifted in the superconducting (SC) state, while the singularity at 40 meV in the anti-nodal direction is shifted by the SC gap. The model predicts a dip-hump structure in the spectral function $A(k_F, \omega)$, which is observed in ARPES.

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Introduction - The pairing mechanism in high-temperature superconductors (HTSC) is still under the debate. However, recent ARPES gives evidence for pronounced phonon effects in the quasiparticle energy, while the theory predicts that strong correlations give rise to a pronounced forward scattering peak (FSP) in the electron-phonon interaction (EPI) and in the non-magnetic impurity scattering - the FSP model. It predicts: (i) d-wave pairing is due to the EPI and the residual Coulomb repulsion, which triggers it; (ii) the transport coupling constant $\lambda$, i.e. $\lambda \ll \lambda_c$; (iii) robustness of d-wave pairing in the presence of non-magnetic impurities, etc. The FSP in the EPI of strongly correlated systems is a general effect which affects electronic coupling to all phonons. Numerical calculations on the Hubbard model with the EPI confirm the theory of Ref.

Recent ARPES on various HTSC families show a kink in the normal (N) state quasiparticle spectrum, $\omega(k_F)$, in the nodal direction $(0, 0) - (\pi, \pi)$ at energy $\omega^{(70)} \approx 70$ meV, which is a characteristic oxygen vibration energy, i.e. $\omega^{(70)} \approx \omega_{ph}$. Surprisingly the kink is not shifted in the SC state, contrary to the standard Eliashberg theory. Furthermore, ARPES on $La_{2-x}Sr_xCuO_4$ and BISCO crystals show that in the anti-nodal direction $(\pi, 0) - (\pi, \pi)$ a singularity appears in $\omega(k_F)$ in the N state $(T > T_c)$ at $\omega^{(40)} \approx 40$ meV, which is also a characteristic oxygen vibration energy $\omega^{(40)} \approx \omega_{ph}$. It is shifted in the SC state (at low $T$) to $\omega \approx 60$ meV ($= \omega_{ph} + \Delta_0$), where $\Delta_0(\approx 20$ meV) is approximately the maximal SC gap at the anti-nodal point. The different shifts of $\omega^{(40)}$ and $\omega^{(70)}$ in the SC state we call the ARPES shift-puzzle.

Why is the anti-nodal singularity $\omega^{(40)}$ shifted in the SC state, but the nodal kink $\omega^{(70)}$ is not? The ARPES shift-puzzle can not be explained by the standard (with the integration also over the whole Fermi surface) Eliashberg (or BCS) theory for any kind of pairing, which predicts that $\omega^{(40)}$ and $\omega^{(70)}$ are shifted in the SC state by the same value $\Delta_0$, i.e. $\omega^{(40)} \rightarrow \omega^{(40)}_\text{SC} + \Delta_0$ and $\omega^{(70)} \rightarrow \omega^{(70)}_\text{SC} + \Delta_0$, where $\Delta_0$ is the maximal gap value. ARPES can not be explained by the spin-fluctuation theory (SF) based on the 41 meV magnetic-resonance mode because of at least two reasons: (i) the kink at 70 meV is present also in the N state, where there is no magnetic resonance mode and (ii) the kink is seen in $La_{2-x}Sr_xCuO_4$, where there is no magnetic resonance mode neither in the N nor in SC state. ARPES gives also evidence for the linear (in $\omega$) contribution to $\text{Im} \Sigma(\omega)$ due to the Coulomb interaction (SF is only part of it). This, i.e. $\text{Im} \Sigma_C(\omega) \sim -\pi \lambda_c \omega/2$ for $T < \omega < \Omega_C$. It is clearly discernable in ARPES for $\omega_{ph} < \omega < \Omega_C$ with $\lambda_C \lesssim 0.4$.

Here we show that the ARPES shift-puzzle implies the FSP model with the following ingredients: (i) the EPI is dominant and its spectral function $\alpha^2 F(k, k', \Omega)$ has a pronounced FSP (at $k \sim k'$) due to strong correlations. Its width is very narrow $|k - k'| \ll k_F$ even for overdoped systems; (ii) the dynamical part (beyond the Hartree-Fock) of the Coulomb interaction is characterized by the spectral function $S_C(k, k', \Omega)$. The ARPES shift-puzzle implies that $S_C$ is either peaked at small $|k - k'|$, or it is so small that it does not affect the shift. Which of these possibilities is realized is a matter of future ARPES. In order to minimize numerical calculations we assume here that the former case is realized.; (iii) The scattering potential on non-magnetic impurities has pronounced FSP, due to strong correlations. In the following we calculate $\Sigma(k, \omega)$ in the N and SC state and show that the anti-nodal singularity at $\omega^{(40)}$ is shifted in the SC state by $\Delta_0$, while the nodal kink at $\omega^{(70)}$ is not. The FSP model predicts also the existence of a dip-hump structure in $A(k, \omega)$.

Eliashberg equations for the FSP model - The normal and the anomalous Matsubara Green’s functions are defined by $G(k) = -[Z(k)\omega_n + \xi(k)]/D(k)$ and $F(k) = Z(k)\Delta(k)/D(k)$ ($k = (k, \omega_n)$, respectively, where $D(k) = (Z(k)\omega_n)^2 + [\xi^2(k) + (Z(k)\Delta(k))^2]$.}
The diagonal odd part of the self energy is $\Sigma(k, \omega_n) = \omega_n[1 - Z(k, \omega_n)](-\Sigma(k, -\omega_n))$, while its even part is $\Sigma_e(k, \omega_n) = \xi(k) - \xi_0(k) = \Sigma_c(k, -\omega_n)$, where $\xi_0(k) = \epsilon_0(k) - \mu$. Since in the following we assume the electron-hole symmetry, then $\Sigma_e(k, \omega_n) \approx \xi(k) - \xi_0(k)$, i.e. it is a dull function of $\omega$ which renormalizes the chemical potential and the bare quasiparticle energy \[3, 10\].

The 2D Fermi surface of HTSC oxides is parametrized by $k = (k_F + k_L, k_F \varphi)$, where $k_F(\varphi)$ is the Fermi momentum and $k_F \varphi$ is the tangential component of $k$ at the point on the Fermi surface \[10\]. In that case $\xi(k) \approx v_F (k_L)$ and $f d^2k[...] = \int d\varphi f(k_F \varphi) d\varphi$ \[10\]. For simplicity we assume that near the Fermi surface the EPI spectral function $\alpha_{ph}^2 F(k, k', \Omega)$ is weakly dependent on energies $\xi$, $\xi'$, i.e. $\alpha_{ph}^2 F(k, k', \Omega) \approx \alpha_{ph}^2 F(\varphi, \varphi', \Omega)$ \[10\] - see the item (i) in the discussion. In the presence of strong correlations one has $\alpha_{ph}^2 F(\varphi, \varphi', \Omega) \sim \gamma_2^2(\varphi - \varphi')$, where the charge vertex $\gamma_2(\varphi - \varphi')$ is strongly peaked at $\delta\varphi(= \varphi - \varphi') = 0$ with the width $\delta\varphi \ll \pi$ even for overdoped hole doping \[3, 5\]. Then in the leading order one has $\alpha_{ph}^2 F(\varphi, \varphi', \Omega) \approx \alpha_{ph}^2 F(\varphi, \varphi', \Omega)$ \[10\] which picks up the main physics \[5\] whenever $\delta\varphi \ll \pi$ - see also the item (i) in the discussion. After integration over $\varphi'$ and for $N_\varphi(\xi) \approx N_\varphi(0)$ one obtains the Eliashberg equations

$$\omega_{n, \varphi} = \omega_n + \pi T \sum_{m} \frac{\lambda_{ph, \varphi}(\omega_n - \omega_m)\tilde{\omega}_{m, \varphi}}{\omega_{m, \varphi}^2 + \Delta_{m, \varphi}^2}$$

$$+ \frac{\lambda_{C, n, \varphi}}{\omega_{n, \varphi}^2 + \Delta_{n, \varphi}^2}$$

$$+ \frac{\gamma_1_{n, \varphi}}{\sqrt{\omega_{n, \varphi}^2 + \Delta_{n, \varphi}^2}}$$

$$+ \frac{\gamma_2_{n, \varphi}}{\sqrt{\omega_{n, \varphi}^2 + \Delta_{n, \varphi}^2}}$$

$$+ \Delta_{n, \varphi} = \pi T \sum_{m} \frac{\lambda_{ph, \varphi}(\omega_n - \omega_m)\Delta_{m, \varphi}}{\omega_{m, \varphi}^2 + \Delta_{m, \varphi}^2} + \Delta_{C, n, \varphi},$$

$$+ \frac{\gamma_1_{n, \varphi}}{\sqrt{\omega_{n, \varphi}^2 + \Delta_{n, \varphi}^2}}$$

$$+ \frac{\gamma_2_{n, \varphi}}{\sqrt{\omega_{n, \varphi}^2 + \Delta_{n, \varphi}^2}}$$

$$+ \frac{\lambda_{ph, \varphi}(\omega_n - \omega_m)}{\omega_{n, \varphi}^2 + \Delta_{n, \varphi}^2}$$

where the EPI coupling $\lambda_{ph, \varphi}(\omega_n - \omega_m)$ is given by

$$\lambda_{ph, \varphi}(\omega_n - \omega_m) = 2 \int_0^\infty d\Omega \frac{\alpha_{ph, \varphi}^2 F(\varphi, \Omega, \Omega)}{\omega_{n, \varphi}^2 + \Delta_{n, \varphi}^2}.$$
Fermi surface, i.e. $\Delta_{n,\sigma}$ is locally “s-wave SC” and globally d-wave pairing, which is also manifested for more realistic interactions, whenever $\delta \varphi_\omega \ll \pi$ - see [2].

(1) $\omega^{(70)}_{kink}$-kink in the nodal direction ($\varphi = \pi/4$) - The kink at $\omega^{(70)}_{kink} \approx 70$ meV in $\omega(\xi_k)$ means that the quasiparticles moving along the nodal direction interact with various phonons with frequencies up to 70 meV [11], i.e. $\delta^2_{ph,\pi/4} F_{\pi/4}(\Omega) \neq 0$ for $0 < \Omega \lesssim 70$ meV. Since it is unknown, a Lorenzian shape centered at $\omega_{ph,70}$ meV is assumed. In this case the theory predicts more singularity-like [11] than the observed kink-like behavior. $\Delta_{\pi/4}(\omega) = 0$ and Eq.(1) imply that $\omega(\xi_k)$ is equal in the N and in the SC state, as it is shown in Fig.1a. It confirms that the kink in the nodal direction is not shifted in the SC state - in a qualitative agreement with ARPES findings [2].

The realistic phonon spectrum will smear the theoretical singularity in $\omega(\xi_k)$ - seen in Fig1a. In Fig.1b is shown $\text{Im} \Sigma(\xi = 0, \omega)$, where a qualitative similarity with ARPES [2] is obvious. For $\omega_{ph} < \omega < \Omega_C$ the linear term $| \text{Im} \Sigma_C(\xi = 0, \omega) | \sim \omega$ is discernable, while near $\omega_{ph}$ Im $\Sigma(\xi = 0, \omega)$ is steeper due to $\lambda_{ph}(= 1) \gg \lambda_C(= 0.3)$.

(2) $\omega^{(40)}_{sing}$-singularity in the anti-nodal direction ($\varphi \approx \pi/2$) - The singularity (not the kink) at $\omega^{(40)}_{sing}$ in $\omega(\xi_k)$ in the anti-nodal direction is observed in ARPES in the N and SC state of La$_{2-x}$Sr$_x$CuO$_4$ and BISCO [3], which means that the quasiparticle moving in the anti-nodal direction interact with a narrower phonon spectrum centered around $\omega^{(40)}_{ph} \approx 40$ meV. So, the assumed (by us) the Lorenzian shape for $\sigma^2_{ph,\varphi=\pi/2} F_{\varphi=\pi/2}(\Omega)$, centered at $\omega_{ph} \approx 40$ meV, is acceptable approximation. Since $\Delta_{\pi/2}(\omega) = \pm \Delta_0$ then Eq.(1) gives that $\omega(\xi_k)$ in the N-state is singular at $\omega_{sing} = \pm \omega_{ph}^{(40)}$, while in the SC state it is shifted to $\omega^{(40)}_{sing} = \pm (\omega_{ph}^{(40)} + \Delta_0)$. This is confirmed by numerical calculations shown in Fig.2a - $\omega(\xi_k)$, and in Fig.2b - $\text{Im} \Sigma(\varphi, \omega)$, for $\lambda_{ph} = 1$ and $\lambda_C = 0.3$.

The $\omega^{(40)}_{sing}$ singularity is shifted in the SC state, contrary to the nodal kink at $\omega^{(70)}_{kink}$ which is not. So, the different shifts of $\omega^{(70)}_{kink}$ and $\omega^{(40)}_{sing}$ in the SC state is a direct consequence of the forward scattering peak in the charge scattering processes. Since we assume a rather narrow phonon spectrum (centered around $\Omega_{ph}$) the behavior of $\text{Im} \Sigma(\xi = 0, \omega)$ at $\omega \ll \Omega_{ph}$ is due to the Coulomb interaction - the small tails in Fig1b and Fig2b.

(3) ARPES dip-hump structure - The FSP-model explains qualitatively the dip-hump structure in $A(\varphi, \omega)(= -\frac{1}{2} \text{Im} G(\varphi, \omega))$. The latter was observed recently in ARPES [3], where the dip is very pronounced in the SC state. In Fig.3a it is seen that the dip-hump structure is realized (also in the presence of impurities) already for
a moderate coupling $\lambda_{ph} = 1$ in the $N$ state, while it is more pronounced in the SC state. $A(\omega)$ is appreciable narrowed in the SC state. It seems that the dip-energy cannot be attached to the (shifted) phonon energy at $\omega_{ph} = 40$ meV only, since the maxima of $-dA/d\omega$ have more universal meaning (than the minima of $A$) - see Fig.3b. The maxima in $-dA/d\omega$ appear near the energies $(-\Delta_0 - n\omega_{ph})$. The calculations give the dip structure also in the anti-nodal density of states $N_{n/2}(\omega)$ (not shown) already for $\lambda_{ph} = 1$, which is much more pronounced for larger $\lambda_{ph}$.

**Discussion and conclusions** - In obtaining Eqs. (1 - 5) in the FSP model several approximations are made: (i) the charge scattering spectral functions are assumed to be $\sim \delta(\varphi - \varphi')$. This extreme limit is never realized in nature, but for the self-energy it is a good starting point. The finite $\delta\varphi_{\omega}$ effects (but $\delta\varphi_{\omega} \ll \pi$) will not change the qualitative picture but only the quantitative one. In previous studies the EPI spectral function was treated in the extreme momentum FSP limit, were they were proportional to $\delta(k - k')$ - the MFSP model. The latter resolves the ARPES shift-puzzle too, but its self-energy is more singular than in the FSP model. In reality the spectral functions are broadened in the interval $|k - k'| < \delta k_c \ll k_F$ and the effects of finite level-spacing ($\sim 1/N$) in $k$-space are absent; (ii) the Migdal theory is assumed to hold and vertex corrections due to the EPI are neglected. However, in the FSP-model vertex corrections may be important for $\lambda_{ph} < 1$, by increasing $T_c$ significantly; (iii) the role of the Coulomb repulsion in the anomalous self-energy Eq. (2) is unknown, but since the calculation of $T_c$ was not the (main) purpose of this paper and because ARPES and other experiments suggest that $\lambda_C \ll \lambda_{ph}$ we have omitted its contribution to the gap equation.

In conclusion, we analyze the quasiparticle self-energy effects for HTSC oxides in the theoretical model with the pronounced forward scattering peak in the electron-phonon interaction (which dominates in HTSC), Coulomb interaction and impurity scattering - the FSP model. The different shifts of the nodal kink (at 70 meV) and anti-nodal singularity (at 40 meV) in the superconducting state, which are observed in the ARPES experiments on HTSC oxides, are explained by the FSP model in a consistent and unique way. However, a quantitative refinement of the FSP model is needed, which must take into account realistic phonon and band structure, bi(multi)layer structure, less than (delta-function) singular spectral functions, etc.

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