Angle-resolved photoemission spectra of $Bi_2Sr_2CaCu_2O_8$ show a Coulomb coupling ≈1 and an electron-phonon coupling of 2–3

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We show that the double kink structure in the electronic self-energy of Bi2212 near the nodal point at low energy $\omega_1 \approx 50-70$ meV and at high energy at $\omega_2 \approx 0.35-0.4$ eV, observed recently in the angle-resolved photoemission spectra (ARPES) measurements can be explained by the electron-phonon interaction (EPI) coupling constant [in the normal part of the self-energy $\mathrm{Re}\,\Sigma(\omega)$] $\lambda_z^{EP} \approx 2.1$ and the Coulomb coupling $\lambda_z^C \approx 1.1$. Additionally, the low-energy slope of the ARPES $\mathrm{Re}\,\Sigma(\omega)$ at $\omega < 20$ meV by Valla *et al.* gives a hint that low-energy phonons might contribute significantly to the EPI coupling, i.e., $\lambda_z^{low,EP} > 1$, thus giving the total EPI coupling constant $\lambda_{z,tot}^{EP} = \lambda_z^{EP} + \lambda_z^{low,EP} > 3$. In order to test the role of low-energy phonons by ARPES measurements much better momentum resolution is needed than that reported by Valla *et al.* Possible pairing scenarios based on ARPES, tunneling, and magnetic neutron scattering measurements are discussed.

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In the past several years angle-resolved photoemission spectra (ARPES) measurements in high temperature superconductors (HTSCs), with much better momentum and energy resolution, made a breakthrough in determining the energy and momentum dependence of the quasiparticle self-energy in HTSCs. Important measurements by Shen and co-workers[1,2] gave evidence for low-energy kink in the quasiparticle spectrum around the phonon energy 40–70 meV, in both nodal and antinodal points. Since above and below T_c the low-energy kink is pronounced practically in all HTSC materials it may be of phononic origin. This possibility is favored by the recently observed ARPES isotope effect in $\mathrm{Re}\,\Sigma$.[3] These results gave an impetus in the HTSC physics by renewing the interest in the electron-phonon interaction (EPI) and its role in the pairing mechanism of HTSCs. In spite of rather convincing evidence in ARPES, tunneling, scanning tunneling microscopy, and optic measurements that strength of EPI in HTSC is appreciable ($\lambda^{EPI} > 1$),[4–7] theories based on the spin-fluctuation (SF) mechanism of pairing still persist to explain main features in the electronic self-energy *solely* by this nonphononic coupling.

One of the central questions in the HTSC physics is the following: Which of the several possible quasiparticle scattering mechanisms, EPI, the direct Coulomb interaction (includes strong correlations, SF, and long-range Coulomb interaction) is important for pairing. To remind the reader, in bosonic and bosoniclike mechanisms of pairing, which are based on the Fermi liquid theory, the strength of the quasiparticle scattering in the normal part of the self-energy $[\Sigma(\mathbf{k},\omega)]$ in the Migdal-Eliashberg theory is characterized by the total coupling constant

$$\lambda_z(\mathbf{k}) = 2\sum_i \int_0^\infty \frac{\alpha_{\mathbf{k},i}^2 F_i(\omega)}{\omega} d\omega, \tag{1}$$

where $\alpha_{\mathbf{k},i}^2 F_i(\omega)$ is the spectral function of the ith bosonic glue and the summation goes over all bosonic modes involved in the scattering mechanism. At low energies usually one has $\Sigma(\mathbf{k},\omega) = -\lambda_z(\mathbf{k})\omega$ for $\omega \ll \omega_b$, where ω_b is the (smallest) characteristic bosonic frequency. We stress the known fact that the Migdal-Eliashberg theory is well defined for the electron-phonon (boson) scattering mechanism with $\lambda\Omega/W \ll 1$, where Ω is the characteristic phonon (boson) energy and W is the bandwidth.

In the SF mechanism $\alpha_{\mathbf{k}}^2 F(\omega)$ can be calculated in the weak coupling limit of the Hubbard model, while in the strong coupling limit a *phenomenological form* for the spectral function $\alpha_{\mathbf{k}}^2 F(\omega)_{SF} \sim g_{SF}^2 \,\mathrm{Im}\,\chi(\mathbf{k},\omega)$ is assumed,[8] where $\chi(\mathbf{k},\omega)$ is the dynamical spin susceptibility. However, in systems where $\mathrm{Im}\,\chi(\mathbf{k},\omega)$ is strongly peaked around some $\mathbf{k}$ points, like in underdoped HTSCs where $\mathbf{k} = \mathbf{Q}_{AF}(\pi/a,\pi/a)$, this approximation for $\alpha_{\mathbf{k}}^2 F(\omega)_{SF}$ is unwarranted, since the vertex correction (terms beyond the Migdal-Eliashberg approximation) can significantly influence the self-energy—the latter is most probably suppressed.[9,10] While the SF mechanism of pairing is physically plausible and very attractive approach since it gives rise to d-wave pairing, the quantitative explanation of high $T_c \sim 100$ K needs rather large coupling $g_{SF} \gtrsim 0.6$ eV.[8] At present there is no microscopic theory which can justify such a large g_{SF}. In that respect, in Ref. 11 it was shown that the SF phenomenology fails to give large $T_c(\sim 100$ K) even for $g_{SF} \gg 1$ eV, if the spectral function $\mathrm{Im}\,\chi(\mathbf{k},\omega)$ is taken from neutron magnetic scattering experiments and not from low frequency NMR spectra—the latter was done in the original SF theory.[8] Additional difficulties arise when one tries to fit the slope $d\rho/dT$ of the resistivity $\rho(T)$, which gives $g_{SF} \lesssim 0.3$ eV.[11] Important evidence for the inefficiency of SF to *solely explain* the self-energy effects in HTSC materials comes from neutron magnetic scattering measurements done by Bourges's group.[12] They have shown that by changing doping from slightly underdoped to optimally doped systems there is a dramatic change in the magnitude and ω shape of the magnetic spectral function $\mathrm{Im}\,\chi(\mathbf{k} \approx \mathbf{Q},\omega)$ in the normal state at $(T > T_c)$. The experiments at $T > T_c$ show[12] that in the *slightly underdoped* $YBa_2Cu_3O_{6.92}$ (YBCO), with $T_c = 91$ K, $\mathrm{Im}\,\chi(\mathbf{Q},\omega)$ is peaked (with *very large value*) at $\omega \approx 35$ meV, while in the *optimally doped* $YBa_2Cu_3O_{6.97}$, with

T_c=92.5 K, Im $\chi(\mathbf{Q},\omega)$ is *drastically suppressed* and practically negligible in the measured energy region $\omega < 70$ meV. These results were confirmed quite recently in Ref. 13 in optimally doped systems where Im $\chi(\mathbf{k},\omega)$ is practically negligible at all $\mathbf{k}$, since the spin fluctuations are spread over the whole Brillouin zone and broad energy range—the situation unfavorable for pairing. The insensitivity of T_c to the large reconstruction and suppression of Im $\chi(\mathbf{k},\omega)$ around the optimal doping systems means that SF does not affect superconductivity significantly and that the corresponding coupling constant g_{SF} and pairing constant $\lambda^{SF}(\sim g_{SF}^2)$ are rather small, i.e., $g_{SF} \ll 1$ eV and $\lambda^{SF} \approx 0.3$. It is worth to mention that the recent numerical calculations on the Hubbard and $t-J$ model render evidence that probably there is *no high temperature superconductivity* (SC) in these models[14]—if SC exists in these models (at all) its T_c is rather low. Therefore, other interactions, such as EPI and other parts of the Coulomb interaction (the long-range part), should be taken into account. However, there is one fundamental problem with EPI in HTSCs, since as the pairing glue EPI alone cannot produce d-wave pairing. Therefore, if EPI is operative in HTSC d-wave superconductors it must be inevitably supported by the Coulomb interaction which triggers d-wave pairing—see discussion below.

What is the experimental situation regarding the strength of the scattering and pairing mechanism in HTSCs? Some hints come from recent ARPES experiments,[1,2] which give that Re $\Sigma(\mathbf{k},\omega)$ at energies $\omega < \omega_{ph}^{\max} \approx 80$ meV ($\omega_{ph}^{\max}$ is the maximal phonon frequency) has a low-energy kink at characteristic phonon energies ω=40–70 meV and that the *effective* EPI coupling[3] is rather strong ~ 1. Furthermore, in Ref. 3 it was shown that there is *oxygen isotope effect* of the kink. This low-energy behavior (below 0.5 eV) of the ARPES $\Sigma(\mathbf{k},\omega)$ in Refs. 1–3 was qualitatively and semiquantitatively explained by the *combined effect* of the EPI and Coulomb interaction.[15–17] We stress, that the EPI self-energy was extracted from ARPES experiments in Refs. 1–3 by subtracting the high-energy slope of the quasiparticle spectrum $\omega(\xi_k)$ at $\omega > 0.3$ eV. The latter is due to the Coulomb interaction. Although the position of the low-energy kink is not affected by this procedure if $\omega_{ph}^{\max} \ll \omega_C$, the above (subtraction) procedure gives, in fact, not real but an *effective* EPI self-energy $\Sigma_{eff}^{EP}(\mathbf{k},\omega)$ and *coupling constant* $\lambda_{z,eff}^{EP}(\mathbf{k})$ only. Let us briefly demonstrate that $\lambda_{z,eff}^{EP}(\mathbf{k})$ is smaller than the real EPI coupling constant $\lambda_z^{EP}(\mathbf{k})$. The total self-energy is $\Sigma(\mathbf{k},\omega) = \Sigma^{EP}(\mathbf{k},\omega) + \Sigma^C(\mathbf{k},\omega)$ where Σ^C is the contribution due to the Coulomb interaction. At very low energies $\omega \ll \omega_C$ one has usually $\Sigma^C(\mathbf{k},\omega) = -\lambda_z^C(\mathbf{k})\omega$, where $\omega_C(\sim 1$ eV) is some characteristic Coulomb energy and λ_z^C the Coulomb coupling constant. The quasiparticle spectrum $\omega(\mathbf{k})$ is determined from the condition

$$\omega - \xi(\mathbf{k}) - \mathrm{Re}[\Sigma^{EP}(\mathbf{k},\omega) + \Sigma^C(\mathbf{k},\omega)] = 0, \quad (2)$$

where $\xi(\mathbf{k})$ is the bare band structure energy. At low energies $\omega \ll \omega_C$ Eq. (2) can be rewritten in the form

$$\omega - \xi^{ren}(\mathbf{k}) - \mathrm{Re}\,\Sigma_{eff}^{EP}(\mathbf{k},\omega) = 0, \quad (3)$$

where $\xi^{ren}(\mathbf{k}) = [1+\lambda_z^c(\mathbf{k})]^{-1}\xi(\mathbf{k})$ and $\mathrm{Re}\,\Sigma_{eff}^{EP}(\mathbf{k},\omega) = [1+\lambda_z^c(\mathbf{k})]^{-1}\,\mathrm{Re}\,\Sigma^{EP}(\mathbf{k},\omega)$. Since at very low energies $\omega \ll \omega_{ph}^{\max}$ one has $\mathrm{Re}\,\Sigma^{EP}(\mathbf{k},\omega) = -\lambda_z^{EP}(\mathbf{k})\omega$ and $\mathrm{Re}\,\Sigma_{eff}^{EP}(\mathbf{k},\omega) = -\lambda_{z,eff}^{EP}(\mathbf{k})\omega$, then the real EPI coupling constant is related to the effective one by

$$\lambda_z^{EP}(\mathbf{k}) = [1+\lambda_z^C(\mathbf{k})]\lambda_{z,eff}^{EP}(\mathbf{k}) > \lambda_{z,eff}^{EP}(\mathbf{k}).$$

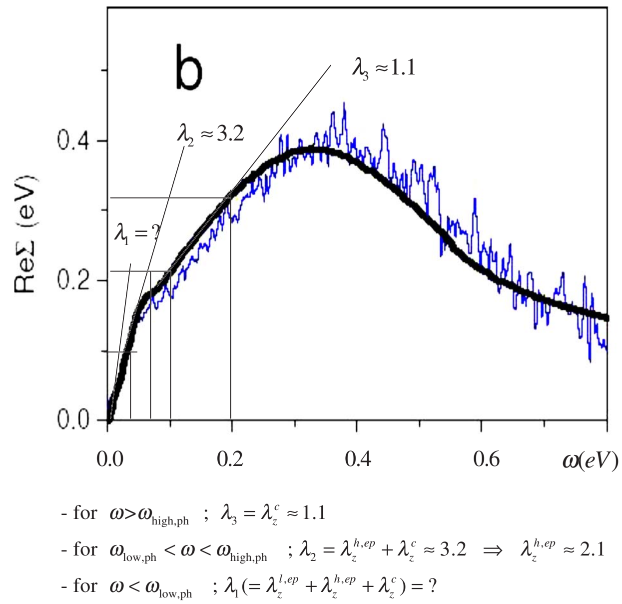

FIG. 1. (Color online) Figure 4(b) from Ref. 18: Re $\Sigma(\omega)$ measured in Bi2212 (thin line) and model Re $\Sigma(\omega)$ (bold line) obtained in Ref. 18. The three thin lines ($\lambda_1, \lambda_2, \lambda_3$) are the slopes of Re $\Sigma(\omega)$ in different energy regions.

At *higher energies* near $\omega_{ph}^{\max}$ one has $\mathrm{Re}\,\Sigma(\mathbf{k},\omega) \approx -\lambda_z^C(\mathbf{k})\omega + \mathrm{Re}\,\Sigma^{EP}(\mathbf{k},\omega_{ph}^{\max})$ and in order to obtain λ_z^C one needs Re $\Sigma(\mathbf{k},\omega)$ at these energies. In recent ARPES measurements on Bi2212 ($Bi_2Sr_2CaCu_2O_8$) and $La_{2-x}Sr_xCuO_4$ by Valla *et al.*[18] $\Sigma(\mathbf{k},\omega)$ was determined in the broad energy interval. The measured $\mathrm{Re}\,\Sigma^{\exp}(\mathbf{k},\omega)$ at T=10 K near and slightly away from the *nodal point* in the optimally doped Bi2212 with T_c=91 K (Ref. 1) is shown in Fig. 1.

It is seen in Fig. 1 that $\mathrm{Re}\,\Sigma^{\exp}(\mathbf{k},\omega)$ has *two kinks*—the first one at *low-energy* $\omega_1 \approx \omega_{ph}^{high} \approx 50-70$ meV which is according to the arguments in Refs. 1–3 most probably of the phononic origin, while the second kink at *higher-energy* $\omega_2 \approx \omega_C \approx 0.35-0.4$ eV is evidently due to the Coulomb interaction. The important result in Ref. 1 is that *near the nodal point* the slopes of $\mathrm{Re}\,\Sigma^{\exp}(\mathbf{k},\omega)$ at low energies ($\omega \ll \omega_{ph}^{high}$) and at higher energies near ω_{ph}^{high} are *rather different*—they are depicted in Fig. 1 by thin lines. From this figure it is obvious that EPI prevails at low energies $\omega \ll \omega_{ph}^{high}$. More precisely digitalization of $\mathrm{Re}\,\Sigma^{\exp}(\mathbf{k},\omega)$ in the interval $\omega \sim \omega_{ph}^{high}$ gives the Coulomb coupling λ_z^C (which is larger than λ_z^{SF})

$$\lambda_z^C \approx 1.1, \quad (4)$$

while the same procedure at $20\text{ meV} \approx \omega_{ph}^{\text{low}} < \omega < \omega_{ph}^{high} \approx 50-70$ meV gives the total coupling constant $\lambda_2 (\equiv \lambda_z) = \lambda_z^{EP} + \lambda_z^C \approx 3.2$ and $\lambda_z^{EP} (\equiv \lambda_z^{high,EP})$

$$\lambda_z^{EP} \approx 2.1. \quad (5)$$

Equations (4) and (5) tell us that at and near the nodal point the EPI *dominates* in the quasiparticle scattering at low energies since $\lambda_z^{EP}(\approx 2.1) \approx 2\lambda_z^C > 2\lambda_z^{SF}$, while at large (compared to *phononic*) energies the Coulomb interaction with $\lambda_z^C \approx 1.1$ dominates. We point out that EPI near the antinodal point can be even larger than in the nodal point, partly due to the higher density of states at the antinodal point.

We emphasize two points. First, comparing the results of Valla *et al.*[18] with the previous ARPES measurements[1,2] it is apparent that the real EPI coupling constant $\lambda_z^{EP}(\mathbf{k})$—obtained from Ref. 1 are at least twice larger than the effective one $\lambda_{z,eff}^{EP}(\mathbf{k})$—from Refs. 1–3, i.e., $\lambda_z^{EP}(\mathbf{k}) \approx 2\lambda_{z,eff}^{EP}(\mathbf{k})$. Second, the ARPES results[18] for $\mathrm{Re}\,\Sigma^{\exp}(\mathbf{k},\omega) \times (=-\lambda_1\omega)$ at *very low energies* $\omega < \omega_{ph}^{low} \approx 20$ meV, which are shown in Fig. 1, hint to an even larger slope giving rise to $\lambda_1 = \lambda_z^{low,EP} + \lambda_z^{EP} + \lambda_z^C > \lambda_2$. This slope gives for $\lambda_z^{low,EP} \gtrsim 0.3-1.3$, while the total EPI coupling is $\lambda_{z,tot}^{EP} = \lambda_z^{low,EP} + \lambda_z^{EP} > 2.4-3.4$—in the following it is called the *L scenario*. It is worth to stress that if the *L scenario* turns out be correct and if the high value of $\lambda_z^{low,EP} \gtrsim 1.3$ is realized, then the *vibrations of heavier atoms* (than oxygen) contribute significantly to pairing in HTSCs. One of the consequence of this result would be a significant reduction (from the canonical value 0.5) of the *oxygen isotope effect* in optimally doped systems, as it was observed experimentally in optimally doped YBCO and other HTSC families[19]—see also Ref. 5 and references therein. Furthermore, the possible value of $\lambda_z^{low,EP} \gtrsim 1.3$ would be compatible with earlier tunneling measurements on $Bi_2Sr_2CaCu_2O_8$ (with $T_c \approx 70$ K),[20] which give the total EPI coupling constant $\lambda_{tunn}^{EP} \approx 3.5$, while $\lambda_{tunn}^{low,EP} \approx 2.1$ for $\omega < 20$ meV, as well as with Ref. 21 where the tunneling experiments from Ref. 22 were analyzed. However, in order to elucidate the role of low energy phonons by ARPES measurements much better momentum resolution (δk) is needed than that reported in Ref. 18, where $\delta k \approx 0.04$ Å^{-1} and $\delta \mathrm{Re}\,\Sigma \approx 20$ meV. This resolution is insufficient for a reliable conclusion on the contribution of low-energy phonons in EPI.

The high-energy kink at $\omega_2 \approx 0.3-0.4$ eV and related waterfall effects are solely due to the Coulomb interaction (at such high energies EPI is ineffective) as it was explained satisfactory in Refs. 23 and 24 by calculating $\Sigma(\mathbf{k},\omega)$ in the tt'-J model. It was shown there that the high-energy waterfall phenomenon in the quasiparticle spectrum is related to the coherent-incoherent crossover in the quasiparticle scattering.

Although it is still premature for giving a definitive pairing scenario in HTSCs, the experimental evidence for d-wave pairing and for rather strong EPI in HTSCs implies inevitably a necessary condition on EPI in HTSCs: EPI in HTSCs must be *peaked* at small transfer momenta, i.e., there is *forward scattering peak* in EPI making it long ranged. Otherwise, if the rather large EPI ($\lambda_z^{EP} \approx 2$) were weakly momentum dependent it would be pair breaking and inevitably destroy d-wave pairing in HTSCs—see more in Ref. 4–7. In that case the nonphononic pairing mechanism should give very large bare critical temperature $T_c^0 \approx T_c \exp\{\lambda_z^{EP}\} = 750-1000$ K. Since this is rather improbable other pairing scenarios must be invoked, which depend on the strength of the EPI coupling in the *d-wave channel*. (1) If one has $\lambda_d^{EP} \lesssim \lambda_z^{EP}$ and the SF coupling is small, $\lambda_z^{SF} \ll \lambda_z^C \sim 1$, then d-wave pairing is dominated by EPI which in conjunction with the Coulomb interaction (by including both the short- and long-range parts) gives d-wave pairing. In that case the s-wave part of the Coulomb interaction, λ_s^C, suppresses s-wave pairing while the d-wave part $\lambda_d^C (\ll \lambda_s^C)$ if $\lambda_d^C > 0$ affects d-wave pairing weakly. T_c can be qualitatively explained in the weak coupling limit where one has $T_{c,d} \approx \langle\omega_{ph}\rangle \exp\{-1/(\lambda_d^{EP} - \lambda_d^C)\}$ and $T_{c,s} \approx \langle\omega_{ph}\rangle \exp\{-1/(\lambda_s^{EP} - \lambda_s^C)\}$ in d-wave and s-wave channels, respectively. Since $(\lambda_s^{EP} - \lambda_s^C) < (\lambda_d^{EP} - \lambda_d^C)$ one has $T_{c,s} < T_{c,d}$. (2) For appreciable large λ_d^{EP} and if the Coulomb interaction is attractive in the d channel,[25] i.e., $\lambda_d^C (<0)$, it strengthens d-wave pairing additionally. (3) Very interesting situation arises if both EPI and the (total) Coulomb interaction give appreciable attraction in the d-channel, with $\lambda_d^{EP} \approx -\lambda_d^C$, thus giving $T_{c,d} \gg T_{c,s}$. If $|\lambda_d^{SF}| \approx \lambda_z^C \approx 1$ is realized then SF and EPI contribute almost equally to T_c. However, as we have already discussed this attractive scenario contradicts magnetic neutron scattering measurements of Bourges and co-workers,[12,13] which imply that $|\lambda_d^{SF}| \ll \lambda_z^C$.

The above discussion raises an important and natural question: What is the physical origin for the appreciable EPI coupling constant in the d-wave channel, λ_d^{EP} (but with $\lambda_d^{EP} \lesssim \lambda_s^{EP}$)? In Refs. 5 and 26 it was shown that strong correlations produce the forward scattering peak in EPI (and other charge scattering processes such as impurity scattering)—see also the reviews in Refs. 5–7. The theory predicts that the EPI coupling in the d-wave channel λ_d^{EP} is appreciable and of the order of λ_s^{EP} around (and below) the optimal doping, while, on the other hand, the transport EPI coupling $[\rho(T) \sim \lambda_{tr}T;\ \lambda_{tr} = \lambda_{tr}^{EP} + \lambda_{tr}^C + \cdots]$ is suppressed by strong correlations, i.e., $\lambda_{tr}^{EP} < (\lambda_z^{EP}/3)$.[5,26] The latter result resolves the long-standing experimental puzzle in HTSCs that the experimental value of λ_{tr} is too small to give high T_c. Contrary to low temperature superconductors, where in most materials $\lambda_{tr} \approx \lambda_z \approx \lambda_z^{EP}$, in HTSC materials one has $\lambda_{tr} \ll \lambda_z$. The latter is explained in a natural way by the presence of the forward scattering peak in EPI and its contribution to λ_{tr} is suppressed, i.e., $\lambda_{tr}^{EP} \ll \lambda_z^{EP}$.[5,26] We point out that the weakly screened EPI Madelung coupling (which may be very strong for a number of phononic modes), which is due to the ionic-metallic quasi-two-demsional structure of HTSCs, supports additionally the forward scattering peak in EPI.[27] The long-range character of the Madelung EPI coupling, which is due to vibrations of the out of plane ions (such as Y, Ba, Bi, etc.), gives rise to the large EPI coupling, as it was first explained in Ref. 28.

In conclusion, we have argued that the recent ARPES measurements of the nodal self-energy in Bi2212 by Valla *et al.*[8] give evidence that the large EPI coupling constant at low energies $\omega < 70$ meV and is at least twice larger than the total Coulomb coupling constant (which includes spin fluctuations too). It turns out that $\lambda_z^{EP} > 2.1$ and $\lambda_z^C \approx 1.1$. These ARPES measurements give also a hint that low-energy phonons can give an appreciable EPI coupling $\lambda^{low,EP} \gtrsim 1$ and $\lambda_{z,tot}^{EP} > 3$. In order to elucidate the role of low-energy phonons in EPI, ARPES measurements need much better resolution in momentum space than that reported in Ref. 18.

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