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High-energy anomaly and self-energy effects in ARPES spectra of cuprates

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We analyze the high-energy anomaly recently observed in ARPES experiments on cuprates within a phenomenological model where electrons are coupled to a bosonic mode in a generic form of a damped oscillator. It is shown that the model allows to describe the main anomalous features found in experiments, such as the broad incoherent spectral weight, the "waterfall dispersion", its doping and temperature dependence. In contrast to the low-energy kink, presence of significant damping is required to account for the anomalies. The "bosonic mode" is related to the incoherent mid-infrared excitation peak observed in optical conductivity spectra of cuprates.

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1. Introduction

Recent reports of the “high energy anomaly" (HEA) [1]-[6] in the ARPES experiments have raised new question concerning properties of high Tc cuprates. A kink appears in the linear dispersion of the spectral density peak at around - 4 eV and is then followed by a broad incoherent \waterfall" tail with almost constant linewidth until at the energy around - 9 eV the dispersion becomes parabolic. However the parabolic bottom of the band is significantly lower than predicted by LDA calculations [4]. The MDC linewidth along the main symmetry directions of the Brillouin zone is almost unchanged within the waterfall energy interval [1, 5]. In some papers its momentum distribution in the Brillouin zone at fixed energy is characterized as diamond-like [1] and in others as more anisotropic, grid-like, when the intensity along the diagonal is suppressed compared to the orthogonal direction [5, 6]. It has been suggested that the latter is indicative of the one-dimensional structure. In contrast, other theoretical explanations of the HEA in terms of selfenergy effects or interaction with a bosonic excitation have been proposed (e.g., spin fluctuations) that can be identified in neutron scattering experiments [3, 7, 8]. In [9] the optical conductivity spectra have been analysed in view of extracting the electron selfenergy. No anomalous \high energy" signature has been obtained in this way while the well known low energy kink at ~60 meV is reproduced in detail. It should be noted that a significant difference in the location of the "high energy kink" has been observed for different symmetry directions of the Brillouin zone [5]. We have analyzed the high-energy anomaly in the photoemission spectra of high-Tc cuprates in the framework of a semi-phenomenological model assuming interaction of electron excitations with a bosonic excitation, parameterized in terms of a damped oscillator. The parameters determined from comparison to the observed spectra allow to connect the bosonic excitation to the other "anomalous" feature observed in optical experiments the incoherent peak in the mid-infrared part of the spectrum. Connection of the latter to another "anomaly", namely that observed by neutron scattering for the inplane bond-stretching phonon mode, is also discussed in this context. The model explains the verticality of the "waterfall" region (0.4 – 0.8 eV), the behavior of the linewidth, anisotropy, location and doping dependence of the HEA, recovering of the "bare" dispersion at larger energies and other properties of the anomaly. We suggest that the HEA should also exist in a broader class of perovskite materials with strong electron correlations [10] where the incoherent mid-infrared excitation has been reported.

2. Model and results

In the present work we propose a model motivated by the presence of a broad incoherent excitation in the mid-infrared (MIR), 0.3 – 0.6 eV, region of the optical conductivity spectra in cuprate superconductors: [11]$La_{1.9}Ca_{1.1}Cu_20_{6+\delta}$ [12] $La_{1.9}Sr_{0.1}CuO_{4+\delta}$ [13]$YBa_2Cu_4O_8$ [14]$YBa_2Cu3O_{6.9}$ [15] $Bi_2Sr_2Ca_2Cu_3O_{10}$ and others . For instance, the Drude-Lorentz analysis of the corresponding dielectric function gives for the frequency and linewidth of this MIR oscillator ω_0= 0.545eV, γ = 0.95eV in $Bi_2\ Sr_2\ CaCu_2\ O_8$ [16], and ω_0 = 0.48eV, γ = 0.9eV respectively in $HgBa_2\ CuO_{4+\delta}$ [17] materials. The spectral weight of the MIR excitation is very large and comparable to the Drude component for the optimally doped materials. Its origin is a matter of debate for many years. Recent magneto-optical experiments [18] do not corroborate that it is magnetic. On the other side, in the paper [19] it has been suggested that a charge excitation in the same region of the spectrum might be responsible for the anomalous

softening of a phonon mode. So, we assume for our model that electron excitations described within a tight binding model and fitted to the low energy properties (e.g. the Fermi surface) are renormalized at these "high energies"by their interaction with bosonic excitation described by retarded propagator in the form of damped oscillator.$B(\omega)= \omega_{0}(\omega^2- \omega_0^2+i\,\gamma\,\omega)^{-1}$

Then the electron selfenergy $\Sigma(\omega)$ is obtained in the usual way [20]. The coupling constant is derived from the slope of experimentally observed dispersion and is close to 1 [3]. Calculation shows that the location of the peaks in electron spectral density and Re $\Sigma(\omega)$ is determined by the effective frequency $\Omega = (12\omega_0^2 - 6_\gamma{}^2 + 6\sqrt{16\omega_0^4 - 4\omega_0^2\gamma^2 + \gamma^4}$ the maximum of the oscillator spectral density. Consequently, the renormalized dispersion acquires a kink at the same frequency. From the above expression it can be seen that for the considered MIR oscillator this frequency is significantly lower than ω_0 and falls in the range typical for the high energy kink. It is a standard exercise to derive the expression for the self-energy without vertex corrections in terms of fermionic and bosonic spectral densities *(F;B)*:

$$\sum{}_R(k,\omega) = \frac{1}{N}\sum_q g^2(k,q)\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\sigma_F(k-q,x) \times \rho_B(q,y)\frac{n_B(y)+n_F(x)}{\omega+y-x+i0}dxdy \qquad (1)$$

where *g(q)* is the coupling constant and $\eta_{B,F}$ are the respective distribution functions. It is also easy to and the spectral density of the damped oscillator corresponding to B *(ω)*

$$\rho_B(\omega) = \frac{\gamma\omega_0\omega/\pi}{(\omega^2-\omega_0^2)+(\gamma\omega)^2}$$

while for the fermionic one we use a simplest form of $\delta(x-\varepsilon_{k-q})$; where the band dispersion is taken from known tight-binding parametrization. In the Fig. 1 ε_k corresponds to LSCO and we show the Re$\Sigma(\omega)$ and Im$\Sigma(\omega)$. The slope of the Re$\Sigma(\omega)$ corresponds to the coupling constant 1:3. One can see that the (-*Im*$\Sigma(\omega)$) behaves as ω^2 at low energies and its injection point corresponds to Ω After reaching its maximum at lower energy (-*Im*$\Sigma(\omega)$) becomes almost at until it starts decreasing closer to the band bottom. The flattening of Im$\Sigma(\omega)$ corresponds to the incoherent "waterfall" region in ARPES with almost constant linewidth. We nd that the large value of the damping parameter is also responsible for the verticality of the dispersion in the waterfall region. Such behavior is in agreement with the data reported in [1, 5] for the linewidth of the ARPES spectral function.

It should however be noted, that optical data refer to the long wave limit, *q = 0*; of the excitation and its parameters at finite *q* are not known. In the present calculation we have neglected the dispersion to analyse the effect of other factors, but it is certainly required for a more detailed comparison. In particular, the anisotropy of the HEA corresponds to a stronger charge response located at lower energy (i.e. lower Ω) for the orthogonal (1,0) direction compared to a weaker response and located at higher energies for the diagonal direction in the Brillouin zone. This also corresponds to the pattern of the bond-stretching in plane phonon softening [19]. In Fig. 2 is shown the dispersion of the spectral density maximum along the diagonal direction, *K = Kx = Ky*.

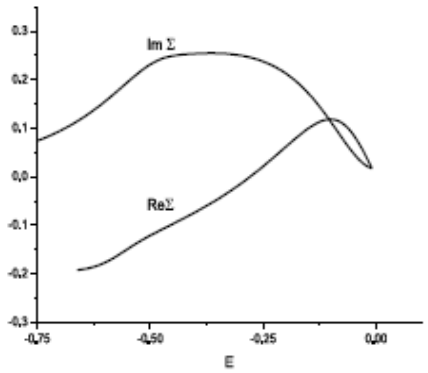

Fig. 1. Real and imaginary parts of the selfenergy Σ (ω) resulting from interaction with the overdamped oscillator with spectral density ρ_B (ω). Parameters are ω_0= 0.18; γ =0.3; λ = 1.3; T = 0.001; δ= 0.15: The flattening of ImΣ(ω) corresponds to the incoherent "waterfall" region in ARPES with almost constant linewidth

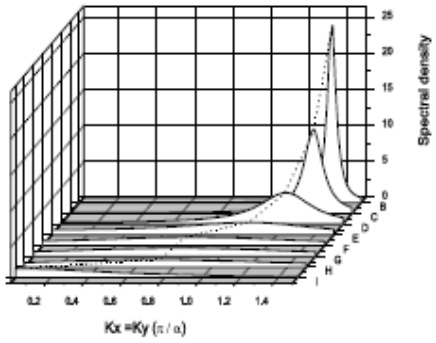

Fig. 2. Momentum distribution curves for different energiesfbelow the Fermi surface of the LSCO. Parameters are ω_0 =0.18 ; γ = 0.21; λ = 1.3; T=0.001; δ = 0.15.

In the full Brillouin zone this dispersion is described by the surface shown in Fig. 3.The momentum of the high energy kink k_0 decreases with doping. This suggests that the band structure is of primary importance for the location and doping dependence of the HEA, as the doping dependence of *k0* follows the shrinking of the Fermi surface. Our calculation indicates the decrease of the linewidth of the spectral function with doping, it would be interesting whether such dependence can also be seen in

experiments. The temperature dependence of $\Sigma(\omega)$ is very weak in the relevant region of energies.

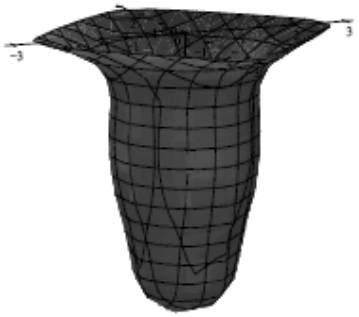

Fig. 3. Dispersion surface of the spectral density peak in the full Brillouin zone for the parameters in Fig. 2

We find a broader linewidth in the (0; 1) and (1; 0) directions as compared to the diagonal in agreement with the measurements presented in [21]. As noted in some papers [3, 5, 6] the ARPES measurements reveal an anisotropic structure of the HEA. These results can be described within the present model by introducing the anisotropy into the parameters of the oscillator. For instance, the difference in energy of the high energy kink for the momentum cuts along different directions of the Brilouin zone found in [5] can be explained by a larger value of along the diagonal direction. In a different context, it has been suggested that the anomalous softening of a bond-stretching in plane phonon mode is related to an overdamped charge excitation in the same MIR part of the spectrum [19] and that the behavior of this mode could serve as a energy-momentum resolved probe for the charge excitation. This opens a possibility that the same overdamped excitation is responsible both for phonon anomaly and the HEA. One of its characteristics implied from the phonon analysis is the anisotropy of the charge response at finite momentum in the energy range that matches the grid-like pattern mentioned in [6]. Namely that anomalous phonon softening occurs in the (0; 1) ; (1; 0) directions and a much smaller effect is observed in the (1; 1) direction. Such behavior is also in agreement with the MIR charge "boson" scenario proposed here. The broad incoherent spectrum below the kink emerges due to the composite nature of electronic excitation with emission of an "overdamped boson". This explains the qualitative difference between high and lowenergy kinks. In the latter case the linewidth of the boson is not more than 10% of its energy scale, while in the case of MIR it is an order of magnitude larger: At the same time, for a comparable coupling constant, such linewidth accounts for the verticality of the dispersion and linewidth of the waterfall and the remains almost at in this region. At lower energies, around 0:9 eV, the $\mathrm{Im}\Sigma$ starts to decrease and the dispersion recovers the bare band parabolic shape. As discussed above, one needs to have a probe for momentum resolved charge excitations in the 0:4 - 0:5 eV range to characterize the "overdamped boson" in sufficient detail. The presented arguments suggest that the HEA in ARPES should also exist in those materials where one observes such an incoherent MIR excitation in the optical conductivity spectra. The latter is known to be the common features of various perovskite materials. Interestingly, most of these materials show an anomaly in the softening of the bond stretching phonon mode, presumably due to coupling to charge fluctuations [22]. According to the presented scenario interesting candidates for the HEA are the nonmagnetic perovskites such as $Ba_{1-x}K_xBiO_3$ with a relatively high Tc that is also known to have an incoherent charge excitation in the MIR about 0:4 - 0:6 eV [23] as well as anomalous bond-stretching phonon branch.

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