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Dispersion anomalies induced by the low-energy plasmon in the cuprates

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We discuss the characteristic effects of the electron plasmon interaction resulting from the ~ 1 eV plasmon, which is a universal feature in the cuprates. Using the framework of a one-band tight binding model, we identify signatures of this low energy plasmon in the electronic structure of metallic overdoped Bi2212 as well as half-filled insulating SCOC. The electron-plasmon interaction is found to yield renormalizations near the Fermi energy in reasonable accord with experimental observations, and to produce dispersion anomalies at higher energies.

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Quasiparticle dispersions near the Fermi energy in the cuprates are renormalized (reduced) by a factor of $Z \sim 0.3 - 0.6$ [1] in comparison to the band theory predictions based on the conventional LDA picture, interrupted by the appearance of low energy ‘kinks’ or dispersion anomalies in the 50-70 meV energy range, which arise from the coupling of the electronic system with phonons[2] and/or magnetic modes[3]. Interestingly, the ‘spaghetti’ of various hybridized and unhybridized Cu and O bands starting around 1 eV in the cuprates seems to remain more or less unrenormalized.[4] Recalling that optical[5] and electron energy loss spectroscopy (EELS) experiments[6, 7] have shown the presence of dispersive plasmons in the cuprates lying at ~ 1 eV, we explore the effects of such a low energy plasmon in this Letter. The plasmon is found to induce renormalizations in the low energy regime in both the metallic and the insulating cuprates, which are in substantial accord with the corresponding experimental results. We emphasize that plasmons in 3D materials typically lie at ~ 10 eV and therefore have little influence on the electronic states in the 0-1 eV range.

We approach the problem within the framework of a one-band tight-binding model and consider the limiting cases of a metal with the example of overdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ (Bi2212)[8, 9] and the insulator with the example of half-filled $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ (SCOC)[10]. The dielectric functions computed via the random phase approximation (RPA) yield loss functions and the associated plasmon dispersions in both Bi2212 and SCOC, which are in reasonable accord with the corresponding EELS data. The generic effects of the electron-plasmon interaction on the electronic structure and how the low energy plasmon in the metal and the insulator induces characteristic dispersion anomalies and renormalizations of the spectrum are then delineated via a first order calculation of the electronic self energy.

We discuss first the metallic case of overdoped Bi2212. Here the magnetic gap has collapsed fully and we take the bare electronic dispersion to be given by a one-band tight-binding model fitted to the LDA-based band structure of Bi2212 in the vicinity of the Fermi energy (E_F)

as follows[1]:

$$\epsilon_{\mathbf{k}} = -2t[c_x(a) + c_y(a)] - 4t'c_x(a)c_y(a) - 2t''[c_x(2a) + c_y(2a)] - 4t'''[c_x(2a)c_y(a) + c_y(2a)c_x(a)], \quad (1)$$

where $c_\alpha(na) = \cos(nk_\alpha a)$ for $\alpha = x$ or y , n is an integer, and a is the in-plane lattice constant. Hopping parameters appropriate for Bi2212 (neglecting bilayer splitting)[1] are: $t=360$ meV, $t' = -100$ meV, $t''=35$ meV, $t''' = 10$ meV. We model the dynamic dielectric function, $\epsilon(q, \omega)$, in the form[6, 11]

$$\epsilon(q, \omega) = \epsilon_0 \left[1 - \frac{\omega_p^2(q)}{\omega(\omega - i\gamma(q))} \right], \quad (2)$$

where $\epsilon_0 = 6$ and the dispersion and damping of the plasmon in Bi2212 obtained from EELS data are given by[6]: $\omega_p = 1.1eV[1 + 4S_{xy}]$, $\gamma = 0.7eV[1 + 16S_{xy}]$, $S_{xy} = \sin^2(q_x a/2) + \sin^2(q_y a/2)$. Notably, due to the large broadening, the experimental plasmon peak lies at a lower energy than the bare value ω_p . Using the bare dispersion of Eq. 1 and the dielectric function of Eq. 2, it is straightforward[12] to obtain the first order correction to the electronic self energy Σ due to the screened Coulomb interaction[13]. The formulas can also be derived from those for the insulator (Eqs. 5-11 below) by letting the magnetic gap $\Delta_m \rightarrow 0$.

Figure 1 displays the spectral density in the overdoped metallic case where effects of the electron-plasmon interaction are included. We consider the low energy region along $\Gamma \rightarrow (\pi, 0)$ shown in (b) first. A region of high spectral intensity depicted by the thin white trace in (b) can be seen clearly (note logarithmic scale), indicating that the LDA band continues to persist in the presence of the plasmon, albeit with some renormalization. An average factor of $Z = 0.5$ is seen to more or less describe the renormalization of the LDA band as seen by comparing the dashed blue line with the whitish trace of high intensity. The $Z = 0.5$ value so determined is in substantial accord with the corresponding experimental value of $Z = 0.28$,[1] indicating that the plasmon constitutes a substantial part of the bosonic dressing of the electron. Moreover, the spectral weight spreads out from the renormalized band towards the bare band (red line), giving the

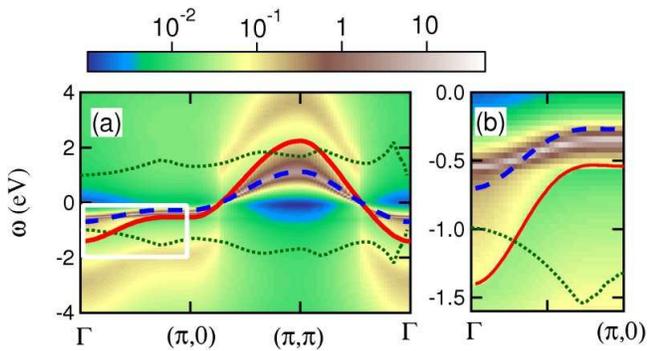


FIG. 1: (Color online) (a) Dressed spectral density function in overdoped (metallic) Bi2212. Bare dispersion (red line) is compared with dispersion renormalized with $Z = 0.5$ (blue dashed line). Dotted lines indicate plasmon dispersion. (b) Blowup of region enclosed by white box in (a). Logarithmic color scale is used to reveal weaker features.

resulting yellowish trace the visual appearance of a 'waterfall' terminating around the Γ point. These results bear some resemblance to 'waterfall'-like anomalies reported recently in the ARPES spectra from the cuprates over the 0.4-0.8 eV energies[8, 9]. However, the waterfall-like features induced by the plasmon and those reported in ARPES differ significantly insofar as their location in energy and momentum is concerned, and therefore, on the face of it, the plasmon would not seem to provide an explanation of the recent ARPES results. We return to comment further on this point below.

We now turn to Fig. 1(a) which exposes effects of the plasmon over a wider energy scale. Here we see that the plasmon induces 'plasmaron' features[14] – a new 'shadow' band lying 1.5 eV below the bare dispersion via the plasmon emission process along the filled portion of the LDA bands along the Γ to $(\pi, 0)$ and the Γ to (π, π) lines. A similar shadow band associated with plasmon absorption appears 1.5 eV above the unfilled part of the LDA band along the $(\pi, 0)$ to (π, π) and Γ to (π, π) lines. At low energies, the plasmon dresses the electrons, making them heavier and renormalizing their dispersion. In contrast, at high energies, the plasmon becomes progressively less effective in dressing the electrons which move with ever increasing speeds, even though the electronic states are still broadened by plasmon emission effects.

We now demonstrate that the experimentally observed plasmon dispersion in Bi2212 is in fact described reasonably well by the band structure of Eq. 1, consistent with the results of Ref. [15]. For this purpose, we directly evaluate the dielectric function from the bare charge susceptibility χ_0 and the Coulomb interaction $V_{\mathbf{q}}$ via

$$\epsilon(\mathbf{q}, \omega) = \epsilon_0[\mathbf{1} + \mathbf{V}_{\mathbf{q}}\chi_0(\mathbf{q}, \omega)]. \quad (3)$$

χ_0 is calculated straightforwardly within the RPA approximation where the band structure of Eq. 1 is renor-

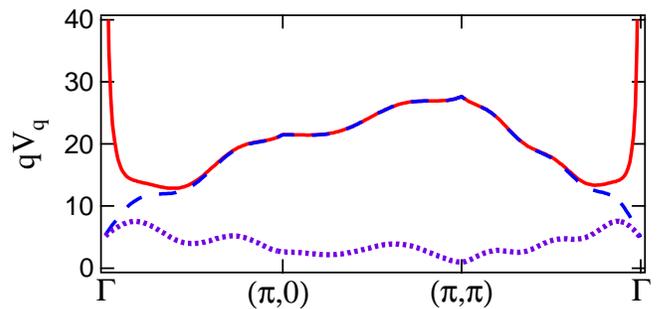


FIG. 2: (color online) Different calculations of the Coulomb potential (see text) in the form of $qV_{\mathbf{q}}$ are compared. Full 3D layered lattice (solid line); A single 2D layer (dashed); and 2D layer without the on-site U term (dotted).

malized by a factor of $Z=0.28$ to account for the renormalization observed in ARPES experiments on Bi2212. The treatment of the long-range Coulomb interaction $V(r)$ for the correlated electronic system in a layered structure requires some care and we model $V(r)$ as an on-site Hubbard $U = 2$ eV term[16] plus a $1/r$ contribution screened by the background dielectric constant ϵ_0 at other lattice sites. $V_{\mathbf{q}}$ is then obtained via a lattice Fourier transform by summing the contributions of all in-plane Cu terms for $r \leq R \equiv 4a$ (a being the in-plane lattice constant) and approximating the remaining in-plane as well as interplane contributions for $r > R$ by a continuum in order to recover the correct $q \rightarrow 0$ limit of $V_{\mathbf{q}}$. Fig. 2 shows $qV_{\mathbf{q}}$ along high symmetry lines in the Brillouin zone (BZ). $V_{\mathbf{q}}$ is seen to display a crossover from 3D behavior $\sim 1/q^2$ to 2D behavior $\sim 1/q$ for $qc > 1$, where c is the distance between successive CuO_2 planes.

The use of $V_{\mathbf{q}}$ and χ_0 in Eq. 3 yields the dielectric function based directly on the band structure of Eq. 1. The plasmon dispersion is found from the peak of the EELS spectrum, which is proportional to the loss function $\text{Im}[-1/\epsilon]$, plotted in Fig. 3. The theoretically predicted plasmon energy given by the maximum of the loss function (white trace in the figure) is compared to the available experimental results in Bi2212 (red dots). Given that the calculation is not self-consistent, the agreement is seen to be reasonable. Notably, our calculations assume purely in-plane excitations ($q_z = 0$).[17]

We consider next the more challenging case of insulating SCOC, where a magnetic gap is present and it has not been clear how the EELS spectra[7] are related to the plasmon excitation. As in the metallic case, the starting point is the dispersion of Eq. 1, except that the hopping parameters are chosen to fit the LDA-based bands in SCOC: $t=420$ meV, $t' = -57$ meV, $t''=52$ meV, $t''' = 26$ meV. The correlated band structure is modeled by introducing an on-site Hubbard term $U=2$ eV and treating the system as a uniform half-filled antiferromagnet[18] with saturated (staggered) moment $m_Q = 0.5$. The band

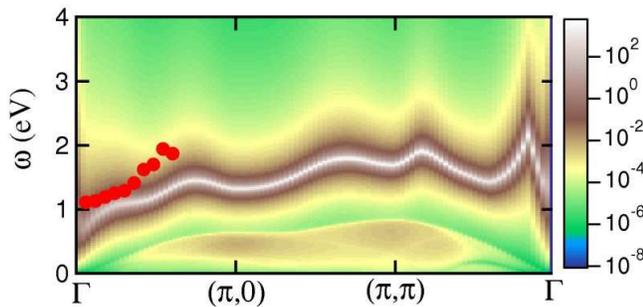


FIG. 3: (Color online) Loss function $\text{Im}[-1/\epsilon]$ as a function of ω and \mathbf{q} in Bi2212 plotted on a logarithmic color scale. Red dots give the experimental plasmon peak positions [6].

structure of Eq. 1 then splits into upper and lower magnetic bands with gap $\Delta_m = Um_Q$. The dielectric response given by Eq. 2 in the metallic case is modified strongly at low frequencies and our analysis indicates that the dielectric function in the insulator can be modeled as

$$\epsilon = \epsilon_0 \left[1 - \frac{\omega_p^2}{\omega(\omega - i\gamma) - \omega_0^2} \right], \quad (4)$$

where $\omega_0 \simeq U$. [19] Taking $\omega_0 = 2$ eV and the same γ as in Eq. 2, the EELS data [7] on SCOC can be fitted to Eq. 4 with $\omega_p = 1.3eV[1 + 3S_{xy}]$. Again, the broadening shifts the peak in $\text{Im}[\epsilon^{-1}]$ from its expected position $\tilde{\omega}_p = [\omega_p^2 + \omega_0^2]^{1/2}$; the experimental peak can be fit to a similar q -dependence, but with $\omega_p^e = 2.4eV[1 + 0.33S_{xy}]$. Note that ω_p is not very different in metallic Bi2212 and insulating SCOC, so that most of the shift in the position $\tilde{\omega}_p$ of the plasmon peak in the loss function is due to the gap ω_0 .

The spectral density for the dressed Green function in the insulator is shown in Fig. 4. The results are similar to those of Fig. 1 for Bi2212 in that the dressed lower magnetic band in Fig. 4 displays the waterfall effect and that it is renormalized in comparison to the bare band (compare red line with dashed blue line). The renormalization of the low energy spectrum by a factor of $Z \sim 0.3$ in SCOC due to the plasmon in Fig. 4 is again comparable to the corresponding experimental value of $Z = 0.64$.

Finally, we consider briefly the calculation of the loss function and the self-energy in the insulating system. With two bands involved in this case, the formalism is less familiar than the one-band metallic case, and therefore, an overview of the relevant results is appropriate. [The metallic case can be recovered by taking the limit $\Delta_m \rightarrow 0$.] The RPA expression for the charge susceptibility χ_0 in the insulator is

$$\chi_0(\mathbf{q}, \omega) = \frac{1}{N} \sum_k [u_-^2 (g_{12} + g_{21}) + u_+^2 (g_{11} + g_{22})], \quad (5)$$

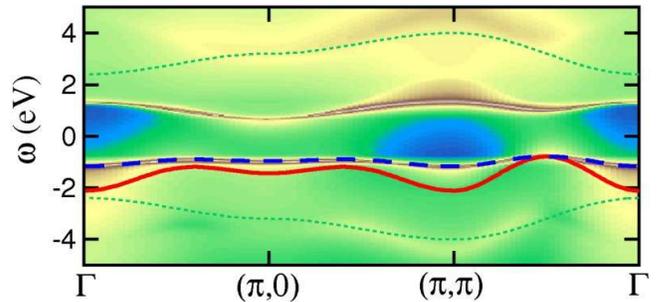


FIG. 4: (Color online) Dressed spectral density function in SCOC at half-filling. Bare dispersion (red line) is compared with dispersion renormalized with $Z = 0.3$ (blue dashed line). Dotted lines indicate plasmon dispersion. Logarithmic color scale is the same as in Fig. 1.

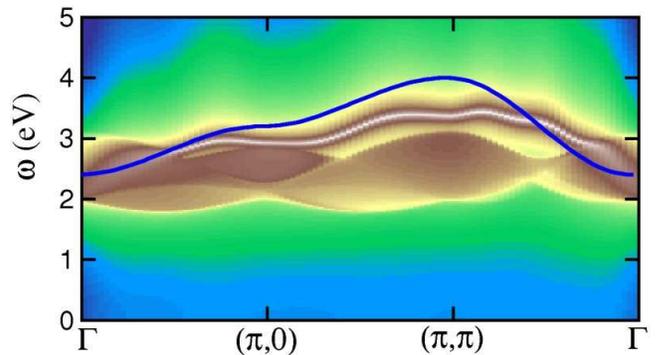


FIG. 5: (Color online) Loss function $\text{Im}[-1/\epsilon]$ as a function of ω and \mathbf{q} in SCOC at half-filling. Solid line gives the experimental plasmon dispersion ($\tilde{\omega}_p$) for SCOC [7]. Logarithmic scale as in Fig. 3.

where the prime means summation over the magnetic Brillouin zone only,

$$g_{ij}^2 = \frac{[1 - f(\epsilon_{i,k})]f(\epsilon_{j,k+q})}{\epsilon_{i,k} - \epsilon_{j,k+q} + \omega + i\delta}, \quad (6)$$

f is the Fermi function,

$$\epsilon_{1,2k} = \epsilon_k^{(+)} \mp E_k, \quad (7)$$

with the 1(2) going with the $-(+)$ sign, $\epsilon_k^{(\pm)} = (\epsilon_k \pm \epsilon_{k+q})/2$,

$$u_{\pm}^2 = \frac{1}{2} \left[1 \pm \frac{\epsilon_k^{(-)} \epsilon_{k+q}^{(-)} + \Delta_m^2}{E_k E_{k+q}} \right], \quad (8)$$

and $E_k = [\epsilon_k^{(-)2} + \Delta_m^2]^{1/2}$. The preceding equations have been applied previously to the Hubbard model [20, 21], but we have extended their usage to include the long-range Coulomb interaction.

In the presence of a gap, the electronic self energy Σ becomes a tensor with indices 1(2) corresponding to the lower (upper)magnetic band[12, 22]:

$$\Sigma_{11}(\mathbf{p}, \omega, \sigma) = \int_{BZ} \frac{d^2q}{(2\pi)^2} [v_m^2 \hat{\Sigma}_1 + u_m^2 \hat{\Sigma}_2], \quad (9)$$

$$\Sigma_{12} = \Sigma_{21} = \int_{BZ} \frac{d^2q}{(2\pi)^2} u_m v_m \sigma [-\hat{\Sigma}_1 + \hat{\Sigma}_2], \quad (10)$$

where

$$\hat{\Sigma}_i = [\Theta(\omega - \epsilon_{i,p+q}) - \Theta(-\epsilon_{i,p+q})] \frac{V_{\mathbf{q}}^2 \chi_0(\mathbf{q}, \omega - \epsilon_{i,p+q})}{\epsilon(\mathbf{q}, \omega - \epsilon_{i,p+q})/\epsilon_0};$$

$$u_m = \sqrt{\frac{1}{2} \left[1 + \frac{\epsilon_{p+q}^{(-)}}{E_{p+q}} \right]}; \quad v_m = \sqrt{\frac{1}{2} \left[1 - \frac{\epsilon_{p+q}^{(-)}}{E_{p+q}} \right]}, \quad (11)$$

and Σ_{22} has the same form as Σ_{11} , but with u_m and v_m interchanged.

The loss function in SCOC computed from Eqs. 5 and 3 is shown in Fig. 5. The experimentally observed plasmon dispersion (solid line) is seen to be in good accord with the theoretical prediction. A comparison of Figs. 3 and 5 reveals how the gap in the underlying spectrum of the insulator shifts the plasmon energy in SCOC to higher values with little weight at energies below ≈ 2 eV in contrast to the metallic case of Bi2212.

The present results have significant implications for the low energy physics of the cuprates and provide a route for connecting this physics to the spectrum at higher energy scales as one encounters the venerable ‘spaghetti’ of Cu and O related bands spread typically over ~ 1 -8 eV binding energies. We have shown that the plasmon induces band renormalizations at low energies in the metallic case of Bi2212 as well as the insulating case of SCOC, and that these renormalization effects are in substantial accord with the corresponding experimental values. Our results clearly establish the importance of the plasmon in the bosonic dressings of the low energy quasiparticles in the cuprates.

There have been several recent calculations of electronically-induced kinks, but these are generally very weak[23] or confined to a restricted doping range[24]. The plasmon by contrast is robust and produces strong kink-like features which extend over several eVs, due to the large broadening of the plasmon[25]. While these characteristic features of the electron-plasmon interaction are reminiscent of those reported in very recent ARPES experiments on several families of cuprates[8, 9, 10], they fall at too high an energy scale. Possible candidates for the intermediate waterfall scale include the acoustic branch of the plasmons and high-energy magnetic excitations. The extent to which low energy plasmons are involved in an electronic mechanism of superconductivity remains unclear, although such suggestions have been made in the literature[26].

In conclusion, we have shown that the low-energy plasmon, which is a universal feature of the cuprates, produces renormalizations and dispersion anomalies in the electronic structure. Our study indicates that the plasmon is a very significant player for understanding the physics of the cuprates.

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