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Strong correlation effects and optical conductivity in electron-doped cuprates

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Abstract – We demonstrate that most features ascribed to strong correlation effects in various spectroscopies of the electron-doped cuprates are captured by a calculation of the self-energy incorporating effects of spin and charge fluctuations. The self-energy is calculated over the full doping range of electron-doped cuprates from half filling to the overdoped system. The self-energy divides the low-energy physics of cuprates into two energy scales: an antiferromagnetic (AFM) “pseudogap” region near the Fermi level and a high-energy “Mott gap region”. The corresponding spectral function reveals four subbands, two widely split incoherent bands representing the remnant of the split Hubbard bands, and two additional coherent, spin- and charge-dressed in-gap bands split by a spin-density-wave, which collapses in the overdoped regime. The incoherent features persist to high doping, producing a remnant Mott gap in the optical spectra, while transitions between the in-gap states lead to AFM pseudogap features in the mid-infrared.

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A key issue in electron-doped cuprate physics is to understand the routes through which cuprates evolve from a “Mott” insulator at half filling to an AFM region at finite doping to a Fermi liquid region at overdoping. Recently, we have introduced a quasiparticle-*GW* or QP-*GW* model to demonstrate that the strong coupling Mott physics model is inappropriate for the cuprates, and that the correct model should be an intermediate coupling model which includes spin-density-wave (SDW) [1,2]. The intermediate correlation strength of electron-doped cuprates is also consistent with experimental observations [3].

Such a model explains many diverse phenomena such as Fermi surface reconstructions [4] and observed quantum oscillations [5], Fermi velocity renormalization [1]. These results indicate that the low-energy pseudogap must collapse with doping. In sharp contrast, optical studies point to a far more complex and puzzling picture in that even in the overdoped case, an absorption peak characteristic of the Mott gap continues to persist [6,7] in the spectra, suggesting that doping introduces new *in-gap states* in which the pseudogap physics resides, but that otherwise the Mott gap persists at all dopings.

Here we show that the same model of the electronic self-energy, where the quasiparticles are dressed with spin-density-wave excitations, captures the key experimentally

observed features of the remarkable doping evolution in optical and other spectroscopies, including in particular the persistence of the Mott gap in the overdoped regime. These findings are also consistent with quantum Monte Carlo (QMC) [8–12] and dynamical mean-field theory (DMFT) [13,14] calculations.

We evaluate the self-energy Σ as a convolution over the green function G and the interaction $W \sim U^2\chi$ (including both spin and charge contributions) [1,2,15],

$$\Sigma(\vec{k}, \sigma, i\omega_n) = \eta U^2 \sum_{\vec{q}, \sigma'} \int_{-\infty}^{\infty} \frac{d\omega_p}{2\pi} \times G(\vec{k} + \vec{q}, \sigma', \omega_n + \omega_p) \Gamma(\vec{k}, \vec{q}, \omega_n, \omega_p) \text{Im}[\chi^{\sigma\sigma'}(\vec{q}, \omega_p)], \quad (1)$$

where σ is the spin index and the prime over the \vec{q} summation means that the summation is restricted to the magnetic Brillouin zone. η is the spin degeneracy factor, taking the value of 1 for the transverse spin flip channel and 1/2 for the longitudinal spin and charge channel. In the underdoped region where the SDW dominates, resulting G , χ and Σ become 2×2 tensors [16]. We define a total self-energy as $\Sigma^t = US\hat{\tau}_1 + \Sigma$, where $\hat{\tau}_1$ is the Pauli matrix along the x -direction and US is the SDW gap defined below. The self-energy Σ^t contains essentially

two energy scales: i) it gives rise to the SDW with an additional renormalization of the overall quasiparticle dispersions in the low-energy region [4,17–19], we call it “pseudogap” region and ii) at higher energies it produces the Hubbard bands, designated as “Mott gap” region [20,21]. We use a modified self-consistent scheme, referred to as quasiparticle-GW (QP-GW)-scheme in which G and W are calculated from an approximate self-energy $\Sigma_0^t(\omega) = US\tilde{\tau}_1 + (1 - Z^{-1})\omega\tilde{\mathbf{1}}$, where the renormalization factor Z is adjusted self-consistently to match the self-energy Σ^t at low energy [20,21].

We find that near optimal doping spin waves [11,12,20, 21]¹ dress the quasiparticles into a coherent *in-gap state*, while the incoherent high-energy features are remnants of the upper and lower Hubbard bands (U/LHBs)². With underdoping the in-gap state develops into a SDW state which opens a gap between the upper and lower magnetic bands (U/LMBs). The model also describes the high-energy kink or the waterfall effect seen in the electronic dispersion [22] as the crossover between coherent and incoherent features.

The present calculations are restricted to the electron-doped cuprates in order to avoid possible complications of nanoscale phase separation. The self-energy Σ_0^t splits the LDA-band, $\xi_{\vec{k}}$ (modelled by tight-binding (TB) parameters [20]) into renormalized UMB ($\nu = +$) and LMB ($\nu = -$): $E_{\vec{k}}^{\nu} = Z \left(\xi_{\vec{k}}^{\pm} \pm \sqrt{(\xi_{\vec{k}}^{\pm})^2 + (US)^2} \right)$, where $\xi_{\vec{k}}^{\pm} = (\xi_{\vec{k}} \pm \xi_{\vec{k}+\vec{Q}})/2$. The AFM magnetization S at $\vec{Q} = (\pi, \pi)$ is calculated self-consistently at each doping, assuming a doping dependent U due to charge screening [17]. In the present formalism U is renormalized by Z . The doping dependency of U is chosen such that ZU reproduces the pseudogap in both angle-resolved photoemission spectroscopy (ARPES) and optical spectra, while x , S , and Z are determined self-consistently solving coupled gap equations [19]. Remarkably, the same set of parameters gives good agreement with ARPES and optical spectra. Finally, the vertex correction $\Gamma(\vec{k}, \vec{q}, \omega, \omega_p)$ in eq. (1) is taken to its first-order approximation (Ward’s identity) as $\Gamma(\vec{k}, \vec{q}, \omega, \omega_p) = 1/Z$. Since the k -dependence of Σ is weak [20], we further simplify the calculation by assuming a k -independent Σ , which we calculate at a representative point $k = (\pi/2, \pi/2)$.

We begin by discussing the optical spectra of fig. 1. The frequency-dependent optical conductivity, $\sigma(\omega)$, is calculated using standard linear response theory in the AFM state [23], for the full doping range from the half-filled state to the quantum critical point (QCP) in the overdoped region. To fit the Drude conductivity, we

¹While the low-energy carriers are mainly dressed by electronic excitations in the magnetic channel [11,20], the charge channel can also contribute [21].

²In reality, the Mott physics lies at a higher energy, comparable to the bonding-antibonding separation of the CuO_2 -hybridized bands, and the bands we refer to as U/LHB are the incoherent high-energy tails of the antibonding (LDA) band.

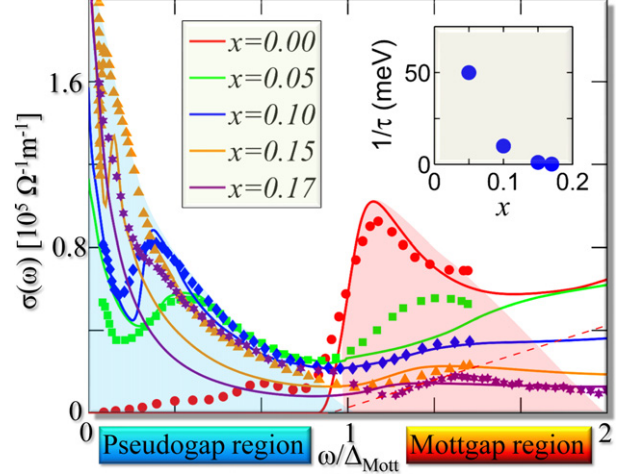


Fig. 1: (Color online) Calculated optical conductivity (solid lines) for electron-doped cuprate compared with experiment (symbols of same color) for dopings $x=0.0$ to $x=0.15$ as taken from ref. [6] and for $x=0.17$ from ref. [7]. The latter data is subtracted by a background contribution to match the former data set³. The dashed line gives the background contribution added to the theoretical spectrum at $x=0$. The blue and red shadings differentiate the “pseudogap” energy scale and “Mott gap” energy scale by a characteristic energy $\Delta_{\text{Mott}} = 1.5$ eV. Inset: inferred doping dependence of the scattering rate.

have introduced an impurity scattering rate τ which is found to have a strong doping dependence (inset). At high energy we include a doping-dependent background contribution (see footnote ³), partially associated with interband transitions to higher-lying bands not included in the present calculations⁴. The background is used to have the same (linear) energy-dependence for all dopings with its slope decreasing smoothly with doping. The red dashed line in fig. 1 shows this interband contribution for the $x=0.0$ spectrum. A very good level of accord is seen with the experimental results [6,7], without any further adjustment of intensity.

Interestingly, the spectra show a nearly isobetic (equal absorption) point near $\Delta_{\text{Mott}} = 1.5$ eV, consistent with the experimental behavior. We show below that the same energy scale for Δ_{Mott} is also consistent with the ARPES data where isobetic point represents “waterfall” region, see fig. 2. The doping evolution is completely different on opposite sides of Δ_{Mott} . Above this point the spectrum is dominated by a broad hump feature, a signature of the Mott gap. At half filling, only this feature is present and the optical spectrum shows an insulating gap whose energy, structure, and intensity match remarkably with measurements [6,7]. As doping increases the high-energy peak shifts to higher energy and broadens.

³The two experimental data set from ref. [6] and ref. [7] are very similar except the high-energy background contribution which suggests that this background may be largely extrinsic.

⁴The high-energy bands are predominantly non-bonding oxygens of the three-band model of cuprates. See Supplemental fig. 3 of Comanac *et al.* [12].

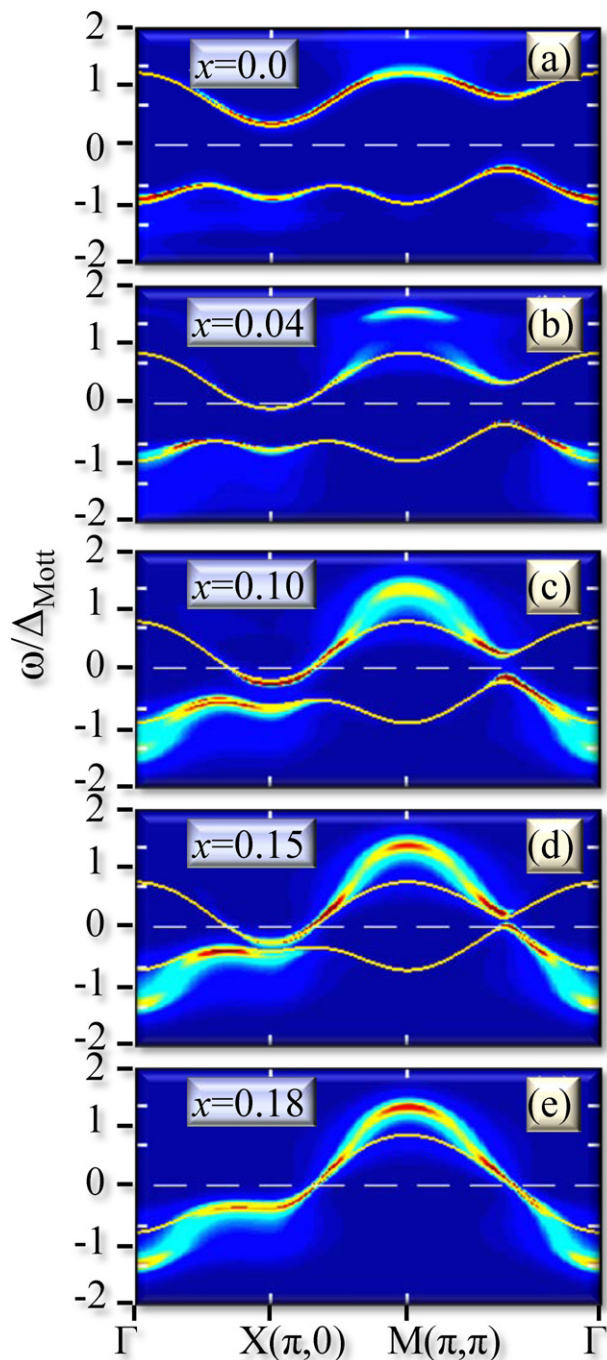


Fig. 2: (Color online) Spectral intensity as a function of ω along the high-symmetry lines for several dopings (at $T = 0$). Blue-to-red color map gives the minimum to maximum intensity. In each panel, the gold lines represent the renormalized magnetic bands (Σ_0 -dressed).

Below the isosbestic point there is little spectral weight at half filling, but as doping increases spectral weight is gradually transferred from the higher-energy region to the mid-infrared (MIR) one. The lower-energy spectrum is associated with a Drude peak related to intraband transitions and a mid-infrared peak associated with transitions across the magnetic gap (the pseudogap for the

electron-doped cuprates). With doping, this peak shifts to lower energy as the magnetic gap collapses and gradually sharpens. Note that at $x = 0.17$, when the pseudogap has collapsed, Mott-gap features still persist in the spectrum. The present mean-field calculation overestimates the Néel temperature T_N , but this can be corrected by including critical fluctuations, *grave à la* Mermin-Wagner theorem [24].

The origin of these features can be understood by looking at the doping dependence of the momentum-resolved spectral weight in fig. 2. In the overdoped case in fig. 2(e), a kink due to the bosonic coupling reproduces the waterfall effect below E_F , with a corresponding effect above E_F , splitting the spectrum into an effective three-band behavior, with UHB, LHB, and in-gap states. The features in the optical spectra are associated with transitions between these bands: The residual Mott gap arises from the transition from the LMB to the incoherent UHB (or from LHB to UMB), while the Drude term is associated with intraband transitions near the Fermi level. At lower doping an AFM gap opens in the coherent in-gap states⁵, leading to the UMB/LMB splitting and a four-band behavior similar to that seen in QMC cluster calculations [10]. Consistent with the QMC calculations, the coherent in-gap bands are dressed by magnetic quasiparticles. As the magnetic gap opens, the MIR feature in the optical spectra, being associated with transitions across this gap, shifts to higher energy.

The quality of self-consistency of our scheme can be assessed by noting that the final coherent bands have nearly the same dispersion as the Σ_0^t -dressed ones (gold lines) used as input to obtain the self-energy. The doping dependence of the two coherent magnetic bands is in excellent agreement with experiments [25] and earlier mean-field calculations [17,18], and captures the incoherent weight (the UHB/LHBs) at higher energies seen experimentally. Note that the incoherent weight is concentrated near the top and bottom of the bare LDA bands, leading to a nearly doping-independent UHB-LHB splitting.

Further insight is provided by fig. 3(a), which compares the full QP-*GW* DOS (blue line) and the Σ_0 -dressed quasiparticle DOS (red line), normalized to the same peak height, for a representative doping $x = 0.04$. The good agreement between various computations over most of the energy range indicates the high degree of self-consistency in the self-energy. The dressed DOS shows four well-separated peaks. A clear leading edge gap of ~ 0.3 eV (~ 1 eV at $x = 0$) can be seen. A gap persists at higher doping up to $x = 0.18$ (fig. 1), although it is obscured in the DOS by band overlap. The importance of the vertex correction is illustrated by the green line in fig. 3(a), which shows that setting $\Gamma = 1$ reduces the weight in the U/LHBs.

Figure 3(b) shows how the calculated imaginary self-energy Σ'' evolves with doping. The solid lines give the

⁵We use a single renormalisation factor for both bands at all dopings.

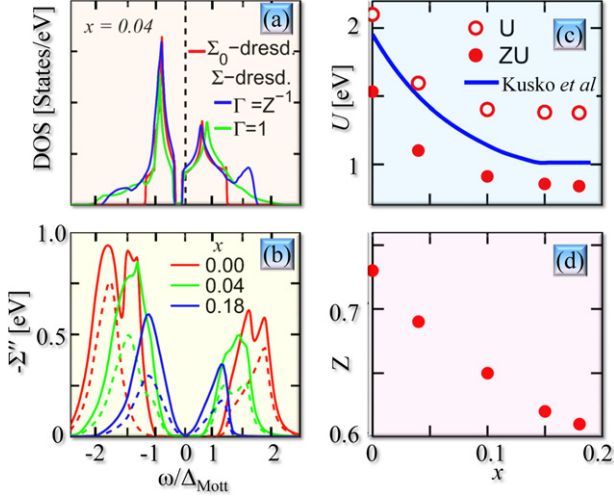


Fig. 3: (Color online) (a) The QP-GW DOS (blue lines) is compared with Σ_0 -dressed DOS (red lines) calculated at $T=0$. The green lines show the DOS without the vertex correction. (b) Solid lines give the imaginary part of the self-energy, while the dashed lines give the corresponding charge contributions. (c) Doping dependence of self-consistent values of U and ZU is compared with earlier mean-field results [17,18]. (d) The renormalization factor Z decreases linearly with doping.

total Σ'' , with the corresponding dashed lines giving the charge contribution. ($\Sigma_{\text{spin}} = \Sigma_{\text{total}} - \Sigma_{\text{charge}}$ is not shown.) In the underdoped region the extra splitting at high energies in the self-energy is related to spin-charge separation. The spin response is significant at low energy for all doping but the charge contribution is nearly zero in the low-energy region for the lower doping and becomes finite only at higher energies above ~ 3 eV. As doping increases, the charge response moves toward the Fermi level and increases in contribution to its total value. At $x=18\%$, when the AFM gap vanishes, the charge and spin susceptibility become equal. Note that the broadening of the self-energy evident in fig. 3(b) is reflected in the increasing broadening of the Mott gap feature with doping. The shift of the peak in the imaginary part of the self-energy towards E_F in fig. 3(b) reflects the doping dependence of the MIR feature in fig. 1.

Figure 3(c) describes the doping dependence of U . Although the renormalized Hubbard parameter ZU follows almost the same doping dependence as in mean-field calculations [17,18], the bare U displays considerably weaker doping dependence away from half filling. The renormalization factor Z in fig. 3(d) actually increases with underdoping⁶. This can be readily understood. As we lower doping, the AFM gap increases leading to a decrease of the spectral weight near the Fermi level. This causes a reduction of the real part of the self-energy,

⁶Recall that this Z parameter represents an average renormalization over the coherent band, and is not necessarily equal to the conventional renormalization factor at E_F .

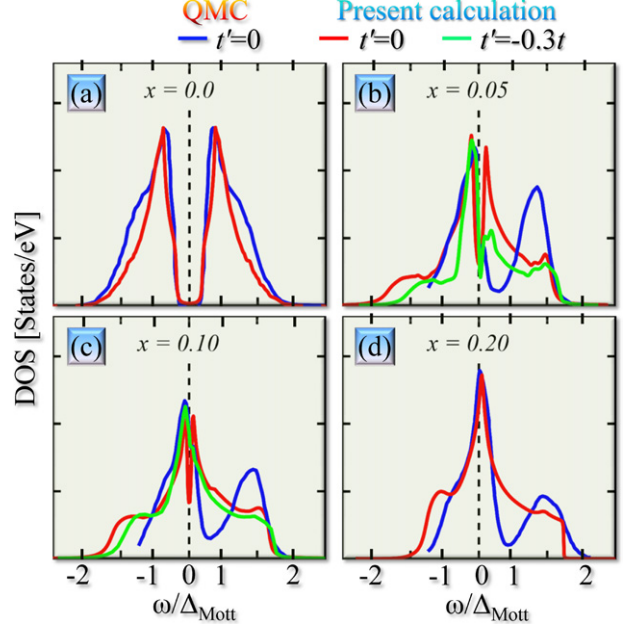


Fig. 4: (Color online) The computed DOS at various dopings are compared with the corresponding QMC results (blue lines) for $x=0.0$ [8] and for $x=0.05$ to $x=0.20$ [9]. The red lines in each panel give our result for $t'=0$, whereas the green lines in (b) and (c) are for $t'=-0.3t$.

shifting the peak in Σ' towards higher energy. The resulting slope decrease leads to a larger Z .

Existing QMC calculations on the cuprates generally employ simpler hopping parameter sets, so we have repeated our calculations with the same band parameters for a quantitative comparison in fig. 4. All the QMC results (blue lines) are obtained for $t'=0$, $U=8t$ with a momentum-dependent self-energy correction [8,9]. We have obtained the corresponding DOSs (red lines) for $t'=0$ for Σ calculated at a fixed momentum of $k=(\pi/2, \pi/2)$, using a doping-dependent renormalized U (ZU) very similar to the one found for the electron-doped case in fig. 3(c). (Note that the QMC automatically generates a renormalized U .) Our result reproduces the QMC very well for $x=0$ in fig. 4(a) where a prominent electron-hole symmetry is observed. At higher doping, the QMC results show a relatively smaller coherent peak above the Fermi level, whereas our result continues to exhibit near electron-hole symmetry in the in-gap region as might be expected for $t'=0$ dispersion. We can mimic a momentum-dependent self-energy by including $t'=-0.3t$, and find that this provides better agreement with the QMC results as shown by the green lines in figs. 4(b) and (c). Finally, at $x=0.20$, the pseudogap collapses and our result with $t'=0$ agrees very well with the QMC in fig. 4(d). As might be expected from our approximate self-energy calculation, the weight of the UHB is generally underestimated.

In summary, we find that spin-wave dressing of the quasiparticles explains the incoherent U/LHB

features seen in various experiments including the recent experiments observing waterfall effects in the cuprate spectra. The self-energy corrections not only renormalize the large widths of the LDA dispersions but also restore the residual incoherent spectral weight associated with U/LHBs. In the underdoped regime, we show that the coherent in-gap bands reproduce both the four-band behavior seen in quantum cluster calculations and the magnetic gap collapse found in the mean-field calculations and a variety of experiments. The puzzling persistence of the Mott gap in optical spectra, even as the magnetic gap collapses, is thus reconciled. The fact that our calculations work so well confirms that the cuprates can be understood within the intermediate coupling regime, with U much less than twice the bandwidth [13,14]. We extend these calculations to multiband systems such as iron-pnictide [26], iron-selenide [27] and heavy-fermion compounds [28] where we find that the magnetic and superconducting properties can also be understood from such intermediate coupling theories.

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