Changes in the self-energy and $d$-wave pairing strength with doping in overdoped La$_{2-x}$Sr$_x$CuO$_4$

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Angle resolved photoemission spectroscopy (ARPES) studies of the overdoped cuprate superconductor La$_{2-x}$Sr$_x$CuO$_4$ find only small changes in the near nodal electron self energy over a spectral range of several hundred meV as the doping increases from $x = 0.2$ to $x = 0.3$ and the superconducting transition temperature $T_c$ decreases from 32K to 0K. These measurements put constraints on the structure of the electron-electron interaction. Here we show that a spin-fluctuation interaction leads to behavior which is consistent with these experimental results.

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A possible way to identify the pairing interaction responsible for superconductivity in a given material is to investigate the structure in the effective self-energy extracted from angle resolved photoemission spectroscopy (ARPES) measurements. Recently Park et al. have reported ARPES measurements on overdoped La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) with different doping levels that raise questions regarding the origin of the pairing interaction. In the present work we provide theoretical calculations within a spin-fluctuation approximation, we believe that it can provide a useful approximation for the overdoped regime. Since we are interested in determining the spectral function and self energy as functions of frequency, we will work on the real frequency axis as described in Ref. This avoids the need of analytic continuation from imaginary Matsubara frequencies to the real axis, which can be numerically unstable.

Within FLEX the imaginary part of the self-energy $\Sigma$ is obtained from

$$\text{Im } \Sigma (k, \omega) = -\frac{1}{N} \sum_{q} \int_{-\infty}^{\infty} d\Omega \left[ n(\Omega) + f(\Omega - \omega) \right] \times \text{Im } \Gamma (q, \Omega) A (k-q, \omega - \Omega).$$

(1)

Here, $f$ and $n$ are the usual Fermi and Bose functions, respectively, and $N$ is the number of lattice sites. The vertex function $\Gamma$ includes the interactions due to spin and charge fluctuations and is given by

$$\Gamma = \frac{3}{2} \frac{U^2 \chi_0}{1-U \chi_0} + \frac{1}{2} \frac{U^2 \chi_0}{1+U \chi_0} - U^2 \chi_0$$

(2)

where the last term removes a double counting. $\chi_0$ is...
The single particle spectral weights obtained from the FLEX calculation for $x = 0.22$ and $x = 0.3$ along the nodal C1 cut are shown in Figs. 2a and b. In the FLEX calculation, we adjust the bandstructure $\epsilon_k$ in such a way that the renormalized Fermi surface at each doping is fixed to the ARPES determined Fermi surface for that doping. This is done by requiring that at each iteration of the FLEX calculation the quantity $\epsilon_k + \text{Re} \Sigma (k, \omega = 0)$ remains equal to $\epsilon_k$ and amounts to setting $\mu = -0.99$. Our calculations are done in energy units of $t$. The parameter $t$ is then determined at the end of the calculation in such a way that the nodal MDC peak position of our FLEX calculation agrees with the experimental one from Park et al. at $\omega = -200$ meV. In this way our value of $t$ represents an unrenormalized hopping in contrast to the renormalized value of $t = 250$ meV found by Yoshida et al. For our numerical calculations we have chosen a moderate value of $U/t = 3$ to stay in a weak coupling regime where FLEX can be assumed to give reliable results.

Results - The single particle spectral weights obtained from the FLEX calculation for $x = 0.22$ and $x = 0.3$ along the nodal C1 cut are shown in Figs. 2a and b, respectively. Here the $y$-axis denotes energy in units of meV and the $x$-axis the wavevector in units of inverse Angstroms. A lattice constant $a = 3.79a$ was used to set the wavevector scale. The solid curves in Figs. 2a and b show the MDC peak and the dashed line is a linear dispersion connecting the MDC peaks at $0.0$ eV and $-2.0$ eV. For $x = 0.22$, we find the bare $t = 500$ meV while for $x = 0.3$, $t = 415$ meV. The dispersions of the MDC peak for the two dopings are compared in Fig. 2c.
Increasing the interaction strength $U/t$ will increase the peak height but takes the system into a stronger coupling regime where the FLEX calculation is less reliable. The C2 and C3 cuts (Figs. 3b and c) show a similar behavior. Overall, the results for $\text{Re } \Sigma_{\text{eff}}(k, \omega)$ shown in Fig. 3 appear similar to what is seen experimentally. In particular, the peak in $\text{Re } \Sigma_{\text{eff}}(k, \omega)$ for $x = 0.3$ is reduced by about 30% from that for $x = 0.22$. Thus just as seen experimentally for the nodal momentum cut and the nearby C2 and C3 cuts, there is only a modest weakening of the peak in $\text{Re } \Sigma_{\text{eff}}(k, \omega)$ when the doping is increased from 0.22 to 0.3.

Next we examine the change in the $d$-wave pairing strength when the doping $x$ is increased from 0.22 to 0.3. While the value of $T_c$ depends upon $U$ as well as the impurity scattering [22] associated with the Sr doping, the change in the $d$-wave pairing strength

$$
\lambda_d = \int_0^\infty \frac{d\omega}{\pi\omega} \frac{\langle g(k) \text{ Im } \tilde{\Gamma}(k-k', \omega) g(k') \rangle_{k,k'}}{\langle g^2(k) \rangle_k}
$$

provides a useful measure of the effect of doping on the pairing. Here $\tilde{\Gamma}$ is the pairing interaction vertex

$$
\tilde{\Gamma} = \frac{3}{2} \frac{U^2 \chi_0}{1-U\chi_0} - \frac{1}{2} \frac{U^2 \chi_0}{1+U\chi_0}
$$

and $g(k)$ the gap function $(\cos k_x a - \cos k_y a)$. The averages in Eq. (7) are taken over the Fermi surface. Although the charge fluctuation contribution to the self-energy interaction $\Gamma$ changes sign in the singlet pairing vertex $\tilde{\Gamma}$, the dominant term in both vertices is the spin-fluctuation interaction given by the first term in Eqs. (2) and (8). For $x = 0.22$ we find that $\lambda_d = 1.10$ while for $x = 0.3$ it is reduced to 0.35. This decrease reflects a redistribution of the spectral weight from the antiferromagnetic ($\pi, \pi$) region of the Brillouin zone to other parts of the Brillouin zone which contribute less or even negatively to the “$d$-wave” average in Eq. (7). Thus as the doping $x$ increases, the strength of the interaction in the anomalous self-energy $d$-wave pairing channel can significantly decrease while the change in its contribution to the normal self-energy in the nodal region is relatively modest. In Fig. 3 we have plotted $\lambda_d(\Omega)$ obtained by cutting off the frequency integration in Eq. (7) at $\Omega$. This plot shows that the contributions to $\lambda_d$ come from modes with energies in a spectral range of several hundred meV.

Conclusions - A variety of ARPES studies [5, 6, 9, 10, 13] of hole doped LSCO observe a 50–80 meV kink in the near nodal MDC dispersion which is reflected as a broad peak in an effective self energy $\text{Re } \Sigma_{\text{eff}}(k, \omega)$ over an energy range of several hundred meV. However, there remains disagreement regarding the origin of this structure and its relationship to the pairing interaction. Here we have focused on recent results for overdoped LSCO, a system which is expected to be more amiable
to a weak coupling analysis. In addition, this is a single layer cuprate whose Fermi surface at the dopings we have studied has been determined by ARPES. Within a FLEX approximation we have calculated the single particle spectral weight for overdoped LSCO and extracted Re $\Sigma_{\text{eff}}(k,\omega)$ in the same manner as done in the ARPES experiment. An important ingredient in this calculation was the adjustment of the bare band parameters such that the renormalized Fermi surface at a given doping was fixed to the ARPES determined Fermi surface for that doping. The results showed that the renormalized nodal Fermi velocity remained the same and the maximum value of Re $\Sigma_{\text{eff}}(k,\omega)$ decreased by $\sim30\%$ as the doping changed from 0.22 to 0.3, similar to what was seen experimentally. Using the same parameters, the pairing strength in the $d$-wave channel was found to decrease from $\lambda_d = 1.10$ ($x = 0.22$) to $\lambda_d = 0.35$ ($x = 0.3$). Thus we conclude that a spin-fluctuation interaction can give rise to the observed structure in Re $\Sigma_{\text{eff}}(k,\omega)$ and also exhibit a significant increase in the $d$-wave pairing strength as the doping increases from $x = 0.22$ to 0.3. The point is that the self-energy is determined by the convolution of the interaction with the spectral weight $A(k,\omega)$, while the pairing strength depends on the $d$-wave projection of the interaction. This $d$-wave projection is more sensitive to the changes in the momentum dependence of the spin-fluctuation interaction and the Fermi surface with doping than is the self-energy. Thus we conclude that the experimental results reported by Park et al. for overdoped LSCO are consistent with a spin-fluctuation pairing mechanism operating in a spectral range of several hundred meV.

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