ELSEVIER

Physica B 284–288 (2000) 983–984

PHYSICA B

www.elsevier.com/locate/physb

Single-particle spectra near a stripe instability

S. Caprara*, C. Di Castro, M. Grilli

Istituto Nazionale per la Fisica della Materia – Unità di Roma 1, and Dipartimento di Fisica - Università di Roma "La Sapienza", P.le A. Moro 2, I-00185 Rome, Italy

Abstract

We analyze the single-particle spectra of a bi-layered electron system near a stripe instability and compare the results with ARPES experiments on the Bi2212 cuprate superconductor near optimum doping, addressing also the issue of the puzzling absence of bonding–antibonding splitting. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Charge and spin fluctuations; Fermi surface

It was proposed that the anomalous normal-state properties of the cuprate superconductors at optimum doping may result from the mixing of the doped holes with the collective charge and spin fluctuations near a stripe instability [1]. To investigate the corresponding quasiparticle spectra, and to compare with experiments on the bi-layered Bi2212 [2], we introduce the Hamiltonian

$$H = \sum_{k;\sigma} \sum_{\ell} (\xi_k - \delta\mu) c^+_{k\sigma\ell} c_{k\sigma\ell} - t_\perp \sum_{k;\sigma} \gamma_k (c^+_{k\sigma 1} c_{k\sigma 2} + h.c.) + \sum_{k,q;\sigma,\rho} \sum_{\ell} \sum_{i} g_i c^+_{k+q\sigma\ell} c_{k\rho\ell} \tau^i_{\sigma\rho} S^i_{-q\ell},$$

where $\xi_k = -2t(c_x + c_y) + 4t' c_x c_y - \mu$, with $c_{x,y} = \cos(k_{x,y} a)$, is the tight-binding dispersion for electrons on a square lattice with nearest and next-to-nearest neighbors hopping, a is the lattice spacing, μ is the bare chemical potential and $\delta\mu$ is the shift in the interacting system. The planes are labelled by $\ell = 1, 2$ and $t_\perp$ is the interplane matrix element modulated by $\gamma_k = \frac{1}{2}|c_x - c_y|$ to account for the suppression at $k_x \simeq \pm k_y$ [3]. The constants g_i couple electrons to charge ($i = 0$) and spin ($i = 1, 2, 3$) fluctuations. The spin structure of the generalized density coupled to $S^i_{-q\ell}$ is accounted for by the Pauli matrix τ^i. The counterterm $\delta\mu \sim O(g^2)$ is determined, order by order in perturbation theory, to fix the number of electrons. The fluctuating fields $S^i_{-q\ell}$ are characterized by the susceptibilities $\chi_{ij\ell\ell'}(q, \omega) = \delta_{ij}\delta_{\ell\ell'} A_i / [\kappa^2 + \eta_{q-Q_{i\ell}} - i\bar{\tau}\omega]^{-1}$, where A_i are constants, the mass κ^2 vanishes at criticality, $\eta_k = 2 - c_x - c_y$ reproduces the k^2 behavior at $ka \ll 1$, preserving the lattice periodicity, $Q_{i\ell}$ are the critical wave-vectors, $\bar{\tau}$ is a characteristic time scale, and the dimensionless coupling constants are $\lambda_i = g_i^2 A_i / t$. In the paramagnetic phase the parameters are the same for $i = 1, 2, 3$, and we label charge and spin fluctuations with c,s. The direction of the charge modulation is debated. As a matter of illustration we analyze the case $Q_{c1} = 0.4(\pi/a, -\pi/a)$, $Q_{s1} = (\pi/a, \pi/a)$, suggested by the ARPES experiments on Bi2212 [2]. We allow for a mismatch of the charge modulation pattern on the two planes and take $Q_{c2} = 0.4(\pi/a, \pi/a)$, while $Q_{s2} = Q_{s1}$. The Hamiltonian is written in a simpler "plane representation", in which the interaction is diagonal, and the decoupling of the two planes as $t_\perp \to 0$ is evident. The alternative "band representation" is obtained by diagonalization of the fermionic part of the Hamiltonian, but the interaction is not diagonal, and the role of $t_\perp$ is less transparent. The two representations are, of course, equivalent.

The $O(\lambda)$ perturbation theory accounts for the main dressing of the electrons by quasicrystal charge and spin fluctuations. An average over $\pm Q_c$ is performed to maintain inversion symmetry, leading to the self-energy $\Sigma_\ell = \langle \Sigma_{c\ell} \rangle + 3\Sigma_s - \delta\mu$. Previous analysis for $t_\perp = 0$ [4] showed that spectral weight is transferred from the

* Corresponding author.
E-mail address: sergio.caprara@roma1.infn.it (S. Caprara)

0921-4526/00/$ - see front matter
PII: S0921-4526(99)02316-9

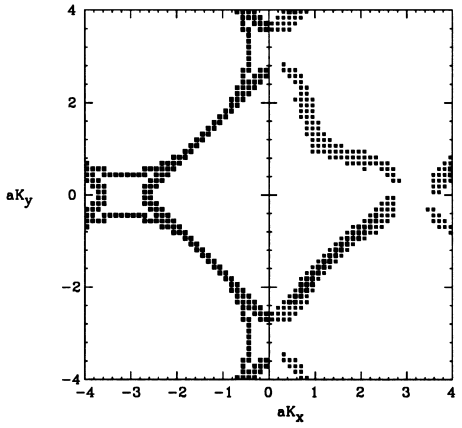

Fig. 1. FS as calculated for electrons on the plane $\ell = 1$, with $t = 200$ meV, $t' = 50$ meV, $t_\perp = 50$ meV, $\mu = -180$ meV, $\kappa^2 \simeq 0$, $\bar{\tau}^{-1} = 200$ meV and $\lambda_{s,c} = 0$ (left), $\lambda_s = 0.5$, $\lambda_c = 0.3$ (right). A half of the FS is plotted in both cases to save space. The full FS is obtained by inverting the data with respect to the point $\Gamma = (0, 0)$.

quasiparticle peak to incoherent shadow resonances. The changes in the single-particle spectra and inthe distribution of low-lying spectral weight are in agreement with the experiment [2]. The suppression of spectral weight at the Fermi level near the M points [i.e. $ak_M = (0, \pm\pi); (\pm\pi, 0)$], due to spin fluctuations, is modulated by charge fluctuations.

Here we address the absence of bi-layer splitting, despite a sizable calculated $t_\perp$ [3]. The contribution of the plane ℓ to the spectral density is

$$A_\ell = -\frac{1}{\pi}\sum_{\alpha=1,2} \mathrm{Im}\frac{1 + (-1)^{\alpha+\ell}\Sigma_-/\tilde{t}_\perp}{\omega - \xi_k - \Sigma_+ + (-1)^\alpha \tilde{t}_\perp}\Bigg|_R,$$

where $\Sigma_\pm = \frac{1}{2}(\Sigma_{\ell=1} \pm \Sigma_{\ell=2})$, $\tilde{t}_\perp = (t_\perp^2\gamma_k^2 + \Sigma_-^2)^{1/2}$ and the subscript R means retarded. For $\lambda_i = 0$ the quasiparticle FS consists of two branches, corresponding to the bonding and antibonding band (Fig. 1, left part of the figure), well separated near the M points, where γ_k is larger. However, a moderate coupling between the electrons and the critical fluctuations is sufficient to eliminate the FS splitting. Indeed, the suppression of spectral weight is stronger near the M points where the splitting is expected to be larger, and is weaker where the splitting is naturally suppressed by γ_k. The effect is enhanced in the case of a mismatch between the fluctuation patterns on the two different planes. The resulting FS, projected onto a single plane (e.g. $\ell = 1$) as it is suitable to interpret ARPES results, is essentially the same as in the absence of interlayer coupling (Fig. 1, right panel). Thus, the absence of the band splitting in ARPES spectra of bi-layered materials can be due to the enhancement of charge and spin fluctuations scattering the quasiparticles near a stripe instability.

Acknowledgements

Part of this Research work was carried out with the financial support of the I.N.F.M. - P.R.A. 1996.

References

[1] C. Castellani, C. Di Castro, M. Grilli, Phys. Rev. Lett. 75 (1995) 4650.
[2] N.L. Saini et al., Phys. Rev. Lett. 79 (1997) 3467.
[3] O.K. Andersen et al., Phys. Rev. B 49 (1994) 4145.
[4] S. Caprara, M. Sulpizi, A. Bianconi, C. Di Castro, M. Grilli, Phys. Rev. B 59 (1999) 14 980.