J. Phys.: Condens. Matter 5 (1993) A377–A380. Printed in the UK

Electronic susceptibility of $YBa_2Cu_3O_7$ and its relation to phonon anomalies

C O Rodriguez, A I Liechtenstein, I I Mazin, O Jepsen and O K Andersen
Max Planck Institüt für Festkörperforschung, Heisenbergstrasse 1, D-7000 Stuttgart 80, Federal Republic of Germany

Abstract. A first-principles prediction of the q dependence of the electronic susceptibility of $YBa_2Cu_3O_7$ and the relation to experimentally observed phonon anomalies is presented.

Density-functional (LDA) frozen-phonon calculations of structural parameters, phonon frequencies, the electronic structure, and electron–phonon interactions in the stoichiometric high-temperature superconductor $YBa_2Cu_3O_7$ have been reported [1–3]. Good agreement was found with the experimental structural parameters and phonon frequencies, as well as with the frequency change, induced by gap formation below T_c, observed for three Raman active phonons. Recently, there has been considerable progress in the experimental determination of the Fermi surface (FS) and the agreement with our [4] and other [5] theoretical predictions is surprisingly good.

The calculated cross sections of the FS, $\epsilon_{nk} = 0$, with the $k_z = 0$, and $k_z = \pi/c$ planes, were shown in figures 2 of [2] and [3]. The FS has four sheets (n), denoted a, b, c, and s. The a and b sheets have *plane* pdσ^* character (O2(p_x)–Cu2($d_{x^2-y^2}$)–O3(p_y)) and are, respectively, antibonding and bonding between the planes. The c sheet has *chain* pdσ^* character (O4(p_z)–Cu1($d_{z^2-y^2}$)–O1(p_y)), and the s sheet, the *stick*, has predominantly *apical-oxygen* (O4) character (O4(p_y)–Cu1(d_{yz})–O1(p_z)–Ba(p_x)) [6]. The low-velocity (high-density-of-states) parts of the FS are the stick, which is centred on the line $k = (\pi/a, \pi/b, k_z)$ (S–R) and whose band maximum is only 35 meV above the Fermi level, the *knuckles* of the a-plane sheet, which are pointing in the [100] direction towards saddle points at $Y_\pm \simeq (0, (1\pm\frac{1}{3})\pi/b, 0)$, and the *cracker* of the a-like part of the c-sheet, running in the [100] direction and with the *necks* centred at the saddle points $X_\pm \simeq ((1\pm\frac{1}{4})\pi/a, 0, 0)$. These X and Y saddle points are, respectively 20 and 10 meV below the Fermi level and their bifurcation away from the X and Y points is caused by dimpling of the planes. The dispersion in the k_z direction is negligible for the b and s sheets, but noticeable for the a and c sheets because these have avoided crossings, except in the $k_z = 0$ plane. The strong a–c hybridization for $k_z \neq 0$ causes the $X_\pm$ saddles to be *minima* as functions of k_z, while the $Y_\pm$ saddles are *maxima*. Near the Y saddle point the FS thus has two sheets (knuckles) on either side, whereas near an X saddle point it has one sheet (the cracker).

The electron–phonon coupling constant λ may be expressed as the sum over coupling constants, $\lambda_{\nu q} \equiv [\pi N(0)]^{-1}\gamma_{\nu q}/\omega_{\nu q}^2$, for each phonon mode. Here, $\omega_{\nu q}$ is the phonon energy, $\gamma_{\nu q}$ the phonon linewidth, and $N(0) \equiv \sum_{nk}\delta(\epsilon_{nk}) = 35$ states/(Ryd×$YBa_2Cu_3O_7$×spin) is the electronic density of states per spin at the Fermi level and $\sum_k \equiv \int d^3k/\text{BZV}$ is the Brillouin-zone average. The linewidth of a phonon due to its interaction with the electrons is given by Fermi's golden rule as

$$\gamma_{\nu q} = 2\pi \sum_{nmk} |g_{\nu q,nk,m(k+q)}|^2 f(\epsilon_{nk})[1 - f(\epsilon_{m(k+q)})]\delta(\epsilon_{m(k+q)} - \epsilon_{nk} - \omega_{\nu q}) \qquad (1)$$

0953-8984/93/SA0377+04$07.50

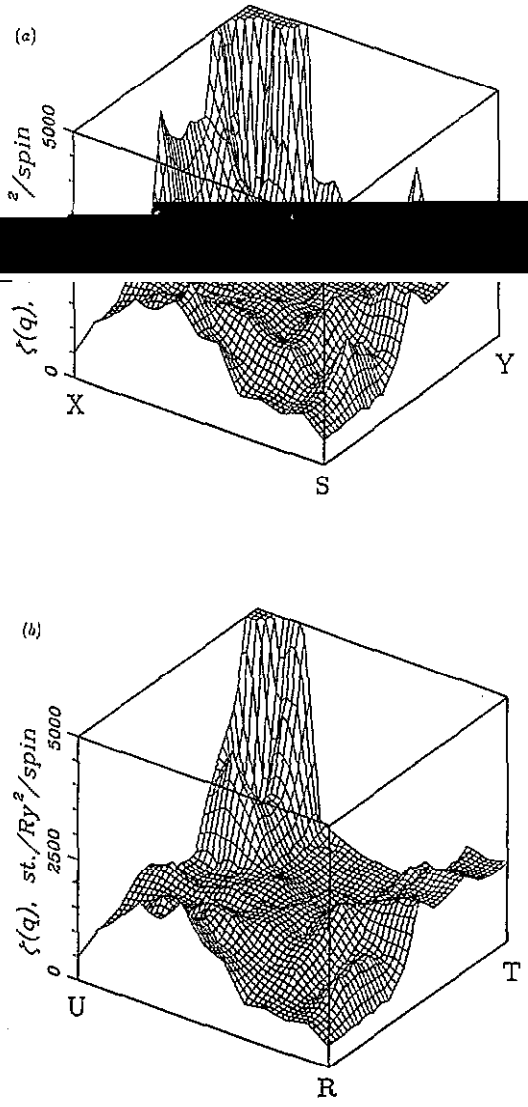

Figure 1. Calculated $\zeta(q)$ (2) in the planes (*a*) $q_z = 0$ and (*b*) $q_z = \pi/c$.

where the factor of 2 originates from the spin degeneracy and g is the electron–phonon matrix element.

To investigate the q dependence in general, we take the matrix element outside the sum in (1) and, first, consider the small-temperature and small-ω limits, that is, we consider the function

$$\zeta(q) \equiv \frac{1}{2\pi g^2} \lim_{\omega \to 0} \frac{\gamma(q,\omega)}{\omega} = \sum_{nmk} \delta(\epsilon_{nk})\delta(\epsilon_{m(k+q)}) = \sum_{nm} \int \frac{\mathrm{d}k/\mathrm{BZV}}{|v_{nk} \times v_{m(k+q)}|} \tag{2}$$

which gives the phase space available for scattering by q from one part of the FS to another and is proportional to $\mathrm{Im}\,\chi^0(q,\omega)/\omega$ in the limit $\omega \to 0$. The line integral in the last expression is along the cut between the n sheet and the m sheet displaced by $-q$. This ζ function is shown in figure 1 for $q_z = 0$ and for $q_z = \pi/c$, and is

seen to have a strong q dependence. Its average over the Brillouin zone is $N(0)^2 \simeq 1200$ [states/(Ryd × $YBa_2Cu_3O_7$ × spin]^2 and the value at S is about one half, while the value at Y is about one and a half times this average. This higher value at Y is mainly caused by stick-to-knuckle nesting. For quantitative estimates matrix-element effects cannot be neglected. This should therefore be kept in mind during the following discussion.

Peaks in $\zeta(q)$ generally occur for values of q which nest high-density-of-states parts of the FS, or which nest large FS areas. For $YBa_2Cu_3O_7$, the neck-to-neck and knuckle-to-knuckle nestings indicated by arrows in figure 2 of [2] cause the peaks near the *points* X_+–$X_- \simeq ((\frac{1}{2})\pi/a, 0, 0)$ and Y_+–$Y_- \simeq (0, (\frac{2}{3})\pi/b, 0)$. The ridges connecting these peaks with the central peak, thus running along the inner parts of the *lines* ΓX and ΓY, are due to sliding nesting of those parts of the a and b sheets which are flat and parallel to the (010) and (100) planes. More importantly, sliding nesting of the cracker contributes to the ΓX ridge and makes it considerably higher than the ΓY ridge.

Conventional nesting [8] and sliding nesting [9–11] are instrumental in current attempts to explain the observed marginal Fermi liquid behaviour.

Since the dominating structure in $\zeta(q)$ is caused by transitions between parts of the FS (knuckles, necks, or stick) which are within phonon energies, as well as within k_BT, of the saddle point or maximum of the corresponding band, the ω and temperature dependences cannot really be neglected. Keep in mind that the calculated position of the Fermi level is not accurate to more than 10 meV.

Support for the reality of neck-to-neck and/or knuckle-to-knuckle nesting comes from neutron scattering experiments on *twinned* single crystals of $YBa_2Cu_3O_7$ [12]: these experiments found anomalously large phonon linewidths (initially described as an extra branch) for q along the [100]/[010] directions and $0.4\pi/a \leqslant q \leqslant 0.8\pi/a$. The ζ function also indicates for which q values the self-energy for a phonon with energy close to the superconducting gap should change when the gap opens up. Indeed, for q along the [100]/[010] direction, it was found for $YBa_2Cu_3O_7$ [13] that the pronounced softening of the Raman 330 cm^{-1} phonon decreases slowly for q increasing up to $0.5\pi/a$ and thereafter it drops abruptly. For $YBa_2Cu_3O_{6.92}$, the softening increased slowly to a maximum for $q \simeq 0.5\pi/a$.

A detailed evaluation of the dependence of phonon linewidths on ω, temperature and oxygen stoichiometry is in progress.

References

[1] Rodriguez C O, Liechtenstein A I, Mazin I I, Jepsen O, Andersen O K and Methfessel M 1990 *Phys. Rev.* B 42 2992

[2] Andersen O K, Liechtenstein A I, Rodriguez C O, Mazin I I, Jepsen O, Antropov V P, Gunnarsson O and Gopalan S 1991 *Physica* C **185–9** 147

[3] Mazin I I, Andersen O K, Liechtenstein A I, Jepsen O, Antropov V P, Rashkeev S N, Anisimov V I, Zaanen J, Rodriguez C O and Methfessel M 1993 *Proc. Lattice Effects in High-T_c Superconductors (Santa Fe, 1992)* ed Y Bar-Yam, T Egami, J T Muestre de Lyon and A R Bishop (Singapore: World Scientific) pp 235–51

[4] Mazin I I, Jepsen O, Andersen O K, Liechtenstein A I, Rashkeev S N and Uspenskii Y A 1992 *Phys. Rev.* B **45** 5103; 1992 *Phys. Rev. Lett.* **68** 3936, and references therein

[5] Pickett W E, Krakauer H, Cohen R E and Singh D J 1992 *Science* **255** 47

[6] Andersen O K, Jepsen O, Rodriguez C O, Liechtenstein A I and Mazin I I to be published

[7] Pickett W E, Krakauer H and Cohen R E 1990 *Physica* B **165–6** 1055

[8] Virosztek V and Ruvals J 1990 *Phys. Rev.* B 42 4064

[9] Markiewicz R S 1991 *Int. J. Mod. Phys.* B 5 2037

[10] Newns D M, Pattnik P C and Tsuei C C 1991 *Phys. Rev.* B 43 3075

[11] Gopalan S, Gunnarsson O and Andersen O K 1992 *Phys. Rev.* B **46** 11 798
[12] Pintschovius L, Pyka N, Reichardt W, Rumiantsev A Yu, Mitrofanov N L, Ivanov A V, Collin G and Bourges P 1991 *Physica* C **185–9** 156
[13] Pyka N, Reichardt W, Pintschovius L, Engel G, Rossat-Mignod J and Henry J Y *Phys. Rev. Lett.* **70** 1457