Density-of-states-driven anisotropies induced by momentum decoupling in $Bi_2Sr_2CaCu_2O_8$

G. Varelogiannis
Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, P.O. Box 1527, Heraklion Crete 71110, Greece

A. Perali, E. Cappelluti, and L. Pietronero
Dipartimento di Fisica, Università di Roma "La Sapienza," Piazzale A. Moro 2, I-00185 Roma, Italy
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Momentum decoupling arises when small-q scattering dominates the pairing interaction and implies density-of-states-driven anisotropies in superconductivity. In this scheme we explain puzzling aspects of the anisotropy in $Bi_2Sr_2CaCu_2O_8$, such as the correlation of gap magnitude and visibility of the dip above the gap, the enhancement of anisotropy with temperature, the presence of gap minima away from the Γ-X direction and a gap maximum in the Γ-$\bar{M}$ direction, the similarity of tunnel and angle-resolved photoemission spectra in the Γ-$\bar{M}$ direction, and the asymmetry in vacuum tunnel spectra where the dip structure is present only at negative sample bias. [S0163-1829(96)52134-X]

The observation by angle-resolved photoemission spectroscopy (ARPES) of the superconducting gap in $Bi_2Sr_2CaCu_2O_8$ (Refs. 1–5) failed in answering the controversial question of the symmetry of the order parameter. Some experimental results support the d-wave hypothesis,[2] while others point to a rather complex mixed state in which the gap has nodes away from the Γ-X ($k_x=k_y$) direction[3] or even has no nodes at all.[1,4] These contradictions, together with the absence of gap observation in $YBa_2Cu_3O_7$ and the weakness of the gap values reported on $Bi_2Sr_2CaCu_2O_8$,[5] illustrate the difficulty in measuring the gap with the ARPES technique.

However in some qualitative points all ARPES experiments are in agreement. The first point is that the higher values of the gap are reached in the direction where the density of electronic states (DOS) on the Fermi level $N(E_F,\mathbf{k})=|v_F(\mathbf{k})|^{-1}$ is maximal, and in general the gap magnitude is correlated with the DOS magnitude. A second point is related with the anomalous dip structure above the gap seen also by tunnel spectroscopy. This dip structure is more visible in the direction in which the gap and the DOS are maximal and the sharpness and magnitude of this structure is correlated with the magnitude of the gap and local DOS. A third important remark is that from the ARPES experiments in the Γ-$\bar{M}$ (0,1) direction where the gap and DOS are maximum, one obtains a spectral function very similar to the tunnel spectrum.[6] In the case of tunneling we see the average of the spectral function over the Fermi surface, and the similarity of ARPES and tunnel data in such anisotropic materials is quite surprising. In addition, some very important experimental trends have been reported recently. In Ref. 4 it is shown that the anisotropy is strongly enhanced when we move from the $T=0$ regime to the $T\rightarrow T_c$ regime. In Ref. 3 it has been shown that the gap has minima about 10° away from the Γ-X direction and a maximum in the Γ-X direction. On the other hand, detailed vacuum tunneling spectroscopy measurements[7] report an asymmetric density of states in $Bi_2Sr_2CaCu_2O_{8+\delta}$, with the dip appearing only at negative sample bias.

In the following, we will give a simultaneous explanation to all the previously cited experimental points. We will see in particular that all the previous points characterize a superconductor in which the isotropic s-wave electron-photon (or other boson) coupling is dominated by forward scattering processes. Dominance of forward scattering could be due for example to the vicinity of a phase separation instability[8] in strongly correlated electronic systems[9] or to an interlayer Josephson tunneling mechanism,[10] or simply due to the two-dimensional character of the electronic system.[11] On the other hand, there is evidence from Raman scattering[12] that small momentum transfer (Raman active) phonons are strongly affected by superconductivity in cuprates. Notice that a somewhat analogous situation has already been considered in discussions of the peak in the microwave conductivity[13] and of the change of sign of the order parameter[14] reported in some experiments on $YBa_2Cu_3O_7$.

When forward scattering is dominant, there is "momentum decoupling" (MD) in the superconducting behavior, implying *a different coupling in different regions of the Fermi surface*. In the case of MD the coupling at each region of the Fermi surface is proportional to the DOS in this region, and therefore *the anisotropies of the superconducting state are induced by the anisotropies of the density of states in the normal state*.

Let us now illustrate briefly how the MD appears for small momentum transfer processes and why it leads to DOS dependent anisotropies. The anisotropic Eliashberg equation in the off-diagonal sector, for an Einstein spectrum can be written with usual notations as follows:

$$\Delta_{\mathbf{k}}Z_{\mathbf{k}}=\pi T\sum_m \int_{S_F}\frac{d^2p}{S_F}\,\frac{N(E_F,\mathbf{p})|g(\mathbf{k}-\mathbf{p})|^2\Omega}{\Omega^2+(\omega_n-\omega_m)^2}F(\Delta_{\mathbf{p}},\omega_n).$$

The $\mathbf{k}$ dependence is contained in the coupling $|g(\mathbf{k}-\mathbf{p})|^2$.

In conventional s-wave superconductors it is assumed that the interaction $|g(\mathbf{k}-\mathbf{p})|^2$ is almost constant on the Fermi surface and it leads to an isotropic gap. On the other hand, if one supposes that $|g(\mathbf{k}-\mathbf{p})|^2$ has a relevant momentum dependence in the vicinity of the Fermi surface (as it is the case in the d-wave scenario where this function reflects electron-spin fluctuation coupling) then from the above equation one can obtain an anisotropic gap. However the anisotropy of the superconducting parameters is mainly imposed by the anisotropy of the interaction and *not* from the anisotropy of the density of states. In order to obtain significant DOS induced anisotropies one has to consider an *isotropic s-wave interaction* dominated by forward scattering processes. This can be illustrated by taking for example an interaction sharply peaked at zero momentum $|g(\mathbf{k}-\mathbf{p})|^2 \approx g^2\delta(\mathbf{k}-\mathbf{p})$. In that case occurs the perfect *momentum decoupling*. We obtain a momentum independent Eliashberg equation which provides the gap function $\Delta(\mathbf{k},i\omega_n)$ for each momentum $\mathbf{k}$ on the Fermi surface. This last equation is analogous to the isotropic Eliashberg equation *with a coupling strength proportional to the density of states at the given point of the Fermi surface* $N(E_F,\mathbf{k})$. We remark that our MD regime is completely different from any separable potential approach which can only lead to potential driven anisotropies.

Of course a δ-function peak at $q=0$ is a rather unrealistic coupling function. In our approach we consider an isotropic interaction that has a finite range in momentum space with a characteristic momentum cut-off q_c that is much smaller than k_F yet sufficiently larger than the level spacing $\approx 1/N$ in k space in such a way that the k integration introduces an average occupancy. However MD occurs even for finite q provided q *is small compared to the characteristic momentum of the DOS variations*. To illustrate this point we performed numerical simulation on a simple two-dimensional BCS model. In that case the gap is given by

$$\Delta(\mathbf{k}) = \sum_{\mathbf{p},|\xi_p|<\Omega_D} \frac{-V(\mathbf{k}-\mathbf{p})\Delta(\mathbf{p})}{2\sqrt{\xi_{\mathbf{p}}^2+\Delta^2(\mathbf{p})}} \tanh\{\sqrt{[\xi_{\mathbf{p}}^2+\Delta^2(\mathbf{p})]}/2T\}.$$

We consider an isotropic s-wave electron-phonon coupling having at small momenta *a* Lorentzian behavior as a function of the norm of the exchanged momentum $V(\mathbf{q}) = -V(1+|\mathbf{q}|^2/q_c^2)^{-1}$. In this spectrum the electron-phonon scattering is dominated by the processes which transfer a momentum smaller than q_c. In our analysis q_c is the relevant parameter and the particular shape of the interaction is irrelevant.

For clarity, we will consider here the simple nearest-neighbor tight-binding dispersion at half-filling $\xi_{\mathbf{k}} = -2t[\cos(k_x)+\cos(k_y)]$ (the lattice spacing is taken equal to unity). The Fermi surface is a square defined by $k_x = k_y \pm \pi$ and $k_x = -k_y \pm \pi$ with saddle points at $(0,\pm\pi)$ and $(\pm\pi,0)$. The minimum of the density of states is obtained at the points $(\pm\pi/2,\pm\pi/2)$ (in the $k_x=k_y$ direction) and therefore the characteristic momentum length of the DOS variations on the Fermi surface is $\pi/\sqrt{2}$. We expect therefore that for $q_c > \pi/\sqrt{2}$ the gap might be isotropic while for q_c sufficiently smaller than $\pi/\sqrt{2}$ MD should manifest leading to DOS induced anisotropies. In fact in Fig. 1 we show the ratio of the gap at $(0,\pi)$ over the gap at the points where the DOS is minimal $(\pi/2,\pi/2)$ as a function of q_c. We can see that for $q_c < \pi/\sqrt{2}$ this ratio begins to be appreciably different from unity indicating the onset of a DOS induced anisotropy because of MD.

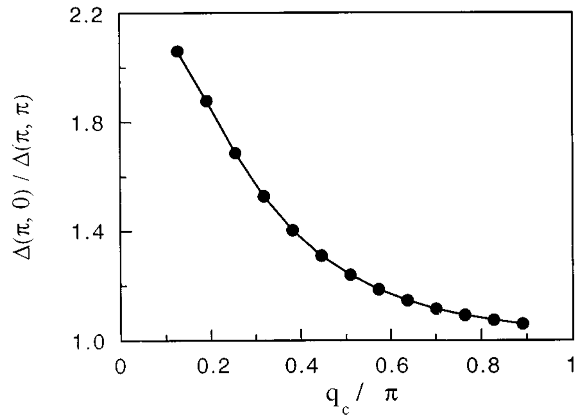

FIG. 1. Evolution of the anisotropy ratio as a function of the characteristic range of the exchanged momenta q_c. For $q_c < \pi/\sqrt{2}$ it increases sharply indicating the onset of MD.

We are now going to see how MD can explain simultaneously all the features of the ARPES and tunnel experiments mentioned in the introduction. We take first the temperature dependence of the anisotropy reported in Ref. 4. If MD was perfect in $Bi_2Sr_2CaCu_2O_{8+\delta}$, roughly speaking the temperature at which the gap disappears in the Γ-X direction should be smaller than the temperature at which it disappears in the Γ-$\bar{M}$ direction. In fact since the DOS is smaller in the Γ-X direction, the coupling and T_c should also be smaller. Therefore, in the case of MD the anisotropy is enhanced close to T_c, and if MD would be perfect it should even diverge.

We will now show how within our BCS model the results of Ref. 4 can be qualitatively reproduced when finite (small) momenta are transferred. In Fig. 2 we report the temperature dependence of the gap at the points $(0,\pi)$ and $(\pi/2,\pi/2)$ [$\Delta(0,\pi)$ and $\Delta(\pi,\pi)$, respectively] for different values of q_c, and in Fig. 3 we give the corresponding temperature dependence of the anisotropy ratio $R = \Delta(0,\pi)/\Delta(\pi,\pi)$. The critical temperatures are obtained by solving numerically the Hermitian eigenvalue problem of the linearized equations near T_c.

When $q_c = \pi/4$ the DOS induced anisotropy, because of partial MD, is already significant ($R \approx 1.7$) but the anisotropy is almost temperature independent (Fig. 3). For smaller values of q_c there is a continuous deformation of the T dependence of $\Delta(\pi,\pi)$ from the large q_c regime to the $q_c \to 0$ regime where, as expected in perfect MD, $\Delta(\pi,\pi)$ should have a BCS behavior going to zero at a temperature of the order $T_c/2$, and therefore the anisotropy ratio should diverge close to T_c. The results of Ref. 4 point to a strong MD regime. But one should bear in mind that, if the small gap is smaller than the temperature at which it is measured, it becomes experimentally inaccessible.[15] Taking into account these damping effects neglected in our BCS model, the results of Ref. 4 can be qualitatively understood even with q_c of the order $\pi/10$.[16] *The enhancement of anisotropy with temperature is an evidence of MD*, and *cannot* be understood in the case of anisotropic interactions such as those considered in the spin fluctuations d-wave scenario.

There is a qualitative feature common to all experiments that certifies that, in agreement with the MD picture, moving

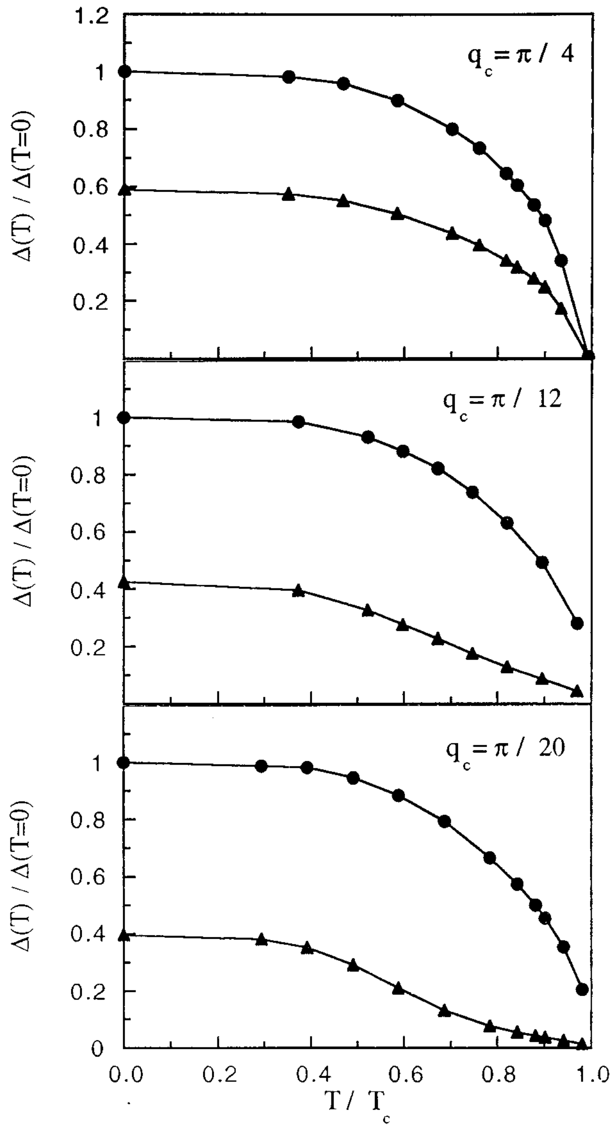

FIG. 2. Temperature dependence of the gap Δ in the $(\pi,0)$ (circles) and in the (π,π) (triangles) directions $[(\pi,0)$ and $(\pi/2,\pi/2)$ points of the FS, respectively$]$ for three characteristic ranges of exchanged momenta q_c.

from the Γ-$\overline{M}$ to the Γ-X direction on the Fermi surface we go from a strong coupling regime to a weak coupling regime. In fact in the Γ-M direction one can observe a dip structure above the gap that is a strong coupling effect independent of the spectral structure of the boson.[17] Such a dip appears when for sufficiently strong couplings the gap Δ is comparable to the boson energies that mediate superconductivity $(2\Delta/T_c \geqslant 5.5)$. The stronger the coupling is, the sharper and deeper is the dip.[17] The visibility of the dip is therefore an effective measure of the coupling strength. It is a common trend of all experiments that, moving from Γ-M towards Γ-X on the Fermi surface, the visibility of the dip follows the reduction of the gap and DOS, indicating that indeed different couplings are present in different regions of the Fermi surface.

In Ref. 3, it has been reported that the gap has minima around 30°–35° and 55°–60° (angles measured from X,Y-M) and a smaller maximum at 45° ($k_x = k_y$ direction).

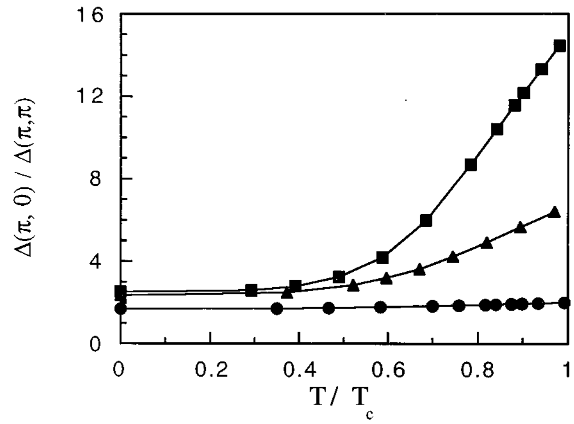

FIG. 3. Temperature dependence of the anisotropy ratio for $q_c = \pi/4$ (circles), $q_c = \pi/12$ (triangles) and $q_c = \pi/20$ (squares). The increase with temperature of this ratio is a clear indication of MD.

The authors claim that there must be a difference between the results in the ΓX and ΓY quadrants (which is not apparent from their data) and that the minima might correspond to nodes. To our analysis instead, these results could be a strong evidence for MD, although MD do not necessarily imply the presence of this local maximum at 45°.

We show in Fig. 4(a), the angular dependence of the density of states [measuring angles exactly as in Ref. 3 starting from the X-M direction around the (π,π) point] for a simple next-nearest neighbor tight-binding dispersion $[E = -0.5(\cos k_x + \cos k_y) + 0.49\cos k_x \cos k_y]$ that accounts qualitatively for the CuO bands seen by ARPES.[18] Fixing the distance from the bottom of the band at ≈350 meV as in the experiment,[5] we consider three different characteristic situations depending on the distance of the Van Hove singularity from the Fermi level δE ($\delta E = 10$ meV, 40 meV, and 90 meV). We can see that the DOS has minima at around 30° and 60° and a maximum at 45° *just due to the bending of the Fermi surface.* To obtain the corresponding anisotropies of the gap, we performed strong coupling calculations for an Einstein phonon spectrum assuming perfect MD. Perfect MD means totally decorrelated physics in the different parts of the Fermi surface, in which case the coupling strength or mass enhancement parameter $\lambda(\mathbf{k})$, for each $\mathbf{k}$, is directly proportional to the local DOS.

We choose a coupling factor or mass enhancement parameter λ that reproduces in the Γ-$\overline{M}$ direction the experimentally reported dip structure $(\lambda \approx 3)$. The absolute value of the gap depends on the considered phonon frequency, that is why we show in Fig. 4(b) only the relative variations of the gap. Considering however $\Omega \approx 40$ meV as the study of the gap ratio spectral dependence[19] and Raman experiments[12] indicate, we reproduced the gap and T_c of these materials.[19]

The local minima of the gap at ≈30° and 60° (Ref. 3) could reflect local minima of the DOS. Notice that, only in the case of an isotropic s-wave interaction in the MD regime, fine structures of the DOS anisotropy such as a local maximum at 45°, could be reflected in the gap anisotropy. If the interaction were not isotropic (as for example in the case of spin fluctuations mediated d waves), the anisotropy of the interaction would completely dominate the fine structures of

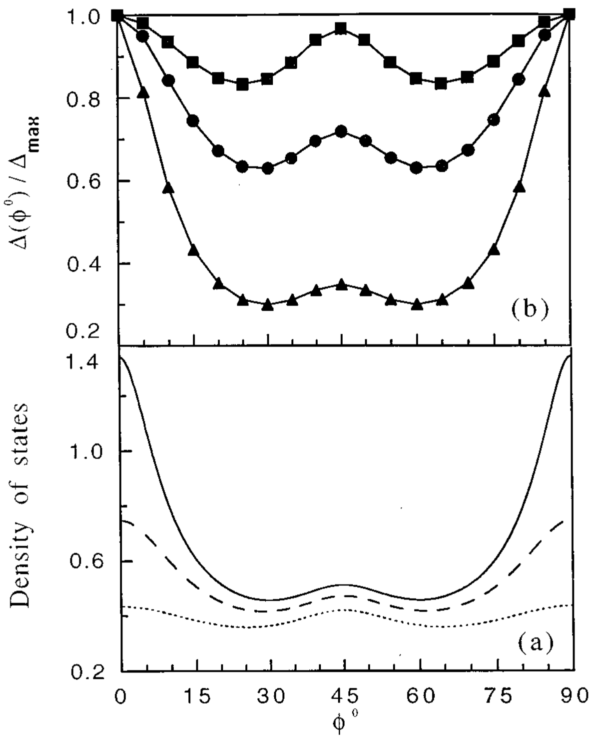

FIG. 4. (a) $N(E_F)$ as a function of the angle ϕ measured from the X-M direction for a simple second nearest-neighbors tight-binding model with a Van Hove singularity at 10 meV (full line), 40 meV (dashed line), and 90 meV (dotted line) below the Fermi level. (b) The corresponding gap anisotropy when the Van Hove singularity is at 10 meV (triangles), 40 meV (circles), and 90 meV (squares) below the Fermi level, obtained by strong coupling calculations assuming perfect MD.

the DOS anisotropy and a local maximum at 45° could not be visible. The magnitude of the anisotropy, is very dependent on the distance of the Van Hove singularity to the Fermi level and is significantly enhanced by the Coulomb pseudopotential.[16] In fact the experimental uncertainty on the value of δE (Ref. 5) is such that one can easily accommodate the gap anisotropies reported by both Refs. 4 and 3, and the momentum dependence of the dip visibility.[16]

As for the qualitative similarity of tunnel spectra and ARPES spectra in the direction optimal for superconductivity, in the case of MD, the tunnel spectrum is a sum of *independent* contributions from various parts of the Fermi surface, and it does *not* reflect an averaged superconducting behavior.[16] The tunnel spectra are dominated by the contribution of the optimal part around Γ-$\overline{M}$, since the Van Hove singularity is extended and covers about 30% of the Brillouin zone and the coupling is much stronger in this region. With this picture we can naturally understand the asymmetry of the tunnel spectra of Ref. 7. In fact, the dip structure is seen only at negative sample bias, because the Van Hove singularity at Γ-$\overline{M}$ is *below* the Fermi level. Measuring at positive sample bias, the dynamic behavior reflects the density of states above the Fermi level (as in inverse photoemission). The presence of the dip at negative sample bias and its absence at positive sample bias,[7] indicates that the density of states at an energy of the order of Δ above the Fermi level, is at least 30% smaller than that at an energy Δ below the Fermi level, and this can be easily obtained given the presence of the Van Hove singularity in the Γ-$\overline{M}$ direction. Because the DOS is smaller above the Fermi surface, the coupling is also smaller and the dip is no more visible.[17,16]

Note added in proof. It was reported recently [R. J. Kelley *et al.*, Science **271**, 1255 (1996)] that overdoped BSCCO has the gap in the (1,1) direction as in Ref. 4, but not the optimally doped. Indeed in our MD scheme nodes may appear or disappear with doping depending on the Coulomb pseudopotential [G. Varelogiannis and M. Peter, Czech. J. Phys. **46**, 1047 (1996); and (unpublished)].

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[18] The local maximum of the DOS at 45° is a quite general feature not specific to the next-nearest neighbors dispersion considered in Fig. 4. For example, one can obtain extended Van Hove singularities and a DOS maximum at $(\pi/2,\pi/2)$ considering a tight-binding model with hopping up to the fourth nearest neighbors and parameters $t_1=-0.4732$, $t_2=0.2224$, $t_3=-0.0095$, and $t_4=0.0031$ (details are given in Ref. 16). Of course such tight-binding fits to the ARPES data are not unique: M. Norman *et al.*, Phys. Rev. B **52**, 615 (1995).
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