Three-dimensional gap structure in layered high-temperature superconductors

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(Received 14 December 1995)

NMR data and electromagnetic response are quantitatively described by a multiband-multiphonon exchange model, which additionally explains why near zeros in the superconducting gap function are shifted away from high symmetry points, as observed by angle-resolved photoemission spectroscopy measurements. The basic idea concentrates on the three-dimensionality of superconductivity, incorporating a coupling of the plane to the c axis via multiphonon exchange leading to a complex gap structure. Band structure related effects and chemistry are consistently included in this approach. [S0163-1829(96)50718-6]

High-temperature superconductivity[1] has mainly been attributed to the existence of the Cu-O planes. Consequently, most gap functions have a two-dimensional (2D) character, neglecting that the onset of high-temperature superconductivity is intimately related to the true three-dimensional character of the system. There are a few attempts to include c-axis coupling to a dominantly 2D-gap function.[2] None of them, however, gives explicit structure-derived relations.

In the following we give an explicit expression for a complex three-dimensional gap function, which is derived from structural considerations, chemical arguments, band structure, phenomenology, and experiment. This gap structure, specifically deduced here for YBCO, self-consistently explains many observations from experiments as electromagnetic response,[3,4] NMR,[5] angle-resolved photoemission spectroscopy (ARPES),[6] extended x-ray-absroption fine structure (EXAFS),[7] and pair-distribution functions (PDF),[8] and is predictive with respect to ARPES, and inelastic neutron scattering and local probes, such as EXAFS, PDF, and NMR.

Common to all cuprate superconductors is a pseudo-two-dimensional structure with (bad) metallic behavior in the planes and nearly ionic properties perpendicular to them. The planes usually show an average static buckling which has the important effect that p-d antibonding bands are lowered in energy, split, shifted away from high symmetry points, and related to broadened van Hove singularities.[9] Simultaneously, the Fermi velocity approaches zero which admits for coupling to the phonons in this specific k-space area. Due to the antibonding character of these bands, doping substantially and smoothly reverses their character and consequently delocalization can occur if reasonable coupling to the lattice is provided. This situation is similar to the superconducting A-15 compounds,[10] where a dynamically driven (nonstatic) lattice instability leads to an energy gain for the antibonding p-d bands.[11] In the case of A-15's there is nevertheless an important difference from the cuprate superconductors, as the van Hove singularities related to the the antibonding bands are quasi-one-dimensional, which strongly reduces their k-space weight, i.e., their weight with respect to T_c. That van Hove singularities, due to their high density of states and the very low Fermi velocity are of extreme importance to high-temperature superconductivity, is clear. However, the van Hove singularities on their own would not lead to three-dimensional superconductivity, if the itinerant electron system and the coupling to it are missing.

From various experiments there is now a consensus that the superconducting energy gap is highly anisotropic with respect to k_x,k_y dispersion, but without addressing k_z dependencies.[6,12] Also it seems clear that $q=0$ phonon modes ''react'' upon the onset of superconductivity, but q dependencies are less investigated. Plane–to–c-axis coupling with the onset of superconductivity has been reported for a few examples only.[13] In the following we address these issues in more detail, and suggest key features to be investigated experimentally.

In our approach, the general gap function is derived from a multiband-multiphonon interaction Hamiltonian which has already been discussed previously in the context of high-temperature superconductivity,[14,15] but also has been used in connection with ''conventional'' superconductors, many years ago.[16,17] The effective interaction Hamiltonian reads in already condensed BCS notation,[14,15] using the transformation techniques of Refs. 2, 17, and 18,

$$H=\sum_{k,i}\epsilon_{ki}c_{ki}^{\dagger}c_{ki}-\sum_{k_i,q}(g_q^{\dagger}a_q^{\dagger}c_{k_i}-qc_{k_i}^{\dagger}+g_qa_qc_{k_i+q}^{\dagger}c_{k_i})$$
$$-\sum_{k_i,k_j,q_1,q_2}\{g_{4q_i}^{\dagger}a_{q_1}^{\dagger}a_{q_2}^{\dagger}(c_{k_i-q_1-q_2}^{\dagger}c_{k_j})$$
$$+g_{4q_i}a_{q_1}a_{q_2}(c_{k_j+q_1+q_2}^{\dagger}c_{k_i})\}, \quad (1)$$

where $a_q^{\dagger},a_q$ and $c_k^{\dagger},c_k$ are phonon and electron creation and annihilation operators, and ϵ_k is the band energy. g_q is the usual Fröhlich electron-phonon interaction term and g_{4q_i} the electron-two-phonon exchange which provides the coupling of a,b-related properties to the c-axis related gap structure. From Eq. (1) it is clear that the phonon-mediated electron-electron interaction is strongly enhanced due to the multiphonon contribution which dominantly acts on the interband interactions, while g_q mainly provides the intraband related coupling.

Proceeding on a BCS-type level, Eq. (1) yields nonlinear coupled gap equations,[19] which have to be solved self-consistently, i.e.,

$$\Delta_i(k)=\sum_{k_i'}\frac{V(k_i,k_i')}{2}\frac{\Delta_i(k_i')}{E_{k_i'}}+\sum_{k_j'}\frac{V(k_i,k_j')}{2}\frac{\Delta_j(k_j')}{E_{k_j'}},\quad(2)$$

where $V(k_i,k_i')$ comes from the second term in Eq. (1), while $V(k_i,k_j')$ comprises the multiphonon interactions and $E_{ki}=[\epsilon_{ki}^2+\Delta_i(k)]^2$.

In the following an explicit gap function is given for YBCO; this function is, of course, material dependent and only some features of it are common to all high-T_c compounds. In YBCO four major contributions to Eq. (2) have to be considered; related to the CuO_2 planes, the interplanar interactions, the plane-chain coupling through the apical oxygen, and the chains. Considering phonon-mediated nearest-neighbor interactions only, the four corresponding pairing potentials from the intraband potential are

$$V(k_1,k_1')=V_1[\cos(k_xa-k_x'a)+\cos(k_yb-k_y'b)],\quad(3a)$$

$$V(k_2,k_2')=V_2\cos(k_xa-k_x'a)\cos(k_yb-k_y'b)\cos(k_zc-k_z'c),\quad(3b)$$

$$V(k_3,k_3')=V_3\cos(k_zc-k_z'c),\quad(3c)$$

$$V(k_4,k_4')=V_4[\cos(k_zc-k_z'c)+\cos(k_yb-k_y'b)],\quad(3d)$$

where $V(k_1,k_1')$ to $V(k_4,k_4')$ refer to the above cited structural elements in YBCO and a,b,c are the unit cell lattice constants. From Eqs. (3) it is obvious that the pairing interactions are all decoupled from each other and act intraband only, yielding separate gaps with one-, two-, and three-dimensional structures.

Coupling of these gaps is provided through $V(k_i,k_j')$ which yields additional contributions to each gap from the multiphonon terms such as $e^{i(k_i+q_i+q_j)}e^{-ik_j}+e^{(k_j-q_i-q_j)}e^{ik_i}$, and simultaneous gap coupling. Quite generally the multiphonon contributions are small, which allows us to approximate them as

$$V(k_i,k_j')=V\cos(\vec{k}_i\cdot\vec{r}_j-\vec{k}_j'\cdot\vec{r}_j)\cos(\vec{k}_i\cdot\vec{r}_i-\delta\vec{k}_j'\cdot\vec{r}_j).\quad(4)$$

Here, δ accounts for the multiphonon contribution and $\vec{r}=a,b,c$. From Eq. (4) the gaps in Eq. (3) are all coupled to each other, and as Eq. (4) explicitly contains the vector $\vec{r}=a,b,c$, all gaps experience influences from three dimensions. This is an extremely important result with numerous consequences.[19] For example, the plane related gap function [Eq. (3a)] disperses in the z direction and still has a small finite component at $k_z=\pi/c$. Also the zeros in the a,b plane are shifted away from $k_xa=k_yb=1$ to low symmetry points; the same happens with the gap related to Eq. (3b). The shifting of the zeros to finite k_x,k_y values should be observed in all high-T_c compounds as the CuO_2 planes are common to all of them. From recent ARPES experiments[6] this indeed seems to be confirmed in the $Bi_2Sr_2CaCu_2O_8$ superconductor. The plane-O(4)-chain related gap experiences the strongest modification as it now yields a dispersion with respect to k_x,k_y and a strong variation in k_z [Fig. 1(c)]. This means that the apex oxygen should show correlated displacements in all three directions, with the z contributions being the strongest. Similarly, the chains show a k_x dispersion in the gap function which, due to the multiphonon contribution, requires that the local structure also has an appreciable x component for the chains [Fig. 2(c)].

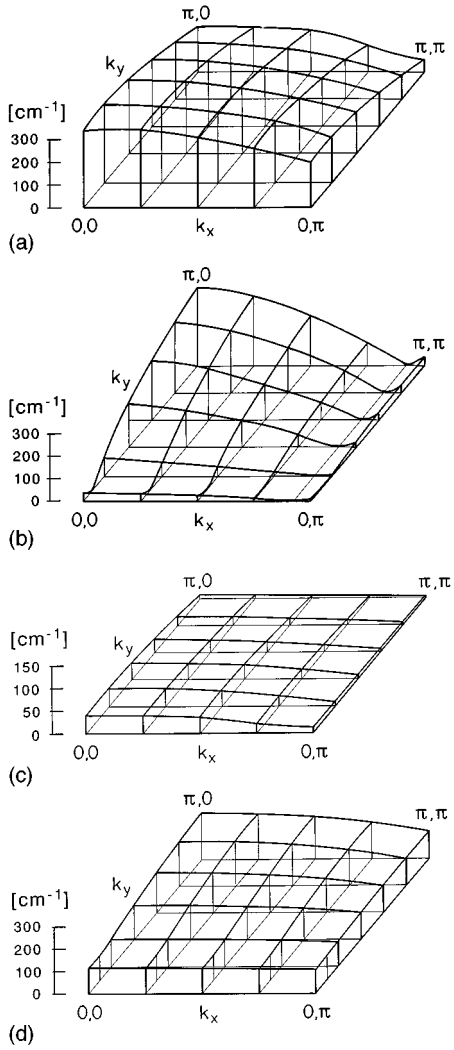

FIG. 1. Gap structures on the Fermi surface as derived from Eqs. 3(a)–3(d) (same order) including the modification through Eq. (4).

The gaps appearing in the $k_z=0$ plane are shown in Fig. 1 with interaction potentials given by $V_1=V_2=42.18$ meV,[20] $V_3=26.05$ meV,[21] and $V_4=9.93$ meV.[23] Note that even though the contribution from the O(4) is rather small, it is crucial for the electromagnetic response and NMR data, as it gives an appreciable contribution to low-energy related excitations, including conductivity. We relate experimental results from penetration depth data which have been interpreted to favor a d-wave-type order parameter[3,22] to this gap. Note that the O(4) related gap strongly couples with the plane coupling gap related to Eq. (3b).

The chain-related gap is rather featureless, with minor dispersion in the k_x,k_y plane, but couples strongly with both plane gaps and yields a large contribution between 100 and 200 cm^{-1}. Experimentally it is probably difficult to detect this gap due to the strong hybridization. But, of course, its k_z dispersion has to be closely examined. In order to calculate NMR and the electromagnetic response, it is necessary

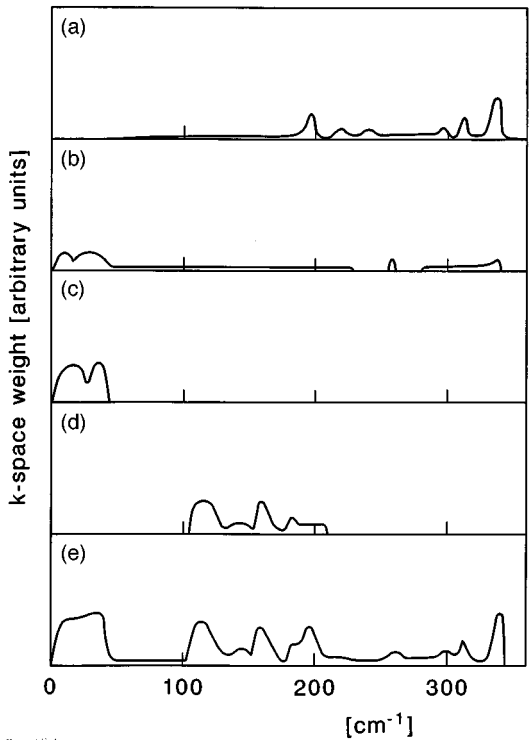

FIG. 2. Energy dependence of the gap functions Eqs. 3(a)–3(d) from top (a) to bottom (d) and total energy dependence (e).

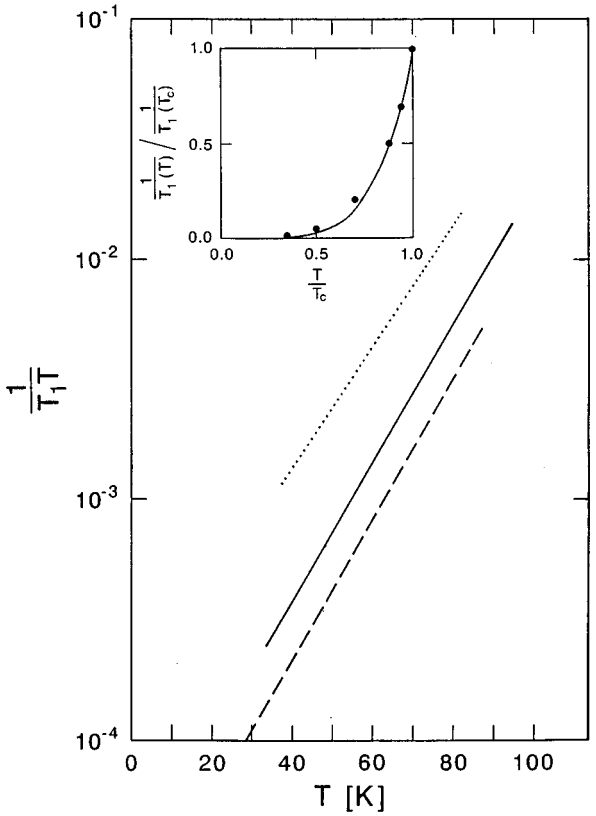

FIG. 3. $\ln 1/T_1T$ versus temperature. Full line corresponds to the calculation as described in the text, dotted line has been taken from Imai (Ref. 25), dashed line from Warren, *et al.* (Ref. 25). The insert compares the calculation (full line) with data from Ref. 5.

to evaluate the coherence factors which, of course, become extremely complicated. To facilitate such calculations, we differentiate the gap structure with respect to k_x, k_y to obtain a continuous gap function which is dependent on energy only. This approach corresponds to representing the gap specific k-space weight on an energy scale. In Fig. 2 the results are shown for the individual gaps, as well as the contribution from the sum over all gaps. It is obvious from Fig. 2 that all four gap structures contribute to very specific energies, i.e., as already outlined above, the O(4) related gap has contributions at small energies only; the chains appear between 100 and 210 cm^{-1}, while the plane gap provides the highest weight around 330–340 cm^{-1} and an appreciable contribution around 200 cm^{-1}. The plane-chain coupling gap appears mainly on the low-energy side, but helps to enhance the high-energy contributions from the pure plane gap.

It is obvious from Fig. 2 that the problem still remains very complex and we limit ourselves to the BCS equations in order to calculate the above cited quantities. We also include in our calculation a temperature-dependent scattering rate ω_τ as deduced from microwave data,[23,3,4] which is given by $\omega_\tau = A + B(T/T_c)^\alpha$ with α between 4.4 and 4.8 and $A=1$ cm^{-1}, $B=67$ cm^{-1}. Note that the T-independent part A reflects scattering due to impurities while the T-dependent term is due to thermal scattering from phonons. The prefactor of the second term together with the exponent are dictated by experiment.

In order to calculate temperature-dependent properties, each term in Eq. (2) has to be multiplied by the corresponding Fermi-Dirac functions. Due to the mapping procedure of Eq. (2) to an energy scale, the calculated nuclear spin lattice relaxation rate $1/T_1$ refers to the in-plane rate and neglects a,b anisotropy. Calculation of $1/T_1$ perpendicular to the planes will be presented elsewhere. The simplest expression for $1/T_1$ within the framework of BCS theory has been used, i.e., $1/T_1 = C\, e^{-\Delta/kT}$ and $C=1$ sec^{-1}, where Δ is given by Eq. (2) with interaction potentials Eq. (3) modified by Eq. (4). The results shown in Fig. 3 agree very well with experimental data from Refs. 5, 24, and 25. Similarly good agreement with experiment is obtained for the electronmagnetic response.[26] Note that for these calculations the O(4) related gap is most important to obtain deviations from BCS results, as this gap structure covers the energy range from zero to small wave numbers (≈ 40 cm^{-1}) dominantly and provides the rather large k-space weight. This gap is clearly the basic reason why features suggestive of d-wave pairing appear in electromagnetic response data.

In this work, high-T_c superconductivity has been attributed to an attractive multiphonon pairing potential where interband, and intraband couplings are considered explicitly. The pairing potentials are specifically given for YBCO, yielding a very complex anisotropic three-dimensional gap structure which has not been considered previously. While the intraband related pairing potentials provide a three-dimensional gap structure for one specific hybridized band only, multiphonon interband interactions give rise to a coupled three-dimensional gap structure from plane-related gap functions; and one attributed to the apex oxygen. The two plane-related gaps have the largest energies near the van Hove singularities, but have practically no significance for experiments testing low-energy properties like NMR, pen-

etration depth, etc. These properties are almost exclusively attributed to a small gap arising from O(4) which has in-plane contributions due to its large anharmonicity. The chain related gap is rather uninteresting experimentally, except that the chains should show correlated displacements in the x direction, thus corresponding strongly with the plane-related gaps.

The suggested model has a variety of aspects which should be tested experimentally and have already been partially observed:

(i) c-axis related phonons should couple to the a,b plane.[13] Due to multiphonon exchange the strongest anomalies in specific phonon modes are predicted to occur at q values around $(0,0),(0,\pi),(\pi,0),(\pi,\pi)\pm 0.05$. For the O(4) related mode the anomaly should be approximately in the middle of the Brillouin zone and has strong coupling to a,b phonons.

(ii) If ARPES is able to measure c axis related effects, we predict that the observed gap structure is strongly dispersive with respect to this axis, and plane-related gaps should nearly vanish at $k_z=\pi/c$. The small finite structure which remains here stems from coupling with the other gaps due to multiphonon exchange.

(iii) The apex oxygen atom has a small gap, but one which crucially influences all small energy sensitive experiments. Systems without ''apex'' oxygen are predicted to behave more like conventional BCS superconductors as they miss this key property.

(iv) The static plane buckling has the important effect of strongly enlarging the k-space weight of the van Hove singularities, which we relate to the largest gap energies. Systems with a single Cu-O layer which is flat, are suggested to contain buckled sandwich layers which again enlarge the k-space weight of the singularities.

(v) The oxygen related isotope effect is site selective as the O(4) is highly anharmonic—much more than the other oxygen atoms—which is known to suppress the isotope effect.[27] A similar argument holds for the other isotope effects for plane and chain oxygen atoms, but is less dramatic.

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