Density of states and the energy gap in superconducting cuprates

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The superconducting density of states for the cuprates, particularly for the Y-Ba-Cu-O compound, has been evaluated, and its dependence on temperature and the oxygen content has been analyzed. The analysis is based on the two-gap model. Moreover, the magnetic scattering and corresponding pair-breaking effect, correlated with the oxygen depletion, is taken into account as a key factor. The temperature dependencies of the energy gaps are calculated. Intensive magnetic scattering leads to gaplessness. The calculation allows us to describe various experimental data. [S0163-1829(97)01237-X]

Many fundamental properties of a superconductor are determined by its density of states (DOS), N_s. One such property is the existence of the energy gap, which corresponds to the region where $N_s=0$. Calculations of transport, optical, and thermodynamic properties require knowledge of N_s as a function of energy. The goal of this paper is to present calculations of the density of states for the high-T_c oxides, primarily the Y-Ba-Cu-O (YBCO) compound. The calculation is based on the model developed by two of us,[1] which has been used to evaluate the penetration depth in high-T_c materials.[2] The basic principles of the model will be described, then the evaluation of the DOS will be presented. The results of the calculation are compared to available data.

Different measurements of the DOS in various cuprates seem contradictory from the point of view of any single theoretical picture. For some cuprates, ($La_{1-x}Sr_xCuO_4$,[3] $Nd_{1.85}Ce_{0.15}CuO_4$,[4] and Hg-based compounds[5]), the measurements indicate a finite energy gap. At the same time, the data on YBCO (Ref. 6) and BSSCO (Ref. 7) compounds show gapless structure in the data. In some cases, the shape of the DOS appears to be sample dependent for the same material.[8] Based on the results shown here, an explanation is presented that can account for the data in different cuprates in a consistent manner.

The major features of the model will be described here, while a more detailed presentation can be found in Ref. 1. The YBCO compound contains two superconducting subsystems: CuO planes (α) and chains (β). Correspondingly, there are two order parameters, $\Delta_\alpha$and Δ_β. In accordance with this, the total density of states is the sum of contributions $N_\alpha(\omega)$ and $N_\beta(\omega)$, where

$$N_i(\omega)=\mathrm{Re}\left[\frac{|\omega|}{[\omega^2-\Delta_i^2(\omega)]^{1/2}}\right] \tag{1}$$

and $i=\alpha,\beta$. As a result, $N(\omega)$ contains two peaks, and this feature is referred to as a ''two-gap'' spectrum, though strictly speaking the presence of two peaks in the DOS does not exclude gaplessness, which is the situation when $N(\omega)$ has a tail down to $\omega=0$ (see below and Ref. 1).

The two-gap model[1] has two important features. First, the pairing in the planes is intrinsic, whereas the superconducting state in the chains is induced by charge transfer (e.g., ''intrinsic'' proximity effect, see Ref. 1). Second, the structure of the density of states, and correspondingly, the energy spectrum, is very sensitive to the oxygen content. Oxygen depletion leads to formation of magnetic moments on the chains (uncompensated Cu^{2+} ions), and the presence of these moments causes pair breaking. It is interesting that, unlike the conventional picture of pair breaking,[9] the appearance of the magnetic moments on the chain side leads to gaplessness without a depression in T_c.

The equations for the order parameter have the form (in the thermodynamic Green's function representation):

$$\Delta_\alpha(i\omega_n)Z_\alpha(i\omega_n)=\lambda_\alpha\pi T\sum_{n'=-\infty}^{\infty}D_{nn'}\frac{\Delta_\alpha(i\omega_{n'})}{K_{n'}^\alpha}+\lambda_{\alpha\beta}\pi T\sum_{n'=-\infty}^{\infty}D_{nn'}\frac{\Delta_\beta(i\omega_{n'})}{K_{n'}^\beta}+\Gamma_{\alpha\beta}\frac{\Delta_\beta(i\omega_n)}{K_n^\beta}, \tag{2}$$

$$\Delta_\beta(i\omega_n)Z_\beta(i\omega_n)=\lambda_{\beta\alpha}\pi T\sum_{n'=-\infty}^{\infty}D_{nn'}\frac{\Delta_\alpha(i\omega_{n'})}{K_{n'}^\alpha}+\Gamma_{\beta\alpha}\frac{\Delta_\alpha(i\omega_n)}{K_n^\alpha}, \tag{3}$$

$$Z_\alpha(i\omega_n)=\left[1+\frac{\lambda_\alpha \pi T}{\omega_n}\sum_{n'=-\infty}^{\infty} D_{nn'}\frac{\omega_{n'}}{K^\alpha_{n'}} + \frac{\lambda_{\alpha\beta}\pi T}{\omega_n}\sum_{n'=-\infty}^{\infty} D_{nn'}\frac{\omega_{n'}}{K^\beta_{n'}}+\Gamma_{\alpha\beta}\frac{1}{K^\beta_{n'}}\right], \quad (4)$$

$$Z_\beta(i\omega_n)=\left[1+\frac{\lambda_{\beta\alpha}\pi T}{\omega_n}\sum_{n'=-\infty}^{\infty} D_{nn'}\frac{\omega_{n'}}{K^\alpha_{n'}}+\Gamma_{\beta\alpha}\frac{1}{K^\alpha_{n'}} +\Gamma_M\frac{1}{K^\beta_{n'}}\right]. \quad (5)$$

Here, $K^i_n=[\omega_n^2+\Delta_i^2(i\omega_n)]^{1/2}$ $(i=\alpha,\beta)$, Γ_{ik} are equal to $|T_{ik}|^2N_k$ where T_{ik} is the tunneling matrix element that describes the ''intrinsic'' proximity effect, λ_α is the in-plane coupling constant describing the pairing in the CuO plane, $\lambda_{\alpha\beta}$ and $\lambda_{\beta\alpha}$ are the off-diagonal coupling constants, $D_{nn'}=\tilde{\Omega}^2/[\tilde{\Omega}^2+(\omega_n-\omega_{n'})^2]$ is the phonon Green's function, $Z_\alpha(i\omega_n)$ and $Z_\beta(i\omega_n)$ are the renormalization functions, and $\tilde{\Omega}$ is the characteristic phonon frequency. The values of the parameters are not all independent, since $\lambda_{\beta\alpha}=\rho\lambda_{\alpha\beta}-1$ and $\Gamma_{\beta\alpha}=\rho\Gamma_{\alpha\beta}-1$ where $\rho=N_\alpha m_\beta/N_\beta m_\alpha$. The last term in Eq. (4) describes the magnetic scattering in the chains, and Γ_M is the amplitude of magnetic scattering, $\Gamma_M\propto n_M$, where n_M is the concentration of magnetic impurities. Γ_M is directly related to the oxygen content.

Based on Eqs. (2)–(5), the temperature dependence of the DOS has been calculated. The values of the parameters used are the same as in Ref. 2, the selection of which were based on the analysis of various experimental data. The parameters used in the calculation for YBCO are $\lambda_\alpha=3.0$, $\lambda_{\alpha\beta}=0.24$, $\lambda_{\beta\alpha}=0.17$, $\Gamma_{\alpha\beta}=90$, $\Gamma_{\beta\alpha}=64$, and $\tilde{\Omega}=385$, though the picture is qualitatively similar for different sets of the parameters. The effect of oxygen depletion on the DOS has also been calculated. The effect is the same as an increase in the magnetic impurity concentration, that is, an increase in Γ_M, since $\Gamma_M\propto n_M$.

The calculations were performed in two ways. The first method is to solve the equations which are the analytical continuation of Eqs. (2)–(5). The second method involves solving directly Eqs. (2)–(5), then performing analytical continuation of the solution, a method first developed in Ref. 10. Both methods gave identical results.

The density of states for the stoichiometric YBCO compound and its temperature dependence is shown in Fig. 1. In the absence of magnetic impurities, there is a region at low energies (the energy gap) within which the density of states is zero. The value of the smaller gap, which is the excitation edge, practically coincides with the position of the lower energy peak. The larger gap, ϵ_α, is associated with a higher energy peak due to the planes. If we associate, by analogy with the usual BCS definition, the energy gaps with the positions of the peaks in the DOS, the values of the energy gaps at $T=0$ K appear to be $\epsilon_\alpha=3T_c$, and $\epsilon_\beta=0.8T_c$. The temperature dependences of the gaps are plotted in Fig. 2. These dependences are drastically different from that of ordinary superconductors (the dependence from BCS theory is plotted for comparison). Unlike conventional superconductors, the energy gaps depend only weakly on temperature over the entire temperature region except in a small interval near T_c. At the same time, the derivative $\delta\epsilon/\delta T$ is much larger than in the BCS theory near $T=T_c$.

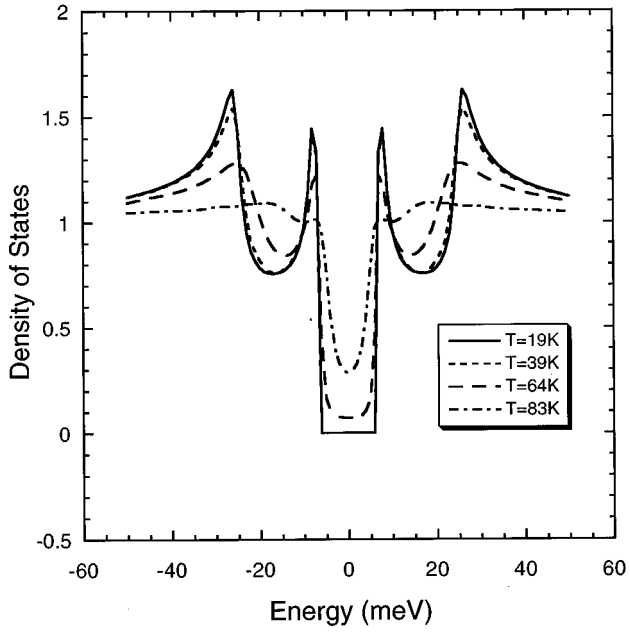

FIG. 1. Temperature dependence of the density of states for the stoichiometric YBCO compound ($\Gamma_M=0$).

One should note that we are calculating the quantity $N_i(\omega)$ which is defined as the ''superconducting'' density of states [Eq. (1)]. This quantity contains the order parameter which depends on temperature through the occupation numbers [these numbers appear explicitly in the equations which are the analytical continuation of Eqs. (2)–(5)]. An increase in T leads to a decrease in the amplitude of the real part of $\Delta_i(\omega)$ and to broadening caused by the imaginary part (see, e.g., Ref. 11 and the review in Ref. 12).

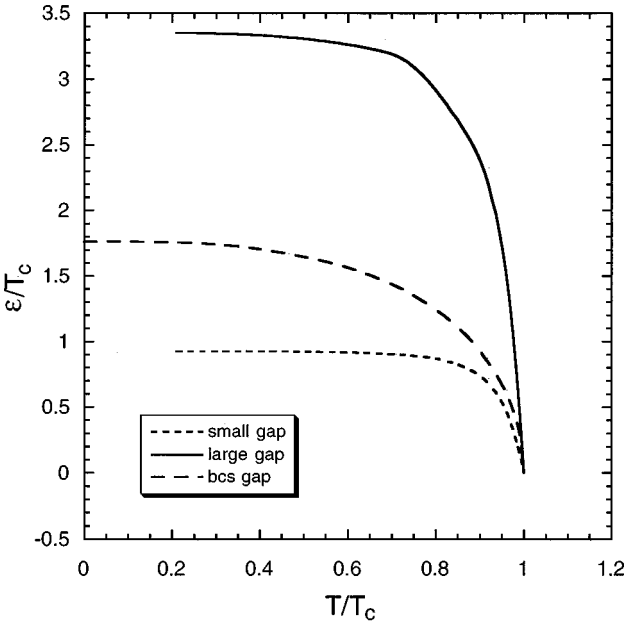

FIG. 2. Temperature dependence of the energy gaps compared to BCS.

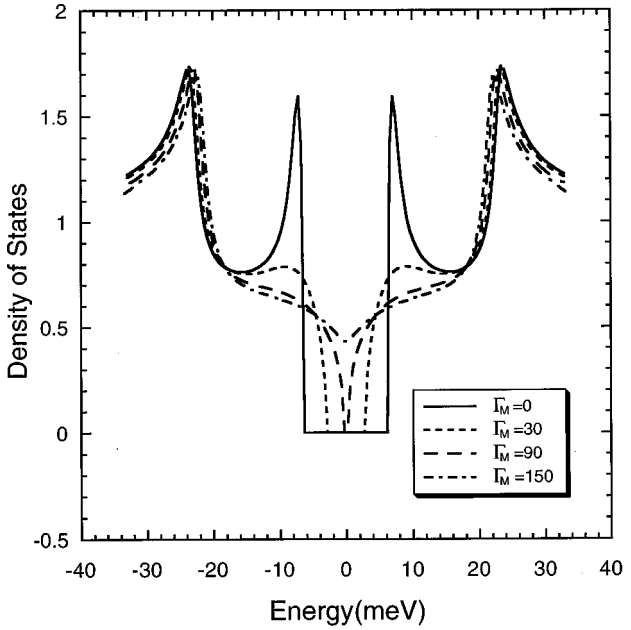

FIG. 3. Density of states for different values of the magnetic scattering parameters.

Oxygen depletion leads to an increase in magnetic impurity scattering (see Ref. 1 and discussion above), and this affects the shape of the DOS. The calculated evolution of DOS (at $T=0$ K) is shown in Fig. 3. An increase in Γ_M leads to a decrease in the energy range where the DOS is zero, though the peaks keep their positions. At $\Gamma_M \approx T_c$ (this corresponds to the criterion $\Gamma_M \approx \epsilon_\beta$, see Ref. 1), the DOS has a tail down to $\omega=0$, so the superconductor is in a gapless state. The temperature dependence of the DOS in the gapless superconductor ($\Gamma_M=100$) is shown in Fig. 4.

For comparison to the calculated curves, tunneling data from YBCO (Ref. 6) are shown in Fig. 5. Evidence for a two-gap structure can be seen in the data. Data from a

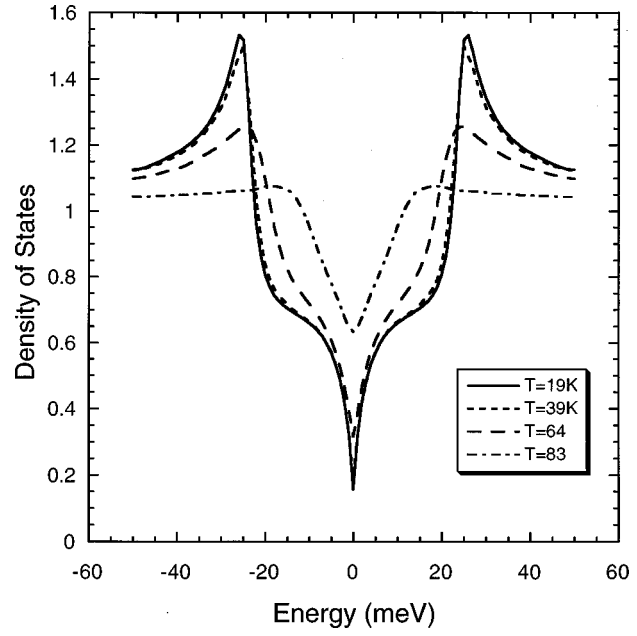

FIG. 4. Temperature dependence of the density of states for gapless YBCO ($\Gamma_M=100$).

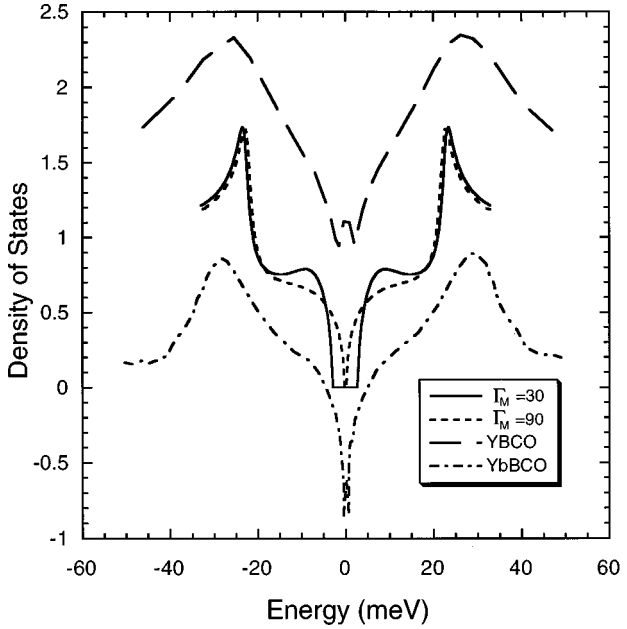

FIG. 5. Calculated density of states compared with data (see Ref. 6).

YbBCO sample are also shown, which more clearly shows the two peaks. Based on the analysis presented above, we conclude that the YbBCO sample in Ref. 6) is in a gapless state, caused by oxygen deficiency. Compared to the calculation, the peak corresponding to the second gap is spread out. This is probably due to either anisotropy of the gaps, which was not part of the calculation, or it is due to inhomogeneity of the sample. Note that the shoulder structure due to the presence of two gaps is also seen in other tunneling data.[13,14]

Other measurements indicate that fully oxygenated YBCO samples (those with an especially high $T_c>92$) are not gapless.[15,16] Exponential behavior has been observed in the temperature dependence of both the penetration depth and the surface resistance. The measured exponent in both cases is small, corresponding to the smaller gap, $\epsilon_\beta \approx 0.8T_c$, of the chains. We think that the sample-dependent DOS in YBCO is directly related to magnetic scattering, which, in turn, depends on the oxygen content. The authors in Ref. 16 note that as the sample ages, the surface resistance increases and no longer displays an exponential temperature dependence. According to Ref. 16, this directly correlates with the loss of oxygen. This observation supports our approach, indicating that oxygen loss leads to gaplessness in the sample.

Specific-heat data on YBCO (Ref. 17) is also consistent with the density of states presented here. For highly oxygenated samples, these measurements show a large specific-heat jump. As oxygen is removed, the specific-heat jump diminishes.

In this paper, we have focused on the YBCO compound and its density of states as a function of temperature and doping level. The presence of oxygen vacancies, especially on the chains, leads to the formation of magnetic moments. The properties of other cuprates will be described in detail elsewhere. However, several qualitative remarks can be made. The Bi-, Tl-, and Hg-based compounds also have a reservoir level, but they do not have a well-developed chain

structure with a large density of states. In addition, these compounds, unlike YBCO, can be readily overdoped. It seems that overdoping leads to magnetic scattering directly in the CuO planes. As a result, one can observe pair-breaking effects and eventually gaplessness. These phenomena are clearly evident in μSR,[18] heat capacity,[19] and penetration depth[20] data, but in these cases, a sharp decrease in T_c is also observed. This decrease in T_c is due to the impact of pair breaking directly on the CuO planes. The magnetic moments are located on the Ba-O layer (O^- ions, see Ref. 21). The formation of magnetic clusters in the CuO planes is also possible.[22] Note that a relatively high value of T_c in the Hg-based compound is due to a relatively small oxygen content in the reservoir layer and to a large distance between the apical oxygen and the CuO planes.[23] Overdoping also leads to an increase in the density of states in the reservoir layer and to the formation of the second small gap (see Ref. 24). The dependence of the density of states on temperature and doping level is qualitatively similar to that in YBCO (see above), but quantitatively is different since magnetic scattering in the CuO planes leads to gapless behavior in the CuO planes.

In summary, the density of states in oxide superconductors has been calculated using a two-band model. The calculations particular to the YBCO compound demonstrate the sensitivity of the DOS to magnetic impurity scattering in the chain band. The magnetic scattering in a second band, which is closely related to the oxygen content, can explain the gapless behavior observed in oxide superconductors.

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