Energy gap dispersion in layered cuprates. Monolayer model

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Self-consistent solutions of the BCS equations were found for different values of the chemical potential. When the Fermi level ϵ_F lies near the bottom (top) of the band, the solutions correspond to s-type pairing and when ϵ_F lies at the center of the band, the solutions are d-type. It was shown that the interaction of the Zhang–Rice singlets via the phonon field gives an energy gap that is in agreement with the experimental data. © *1995 American Institute of Physics.*

One of the most important problems in high-T_c superconductivity is the investigation of the energy gap in cuprates as a function of the wave vector. This topic was the central issue of the discussions at a recent Stanford conference on the spectroscopy of the new superconductors.[1] Three types of dependences attracted special attention:

1) $\Delta_1(k)=\Delta_0[\cos(k_x a)-\cos(k_y a)]$ — so-called d-type pairing, ordinarily associated with spin fluctuations of the copper spins;[2,3]

2) $\Delta_2(k)=\Delta_0[\cos(k_x a)-\cos(k_y a)]$ — anisotropic s-type pairing, proposed in Ref. 4 in connection with the possibility of tunneling of Cooper pairs from one layer into another;

3) $\Delta_3(k)=\Delta_{xy}\cos(k_x a)\cos(k_y a)$ — so-called s_{xy}-type pairing, introduced by Norman *et al.*[5] on the basis of recent photoemission data for $Bi_2Sr_2CaCu_2O_8$ (Ref. 6).

Calculations have shown[7] that the last dependence is admitted by the BCS equation for a monolayer, but with the strange assumption that the interaction of two neighbors in the planar copper-atom lattice is approximately 1.5 times stronger (!) than the interaction of the closest copper atoms, and the magnitude of this interaction must be of the order of 0.15 eV, i.e., very large. For comparison, we point out that the superexchange interaction of the copper spins [between the first neighbors (!)] does not exceed 0.13 eV. In the present paper we report the results of our numerical solutions of the BCS equation, but with reasonable values of the pairing potential. As a supplement to the results of Ref. 7 for a monolayer, we investigated the behavior of the solution with weak doping and found unexpectedly that the BCS equation admits a s-type solution even for a pairing potential of the type

$$-2|V_1|[\cos(q_x a)+\cos(q_y a)], \tag{1}$$

which, as is often assumed, can lead only to a d-type gap.

We also investigated the character of the solutions for the energy gap in the class of pairing potentials of the form

$$V(\mathbf{q}) = -2|V_1|[(1+\alpha)\cos(q_x a) + (1-\alpha)\cos(\mathbf{q}_y a)] - 4|V_2|\cos(\mathbf{q}_x a)\cos(\mathbf{q}_y a), \tag{2}$$

where the parameters V_1 and V_2 are the interaction potentials between the first and second nearest neighbors via the deformation field, and α is an orthorhombicity parameter. In the case of sufficiently strong doping, when the Fermi level lies near the center of the band, the solutions are mixed (s and d type). The computed values of the gap width and T_c agree in order of magnitude with the available experimental data.

In Ref. 8 it was shown that the elementary excitations of the normal phase of cuprates can be described as a motion of singlet-correlated oxygen holes. The numerical results[8] were confirmed in Ref. 9 by the method of successive canonical transformations. This method made it possible to write the energy spectrum of the excitations in the analytic form

$$\epsilon_{1k} = \frac{\epsilon_{pk} + \epsilon_{dk}}{2} + \frac{1}{2}\{(\epsilon_{pk} - \epsilon_{dk})^2 - (1-\delta^2)(t_k^{(12)})^2\}^{1/2}, \tag{3}$$

where δ is the number of doped holes per copper site and

$$\epsilon_{pk} = \epsilon_p^* + \tfrac{1}{2}(1+\delta)\sum_j t_{ij}^{(1)} \exp[-\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)],$$

$$\epsilon_{dk} = \epsilon_d + \tfrac{1}{2}(1-\delta)\sum_j t_{ij}^{(2)} \exp[-\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)], \tag{4}$$

$$t_k^{(12)} = \sum_j t_{ij}^{(12)} \exp[-\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)].$$

The values of the effective transfer integrals t_{ij} are presented in Ref. 9 and $\epsilon_p^* - \epsilon_d = 0.4$ eV. Expression (3) describes satisfactorily the two-peak density of states calculated in Ref. 8. One peak is associated with the so-called saddle points along the coordinate axes $\mathbf{k}_x$ and $\mathbf{k}_y$, and the other peak lies near the bottom of the band and corresponds to the "wings" of the energy surface ϵ_{1k}.

In the compounds such as $La_{2-x}Sr_xCuO_2$ the Fermi level, in our views, lies near the bottom of the band, while in the bilayer compounds $YBa_2Cu_4O_8$ or $Bi_2Sr_2CaCu_2O_8$ the Fermi level lies near the center of the bottom bonding band. In the case at hand we ignore the upper antibonding band, and therefore we study the mono- and bilayer compounds on the basis of a single isolated band with different degrees of filling.

Two important interactions were ignored in the calculation of the energy spectrum of the normal phase:[8,9] the superexchange interaction of the copper spins in the CuO_2 planes

$$V_1^{(ij)} = J_{ij}[1/2 - 2(\mathbf{S}_i\mathbf{S}_j)], \tag{5}$$

and the interaction of the Zhang–Rice singlets via the tetragonal deformation modes[10]

$$V_2(ij) = -\frac{d^i d^j}{8\pi C_{44} R_{ij}^3}\left[4(1-2\gamma^2) - 6(3-4\gamma^2)\frac{X_{ij}^2 + Y_{ij}^2}{R_{ij}^2} + 15(1-\gamma^2)\frac{(X_{ij}^2 + Y_{ij}^2)^2}{R_{ij}^4}\right]. \tag{6}$$

The superexchange coupling parameter is $2J_{ij} \approx 0.12$ eV (Ref. 11). The elastic modulus $C_{44} = 48.3 \times 10^{10}$ dynes/cm^2 for a $YBa_2Cu_3O_7$ crystal was recently measured by Ledbetter *et al.*[12] They also measured the longitudinal and transverse sound velocities $\gamma = 0.582$. The value of the parameter in the deformation potential with a tetragonal mode ($d_i = d_j \approx 6$ eV) was estimated previously in Ref. 10.

Using the values indicated above, we find that the interaction potentials between the first and second neighbors are $V_1 = -0.1$ eV and $V_2 = -0.036$ eV, respectively.

The equation for the energy gap $\Delta(\mathbf{k})$ is

$$\Delta(\mathbf{k}) = \cos^2\theta_{\mathbf{k}} \sum_{\mathbf{k}'} V(\mathbf{k}-\mathbf{k}')\cos^2\theta_{\mathbf{k}'} \frac{\Delta(\mathbf{k}')}{2E_{\mathbf{k}'}} \tanh\frac{E_{\mathbf{k}'}}{2kT}, \tag{7}$$

where

$$E_{\mathbf{k}'} = \sqrt{(\epsilon_{1k}-\mu)^2 + \Delta^2(\mathbf{k}')}. \tag{8}$$

The factor

$$\cos^2\theta_{\mathbf{k}} = \frac{\epsilon_{1k} - \epsilon_{kd}}{\sqrt{(\epsilon_{kp}-\epsilon_{kd})^2 + (t_k^{(12)})^2(1-\delta^2)}} \tag{9}$$

is associated with the hybridization of the singlet-correlated oxygen-hole band ϵ_{pk} with the lower Hubbard copper-hole band ϵ_{dk}. It is obvious from Eqs. (2) and (7) that the wave-vector dependence of the gap must have the general form

$$\Delta(\mathbf{k}) = \{\Delta_x \cos k_x a + \Delta_y \cos k_y a + \Delta_{xy} \cos k_x a \cdot \cos k_y a + \Delta'_x \sin k_x a + \Delta'_y \sin k_y a + \Delta'_{xy} \sin k_x a \cdot \sin k_y a\}\cos^2\theta_{\mathbf{k}}, \tag{10}$$

where Δ_x, Δ_y, Δ_{xy}, Δ'_x, Δ'_y, and Δ'_{xy} are constants which are determined self-consistently.

Just as in Ref. 7, we found that the self-consistent sine amplitudes Δ'_x, Δ'_y, and Δ'_{xy} are negligibly small. The computed values of Δ_x, Δ_y, and Δ_{xy} are presented in Table I. The energy is measured from the top of the band. The peak in the density of states, which is associated with the saddle points, corresponds to $\epsilon = -0.2$ eV. It is obvious from the data presented that near the bottom of the band the solution is always of the s type, while near the center of the band the solution is predominantly of the d type. The mixing of d- and s- type solutions is due to the orthorhombic symmetry of the crystal. In the case of tetragonal symmetry solutions of the s and d type are mutually exclusive.

Our determination of the manner in which the solutions for the gap change as a function of the position of ϵ_F correlates with the existing experimental data. In the so-called electronic superconductors $Nd_{2-x}Ce_xCuO_4$ the Fermi level is split off from the saddle peak by 0.35 eV (i.e., it lies at the bottom of the band).[13] All methods employed for determining the symmetry of the gap show[1] that s-type pairing is realized in them. In $YBa_2Cu_4O_8$, $Bi_2Sr_2CaCu_2O_8$, and other superconductors the Fermi level is removed from the saddle peak by 0.03 eV (i.e., it lies at the center of the band).[13] In most experiments[1] these superconductors exhibit d-type pairing. The photoemission data,[6] shown in Fig. 1, are considered to be exceptions. The ordinates enumerate different

TABLE I. Computed values of the energy gap parameters for different values of V_2, α, and μ.

μ, eV	$V_1=-0,1$, $V_2=0$ $\alpha=0$		$V_1=-0,1$, $V_2=-0,036$ $\alpha=0$			$V_1=-0,1$, $V_2=-0,036$ $\alpha=0,1$		
	Δ_x	Δ_y	Δ_x	Δ_y	Δ_{xy}	Δ_x	Δ_y	Δ_{xy}
−0,10	1,4	1,4	2,3	2,3	1,3	2,7	1,9	1,3
−0,12	2,2	2,2	3,2	3,2	1,7	3,9	2,7	1,7
−0,14	2,2	2,2	3,5	3,5	1,6	4,4	2,7	1,7
−0,16	3,0	3,0	4	4	1,5	6	2,5	1,6
−0,18	12	−12	12	−12	0	16	−9	0,8
−0,20	18	−18	18	−18	0	22	−15	0,5
−0,23	20	−20	20	−20	0	24	−17	0,3
−0,25	18	−18	18	−18	0	21	−16	0,2
−0,30	11	−11	11	−11	0	12	−9	0
−0,35	3,2	−3,5	3,5	−3,5	0	4,2	−3	0
−0,40	0,8	−0,8	0,8	−0,8	0	1,8	0,5	−0,2
−0,42	−3	−3	−3,8	−3,8	1,2	−4,5	−3	1,2
−0,44	−6	−6	−7,5	−7,5	3,2	−9	−6,5	3,3
−0,46	−8	−8	−9,5	−9,5	5	−11	−8	5
−0,48	−8	−8	−9	−9	5	−10	−7,5	5
−0,50	−2	−2	−4	−4	2,5	−4,5	−3,5	2,5

points in the Brillouin zone. The value of a division on the abscissa is the same as in Ref. 6. The solid line represents the results of our calculation for $\mu=-0.2$. Obviously, the calculations and experiment disagree only near the points 1–6. This question obviously requires further theoretical and experimental investigations. On the whole, however, the

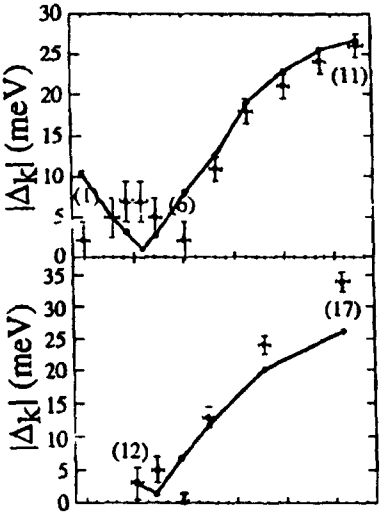

FIG. 1.

computed curve agrees with the photoemission data of Ref. 6 . We note that our computed value of the critical temperature T_c for $\mu = -0.2$ is 90 K, i.e., it corresponds to the real critical temperatures of these compounds: $T_c = 92$ K and 85 K for $YBa_2Cu_4O_8$ and $Bi_2Sr_2CaCu_2O_8$, respectively.

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