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Importance of Out-of-Plane Dispersion of the Excitation Spectrum of Superconducting Bilayers with Josephson Coupling

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We study the effect of Josephson coupling between adjacent superconducting layers on the BCS energy spectrum. We find that the interference between the gap functions of two layers can lead to vanishing condensation energy for perpendicular momenta corresponding to the formation of standing waves. We therefore predict a conventional energy spectrum for large interlayer spacings, if the gap of the single layers has no nodes, and in all cases a gapless spectrum for small spacings. Within the experimental error, our numerical results account for the low-temperature dependence of the penetration depth reported in $Nd_{1.85}Ce_{0.15}CuO_4$ and $YBa_2Cu_3O_{6.9}$.

KEY WORDS: Superconducting gap; Josephson effect; gapless superconductivity; perovskite phase superconductors.

An important yet unresolved aspect of high-temperature superconductivity in the cuprates is the qualitatively different low-temperature dependence of the normal density $\rho^{(n)}$ found in different compounds. In $Nd_{1.85}Ce_{0.15}CuO_4$ (NCCO), for example, measurements of the magnetic penetration depth λ_{ab} in the CuO_2 (ab) plane [1] show the characteristic exponential dependence $\lambda_{ab}(T)-\lambda_{ab}(0)\sim\rho^{(n)}\sim\exp(-\Delta/T)$ expected for conventional BCS superconductors with no nodes in the gap Δ. On the other hand, in $YBa_2Cu_3O_{6.9}$ (YBCO), the same measurements show a linear dependence $\rho^{(n)}\sim T$ [2] which gives evidence for the presence of lines of nodes. This possibility is supported for the cases of YBCO and $Tl_2Ba_2CuO_6$ by recent results on tricrystal Josephson junctions [3] and for the case of $Bi_2Sr_2CaCu_2O_8$ (BSSCO) by the linear dependence of the differential conductance of tunnel junctions on bias voltage [4] and of the optical conductivity on frequency [5]. While such gapless behavior of the excitation spectrum is of fundamental importance for applications, it has attracted attention mostly for the implications for the pairing mechanism in the cuprates. This is because the above linear temperature dependence of $\rho^{(n)}$ is consistent with a gap with d-wave symmetry $\Delta_{\mathbf{k}_\parallel}\sim\cos(k_x a)-\cos(k_y a)$, a being the lattice constant in the ab plane, which has been predicted by the spin-fluctuation theory of superconductivity [6]. Since one would expect that the pairing mechanism is the same for all cuprates given their similar structural and electronic properties, it is of interest to find a model which accounts for the diversity in the excitation spectrum found in different compounds. Proposed models are based on the existence of normal layers in the layered structure [7], thermal fluctuations of the phase of the order parameter [8], magnetic impurities in a two-gap structure [9], the inclusion of a weak repulsive interaction [10] in the BCS Hamiltonian or interlayer coupling via multiphonon exchange [11]. Another possibility is that nodes in the gap appear due to residual antiferromagnetic correlations which coexist with the superconducting state, as suggested by Ismagilov and Kopaev

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[12] and by Kulic' *et al.* [13]. Their argument is based on a generalization of the predictions by Larkin and Ovchinnikov [14] and by Fulde and Ferrel [15] that residual ferromagnetic order in a conventional BCS superconductor can produce a spatially inhomogeneous gap function which vanishes at certain points of the Fermi surface.

In this paper we study the effect of Josephson coupling between two neighboring superconducting layers on the BCS energy spectrum. We show that this coupling also leads to a spatially inhomogeneous gap. This corresponds to a dispersion of the gap along the direction z perpendicular to the layers and arises from the interference between the gap functions of the two layers. We find that, for strong couplings, this interference leads to a vanishing condensation energy for Cooper pairs with momenta k_z and $-k_z$ corresponding to the formation of standing waves. The application of this result to NCCO and YBCO, which have respectively one and two CuO_2 layers per unit cell, accounts quantitatively for the exponential and linear low-temperature dependences of λ_{ab} found experimentally.

Our result is based on two assumptions which are well established experimentally for the cuprates: (1) the two-dimensional character of the single-particle electronic states in the CuO_2 planes. This is demonstrated by the incoherent character of normal transport along the c-axis [16,17] and is confirmed by band structure calculations [18]. (2) The existence of Josephson coupling between adjacent CuO_2 layers, which is demonstrated by recent experiments on YBCO single crystals [19]. We note that the absence of bilayer effects in photoemission experiments on BSSCO [20] suggests that the two-dimensional normal electron states are confined in one single CuO_2 layer and that there exists no coherent coupling of the wavefunctions of neighboring planes. This can be understood by noting that the interlayer tunneling matrix element t_c is small as compared to the characteristic energy of in-plane fluctuations [16,21,22]. A small value of t_c is nonetheless necessary to account for the existence of Josephson coupling in the superconducting state. We conclude that the normal electron states are determined only by the in-plane momentum (and by the spin index σ). We therefore write for the creation and annihilation operators for the electrons confined in the layer located at $z=0$:

$$\langle \hat{a}^{+(0)}_{\mathbf{k}_\parallel,\sigma} \hat{a}^{(0)}_{\mathbf{k}_\parallel,\sigma}(z) \rangle = n_{\mathbf{k}_\parallel,\sigma}\delta(z) \tag{1}$$

where δ denotes the delta distribution and $n_{\mathbf{k},\sigma}$ is the number of quasiparticles. Obviously, the δ-distribution does not correspond to the real distribution. In particular, the δ-distribution is incompatible with the existence of normal transport and of Josephson effect along the out-of-plane direction. The δ-distribution is an effective distribution which simplifies the calculations without affecting the final result. It is straightforward to verify that a more realistic distribution, such as a gaussian distribution, with a characteristic width of ~ 1 Å, would simply contribute to an additional small k_z-dispersion in Eq. (4). Moreover, the use of the δ-distribution shows the qualitative difference between the two cases of purely two-dimensional and purely three-dimensional superconductors. These two cases correspond to respectively zero and strong interlayer couplings. Indeed, it is straightforward to verify that, in the absence of interlayer coupling or, equivalently, in the case of one single layer, also the BCS gap function is a delta distribution at $z=0$. The contrary situation is found in the case of particles with well-defined momentum in three dimensions. In this case the gap function is approximated by a delta distribution at the Fermi surface in k-space rather than in real space. The existence of Josephson coupling between layers produces the intermediate situation in which the k_z-dispersion of the gap function of two layers is no longer trivial, as it is in the above limiting cases of purely two- and purely three-dimensional systems. To find this dispersion, according to (1), we write the z-dependence of the gap as follows:

$$\Delta_{\mathbf{k}_\parallel}(z) = \tfrac{1}{2}\Delta_{\mathbf{k}_\parallel,0}\, e^{i\varphi(z)}[\delta(z-s/2)+\delta(z+s/2)] \tag{2}$$

where $\Delta_{\mathbf{k}_\parallel,0}$ is the gap of one single layer, φ expresses the variation of the phase along z, s is the interlayer spacing, and the factor $1/2$ is needed for normalization.

The physically relevant quantity that enters in the expression of the BCS excitation spectrum [see Eq. (6) below] is the spectral density $|\Delta_{\mathbf{k}}|^2$. Its physical meaning is the condensation energy for a Cooper pair with momenta $\mathbf{k}$ and $-\mathbf{k}$ times the coupling constant [23]. In our case, the above quantity is obtained by taking the Fourier transform of (2):

$$\Delta_{\mathbf{k}} = \int_{-\infty}^{+\infty} e^{-ik_z z}\Delta_{\mathbf{k}_\parallel}(z)dz = \Delta_{\mathbf{k}_\parallel,0}\, e^{i\langle\varphi\rangle}\cos\frac{\Delta\varphi - k_z s}{2} \tag{3}$$

where

$$\langle\varphi\rangle \equiv [\varphi(s/2)+\varphi(-s/2)]/2$$

and

$$\Delta\varphi \equiv \varphi(s/2)-\varphi(-s/2)$$

It follows that

$$|\Delta_{\mathbf{k}}|^2 = \tfrac{1}{2}|\Delta_{\mathbf{k}_\parallel,0}|^2[1+\cos\Delta\varphi\cos(k_z s)] \qquad (4)$$

where the odd powers of $\Delta\varphi$ do not appear if no net Josephson current flows across the layers. The physical meaning of (4) is as follows; if the phases of the gap function of two layers are strongly correlated ($\cos\Delta\varphi\approx 1$), the operation of spatial translation of a Cooper pair with perpendicular momenta k_z and $-k_z$ from one layer to the other corresponds to multiplying the gap function by the phase factor $e^{ik_z s}$. Hence the gap functions of the two layers interfere with opposite sign if the condition for the formation of standing waves $k_z = \pi/s$ is satisfied (see Fig. 3). The condensation energy is thus redistributed in k_z-space, becoming larger (smaller) when the interference is constructive (destructive). The total condensation energy is conserved [23]:

$$E_{cond} = 2\int |\Delta_{\mathbf{k}}|^2 \frac{d^3k}{(2\pi)^3}\frac{dg}{g^2} = \int |\Delta_{\mathbf{k}_\parallel}|^2 \frac{d^2k_\parallel}{(2\pi)^2}\frac{dg}{g^2} \qquad (5)$$

where g is the coupling constant for a single layer. We note that the above interference effect is analogous to the Fano effect [24]. In the latter case, the transition probability in atomic spectra can vanish at certain values of transition energy due to the interference between two transition amplitudes with opposite sign.

In the following section we verify whether Eq. (4) accounts for the experimental low-temperature dependence of λ_{ab} reported in NCCO [1] and YBCO [2]. We calculate λ_{ab} by using the expression for the normal density tensor $\rho_{ij}^{(n)} \sim \lambda_{ij}(T) - \lambda_{ij}(0)$ derived from the two-fluid model [23]:

$$\rho_{ij}^{(n)} m_{jk} = -n\hbar^2 \int k_i k_k \frac{\partial f(\varepsilon_{\mathbf{k}})}{\partial \varepsilon_{\mathbf{k}}}\frac{d^3k}{(2\pi)^3} \qquad (6)$$

where m_{jk} is the effective mass tensor, n is the electron density, f is the Fermi distribution, $\varepsilon_{\mathbf{k}} = \sqrt{|\Delta_{\mathbf{k}}|^2 + \eta_{\mathbf{k}}^2}$ is the BCS energy spectrum, and $\eta_{\mathbf{k}}$ is the quasi-particle energy. The application of our result in the calculation of (6) consists of using expression (4), instead of the gap $\Delta_{\mathbf{k}_\parallel,0}$ of one single CuO_2 layer, in the expression of $\varepsilon_{\mathbf{k}}$. We extract $\eta_{\mathbf{k}}$ from photoemission data available for BSSCO [25–26], which is in agreement with band structure calculations for NCCO [27] and YBCO [18]. For all these compounds, $\eta_{\mathbf{k}}$ is known to be well described by the following tight-binding form:

$$\eta_{\mathbf{k}} = -2t_{ab}[\cos(k_x a) + \cos(k_y a)] \qquad (7)$$

with $t_{ab} \approx 0.25$ eV and where we have neglected the weak dispersion along the c-axis which is estimated to be $t_c \approx 0.07 t_{ab}$ in YBCO from band structure calculations [18]. We take for the in-plane effective mass $m_{ab} \approx 5$–$6 m_e$ (electron mass) according to electrical resistivity and optical measurements [28] and n consistent with the experimental value of the zero-temperature penetration depth $\lambda_{ab}(0) \approx 1500$ Å [29]. To calculate (6) numerically, we have employed an autoadaptive algorithm [30] which controls the truncation error below 0.001 in relative units. The main point of our analysis concerns the value of the phase coupling factor $\cos\Delta\varphi$ in Eq. (4) to be chosen for the two compounds NCCO and YBCO. The large distance (≈ 12 Å) between adjacent CuO_2 layers in the unit cell of NCCO implies weak coupling, hence $\cos\Delta\varphi \approx 0$. However, in YBCO $\cos\Delta\varphi \approx 1$ because in this case the two adjacent layers are separated by the small yttrium ion. Figure 1 shows that, by assuming a conventional isotropic gap without nodes for one single layer, a crossover from exponential to linear behavior of $\Delta\lambda_{ab} \equiv \lambda_{ab}(T) - \lambda_{ab}(0)$ is observed as $\cos\Delta\varphi$ increases from 0 to 1. Hence, Eq. (4) with $\cos\Delta\varphi = 0$ does indeed account for the experimental temperature dependence of λ_{ab} found in NCCO, since it has been already shown in [1] that quantitative account for this dependence is given by assuming a conventional isotropic gap $\Delta_0 \approx 2T_c$. For the gap of YBCO we assume two forms: (1) the d-wave $\Delta_{\mathbf{k}_\parallel,0} = \Delta_2[\cos(k_x a) - \cos(k_y a)]$ in one single layer [$\cos\Delta\varphi = 0$ in Eq. (4)], according to the spin fluctuation picture; (2) the "extended s-wave" proposed by Mahan [31] $\Delta_{\mathbf{k}_\parallel,0} = \Delta_0 + \Delta_4\cos(4\alpha)$ [$\alpha \equiv \arctan(k_y/k_x)$]

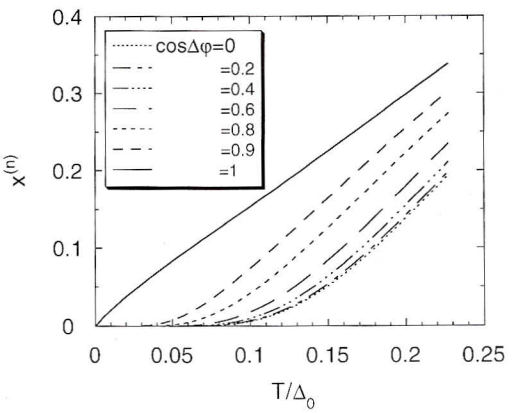

Fig. 1. Dependence of the normal fraction $x^{(n)} \approx 2\Delta\lambda/\lambda(0)$ of a superconducting bilayer as a function of reduced temperature for different values of the phase coupling factor $\cos\Delta\varphi$ in Eq. (4). The in-plane gap function has been taken isotropic with $\Delta_{\mathbf{k}_\parallel,0} = \Delta_0 = 1.76T_c$. The other numerical parameters used for the calculations are $m_{ab} = 6m_e$, $\lambda_{ab}(0) = 1500$ Å, $t_{ab} = 0.25$ eV, and $a = 3.85$ Å (in-plane lattice parameter).

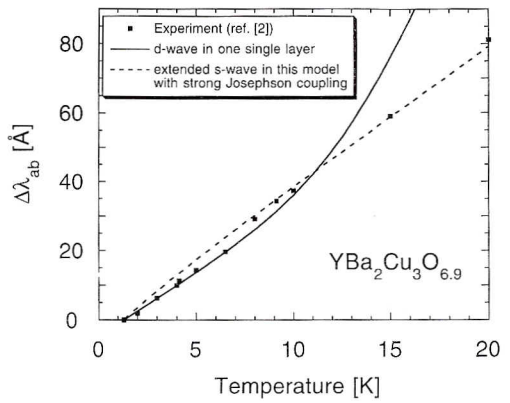

Fig. 2. Comparison between the experimental data of the variation of the in-plane penetration depth of YBCO reported in [2] and our numerical calculations in the case of: (1) "*d*-wave" gap in one single layer [$\cos\Delta\varphi=0$ in Eq. (4)]; (2) "extended *s*-wave" gap with strong Josephson coupling between two adjacent layers [$\cos\Delta\varphi=1$ in Eq. (4)]. The parameters used for the calculations are $\Delta_2=8$ meV and $m_{ab}=5m_e$ in the first case and $\Delta_0=13$ meV, $\Delta_4=7$ meV, and $m_{ab}=6m_e$ in the second case. The other numerical parameters are as in Fig. 1.

with strong coupling between adjacent layers [$\cos\Delta\varphi=1$ in Eq. (4)], according to our picture. We recall that both forms are in quantitative agreement, within the experimental error, with angular resolved photoemission data on BSSCO by setting $\Delta_0\approx 14\pm5$ meV, $\Delta_4\approx6\pm5$ meV, and $2\Delta_2\approx20\pm5$ meV [25–26]. We also use these values for YBCO as T_c differs in the two compounds by only ≈5 K≈0.4 meV, while the resolution of photoemission data is ≈5 meV. The above values refer precisely to the in-plane gap $\Delta_{\mathbf{k}_\parallel,0}$, since the light beam is incident onto the *ab* plane in photoemission experiments.

In Fig. 2 we compare our numerical result with the experimental data given in [2]. We note that quantitative agreement is obtained within the experimental error for both forms of the gap described above, although the prediction based on the *d*-wave form deviates from the experimental data at temperatures above ≈10 K. We conclude that our picture of Josephson-coupled superconducting bilayers accounts for the diversity in the low-temperature behavior of the normal density observed in NCCO and YBCO by simply assuming that this coupling is respectively weak and strong. It would, therefore, be important to verify whether this picture could account for the experimental behavior of other cuprates, both with and without adjacent CuO_2 layers in their unit cell. Since there exists several compounds with three and four layers per unit cell, it might be of interest to generalize Eq. (4) to the case of N layers. The result is straightforward:

$$|\Delta_{\mathbf{k}}|^2=\frac{1}{N^2}|\Delta_{\mathbf{k}_\parallel,0}|^2 \times\left[N+2\sum_{m=1}^{N-1}(N-m)\cos\Delta\varphi_m\cos(mk_zs)\right] \quad (8)$$

where $\Delta\varphi_m$ is the phase difference between two layers separated by ms. Figure 3 shows that, in the above general case, the spectral density (8) is peaked around $k_z=0$ if the phase correlation extends over several times the interlayer distance ($\cos\Delta\varphi_m\approx1$ for all m up to $N\gg1$), because the oscillating terms with wavevector mk_z cancel one another at $k_z\neq0$. This corresponds to the limit of a three-dimensional superconductor with large coherence length $\xi_z\sim1/\Delta k_z$, where Δk_z is the width of the peak of the spectral density.

In conclusion, we have shown that the interference between the gap functions of two adjacent superconducting layers which arises from the Josephson coupling can lead to vanishing spectral density $|\Delta_{k_z}|^2$ of the BCS energy gap at certain values of the perpendicular momentum k_z. By applying this result to the cuprates, we predict that the compounds with large spacing between adjacent CuO_2 layers, such as the systems with one layer per unit cell $La_{2-x}Sr_xCuO_4$, NCCO, $TlBa_2Ca_{n-1}Cu_nO_{2n+3}$, $Tl_2Ba_2Ca_{n-1}Cu_nO_{2n+4}$,

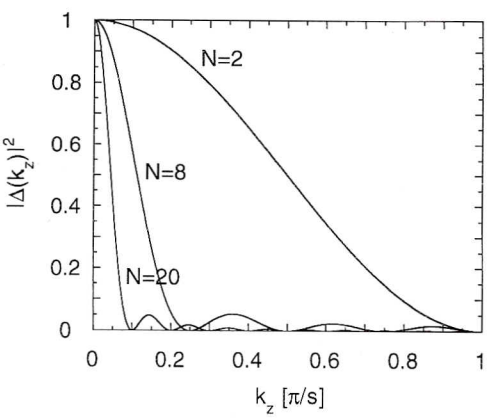

Fig. 3. Dispersion of the spectral density $|\Delta_{k_z}|^2$ of the energy gap of N superconducting layers as a function of the perpendicular momentum k_z in the case of complete phase locking through the Josephson effect [$\cos\Delta\varphi_m=1$ for all $m\leq N$ in Eq. (8)]. Note that the flat dispersion that corresponds to a single layer collapses progressively into a delta distribution at large N. This corresponds to the limit of a three-dimensional superconductor. In a bilayer, the spectral density vanishes when the momentum satisfies the condition for the formation of standing waves $k_z=\pi/s$, where s is the interlayer spacing.

and $Bi_2Sr_2Ca_{n-1}Cu_nO_{2n+4}$ with $n=1$, always exhibit conventional BCS behavior if the gap of the single layers has no nodes. On the other hand, all the systems with two or more adjacent layers per unit cell, such as YBCO, BSSCO, and the above compounds with $n>1$, are expected to exhibit in all cases gapless behavior. Within the experimental error, our numerical results account for the exponential and linear low-temperature dependences of the penetration depth reported in NCCO and YBCO.

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