Transition temperature and a spatial dependence of the superconducting gap for multilayer high-temperature superconductors

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We derive the expressions for the transition temperature ($T_c$), and the spatial dependence of the superconducting gap for a multilayer high-$T_c$ superconductor composed of groups of tightly spaced planes separated by a larger distance. The results are compared with experiment and provide a strong support for an interlayer hopping as the driving force of the large $T_c$ enhancement in multilayered compounds. Our results are universal in the sense that they are valid for an arbitrary pairing potential $V_{kk'}$ in the CuO$_2$ planes, as well as for both Fermi and non-Fermi liquids.

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The physical origin of pairing in high temperature superconductors has not been determined as yet. Therefore, it is very important to formulate a language describing those systems, which is independent of the detailed underlying electronic structure, but still concrete enough to allow for an extensive experimental test. We believe that the model proposed by Anderson and his coworkers [1] and based on the pairing enhancement due to an interlayer Cooper-pair tunneling provides such a crucial feature, on the basis of which one can construct an appropriate quantitative language. Universal features of this model not discussed so far are detailed below and compared with experiment.

In this paper we derive analytically the space profile of the superconducting gap parameter assuming only that we have a \( k \)-dependent pairing potential \( V_{kk'} \) in the two spatial dimensions (for a square planar configuration), and a coherent (Josephson) pair tunneling between the planes [1,2]. Moreover, we analyze explicitly the periodic arrangement of groups of planes, each of them containing \( p \) tightly spaced identical \( \text{CuO}_2 \) planes, and separated by a larger distance, but in contact with each other also by, albeit weaker, Cooper pair tunneling. Such a configuration is drawn schematically in Fig. 1a for the high temperature superconductor. The system is thus characterized by the intragroup \( T^{(I)}(k) \) and intergroup \( (\tilde{T}(k)) \) tunneling amplitudes. Hence, our approach can be applied to both mono- and multilayer high-\( T_c \) systems and thus generalizes previous treatments [1,3,4]. The calculated below space profile of the superconducting gap is shown schematically in Fig. 1b. Our results for the transition temperature \( T_c \) for either Fermi, or Luttinger or statistical spin liquid, the three universality classes appearing for the interacting fermion systems [5].

We label the single electron states by the in-plane component of the wave vector \( k \equiv (k_x, k_y) \) and by spin quantum number \( \sigma = \pm 1 \), as well as by the two discrete numbers \((s, j)\), where \( j = 1, \ldots, p \) characterizes the plane position within the group of tightly spaced planes, and \( s = 1, \ldots, N \) labels the groups. The simplest Hamiltonian describing such a nontrivial structure can be written as follows:

\[
H = \sum_{s=1}^{N} \sum_{k\sigma} \sum_{j=1}^{p} \epsilon_{k,j,s} b_{j,s,k\sigma}^+ b_{j,s,k\sigma} - \frac{1}{N} \sum_{s=1}^{N} \sum_{k} \sum_{j=1}^{p} V_{kk'} b_{j,s,k\uparrow}^+ b_{j,s,k\downarrow} b_{j',s,k'\downarrow}^+ b_{j',s,k'\uparrow}
\]
\[
- \sum_{s=1}^{N} \sum_{k} \sum_{j=1}^{p} \sum_{l=1}^{j+l\leq p} T^{(l)}(k) \left[ b_{j,k}^{+} b_{j,-k}^{+} b_{j+l,-k} b_{j+l,k}^{+} + H.C. \right] \\
- \sum_{s=1}^{N} \sum_{k} \sum_{j=1}^{p} \sum_{l=1}^{1\leq j-l\leq p} T^{(l)}(k) \left[ b_{j,k}^{+} b_{j,-k}^{+} b_{j-l,-k} b_{j-l,k}^{+} + H.C. \right] \\
- \sum_{s=1}^{N-1} \sum_{k} \bar{T}(k) \left[ \left( \sum_{j=1}^{p} b_{j,k}^{+} b_{j,-k}^{+} \right) \left( \sum_{j=1}^{p} b_{j,-k}^{+} b_{j,k}^{+} \right) + H.C. \right].
\]

(1)

The first two terms describe the BCS-type Hamiltonian for \(N \cdot p\) independent planes, the second and the third express the pair tunneling (with the matrix element \(T^{(l)}(k)\)) between the planes in the same group, separated by \((l-1)\) superconducting planes in between, whereas the last term represents the tunneling between neighboring groups. We have assumed that the intergroup tunneling matrix element \(\bar{T}(k)\) is independent of the pair of planes selected in those two groups, since the detailed balance within the group must be achieved much faster than between the groups.

In the following we make the mean field (BCS-like) approximation, \(i.e.,\) assume that the superconducting gap is characterized by the nonvanishing average \(d_{j,k} \equiv \langle b_{j,k}^{+} b_{j,-k}^{+} \rangle\), which will not depend on group index \(s\), as each group is in identical environment and \(N \to \infty\) (this, however, is not the case for the individual planes within the group!) In effect, the gap function can be defined as follows

\[
\Delta_{j,k} = \sum_{j=1}^{p} 2\bar{T}(k)d_{j,k} + \frac{1}{N} \sum_{k'} v_{k'k} d_{j,k'} + \sum_{l=1}^{j+l\leq p} T^{(l)}(k)d_{j+l,k} + \sum_{l=1}^{1\leq j-l\leq p} T^{(l)}(k)d_{j-1,k}.
\]

(2)

The selfconsistency condition for the mean-field solution requires that

\[
d_{j,k} = \Delta_{j,k} \chi_{j,k}.
\]

(3)

The generalized susceptibility \(\chi_{j,k}\) in this universal relation depends on the nature of the normal state. In the case of the Fermi liquid (FL) it takes the usual form \([3]\).

\[
\chi_{j,k} = \frac{1}{2E_{j,k}} \tanh \left( \frac{\beta E_{j,k}}{2} \right),
\]

(4)

where the quasiparticle energy is \(E_{j,k} = \sqrt{(\epsilon_k - \mu)^2 + |\Delta_{j,k}|^2}\). In the case of the spin-charge separated Luttinger liquid (LL), \(i.e.,\) if we have the linear dispersion relation \(\epsilon_k - \mu \sim (k-k_F)\)
for bare particles and two Fermi velocities corresponding to charge \((v_c)\) and spin \((v_s)\) degrees of freedom, the function \(\chi_{j,k}\) is [4]

\[
\chi_{j,k} = \frac{|\Delta_{j,k}|^2}{\sqrt{\nu_c^2 + 4|\Delta_{j,k}|^4}} \frac{\tanh(\beta E_{j,k}/2)}{E_{j,k}} + \frac{1}{\pi} \int_{-\pi}^{\pi} dx \tanh \left( \frac{\beta x}{2} \right) \frac{h_s h_c}{\hbar^2 h_c^2 + |\Delta_{j,k}|^4}
\]

(5)

where \(E_{j,k} = \frac{1}{2} [\nu_+ + \sqrt{\nu_c^2 + 4|\Delta_{j,k}|^4}], h_{c,s} \equiv \sqrt{|x^2 - (v_{c,s}k)^2|}, \text{ and } \nu_\pm \equiv (v_c^2 \pm v_s^2)k^2.\) Finally, for the strongly correlated liquids with non-standard anticommutation relations for the fermion operators [5] the mean-field approximation of the BCS-type leads also to Eq. (2), in which rhs is renormalized only by the factor \(A_k \equiv 1 - \bar{n}_k/2,\) which near the Fermi energy has the value \(1/2.\)

We take into account only the coupling between the nearest neighbors, \(i.e.,\) assume that \(T(l)(k) = T(k)\delta_{l,j\pm 1}.\) This approximation means that we can seek a solution in a simple exponential or trigonometric form. In that situation the gap \(\Delta_{j,k}\) is determined by the system of universal difference equations

\[
\Delta_{1k} - \frac{1}{N} \sum_{k'} V_{kk'} \chi_{1,k'} \Delta_{1,k'} = T(k) \chi_{2,k} \Delta_{1,k} + 2 \tilde{T}(k) \sum_{j'=1}^p \chi_{j',k} \Delta_{j',k},
\]

\[
\Delta_{j,k} - \frac{1}{N} \sum_{k'} V_{kk'} \chi_{j,k'} \Delta_{j,k'} = T(k) (\chi_{j+1,k} \Delta_{j+1,k} + \chi_{j-1,k} \Delta_{j-1,k}) + 2 \tilde{T}(k) \sum_{j'=1}^p \chi_{j',k} \Delta_{j',k},
\]

\[
\Delta_{p,k} - \frac{1}{N} \sum_{k'} V_{kk'} \chi_{p,k'} \Delta_{p,k'} = T(k) \chi_{p-1,k} \Delta_{p-1,k} + 2 \tilde{T}(k) \sum_{j'=1}^p \chi_{j',k} \Delta_{j',k}.
\]

(6)

The shape of the spatial profile of \(\Delta_{j,k}\) \((i.e.,\) its dependence of \(j)\) should not depend on the system temperature, but only on the form of the boundary conditions. Therefore, we solve this system of equations close to the transition temperature \(T_c,\) where the generalized susceptibility \(\chi_{j,k}\) can be linearized in the following way

\[
\chi_{j,k} \simeq \frac{\tanh \left( \frac{\beta \epsilon_k}{2} \right)}{2\epsilon_k} + O(\Delta_{j,k}^2),
\]

(7)

for FL, and

\[
\chi_{jk} \simeq \frac{1}{\pi} \int_{v_{c,k}}^{v_{c,k}} dx \tanh \left( \frac{\beta x}{2} \right) \frac{1}{h_s h_c} + O(\Delta_{j,k}^4),
\]

(8)

for LL. To zero order in the gap parameter the generalized susceptibilities do not depend on the layer index \(j.\) With this expansion, the system (6) represents a system of linear
and inhomogeneous difference equations with respect to index \( j \). In order to solve them we introduce two additional fictitious layers labeled by \( j = 0 \) and \( j = p+1 \) [6]. The natural boundary conditions are expressed in terms of the vanishing gap on these limiting layers, \( i.e., \) we set
\[
\Delta_{0,k} = \Delta_{p+1,k} = 0.
\] (9)
These boundary conditions express the physical equivalence of all \( p \) layers within the group, \( i.e., \) we do not introduce the surface layers, which differ from those inside. In such a situation, the system of equations (6) can be rewritten in a more symmetric form, both for the FL and the LL cases, namely
\[
\Delta_{j,k} - \frac{1}{N} \sum_{k'} V_{kk'} \chi_{k'} \Delta_{j,k'} = T(k) \chi_{k} (\Delta_{j+1,k} + \Delta_{j-1,k}) + Z_{k},
\] (10)
where \( Z_{k} \equiv 2 \tilde{T}(k) \chi_{k} \sum_{j'=1}^{p} \Delta_{j',k}, \) and \( j = 1 \ldots p \).

We solve first the homogeneous part of Eq. (10) (\( i.e., \) put \( Z_{k} \equiv 0 \)). The spatial dependence of the solution for the gap can be taken in the form \( \Delta_{j,k} = \Delta^{(\pm)}_{k} e^{\pm i\alpha j} \), where the constants \( \Delta^{(\pm)}_{k} \) fulfill the set of self-consistent equations
\[
\Delta^{(\pm)}_{k} (1 - 2T(k) \chi_{k} \cos \alpha) = \frac{1}{N} \sum_{k'} V_{kk'} \chi_{k'} \Delta^{(\pm)}_{k'}.
\] (11)
Thus, the general solution of the homogeneous part is
\[
\Delta_{j,k} = \Delta^{(\pm)}_{k} e^{\pm i\alpha j},
\] (12)
where the wave vector of the oscillating gap is determined from the boundary conditions (1), and takes the form
\[
\left( \begin{array}{cc}
1 & 1 \\
e^{i\alpha(p+1)} & e^{-i\alpha(p+1)}
\end{array} \right) \left( \begin{array}{c}
\Delta^{(\pm)}_{k} \\
\Delta^{(-)}_{k}
\end{array} \right) = 0.
\] (13)
The vanishing determinant of the above matrix provides a nontrivial solution only when \( \alpha = n\pi/(p+1) \), where \( n \) is an integer. Substituting back the value of \( \alpha \) to (13) we find \( \Delta^{(\pm)}_{k} = -\Delta^{(-)}_{k} \equiv \Delta_{k} \); so the solution (12) takes the explicit form
\[ \Delta_{j,k} = 2i\Delta_k \sin \left( \frac{n\pi j}{p+1} \right). \] (14)

Physically, the admissible solution is that with \( n = 1 \), as the solution with no nodes inside \( p \) layers should have the lowest energy. The shape of the spatial dependence of the gap has been drawn already in Fig. 1b. Finally, the gap magnitude \( \Delta_k \) is determined from Eq. (10) with \( Z_k = 0 \), which reduces to the integral equation:

\[ \Delta_k = \frac{1}{1 - 2\chi_k \cos \left( \frac{\pi}{p+1} \right)} \frac{1}{N} \sum_{k'} V_{kk'} \chi_{k'} \Delta_{k'}. \] (15)

The solution of the full Eq. (10) is found by superposing the general solution (14) of the homogeneous part of (11) with a particular solution of the full equation, \( i.e. \), by taking

\[ \Delta_{j,k} = \Delta_k' + \Delta_k^{(0)} \sin \left( \frac{\pi}{p+1} j \right), \] (16)

where \( \Delta_k^{(0)} = 2i\Delta_k \), and \( \Delta_k' \) is treated as a small perturbation. The part \( \Delta_k' \) does not depend on \( j \) because the periodic boundary conditions can be taken for \( N \) groups of layers. Substituting the solution (16) into (10) and omitting higher-order terms (\( i.e. \), those \( \sim \Delta_k' \cdot \overline{T}(k) \)), we have the equation for \( \Delta_k^{(0)} \)

\[ \Delta_k^{(0)} = \frac{1}{1 - 2\overline{T}(k)f(p) + T(k) \cos \left( \frac{\pi}{p+1} \right)\chi_k} \frac{1}{N} \sum_{k'} V_{kk'} \chi_{k'} \Delta_{k'}. \] (17)

The equation for \( \Delta_k' \) is

\[ \Delta_k' = \frac{1}{1 - 2\overline{T}(k)\chi_k} \frac{1}{N} \sum_{k'} V_{kk'} \chi_{k'} \Delta_{k'}. \] (18)

where \( f(p) \equiv \sin(\pi p/2(p+1))/\sin(\pi/2(p+1)). \)

The physical \( T_c \) is provided by the larger transition temperatures determined from Eqs. (17) and (18). Hence, it is always determined from Eq. (17). This feature of the theory illustrates the importance of the intergroup hopping \( \overline{T}(k) \) and formally appends the ideas of [1]. Also, it reduces to that of Chakravarty et al. [1] in the limit of \( \overline{T} = 0 \) and \( p = 1 \). Most importantly, our result is the same for both Fermi and Luttinger liquids, as well as for the liquids with a generalized exclusion statistics described in [5,7].
To discuss the implications of our approach let us consider first the monolayer case $(p = 1)$, i.e., a material with the interlayer hopping $\tilde{T}(\mathbf{k}) \equiv (t')^2/t$, for which $t$ is the magnitude of the bare single-particle hopping in the plane. In that case a simple estimate of the denominator of Eq. (17) is:

$$1 - \tilde{T}(\mathbf{k})\chi_{\mathbf{k}} \sim 1 - r \frac{t'}{t} \cdot \frac{t'}{k_B T_c},$$

where $r$ is a numerical constant of the order of unity. Hence, the tunneling can strongly enhance the pairing potential, since $k_B T_c \sim r (t')^2/t$ [1].

To calculate explicitly the value of $T_c$ we consider explicitly the $p \geq 1$ case with a constant pairing potential $V_{\mathbf{k}\mathbf{k}'} = V$ in the energy regime of the width $\omega_D \ll \mu$. Introducing the density of states $N(0)$ at the Fermi level we find from (17)

$$1 = VN(0) \int_{-\omega_D}^{\omega_D} d\epsilon \frac{\chi(\epsilon)}{1 - 2[\tilde{\alpha} f(p) + \cos(\pi p + 1)]\chi(\epsilon)(t')^2/t},$$

where $\tilde{\alpha}$ is the ratio of intergroup to intragroup tunneling amplitudes. In the extreme situation, when the interplanar tunneling provides a dominant contribution to the effective pairing, we can make the assumption $\omega_D/k_B T_c \ll 1$ and thus approximate $\tanh(x) \approx x$. Here, we provide the $T_c$ derivation for the Luttinger liquid [4] using the expression (8) for $\chi_{\mathbf{k}}$. In that case, Eq. (20) reads

$$1 = VN(0) \int_0^{\beta \omega_D/2} dx \frac{I(x)}{1 - \beta T(p)I(x)},$$

where $T(p) \equiv [\tilde{\alpha} f(p) + \cos(\pi p/(p+1))](t')^2/t$, and

$$I(x) = \frac{1}{\pi x} \int_0^1 du \frac{\tanh(xu)}{\sqrt{u^2 - (u_s/u_c)^2} \sqrt{1 - u^2}}.$$

In the limit $\beta \omega_D \ll 1$ the last integral is of elliptic form, which has a property $\int_a^b dz/(\sqrt{z - a} \sqrt{b - z}) = \pi$; hence $I(x) = 1$. In effect, we obtain a remarkably simple expression for $T_c$

$$T_c = VN(0) \frac{\omega_D}{2} + \frac{1}{2} \frac{(t')^2}{t} \left[ \cos \left( \frac{\pi}{p + 1} \right) + \tilde{\alpha} f(p) \right] \equiv T_c^0(p) + T_c' \cos \left( \frac{\pi}{p + 1} \right).$$
This result is of the same type as the formula derived for $\tilde{\alpha} = 0$ in the Fermi liquid case [1] (it can be extended to the case $\tilde{\alpha} \neq 0$ in straightforward manner). Hence, the transition temperature expression is universal and contains a combined effect of the intrinsic in-plane pairing and the two interplanar Josephson tunneling processes.

To test the relative role of the two tunneling contributions we have fitted the tabulated [8] $T_c$ values to the expression (22). Table I displays the detailed comparison, together with the $T_c^0$ and $T'_c$ values. The agreement between the theory and experiment is excellent for $p > 1$ systems. For $p = 1$ systems we have chosen $T_c^0$ as the middle point of the allowed interval; at least part of the $T_c^0$ value must be ascribed to the interplanar tunneling $\sim \tilde{\alpha} f(p)$. In connection with this, one can say that to have a proper behavior in the limit of large $p$ one must assume that $\tilde{T}(k) \sim p^{-1}$; then $\tilde{\alpha} f(p) \sim 1/p$, and the contribution due to the intergroup tunneling is substantially smaller for larger $p$. This is the reason why $T_c^0$ value is essentially constant for $p > 1$. From this point of view, uncertainty in the $T_c$ values for the $p = 1$ systems can be understood by the planes intersection due to the sample imperfection thus hampering the tunneling. Also, because of $T_c^0$ independence on the systems with larger $p$, the coherence length along the axis must exceed the smallest distance between the two neighboring groups. Finally, the maximal available $T_c$ for each family is for $p \to \infty$, and is also listed in Table I.

From our results, one can draw a very important prediction: the $T_c$ should increase substantially by applying the pressure along the $c$ axis, as the pressure will increase it towards the value $T_c(\infty)$.

In summary, we have derived analytically the explicit forms of the space profile of the superconducting gap, and the transition temperature; these results were obtained without the need of specifying the pairing potential in the plane, and independently of the nature of the normal state.

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## TABLE I. Critical temperatures for various single and multilayer superconductors

| Material                      | $p$ | $T_c^{\text{exp}}$ | $T_c^{\text{θ}}$ | $T_c'$ | Theory: $T_c$ |
|-------------------------------|-----|--------------------|------------------|-------|---------------|
| Bi$_2$Sr$_2$CuO$_6$           | 1   | 0-20               | 10               | 148   | 10            |
| Bi$_2$Sr$_2$CaCuO$_8$         | 2   | 85                 | 10               | 148   | 84            |
| Bi$_2$Sr$_2$Ca$_2$Cu$_3$O$_{10}$ | 3   | 110                | 10               | 148   | 112           |
| —                             | $\infty$ | –                 | 10               | 148   | 158           |
| Tl$_2$Ba$_2$CuO$_6$           | 1   | 0-80               | 41               | 126   | 41            |
| Tl$_2$Ba$_2$CaCuO$_8$         | 2   | 108                | 41               | 126   | 103           |
| Tl$_2$Ba$_2$Ca$_2$Cu$_3$O$_{10}$ | 3   | 125                | 41               | 126   | 128           |
| —                             | $\infty$ | –                 | 41               | 126   | 167           |
| Tl$_2$Ba$_2$CuO$_5$           | 1   | 0-50               | 24               | 121   | 24            |
| Tl$_2$Ba$_2$CaCu$_2$O$_7$     | 2   | 80                 | 24               | 121   | 84            |
| Tl$_2$Ba$_2$Ca$_2$Cu$_3$O$_9$ | 3   | 110                | 24               | 121   | 107           |
| Tl$_2$Ba$_2$Ca$_3$Cu$_4$O$_{11}$ | 4   | 122                | 24               | 121   | 122           |
| —                             | $\infty$ | –                 | 24               | 121   | 145           |
| HgBa$_2$CuO$_4$               | 1   | 94                 | 94               | 59    | 94            |
| HgBa$_2$Ca$_2$Cu$_3$O$_8$     | 3   | 135                | 94               | 59    | 135           |
| —                             | $\infty$ | –                 | 94               | 59    | 153           |
FIGURES

Fig. 1. Schematic plot of the gap magnitude (top, a) for a multilayer situation (bottom, b) involving groups of $p \geq 1$ tightly spaced planes.