Possibility of reconciliation on the type of the order parameter in high-temperature superconductors

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A model of high-T_c superconductivity is proposed based on the following assumptions: (a) There are extended saddle-point singularities in the spectrum of electrons with a strongly enhanced density of states; (b) the interaction between electrons consists of a large and long-ranged phonon attraction and a small and short-ranged repulsion. It is shown that this model, having properties of both the *s*-wave and the *d*-wave approaches, can effectively explain most of the rather contradictory properties of these substances.

One of the hottest topics in the theory of high-T_c cuprates is the type of the order parameter. One point of view is that the pairing is of "*s*-type," possibly anisotropic. According to this hypothesis the order parameter does not change its sign along the Fermi surface, and the energy gap has no nodes. This is confined by several experiments which definitely demonstrate a finite energy gap, e.g., the Knight shift,[1] tunneling conductance in BiSCCO,[2] and HgBCCO.[3] The most convincing argument in favor of this point of view is the strong isotope shift of the critical temperature in YBCO with a partial substitution of constituents (Y$\rightarrow$Pr, or B$\rightarrow$La).[4,5] This is a clear evidence of a phonon mechanism of superconductivity which leads to an order parameter with no nodes. The weakness of the isotope shift for pure YBCO can be explained by the influence of "extended saddle point singularities,[6,7] (see below). The same, together with the assumption of a weak screening of Coulomb forces, can explain the observed anisotropy of the gap.[8]

On the other hand there exists also strong evidence in favor of the so-called "*d*-wave" pairing. These are the linear temperature dependence of the penetration depth at low temperatures,[9] the Josephson experiments on single crystals[10] and rings, consisting of several grains.[11] One must have in mind, however, that these experiments demonstrate actually only the fact that the order parameter, as a function of momentum, changes sign and has nodes but does not exclude dependencies differing from the form $\Delta(\mathbf{k})=\cos k_x-\cos k_y$, which is usually advocated by the proponents of the *d*-wave hypothesis. Recent direct measurements of the angular dependence of the energy gap by photoemission[12] did not confirm this form. The only result, which favors it, is the absence of the Josephson effect in a BiSCCO-Pb tunnel junction (surface $\perp c$)[13] but this result, which could mean that the integral of $\Delta(\mathbf{k})$ over the whole Fermi surface vanishes, is in contradiction with the observation of the Josephson effect in the same geometry with YBCO instead of BiSCCO and with the gap measurements already mentioned.

The goal of this paper is to demonstrate that most of the observations can be explained by a very simple idea which is a development of the model proposed recently.[8] It is based on two assumptions, which we call the *E-L* model: (a) the existence of extended saddle point singularities and their dominant role in defining the order parameter and (b) the existence of a large dielectric constant ε_∞ associates with the ion cores which results in weak screening of the Coulomb forces and long range of Coulomb-based interactions of conduction electrons, namely the direct Coulomb repulsion and the electron-phonon interaction.

In order to avoid misunderstanding, I would like to stress the difference of this approach with the one based on "simple" saddle points (see references in Ref. 14). The latter leads to a slight increase of T_c if the Fermi level coincides with the saddle point. This cannot be the case for differently doped materials. The "extended" saddle point (actually a line) means that the spectrum in a certain region of momentum space is quasi-one-dimensional and this leads to a considerable enhancement of the density of states in some energy interval in the vicinity of the saddle point and to the convergence of the integral in the BCS self-consistency equation defining the order parameter (see Ref. 6).

Everywhere we will consider electrons as two-dimensional, and phonons as three-dimensional. Compared to Ref. 8 we introduce the following changes. First of all, for the sake of generality we will write the phonon-mediated electron interaction in the form

$$V(\mathbf{k})=g\left[\frac{\kappa^2}{k^2+\kappa^2}\right]^n\frac{\omega_0^2(\mathbf{k})}{(\xi-\xi')^2-\omega_0^2(\mathbf{k})}\,, \tag{1}$$

where κ is the reciprocal Debeye screening radius, ξ and ξ' are the electron energies before and after the emission of the phonon, $n>1$ is some unknown power (in Ref. 8 we assumed $n=1$), and $\mathbf{k}$ is the 3D phonon momentum. In the case $|\xi-\xi'|\ll\omega_0(\mathbf{k})$ the second factor in Eq. (1) is equal to -1. We will also assume that in addition to this attraction there exists a small and short-ranged repulsive interaction $U=$const which can represent either the renormalized Hubbard repulsion at the copper sites or the interaction mediated by spin fluctuations (taken alone, such an interaction would lead to *d*-wave pairing). If the Fermi level is close to the saddle-point energy, the spectrum in the corresponding part of the momentum space is quasi-one-dimensional (see Ref. 6). As in Ref. 8 we will presume the following inequalities:

$$p_{F1} \ll \kappa \ll P_{0y} \ll 1/d \ll K \ , \tag{2}$$

where $p_{F1}=(2m_x\mu_1)^{1/2}$ is the 1D Fermi momentum in the singular region, $\mu_1=\mu-\varepsilon_0$ is the Fermi energy with respect to the saddle point, P_{0y} is the length of the singularity (as an example, we assume that the saddle point extended along the p_y axis, and the energy to depend only on p_x), d is the lattice period along the c axis, and K is the reciprocal-lattice period in the (ab) plane. As shown in Ref. 8, under conditions (2) Δ is constant in the singular region. Substituting $V(\mathbf{k})+U$ into the BCS self-consistency equation, assuming the density of states and Δ in the singular region to be much larger than beyond it and integrating over k_y and k_z, we obtain

$$1=\frac{\lambda}{2}\int_{-\mu_1}^{\infty}\frac{d\xi\mu_1^{1/2}}{(\xi+\mu_1)^{1/2}}\frac{\tan[(\xi^2+\Delta_1^2)^{1/2}/2T]}{(\xi^2+\Delta_1^2)^{1/2}} \ , \tag{3}$$

where Δ_1 is the value of Δ in the singular region, and

$$\lambda=\frac{(2m_x)^{1/2}}{(2\pi)^2\mu_1^{1/2}}\left[\frac{g\kappa^2}{n-1}-\frac{2UP_{0y}}{d}\right] . \tag{4}$$

We will assume the second term in the brackets to be much less than the first one, and neglect it. The solution of Eq. (3) at $T=0$ in the limit $\Delta \ll \mu_1$ is

$$\Delta_1=8\mu_1 e^{-1/\lambda} . \tag{5}$$

Now let us consider some point at the Fermi surface, distant from the singularity. For simplicity we consider a circular Fermi surface (there is no dependence on k_z), and φ will be the angular distance from one of the singular "points" (the length of the singularity, P_{0y}, and the z size of the Brillouin zone, $2\pi/d$, are assumed to be small compared to the radius of the cylindrical Fermi surface, p_0, which is of the order of K). The integral in the BCS equation consists of two parts: along the singularity and beyond it. Since the density of states in the singular region as well as the value of $\Delta=\Delta_1$ are large, we will assume that this part of the integral dominates (estimate of the other part's contribution; see below), and hence $\Delta(\varphi)$ beyond the singularity will be defined by its value in the singular region. The integral over ξ will be the same, as in Eq. (3), and we can replace it using this equation. Eventually we obtain the equation

$$\frac{\Delta(\varphi)}{\Delta_1}=\frac{2(n-1)P_{0y}}{\kappa^2 d}\left\{\left[\frac{\kappa}{2p_0}\right]^{2n}\left[\sin^{-2n}\left[\frac{\varphi}{2}\right]+\sin^{-2n}\left[\frac{\varphi-\varphi_0}{2}\right]\right]-\frac{U}{g}\right\} , \tag{6}$$

where p_0 is the Fermi momentum and φ_0 is the location of the next singularity (in general a sum over locations of all singularities has to be taken). This formula describes the behavior of $\Delta(\varphi)$ far from the singularities, i.e., at not too small values of φ. For description at any angle a simple interpolation

$$\sin^2\varphi/2 \rightarrow \sin^2\varphi/2+\text{const} ,$$

with the constant chosen so that $\Delta(0)=\Delta_1$ can be used. The minimal value of the first term in the curly brackets of Eq. (6) is at $\varphi=\varphi_0/2$, and its value is $2[\kappa/(2p_0\sin(\varphi_0/4))]^{2n}$. If this is smaller than U/g, then $\Delta(\varphi)$ has a negative value somewhere between the maxima, and hence the gap has two nodes in this region. In the case $\varphi_0=\pi/2$, as it happens in BiSCCO, the nodes have to be located symmetrically around $\pi/4$, and this corresponds to the observations of J.-C. Campuzano *et al.*[12] If $\varphi_0=\pi$, which is most likely to be the case in YBCO, the negative values of Δ are located around $\pi/2$, i.e., if the positive maxima correspond to the a direction, the negative values are around the b direction, which is exactly what is seen in experiments measuring the phase of the order parameter.

The necessary conditions for all that to be true is a sufficiently small value of U:

$$U \ll g\kappa^2 d/P_{0y} . \tag{7}$$

If this condition is fulfilled, Δ_0 in the singular region will be defined self-consistently by Eq. (4), and hence the critical temperature will be also defined by this equation. As shown in Ref. 7, in the case when the characteristic phonon frequency $\omega_0 \lesssim \mu_1$ (ω_0 is an optical frequency, or acoustical frequency at $k=\kappa$), the integration in Eq. (3) has to be cut off at ω_0, and a regular isotope effect appears. Since this is observed in experiment, we believe that the condition (7) is reasonable. Another concern could be the part of the integral in the equation for $\Delta(\varphi)$ outside the singular region. With respect to the terms, which we have kept, it is either of the order of p_{F1}/p_0, or $[UP_{0y}/(g\kappa^2 d)]\times(p_{F1}/P_{0y})$. Both quantities are small.

Since there is no reason for the integral $\int\Delta(\varphi)d\varphi$ to vanish, there should be a Josephson current in the HTSC-Pb junction if the boundary is normal to the c axis, although it may be smaller than what could be expected from an estimate based on Δ_1. The failure to observe it in a BiSCCO-Pb contact could be due to the weak hopping between the CuO_2 layers. The Fermi surface in this case is an almost straight cylinder, and the c component of the electron velocity is very small. If the electron crosses the barrier keeping the direction of its velocity, it has to go a very long path. This decreases drastically the tunneling probability and can destroy the Josephson current. This does not happen if the boundary is parallel to the c axis, because then the velocity normal to the boundary is large, and also in YBCO, where due to the chains the hopping between the CuO_2 layers is stronger, and hence the c component of the velocity is much larger. In these cases the Josephson effect was really observed.[13,15]

The idea presented above also solves an important problem about the suppression of superconductivity by nonmagnetic impurities. In the case of d-wave pairing one would expect the necessary condition to be $\tau\Delta \lesssim 1$,

whereas in the case of s-wave pairing it could happen only at $\tau\varepsilon_F \lesssim 1$. This criterion is rather difficult to apply, because in the HTSC the ratio Δ/ε_F is not so small as in low-temperature superconductors, and it is also not very clear which impurities behave as nonmagnetic. Nevertheless the general opinion is more inclined to interpret experimental data in terms of the condition $\tau\varepsilon_F \lesssim 1$.[16] In our scheme it would be rather natural, since the impurities are most likely ionized, the interaction of electrons with them is weakly screened and long ranged, and it would not mix the singular and remote regions of momentum space. This, however, has to be checked.[17]

There is also a question about the tunneling conductance. Experiments on BiSCCO (Ref. 2) and HgBCCO (Ref. 3) show a small conductance at eV less than some large gap with $2\Delta(0)/T_c \sim 6-8$. This seems in contradiction with the present results, as well as with the d-wave and anisotropic s-wave concepts. Our scheme can explain the tunneling results as follows. The tunneling conductance is proportional to the density of states. In the nonsingular regions not only the gap, but also the density of states (per unit solid angle), is much lower than in the singular region. Therefore it contributes a small background; only, when $eV=\Delta_1$ is reached, the conductance becomes large (the background is usually attributed to normal inclusions).

The model presented here cannot explain all the data. Even with an energy-dependent one-dimensional density of states the maximal value of $2\Delta(0)/T_c$, which can be obtained from Eq. (4), is less than 4 (see Ref. 6), whereas the experimental values are around 6 to 8. This contradiction can be due to the fact that we apply the simple BCS-type theory, whereas the increased density of states makes the effective interaction strong. This has to be resolved in future studies.

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