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Existence of both *s* and *d*-wave solutions of Eliashberg equations

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We solve Eliashberg equations in the case of strong anisotropic electron-phonon coupling and low energy cutoff. In a simplified model representing the Fermi Surface of $(CuO_2)_n$ planes, we exhibit a *d*-wave solution as well as a generalized *s*-wave one.

KEY WORDS: Eliashberg equations, electron-phonon.

1. Introduction

The basic mechanism of high-temperature superconductivity is not yet known. Possibilities are the BCS phonon-mediated interaction, exchange of paramagnons, or some other Coulomb interaction, described for example by the t-J model, or the Pines theory [1]. It is frequently argued that when the superconducting gap parameter Δ has a *d*-wave symmetry [2], this implies a Coulomb mechanism, while a phonon-mediated interaction causes an *s*-wave (or extended *s*-wave) symmetry of Δ [3]. This argument is based on a long experience with the phonon-mediated mechanism, since the work of BCS, Gorkov, Nambu and Eliashberg [4]. The electron-phonon interaction in normal metals is local in ordinary space [5] and consequently the $\boldsymbol{k}$-dependence of the interaction $D(\boldsymbol{k},\boldsymbol{k}', i\omega - i\omega') = g^2(\boldsymbol{k},\boldsymbol{k}')\,2\omega_{ph}/\left[(\omega-\omega')^2+\omega_{ph}^2\right]$ is weak and usually averaged over the FS [6]. This locality is due to strong screening; $g(\boldsymbol{k},\boldsymbol{k}')$ is proportional to the ion-electron potential given by [7] $V(\boldsymbol{k},\boldsymbol{k}') = 4\pi e^2/\left[(\boldsymbol{k}-\boldsymbol{k}')^2+\kappa_{TF}^2\right]$ and the Thomas-Fermi screening parameter κ_{TF} is large, and therefore V is nearly isotropic. In normal metals, $\kappa_{TF}^2 = 0.66\, r_s\, k_F^2$, where r_s ($\approx$3) is the average distance between electrons in units of the Bohr radius. In the high-T_c cuprates, the oxide background has a very large dielectric constant $\varepsilon_0 = 60$ [8], therefore $\kappa_{TF}^2 = 4\pi e^2 n(E_F)/\varepsilon_0$ is much smaller, and a typical value is $\kappa_{TF} \approx 0.3 k_F$. Consequently V is very anisotropic, with predominantly forward scattering. This favors superconductivity with *d*-wave symmetry of Δ, even for the phonon-mediated process.

In the present work, we present solutions of the Eliashberg equations, generalized for an interaction $D(\boldsymbol{k},\boldsymbol{k}', i\omega - i\omega')$ with a strong $\boldsymbol{k}$-dependence, for an electron-phonon matrix element $g(\boldsymbol{k},\boldsymbol{k}')$ proportional to $V(\boldsymbol{k},\boldsymbol{k}')$. We find that there are solutions with *d*-wave and *s*-wave symmetries that are nearly degenerate in energy, and thus small changes in the parameters cause a crossover between the two symmetries, without a large change in T_c.

In previous publications [9] we solved the generalized Eliashberg equations for an electron-phonon coupling $g(\boldsymbol{k},\boldsymbol{k}')$ possessing a cutoff at an energy ξ_{ph} close to the energy ω_0 at which the dielectric constant $\varepsilon(\omega)$ of the background falls significantly, i.e. about 10-20 meV [6]. We found that this small cutoff $\xi_{ph} < \omega_{ph}$, where $\omega_{ph} \approx 40$ meV is the energy of the phonons responsible for the pairing, changes the nature of the solutions of the Eliashberg equations in a very essential way. The well-known relationship $Z = 1 + \lambda$ (for the renormalization at the FS) and $h/2\pi\tau = 2\pi\lambda k_B T$ (the Hopfield relation between the electron-phonon scattering rate τ^{-1} and the McMillan constant λ) no longer hold, even approximately; thus a very large λ ($\approx$10) gives rise to a value of Z of about 2-3, and a very small τ^{-1}. We found that we can account for the high value of T_c, the insensitivity to the very strong Coulomb interaction, the suppression of the isotope effect, the large value of $2\Delta(0)/T_c$, the zero-bias-anomaly, and several other features of the superconductivity of the cuprates, as well as some other exotic superconduc-

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tors, such as the organics. We developed a computer program that solves the generalized Eliashberg equations, incorporating the strong $\boldsymbol{k}$-dependence. The present calculation is a continuation of this work.

2. Description of the model

In our calculations, we consider a simple model of the Fermi surface (FS). It is divided into 3 pieces, in which FS piece number 2 has a different coupling from pieces 1 and 3. This choice is made to remind of the FS of BiSCO, so that number 2 corresponds to the rounded corners while 1 and 3 correspond to the planar sections [11]. The tetragonal crystal symmetry is such that pieces 1 and 3 are equivalent. We restrict ourselves to a 2-dimensional momentum space, thus the momentum can be defined as $\boldsymbol{k} \equiv (k_\perp, k_\parallel)$ where $k_\perp$ is the component perpendicular to the FS and $k_\parallel$ the parallel one.

The gap equation that we solve self-consistently can be written as [12] (in the Matsubara representation where $\omega_n = (2n+1)\pi T$)

$$\Phi(\boldsymbol{k}, i\omega_n) = -T\sum_{n'}\int\int d^2\boldsymbol{k}' G(\boldsymbol{k}', i\omega_{n'}) \times [D(\boldsymbol{k}, \boldsymbol{k}', i\omega_n - i\omega_{n'}) - \mu(\boldsymbol{k}, \boldsymbol{k}')]\ \Phi(\boldsymbol{k}', i\omega_{n'}) \quad (1)$$

where G is the renormalized electronic Green function, D is the phononic one and μ represents the Coulomb potential. We consider an electron-phonon interaction that is cut off in $k_\perp$, i.e. the coupling falls to zero for $|\xi(k_\perp) - \xi(k'_\perp)| > \xi_{ph}$ [13]. This cutoff ξ_{ph} is small except for the FS piece corresponding to the corner. Indeed, since the density of states is larger there (we are near a Van Hove singularity), the elastic scattering rate τ_{el}^{-1} being therefore larger too, and since the cutoff ξ_{ph} must be greater than τ_{el}^{-1}, ξ_{ph} cannot be so small [9]. Another essential feature of our coupling is that it decreases rapidly with $k_\parallel - k'_\parallel$, i.e. the coupling is very weak between two different FS pieces. This follows from the small value of κ_{TF}. Morover, in order to simplify the calculations, we choose the phonon spectrum as an Einstein spectrum of frequency ω_{ph}. The Coulomb repulsion is chosen to have a similar behavior with a cutoff ξ_c and being peaked in $k_\parallel$ (but not so sharply as the electron-phonon interaction).

Since eq.(1) has to be solved self-consistently, we have to choose the initial values for $\Phi(\boldsymbol{k}, i\omega_n)$. We will show that 2 different initial conditions lead to 2 different solutions of the Eliashberg equations even with exactly the same coupling parameters. As we said above, we take 3 FS pieces that are labelled with the discretized $k_\parallel$ coordinate: $q = 1, 3$ for the two planar sections and $q = 2$ for the corner. The s-wave like initial condition is simply

$$\Phi_0^{(s)}(\boldsymbol{k}, i\omega_n) = 1 \qquad \forall \boldsymbol{k}, n \quad (2)$$

wheras the d-wave like one is

$$\Phi_0^{(d)}(\boldsymbol{k}, i\omega_n) = \begin{cases} -1 & \text{if } q = 1 \\ 0 & \text{if } q = 2 \\ 1 & \text{if } q = 3 \end{cases} \qquad \forall k_\perp, n \quad (3)$$

3. Results

The corresponding solutions of the Eliashberg equations are shown in Fig.1. We immediately see that the initial symmetry is preserved. Since we take only a few FS pieces in account, it is more convenient to use a matrix notation to denote the (q, q') dependence of the parameters. The $(k_\perp, k_\perp')$ part is defined through the cutoff matrices ξ_{ph} and ξ_c. The strength of electron-phonon interaction is given by the matrix of McMillan [14] constants λ_{ph} and the coulomb repulsion is defined by μ. The parameters we used for these calculations are:

$$\lambda_{ph} = \begin{bmatrix} 5 & 0.25 & 0.05 \\ 0.25 & 1 & 0.25 \\ 0.05 & 0.25 & 5 \end{bmatrix}, \quad \xi_{ph} = \begin{bmatrix} 0.4 & 2 & 4 \\ 2 & 2 & 2 \\ 4 & 2 & 0.4 \end{bmatrix}$$
$$\mu = \begin{bmatrix} 3 & 0.75 & 0.25 \\ 0.75 & 3 & 0.75 \\ 0.25 & 0.75 & 3 \end{bmatrix}, \quad \xi_c = \begin{bmatrix} 2 & \infty & \infty \\ \infty & 2 & \infty \\ \infty & \infty & 2 \end{bmatrix} \quad (4)$$

Fig.2 shows the density of states (DOS) of the quasiparticles in the two cases considered. We can see that both of these DOS roughly reproduce the measured DOS with ARPES [15] or STM [16]. Indeed the difference between the d-wave and the s-wave DOS is very small and they could equally well explain experimental data.

We considered a situation where the non-diagonal coupling was very small. Following the discussion of Combescot [3], one can think that this is due to the weakness of the coupling. Indeed, we found that the solution possesses s-wave symmetry as soon as the non-diagonal coupling is strong enough. This occurs approximately when the non-diagonal terms of the electron-phonon coupling λ_{ph} become equal to the corresponding terms in the coulomb repulsion μ, and this is completely independent of the choice of the initial condition $\Phi_0^{(s)}$ or $\Phi_0^{(d)}$.

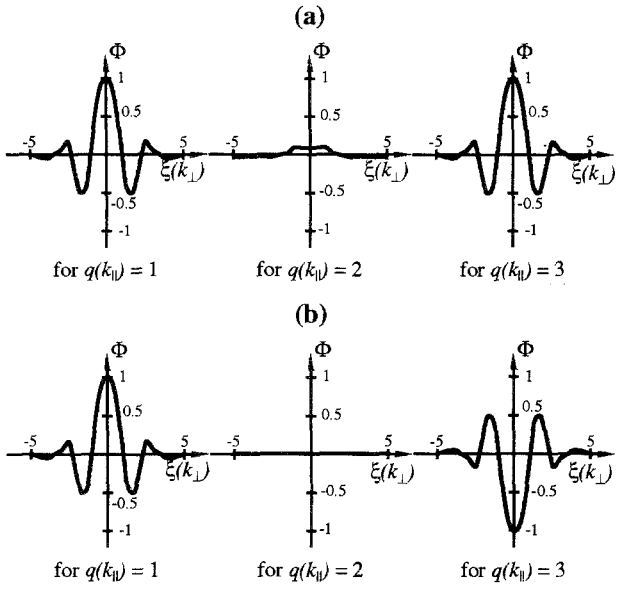

Fig. 1. Gap parameter $\Phi(\boldsymbol{k}, i\omega_n)$ for $n = 0$ as function of $\xi(k_\perp)$ and $q(k_\parallel)$ for **(a)** s-wave case and **(b)** d-wave case. The temperature is $T = 0.016$ (all energies are in units of ω_{ph}).

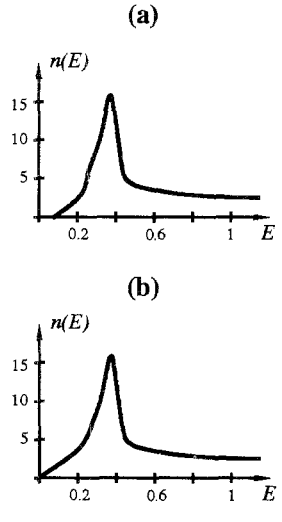

Fig. 2. DOS $n(E)$ of the quasiparticles (approximated as in [9]) as function of their energy E in the case of **(a)** s-wave and **(b)** d-wave (all energies are in units of ω_{ph}).

The solution with the lowest free energy will be the stable one, and it is likely that this is also the one with the highest T_c. This is because high T_c is correlated with a large gap, which in turn lowers the energy more than a small gap. We calculated T_c and found the same temperature of $T_c \approx 0.135\ \omega_{ph}$ in both cases. There seems then at first sight to be a degeneracy in the two symmetries. This is not surprising as long as the coupling is very weak between different FS pieces. In this case the gap equation is in practice decoupled between the different FS pieces and the sign of the gap of one FS with large local coupling can take any value independent of the phase of the gap at neighboring FS pieces.

4. Discussion

We find solutions of the Eliashberg equations with s- and d-wave symmetry are nearly degenerate. This result can also be understood qualitatively within the framework of the weak-coupling limit, where the gap equation is given by [10]:

$$\Delta(k_\parallel) = \frac{1}{\int dk_\perp dk_\parallel} \int \frac{dk'_\parallel}{v(k'_\parallel)} \Delta(k'_\parallel) \ln\left(\frac{2\omega_{ph}}{\Delta(k'_\parallel)}\right) \times [V(k_\parallel - k'_\parallel) - \mu^*(k_\parallel - k'_\parallel)] \quad (5)$$

We consider now an isotropic Coulomb interaction μ^*, an isotropic Fermi velocity $v(k'_\parallel)$, and an anisotropic phonon-mediated interaction $V(k_\parallel - k'_\parallel)$ that vanishes for a scattering angle $(k_\parallel - k'_\parallel)/k_F$ larger than $\Delta\theta$. There is a solution with s-wave symmetry, with: $\Delta_s = 2\omega_{ph} e^{-1/(\lambda - \mu^*)}$, where $\lambda = n(E_F) V_0$, $V_0 = \int V(k_\parallel - k'_\parallel)\, dk_\parallel dk'_\parallel / \int dk_\parallel dk'_\parallel$. There is also a solution with d-wave symmetry, with nodes at $\theta = k_\parallel/k_F = \pm\pi/4, \pm 3\pi/4$. If $\Delta\theta < \pi/4$, then at $\theta = 0$, $\Delta_d = 2\omega_{ph} e^{-1/\lambda}$. We illustrate Δ_s and Δ_d as function of θ in Fig.3a. We plot Δ_s, Δ_d as function of $\Delta\theta$ in Fig.3b, for the "normal" case in which $\mu^* < \lambda$, but μ^* not very small, and for the case in which μ^* is very small. We see that when $\Delta\theta < \pi/4$, and also $\mu^* \ll 1$, the solutions with s- and d-wave symmetry are nearly degenerate.

In our case, $\Delta\theta \approx (\kappa_{TF}/k_F)^2 \approx 0.1$, therefore the condition that there is virtually no scattering for $\theta > \pi/4$ is well satisfied. For a "normal" metal, where $\kappa_{TF} > k_F$, this is not the case. As for μ^*, we estimate for the cuprates that $\mu^* \approx 0.3 - 0.4$, since the bare μ is very large, and $\ln(E_F/\omega_{ph})$ is not very large because of the large value of ω_{ph}. Thus the condition $\mu^* \ll 1$ is not satisfied. However, we saw [9] that because of the small cutoff ξ_{ph}, μ^* has to be replaced by μ^{**} given by: $\mu^{**} = \mu/\{1 + \mu \ln[(E_F/\omega_{ph})(E_F/\xi_{ph})]\}$, and μ^{**} is very small (≈ 0.1). Thus the two conditions for the near-degeneracy are indeed satisfied. This is not the case in the theory of Monthoux et al [1], where the d-wave solution is due to the very large value of μ (1, 3), and no solution with s-wave symmetry is present.

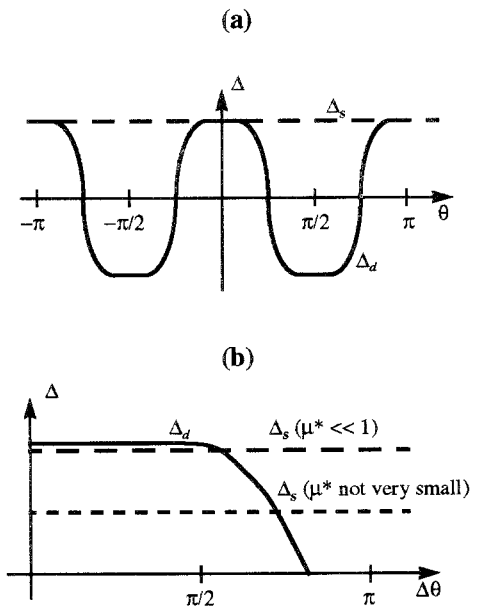

Fig. 3. General shape of the gap parameters Δ_s (dashed line) and Δ_d (plain line) as function of **(a)** the angle θ, and **(b)** Δθ determining the angular range of the interaction.

5. Conclusion

The conventional belief that the phonon-mediated (BCS) mechanism gives rise to solutions with *s*-wave symmetry, depends on a nearly-isotropic electron-ion potential. This is the case in "normal" metals, where the screening parameter κ_{TF} is large. In the cuprates, and some other "exotic" superconductors, κ_{TF} is very small because of the large static polarizability of the oxygen background, and therefore the potential is extremely anisotropic, giving rise to predominantly forward scattering. We found that this causes solutions of the Eliashberg equations with *s*- and *d*-wave symmetry to be nearly-degenerate, so that a small change in parameters (such as the elastic scattering rate due to defects) can cause a cross-over between the two symmetries without a large change in T_c. This seems to be in accord with experiment.

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