Mixed $(s+id)$-wave order parameters in the Van Hove scenario

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In the Van Hove scenario including orthorhombic distortion effect, we develop a pair of coupled gap equations for the mixed $(s+id)$-wave order parameter. It is found that a mixed $s+id$ symmetry state is realized in a certain range of relative strength of the s and d interactions, and there are two second-order transitions between the mixed and the pure symmetry states. Particular attention is paid to the temperature dependence of two components in the mixed order parameter as well as their evolution from a pure s to a pure d symmetry state. [S0163-1829(97)02305-9]

The question of the order parameter symmetry in high-temperature superconductors is presently the subject of a vivid debate.[1] It is widely accepted that the superconducting gap is highly anisotropic, but there is much controversy about whether the order parameter has an extended s-wave symmetry, or a pure d-wave one, or a mixed $(s+e^{i\theta}d)$-wave one (θ being the relative phase of s- and d-wave components). Recent experiments seem to increasingly favor the order parameter having dominantly $d_{x^2-y^2}$-wave symmetry and mixing with the s-wave component near the surface of a superconductor. Experiments that directly probe the pairing symmetry using tricrystal junctions by Tsuei *et al.*[2] and corner junction by Wollman *et al.*[3] provide strong evidence supporting a d-wave pairing state. In addition, very recent angle-resolved photoemission spectroscopy study also suggests a d-wave state.[4] However, there exist some experimental results, such as the measurements of Josephson supercurrent for tunneling between Pb and $YBa_2Cu_3O_7$ (YBCO) (Ref. 5) and critical current of YBCO-YBCO grain boundary junctions in the a-b plane,[6] which are difficult to be understood in the context of a pure d-wave symmetry. Similarly, some photoemission studies on $Bi_2Sr_2CaCu_2O_{8+x}$ (Ref. 7) are inconsistent with the pure d wave but more consistent with a mixed state of s- and d-wave components.

The concept of mixed $s+d$ and $s+id$ symmetries of the superconducting gap was first discussed by Ruckenstein *et al.*[8] and Kotliar.[9] This idea has been used to interpret the NMR and NQR data in the superconducting state of YBCO,[10] as well as the Josephson critical current observed in YBCO SNS junctions and YBCO/Pb junctions.[11] Recently, a two-dimensional tight-binding model, together with the electron spin susceptibility model of Mills, Monier, and Pines (MMP),[12] has been used to study the effects of filling, band structure, and pair potential on the symmetry of the gap with particular emphasis on possible mixed configurations.[13] On the other hand, a two-dimensional Fermi liquid model with free-particle dispersion relation and with attractive interaction in both s and d channels has been used to examine the possibility of a superconducting state with mixed s and d symmetry of the order parameter.[14,15] It was shown that both in the weak-coupling limit and at strong coupling, a mixed $s+id$ symmetry state can be realized in a certain range of interaction, but there is no stable mixed $s+d$ symmetry state in tetragonal systems. In the presence of orthorhombic distortion, however, the $(s\pm d)$ mixed state may occur.[13] A study of the Ginzberg-Landau equations for a d-wave superconductor with inhomogeneity indicates that the s-wave component is always induced near the inhomogeneous regions.[16]

An important feature of high-T_c oxide superconductors found by experiments is that there exist flat bands near the Fermi level E_F. High-resolution angle-resolved photoemission spectroscopy experiments[17,18] suggest that an extended region of flat CuO_2 derived bands close to E_F exists for YBCO as well as other high-T_c cuprates with optimal doping, providing a strong support for the idea of Van Hove scenario.[19] The flat regions of the energy dispersion is associated with the logarithmic singularity in the density of states (DOS), known as the Van Hove singularity (VHS), which comes from two-dimensional (2D) nature of electronic dynamics. An analytical formula for the density of state (DOS) having VHS was exactly derived from a tight-binding model on a 2D rectangular lattice,[20] where the orthorhombic distortion, second-nearest-neighbor, and interlayer hopping have been taken into account. Previous works on the Van Hove scenario are based on an assumption of the conventional s-wave symmetry. They have accounted for many anomalous superconducting and normal-state properties of the high-T_c cuprate superconductors, including the high-T_c and reduced isotope effect,[19,20] the linearly temperature-dependent resistivity,[21] the specific heat jump at T_c,[22] and the uniaxial stress effect on T_c.[23] Recently, the VHS theory has been extended to the pure d-wave pairing,[24–26] indicating that the d-wave version of the Van Hove scenario is fully viable.

In this work we apply the Van Hove scenario to the superconducting state with a mixed s and d symmetry. The 2D tight-binding model is considered as our starting point since it can well describe VHS in the DOS. Based on the same model, we consider the two-body interaction to contain an on-site repulsion and a nearest-neighbor attraction, which may provide two attractive interaction channels for s- and d-wave pairing. The antiferromagnetic superexchange is the most plausible candidate of the nearest-neighbor attractive interaction. However, a phonon-mediated attraction can also contribute to the high-T_c superconductivity in a dominant d-wave superconductor. For example, two holes on adjacent copper sites may experience an attractive interaction due to motion of the intervening oxygen atom.[27] A competition of the s and d interaction channels can give rise to either of the pure s- and d-wave pairing, or the mixed $(s+id)$-wave pairing. The present discussion will be restricted to the $(s+id)$-wave symmetry, i.e., the relative angle between the s- and d-wave components is taken to be $\pi/2$. Such a state has been shown to be a stable solution of the gap equation at least in the tetragonal case.[14,15] Using a pair of coupled equations for s- and d-wave components of order parameter, we calculate the phase diagram of consisting of three regions corresponding to the pure s- and d-wave pairing as well as the mixed $(s+id)$-wave pairing. It is found that both s- and d-wave states can coexist only in a small range of relative strength of the two attractive interactions. Particular attention will be paid to the temperature dependence of the s- and d-wave components of the order parameters in a $(s+id)$-wave state.

We start from a tight-binding model on a 2D rectangular lattice with nearest- and second-nearest-neighbor hopping integrals. The quasiparticle energy is given by

$$E_{\mathbf{k}}=-2t[\cos k_x+\gamma_1\cos k_y-\gamma_2\cos k_x\cos k_y]. \tag{1}$$

Here t and $t\gamma_1$ are the nearest-neighbor hopping integrals along the a and b axes, respectively, and $t\gamma_2/2$ is the second-nearest-neighbor hopping integral. It has been shown[20] that such a tight-binding model yields the VHS in DOS. In the presence of orthorhombic distortion ($\gamma_1<1$), there are two singular peaks in the DOS at the energies $E_+=2t(1-\gamma_1-\gamma_2)$ and $E_-=-2t(1-\gamma_1+\gamma_2)$, the distance between them being equal to $E_+-E_-\ =4t(1-\gamma_1)$. For a square lattice ($\gamma_1=1$) the two singular peaks in the DOS merge into one at $E_s=-2t\gamma_2$. With the aid of the same model we consider the two-body interaction which governs the spatial variation of the order parameters. Supposing an on-site repulsion v_0 and an attraction v_1 between the nearest-neighbor sites, the two-body interaction is given by

$$v(\mathbf{k}-\mathbf{k}')=-v_0+v_1[\cos(k_x-k_x')+\beta^2\cos(k_y-k_y')]. \tag{2}$$

Here $\beta=1$ for a square lattice and its deviation from 1 stands for an orthorhombic distortion. If one expands the interaction $v(\mathbf{k}-\mathbf{k}')$, one finds it to contain the s-wave, d-wave and p-wave channel interactions. The terms of the p-wave channel interaction, such as $\sin k_x\sin k_x'$ and $\sin k_y\sin k_y'$ can be neglected since they do not contribute to the spin-singlet pairing state. The dominant interaction causing the superconductivity is given by

$$v(\mathbf{k}-\mathbf{k}')=v_s+v_d(\cos k_x-\beta\cos k_y)(\cos k_x'-\beta\cos k_y'), \tag{3}$$

where $v_s=-v_0+(1+\beta)^2v_1/2$ and $v_d=v_1/2$ corresponds to the effective s- and d-wave channel interactions, respectively. In this model both v_s and v_d are positive only if $2v_0<(1+\beta)^2v_1$, which is a necessary condition of coexisting the s- and d-wave states.

The present calculations are confined to the weak-coupling limit in which the BCS theory is valid. It is straightforward to extend our calculations to the strong-coupling case in terms of the Eliashberg formalism. For the momentum-dependent interaction $v(\mathbf{k}-\mathbf{k}')$ the BCS gap equation has the following form:

$$\Delta(\mathbf{k})=\sum_{\mathbf{k}'}v(\mathbf{k}-\mathbf{k}')\frac{\Delta(\mathbf{k}')}{2W_{\mathbf{k}'}}\tanh\left(\frac{W_{\mathbf{k}'}}{2T}\right), \tag{4}$$

where $W_{\mathbf{k}}^2=\xi_{\mathbf{k}}^2+|\Delta(\mathbf{k})|^2$ with $\xi_{\mathbf{k}}\equiv E_{\mathbf{k}}-E_F$ as the quasiparticle energy measured from the Fermi level, and T is the temperature. In Eq. (4) both Δ and v have been regarded as a function of momentum $\mathbf{k}$, which allows for more general than in the conventional s-wave case. We now focus attention on the superconducting state with a mixed $s+id$ symmetry of the gap. Corresponding to the interaction (3), the $(s+id)$-wave order parameter is taken to be

$$\Delta(\mathbf{k})=\Delta_s+i\Delta_d(\cos k_x-\beta\cos k_y), \tag{5}$$

which is a sum over the s- and d-wave components with a relative phase of $\pi/2$ between them. Substituting Eqs. (3) and (5) into Eq. (4), and separating the real and imaginary parts of the equation, we obtain a pair of coupled equations

$$\Delta_s=v_s\int\frac{d^2\mathbf{k}}{(2\pi)^2}\frac{\Delta_s}{2W_{\mathbf{k}}}\tanh\left(\frac{W_{\mathbf{k}}}{2T}\right), \tag{6}$$

$$\Delta_d=v_d\int\frac{d^2\mathbf{k}}{(2\pi)^2}\frac{\Delta_d(\cos k_x-\beta\cos k_y)^2}{2W_{\mathbf{k}}}\tanh\left(\frac{W_{\mathbf{k}}}{2T}\right), \tag{7}$$

with

$$W_{\mathbf{k}}^2=\xi_{\mathbf{k}}^2+\Delta_s^2+\Delta_d^2(\cos k_x-\beta\cos k_y)^2, \tag{8}$$

from which Δ_s and Δ_d in a mixed $(s+id)$-wave state can be self-consistently solved. Obviously, when only one of the two interaction channels is present, i.e., either $\Delta_s=0$ or $\Delta_d=0$, the coupled gap equations above reduce to a single one for a pure symmetry order parameter. In Eqs. (6) and (7) we have assumed that the attractive interactions in both s and d channels are energy-independent in a energy range bounded by the cutoff energy k_BT_{c0}, and are zero for $|\xi_{\mathbf{k}}|>k_BT_{c0}$. To embody the cutoff of the energy, the following integral,

$$\int_{-k_BT_{c0}}^{k_BT_{c0}}\delta(\xi-\xi_{\mathbf{k}})d\xi, \tag{9}$$

needs to be added to the right-hand sides of Eqs. (6) and (7). Substitute Eq. (1) into Eqs. (6)–(8) and make a change of integral variables $u=\cos k_x$ and $v=\cos k_y$. The δ function in Eq. (9) can be used to integrate over u, and the remainder is a double integral over v and ξ, yielding

$$\Delta_s=v_s\Delta_s\int_{-k_BT_{c0}}^{k_BT_{c0}}d\xi\int_c^b dv\frac{N(\xi,v)}{2W(\xi,v)}\tanh\left(\frac{W(\xi,v)}{2T}\right), \tag{10}$$

$$\Delta_d=v_d\Delta_d\int_{-k_BT_{c0}}^{k_BT_{c0}}d\xi\int_c^b dv\frac{N(\xi,v)D(\xi,v)^2}{2W(\xi,v)}\tanh\left(\frac{W(\xi,v)}{2T}\right), \tag{11}$$

where

$$W(\xi,v)^2=\xi^2+\Delta_s^2+\Delta_d^2D(\xi,v)^2,$$

$$N(\xi,v)=\frac{N_0}{\sqrt{(a-v)(b-v)(v-c)(v-d)}},$$

$$D(\xi,v)=\frac{\epsilon+(\beta+\gamma_1)v-\beta\gamma_2v^2}{1-\gamma_2v},$$

with $N_0=1/(2t\pi^2\sqrt{\gamma_1^2-\gamma_2^2})$ and $\epsilon=(\xi+E_F)/(2t)$. Here $a,b,c,$ and d are functions of ϵ, having different function forms in different ϵ regions. They are

$$a=(1-\epsilon)/(\gamma_1+\gamma_2),\quad b=1,\quad c=-(1+\epsilon)/(\gamma_1-\gamma_2),\quad d=-1\quad \text{for}\ -1+\gamma_1-\gamma_2\geqslant\epsilon\geqslant-1-\gamma_1+\gamma_2,$$

$$a=(1-\epsilon)/(\gamma_1+\gamma_2),\quad b=1,\quad c=-1,\quad d=-(1+\epsilon)/(\gamma_1-\gamma_2)\quad \text{for}\ 1-\gamma_1-\gamma_2>\epsilon>-1+\gamma_1-\gamma_2,$$

$$a=1,\quad b=(1-\epsilon)/(\gamma_1+\gamma_2),\quad c=-1,\quad d=-(1+\epsilon)/(\gamma_1-\gamma_2)\quad \text{for}\ 1+\gamma_1+\gamma_2\geqslant\epsilon\geqslant1-\gamma_1-\gamma_2.$$

We wish to point out that in gap equations (10) and (11) the VHS is embodied in the function $N(\xi,v)$. As $a=b$ at $\epsilon=1-\gamma_1-\gamma_2$ or $c=d$ at $\epsilon=-1+\gamma_1-\gamma_2$, the integral of $N(\xi,v)$ over v exhibits logarithmic singularity. To see clearer the physical meaning of $N(\xi,v)$, we examine the T_c formula. Taking $\Delta_s=\Delta_d=0$ at T_c in Eqs. (10) and (11), we obtain

$$\Delta_s=v_s\Delta_s\int_{-k_BT_{c0}}^{k_BT_{c0}}\frac{d\xi}{2\xi}\tanh\left(\frac{\xi}{2T}\right)N_s(\xi), \tag{12}$$

$$\Delta_d=v_d\Delta_d\int_{-k_BT_{c0}}^{k_BT_{c0}}\frac{d\xi}{2\xi}\tanh\left(\frac{\xi}{2T}\right)N_d(\xi), \tag{13}$$

with

$$N_s(\xi)=\int_c^b N(\xi,v)dv, \tag{14}$$

$$N_d(\xi)=\int_c^b N(\xi,v)D(\xi,v)^2dv. \tag{15}$$

Notice that $N_s(\xi)$ is the exact DOS of the tight-binding model under consideration. It can be expressed as a complete elliptic integral of the first kind and its explicit expression has been given in Ref. 20. $N_d(\xi)$ is not a real DOS, but can be regarded as an effective DOS in the T_c formula for the d-wave pairing. It cannot be expressed as a simple elliptic integral function, but its singular behavior is similar to that of $N_s(\xi)$. It has been found that the VHS peaks in $N_d(\xi)$ for d-wave pairing are much higher and narrower than those in the s-wave case. This behavior will be favorable for the high-T_c superconductivity if E_F is located right at or very close to the VHS.

Unlike the gap equations (10) and (11), Eqs. (12) and (13) are two independent T_c formulas. Only one of them determines T_c of the superconductor, depending on which has the higher transition temperature. The competition between the s and d interaction channels can lead to either one of the two pure symmetry superconducting states, or a mixed $(s+id)$-wave state. Our calculation shows that there exists a narrow range of interaction ratio, $r_{\min}<v_d/v_s<r_{\max}$, where the s- and d-wave states coexist. For $v_d/v_s<r_{\min}$, only s-wave superconductivity appears and its T_c is determined by Eq. (12). On the contrary, for $v_d/v_s>r_{\max}$, it is a pure d-wave superconductor whose T_c is determined by Eq. (13). It is interesting to point out that in the range of a mixed $(s+id)$-wave pairing the value of T_c is also determined by Eq. (13) if v_s is fixed and v_d is changed.

We now perform numerical calculations by choosing a set of parameters. For ease of comparison, the parameters used in the present calculation are taken to be the same as those in the pure s-wave case.[20] They are $t=0.46$ eV, $T_{c0}=400$ K, $\gamma_2=0.35$, and $v_sN_0=0.056$. We first consider a square lattice of $\gamma_1=1$ and $\beta=1$, in which there is only one VHS peak in the DOS centered at $\epsilon=-\gamma_2$, and assume the Fermi level to be located right at the VHS. Figure 1 shows the phase diagram of the superconductor at zero temperature. What is plotted is the zero-temperature order parameters as a function of the interaction ratio v_d/v_s with fixed v_s. The dotted line indicates Δ_s of the solution of the gap equations (10) and (11) at zero temperature, while the solid line stands for Δ_d. We see that the s-wave solution exists at $0<v_d/v_s<0.39$ and the d-wave solution exists at

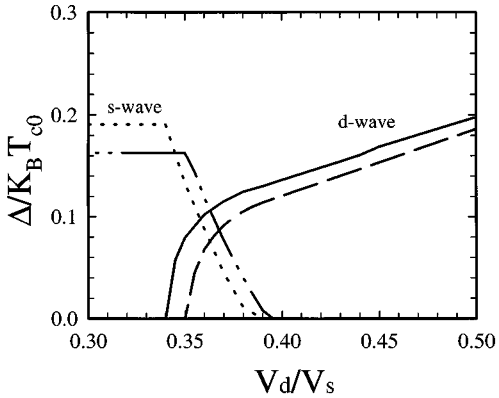

FIG. 1. Phase diagram of the superconductor at zero temperature with v_s fixed. Δ_s (dotted line) and Δ_d (solid line) as functions of v_d/v_s for $\beta=\gamma_1=1$, and Δ_s (dot-dashed line) and Δ_d (long-dashed line) for $\beta=\gamma_1=0.99$.

$v_d/v_s>0.34$. As a result, the phase diagram is divided into three parts: the pure s-wave region for $v_d/v_s<0.34$, the pure d-wave region for $v_d/v_s>0.39$, and the mixed $(s+id)$-wave region for $0.34<v_d/v_s<0.38$. Next, we discuss the effect of orthorhombic distortion.[28] By taking $\gamma_1=0.99$ and $\beta=0.99$, and keeping other parameters unchanged, we obtain Δ_s and Δ_d as functions of v_d/v_s, respectively, as shown by dot-dashed and long-dashed lines of Fig. 1. Their behavior is qualitatively similar to that in a tetragonal structure, having only a quantitative difference. In the presence of orthorhombic distortion, the mixed $(s+id)$-wave region shifts toward right, but its width between r_{max} and r_{min} appears to be almost unchanged.

We now focus attention on the intermediate region where Δ_s and Δ_d coexist and study their temperature dependence. Figure 2 shows the calculated results of Δ_s and Δ_d as a function of temperature for several values of v_d/v_s between $r_{min}=0.34$ and $r_{max}=0.39$. At $v_d/v_s=0.38$ just below r_{max}, the mixed $(s+id)$-wave state has a dominant d-wave component and a small s-wave component, as shown in Fig. 2(a). At zero temperature the d wave coexists with the s wave, but $\Delta_d(0)$ is much greater than $\Delta_s(0)$. At low temperatures Δ_s decreases rapidly with temperature while Δ_d changes smoothly. When the temperature comes up to a certain value T^* ($T^*\ll T_c$), Δ_s first vanishes. After then, only the d wave appears and Δ_d decreases gradually with temperature until T_c. This basic feature of the variation in Δ_s and Δ_d remains almost unchanged in the whole range of the mixed $(s+id)$-wave state. The major change is that with decreasing v^d/v^s, the s-wave component grows up gradually while the d-wave component reduces, and T^* moves towards right and gradually close to T_c. It is worth mentioning that, for smaller v_d/v_s, Δ_s is greater than Δ_d in most range of temperatures, but still first goes to zero at T^* which is always lower than T_c, as shown in Fig. 2(c) . This indicates that, for a fixed v_s, the T_c formula (13) is suitable not only to the pure d-wave superconductors, but also to the superconducting state with mixed $(s+id)$-wave symmetry.

For the $(s+id)$-wave state, the maximum value of the gap at zero temperature is given by $\Delta_{max}(T=0)=[\Delta_s^2(T=0)+4\Delta_d^2(T=0)]^{1/2}$. In Fig. 3, we show the ratio $R=2\Delta_{max}(T=0)/k_BT_c$ as a function of v_d/v_s, together with T_c vs v_d/v_s curve. In the pure s-wave case the present calculated value $2\Delta_s(T=0)/k_BT_c=3.72$ is slightly greater than the standard BCS value 3.52, which arises from the VHS

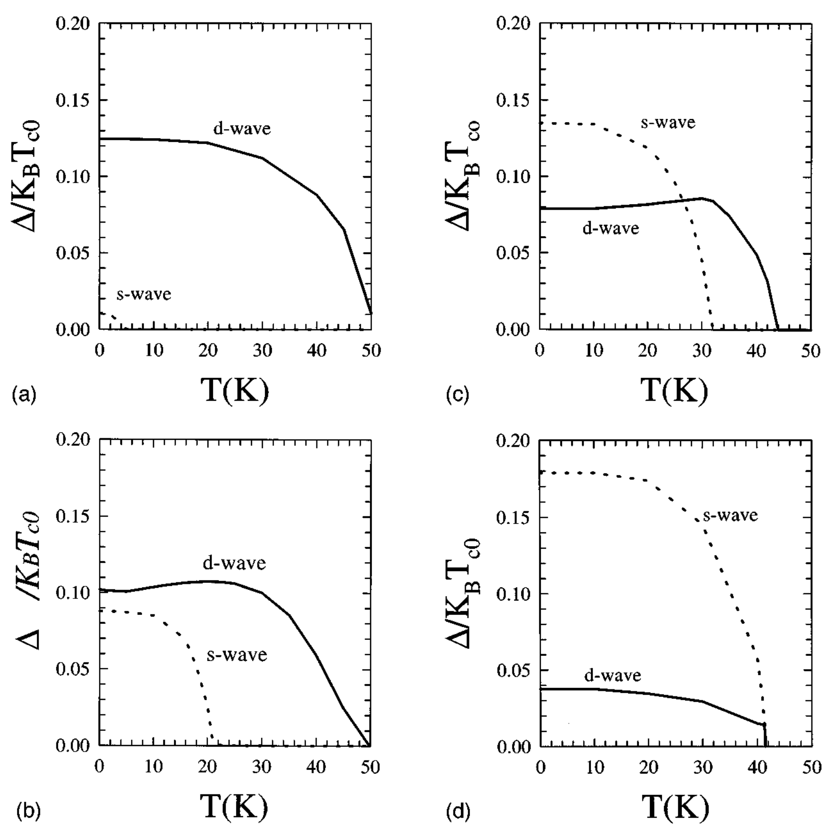

FIG. 2. Δ_s (dashed line) and Δ_d (solid line) plotted vs temperature for several values of v_d/v_s: (a) 0.38, (b) 0.36, (c) 0.35, and (d) 0.342.

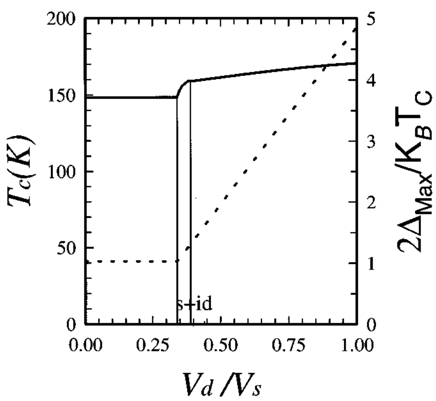

FIG. 3. $R=2\Delta_{\max}(T=0)/k_BT_c$ (solid line) and T_c plotted vs v_d/v_s with v_s fixed.

effect. For the d-wave pairing $2\Delta_d(T=0)/\ k_BT_c$ is found to be weakly v_d/v_s dependent, increasing slowly with v_d/v_s. Its values between 4.0 and 4.26 are greater than that in the s-wave case. In the intermediate region with mixed $s+id$ symmetry there is a continuous change in R from the pure d state to the pure s state. From Figs. 1 and 3, one sees that the order parameter changes continuously either at $r_{\min}$ or $r_{\max}$, while the change in its derivative is uncontinuous. It then follows that the two phase transitions between the mixed and the pure symmetry states are second order. The transition at $r_{\min}$ from s to $s+id$ is one from isotropic symmetry to anisotropic symmetry, while the transition at $r_{\max}$ from d to $s+id$ is one from a state with zero gap nodes to a nodeless state.

In summary, we have studied the coexistence of s- and d-wave states and the temperature dependence of the $s+id$-wave order parameters in the Van Hove scenario including the orthorhombic distortion effect. A competition between s- and d-wave pairing is found to depend strongly on the relative strength of interactions in the two channels.

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