Enhancement of broken-time-reversal-symmetry pairing state in d-wave superconductors with nonmagnetic impurities

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The phase diagrams of a superconductor with dominant d-wave and minor s-wave pairing interactions are obtained with the self-consistent gap equations. A possible broken-time-reversal-symmetry $s+id$ state in an appropriate interaction/temperature range is shown. We point out that a minor s-wave pairing interaction normally cannot compete with the dominant d-wave pairing so that the bulk state usually has a pure d-wave symmetry. Moreover, we show that the possibility to observe the $s+id$ state in a bulk system can be enhanced greatly if nonmagnetic impurity scatterings are introduced. Also interestingly, the amplitude of d-wave order parameter in the $s+id$ phase is shown to decrease with lowering temperature. [S0163-1829(98)00321-X]

An important issue regarding high-temperature superconductivity has been the symmetry of pairing state. Although it has been widely accepted that the pairing state of cuprates has a dominant d-wave symmetry,[1] an admixture of s-wave component to the order parameter (OP) is still a hot topic theoretically and experimentally. More recently, by measuring the tunneling current through copper/insulator/(110) Y-Ba-C-O in-plane junction, Covington *et al.*[2] observed that the zero-bias conductance peak splits at a very low temperature even in the absence of a magnetic field. Such an unexpected behavior indicated the broken-time-reversal symmetry (BTRS) of the pairing state. Several previous works predicted[3,4] that a subdominant OP, which has a relative phase $\pi/2$ with respect to the dominant d-wave OP, could appear near the surface. To fit the experimental data,[2] an s-wave subdominant pairing interaction is estimated[5] to have such a value which gives the superconducting transition temperature of the subdominant OP about 15% of that of the dominant d-wave OP. This s-wave pairing interaction normally cannot compete with the d-wave pairing in the bulk so that the bulk state usually has a pure d-wave symmetry. Here we study the possibility of a bulk BTRS state in a superconductor with attractive interactions from both s and d channels. It is found that the possibility to observe a bulk BTRS state could be greatly enhanced by introducing nonmagnetic impurity scatterings to the system. Also interestingly, we find that as the temperature is lowered below the second phase-transition temperature at which the $s+id$ state occurs, the amplitude of the d-wave component begins to decrease.

For simplicity, we assume the zero-range interaction between an electron and a nonmagnetic impurity at position $\mathbf{R}_i$, and the scattering potential experienced by the electron at $\mathbf{r}$ is

$$U(\mathbf{r})=u_0\sum_{i\in I}\delta(\mathbf{r}-\mathbf{R}_i), \tag{1}$$

where u_0 is the scattering strength and I denotes the set of impurity sites. The system of Gorkov's equations are written as

$$\left[i\omega_n+\frac{\nabla^2}{2m}+\mu-U(\mathbf{r})\right]\mathcal{G}(\mathbf{r},\mathbf{r}';\omega_n)+\int d\mathbf{r}''\Delta(\mathbf{r},\mathbf{r}'')\mathcal{F}^\dagger(\mathbf{r}'',\mathbf{r}';\omega_n)=\delta(\mathbf{r}-\mathbf{r}'), \tag{2}$$

$$\left[-i\omega_n+\frac{\nabla^2}{2m}+\mu-U(\mathbf{r})\right]\mathcal{F}^\dagger(\mathbf{r},\mathbf{r}';\omega_n)+\int d\mathbf{r}''\Delta^*(\mathbf{r},\mathbf{r}'')\mathcal{G}(\mathbf{r}'',\mathbf{r}';\omega_n)=0. \tag{3}$$

Here $\omega_n=(2n+1)\pi T$ with n any integer is the Matsubara frequency (Hereafter the convention $\hbar=k_B=c=1$ is made), μ is the chemical potential, $\mathcal{G}$ and $\mathcal{F}^\dagger$ are the normal and anomalous Green's functions. The pair potential is given by

$$\Delta^*(\mathbf{r},\mathbf{r}')=V(\mathbf{r}-\mathbf{r}')T\sum_{\omega_n}\mathcal{F}^\dagger(\mathbf{r},\mathbf{r}';\omega_n). \tag{4}$$

Note that $V(\mathbf{r}-\mathbf{r}')$ is positive and the pairing interaction is $-V(\mathbf{r}-\mathbf{r}')$. By making use of the standard impurity averaging technique, the system of equations in the momentum space can be obtained[6]

$$[i\omega_n-\xi_\mathbf{p}-\overline{\mathcal{G}}_{\omega_n}]\mathcal{G}_{\omega_n}(\mathbf{p})+[\Delta(\mathbf{p})+\overline{\mathcal{F}}_{\omega_n}]\mathcal{F}^\dagger_{\omega_n}(\mathbf{p})=1, \tag{5}$$

$$[i\omega_n+\xi_\mathbf{p}+\overline{\mathcal{G}}_{-\omega_n}]\mathcal{F}^\dagger_{\omega_n}(\mathbf{p})+[\Delta^*(\mathbf{p})+\overline{\mathcal{F}}^\dagger_{\omega_n}]\mathcal{G}_{\omega_n}(\mathbf{p})=0, \tag{6}$$

where $\xi_\mathbf{p}=\mathbf{p}^2/2m-\mu$ and

$$\overline{\mathcal{G}}_{\omega_n}=\frac{n_iu_0^2}{(2\pi)^2}\int\mathcal{G}_{\omega_n}(\mathbf{p}')d\mathbf{p}', \tag{7}$$

$$\overline{\mathcal{F}}^\dagger_{\omega_n}=\frac{n_iu_0^2}{(2\pi)^2}\int\mathcal{F}^\dagger_{\omega_n}(\mathbf{p}')d\mathbf{p}', \tag{8}$$

with n_i as the density of nonmagnetic impurities. A little algebra yields

$$\mathcal{G}_{\omega_n}(\mathbf{p})=-\frac{i\omega_n-\overline{\mathcal{G}}_{\omega_n}+\xi_{\mathbf{p}}}{-(i\omega_n-\overline{\mathcal{G}}_{\omega_n})^2+\xi_{\mathbf{p}}^2+|\Delta^*(\mathbf{p})+\overline{\mathcal{F}}^{\dagger}_{\omega_n}|^2}, \quad (9)$$

$$\mathcal{F}^{\dagger}_{\omega_n}(\mathbf{p})=\frac{\Delta^*+\overline{\mathcal{F}}^{\dagger}_{\omega_n}}{-(i\omega_n-\overline{\mathcal{G}}_{\omega_n})^2+\xi_{\mathbf{p}}^2+|\Delta^*(\mathbf{p})+\overline{\mathcal{F}}^{\dagger}_{\omega_n}|^2}, \quad (10)$$

where we have used $\overline{\mathcal{F}}^{\dagger}_{\omega_n}=(\overline{\mathcal{F}}_{\omega_n})^*$. Substituting them into Eqs. (7) and (8), and incorporating an additive term in $\overline{\mathcal{G}}_{\omega_n}$ into the chemical potential, we have

$$\overline{\mathcal{G}}_{\omega_n}=\frac{n_i u_0^2}{(2\pi)^2}\int\frac{-(i\omega_n-\overline{\mathcal{G}}_{\omega_n})}{-(i\omega_n-\overline{\mathcal{G}}_{\omega_n})^2+\xi_{\mathbf{p}'}^2+|\Delta^*(\mathbf{p}')+\overline{\mathcal{F}}^{\dagger}_{\omega_n}|^2}d\mathbf{p}', \quad (11)$$

$$\overline{\mathcal{F}}^{\dagger}_{\omega_n}=\frac{n_i u_0^2}{(2\pi)^2}\int\frac{\Delta^*(\mathbf{p}')+\overline{\mathcal{F}}^{\dagger}_{\omega_n}}{-(i\omega_n-\overline{\mathcal{G}}_{\omega_n})^2+\xi_{\mathbf{p}'}^2+|\Delta^*(\mathbf{p}')+\overline{\mathcal{F}}^{\dagger}_{\omega_n}|^2}d\mathbf{p}'. \quad (12)$$

On the other hand, the pair potential in the momentum space is given by

$$\Delta^*(\mathbf{k})=T\sum_{\omega_n}\int\frac{d\mathbf{p}}{(2\pi)^2}V(\mathbf{k}-\mathbf{p})\mathcal{F}^{\dagger}_{\omega_n}(\mathbf{p}). \quad (13)$$

In the weak-coupling limit, the effective attractive electron-electron interaction occurs in a small range near the Fermi surface. When the pairing interaction comes from both the s channel and d channel, it could have the following form:

$$V(\mathbf{k}-\mathbf{k}')=V_s+V_d\cos 2\phi\cos 2\phi', \quad (14)$$

where both V_s and V_d are positive, the angle $\phi=\tan^{-1}(k_y/k_x)$ with $k_{x,y}$ as two components of the Fermi wave vector. The general form of the pair potential can be written as

$$\Delta^*(\mathbf{k})=\Delta_s+e^{i\theta}\Delta_d\cos 2\phi, \quad (15)$$

where Δ_s and Δ_d are now real variables, θ is the relative phase angle between s-wave and d-wave components. In the clean limit, it has been shown based on the Ginzburg-Landau theory[7] and the self-consistent field approximation at zero temperature[8] that only $\theta=\pi/2$ is allowed. In the presence of nonmagnetic impurity scattering, we find that the relative phase angle $\theta=\pi/2$ is most suitable to give the relevant coupled equations for s-wave and d-wave components. With such an observation, we obtain the self-consistent equations for s-wave and d-wave components in the presence of nonmagnetic impurity scatterings

$$\Delta_s=2g_s\pi T\sum_{\omega_n}\int\frac{d\phi'}{2\pi}\frac{(1+\eta_{\omega_n})\Delta_s}{\sqrt{(\omega_n^2+\Delta_s^2)(1+\eta_{\omega_n})^2+(\Delta_d\cos 2\phi')^2}}, \quad (16)$$

$$\Delta_d=2g_d\pi T\sum_{\omega_n}\int\frac{d\phi'}{2\pi}\frac{\Delta_d\cos^2 2\phi'}{\sqrt{(\omega_n^2+\Delta_s^2)(1+\eta_{\omega_n})^2+(\Delta_d\cos 2\phi')^2}}, \quad (17)$$

$$\eta_{\omega_n}=\frac{1}{2\tau}\int\frac{d\phi'}{2\pi}\frac{1+\eta_{\omega_n}}{\sqrt{(\omega_n^2+\Delta_s^2)(1+\eta_{\omega_n})^2+(\Delta_d\cos 2\phi')^2}}, \quad (18)$$

where $g_{s,d}=N(0)V_{s,d}/2$ with $N(0)$ as the density of states per electron spin at the Fermi surface, $\tau^{-1}=2\pi n_i u_0^2 N(0)$ is the impurity scattering rate. Note that in the summation over the Matsubara frequency ω_n, the cutoff frequency ω_c should be introduced.

In the clean limit ($\tau^{-1}=0$), the zero-temperature energy gap and the critical temperature for pure s-wave and pure d-wave superconductors can be obtained analytically. We give them here for completeness: $\Delta_{s0}=2\omega_c e^{-1/2g_s}$, $T_{s0}=(2e^{\gamma}\omega_c/\pi)e^{-1/2g_s}$, and $\Delta_{d0}=4\omega_c e^{-1/g_d-1/2}$, $T_{d0}=(2e^{\gamma}\omega_c/\pi)e^{-1/g_d}$, where $\gamma\approx 0.577$ is Euler's constant. The ratios for pure s-wave and pure d-wave superconductors are $2\Delta_s/T_s=3.53$ and $2\Delta_d/T_d=4.28$, respectively. The larger value of the ratio for pure d-wave superconductor comes from the anisotropic pairing. For a superconductor with the mixed s- and d-wave symmetry, the $s+id$ state can never be achieved if the interaction from the s channel is larger than one half of that from the d channel (i.e., $T_{s0}>T_{d0}$). It can be seen clearly by the fact that Eqs. (16) and (17) (with $\eta_{\omega_n}=0$) can never give a solution with nonzero Δ_s and Δ_d when $g_s/g_d>1/2$. This means that in the region $g_s/g_d>1/2$, the only possible pairing state is of pure s-wave symmetry. When $g_s/g_d\leqslant 1/2$, the phase boundary between the pure d-wave state and the mixed $s+id$ state is determined by the following set of equations:

$$1=2g_s\pi T\sum_{\omega_n}\int\frac{d\phi'}{2\pi}\frac{1}{\sqrt{\omega_n^2+(\Delta_d\cos 2\phi')^2}}, \quad (19)$$

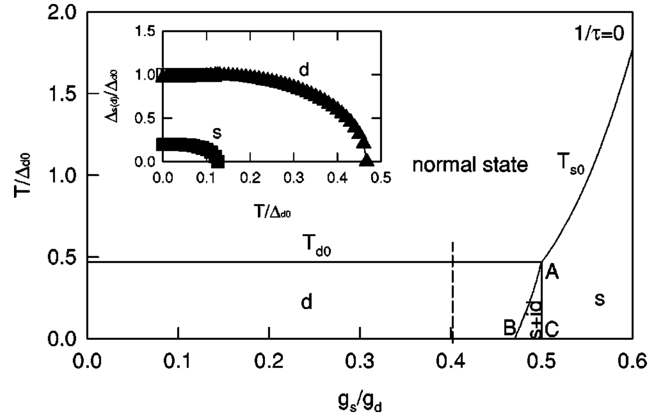

FIG. 1. Phase diagram for clean superconductors with mixed s-wave and d-wave symmetry. The values of g_s/g_d at points A, B, and C are, respectively, 0.5, 0.47, and 0.5. The inset shows the temperature dependence of the d-wave (filled triangle) and s-wave (filled square) components with $g_s/g_d = 0.48$. The pure d-wave OP with $g_s = 0$ (open square) is shown for comparison.

$$1 = 2g_d \pi T \sum_{\omega_n} \int \frac{d\phi'}{2\pi} \frac{\cos^2 2\phi'}{\sqrt{\omega_n^2 + (\Delta_d \cos 2\phi')^2}}. \qquad (20)$$

In general, the above set of equations could only be solved numerically. In Fig. 1, we plot the phase diagram in the T-g_s/g_d parameter space. Within the validity of the weak-coupling theory, $g_d = 1/8$ is chosen throughout the work. In this phase diagram, one can see that the mixed $s+id$ state appears between the pure d-wave and s-wave states. In the clean limit, the boundary delimiting the $s+id$ state and the pure s-wave state is a vertical line, which is located at $g_s/g_d = 1/2$. At zero temperature, the dividing line between the pure d-wave state and the mixed $s+id$ state can be found analytically, $g_s/g_d = 1/(2+g_d)$. To obtain a mixed $s+id$ pairing state, the lower bound of T_{s0}/T_{d0} is about 0.6 regardless of the pairing strength g_d. If we take $T_{d0} = 90$ K, $T_{s0} = 54$ K is required to observe the $s+id$ state in the bulk system which seems too large if the s-wave pairing originates from the electron-phonon interaction. As shown by a dashed line in Fig. 1, g_s/g_d is about 0.404 from the experimentally estimated value $T_{s0}/T_{d0} = 0.15$. In the inset of Fig. 1, the temperature dependence of the two components of the order parameter is plotted with $g_s/g_d = 0.48$. As the temperature is lowered below T_{d0}, the d-wave component appears and increases with lowered temperature. When the temperature is lowered further below the second transition temperature, the system enters into the $s+id$ pairing state. In this region, if we decrease the temperature, the s-wave component increases while the d-wave component decreases. For comparison, the temperature dependence of the pure d-wave OP below the second phase transition temperature is also shown in the figure (open square). The decreasing behavior of d-wave OP in the mixed region is caused by the competition between the s- and d-wave pairing symmetries. However, it is difficult to experimentally observe this behavior in a bulk clean system because a large g_s/g_d ratio is required.

We now turn to the effect of nonmagnetic impurity scattering. In the pure s-wave case, one can see from Eq. (16) (setting $\Delta_d = 0$) that the energy gap is still the same as the clean s-wave superconductor. In the pure d-wave superconductor, the energy gap [see Eq. (17) with $\Delta_s = 0$] is directly affected by the nonmagnetic impurity scattering. Physically, for the s-wave superconductor, $\overline{\mathcal{G}}_{\omega_n}$ is simply proportional to $i\omega_n$ and $\overline{\mathcal{F}}^{\dagger}_{\omega_n}$ is proportional to Δ_s, their proportionality constants are the same. Therefore, the effect of nonmagnetic impurity scatterings can be taken as a simple renormalization of the energy scale so that the thermodynamic properties are not influenced. However, for d-wave superconductor, $\overline{\mathcal{G}}_{\omega_n}$ is still proportional to $i\omega_n$ while $\overline{\mathcal{F}}^{\dagger}_{\omega_n}$ is zero so that simple scaling does not exist. This leads to the depairing effect on the d-wave superconductivity. The superconducting transition temperature T_d for a pure d-wave superconductor in the presence of nonmagnetic impurity scatterings is determined by the following equation:

$$\ln(T_{d0}/T_d) + \psi(1/2) - \psi(1/2 + 1/4\pi T_d \tau) = 0, \qquad (21)$$

where $\psi(x)$ is the digamma function. The phase boundary between $s+id$ and pure s-wave states are determined by

$$1 = 4g_s \pi T \sum_{\omega_n > 0} \frac{1}{\sqrt{\omega_n^2 + \Delta_s^2}}, \qquad (22)$$

$$1 = 2g_d \pi T \sum_{\omega_n > 0} \frac{1}{\sqrt{\omega_n^2 + \Delta_s^2} + 1/2\tau}. \qquad (23)$$

The above two coupled equations show that in the presence of nonmagnetic impurity scattering, the boundary between $s+id$ and pure s-wave states is no longer a straight line. As for the boundary between $s+id$ and pure d-wave states, it is given by

$$1 = 4g_s \pi T \sum_{\omega_n > 0} \int \frac{d\phi'}{2\pi} \frac{1+\eta_{\omega_n}}{\sqrt{\omega_n^2 (1+\eta_{\omega_n})^2 + \Delta_d^2 \cos^2 2\phi'}}, \qquad (24)$$

$$1 = 4g_d \pi T \sum_{\omega_n > 0} \int \frac{d\phi'}{2\pi} \frac{\cos^2 2\phi'}{\sqrt{\omega_n^2 (1+\eta_{\omega_n})^2 + \Delta_d^2 \cos^2 2\phi'}}, \qquad (25)$$

$$\eta_{\omega_n} = \frac{1}{2\tau} \int \frac{d\phi'}{2\pi} \frac{1+\eta_{\omega_n}}{\sqrt{\omega_n^2 (1+\eta_{\omega_n})^2 + \Delta_d^2 \cos^2 2\phi'}}. \qquad (26)$$

By numerically solving these equations, we obtain the phase diagram in Fig. 2 for mixed symmetry superconductors with nonmagnetic impurity scatterings. In our calculation, the impurity scattering strength is taken to be $\tau^{-1} = 0.7\Delta_{d0}$, which gives $T_d \approx 0.30 T_{d0}$. By comparing Figs. 1 and 2, one can find that the pure s-wave phase and the $s+id$ phase are shifted to the smaller g_s/g_d region so that $g_s/g_d = 0.404$ line crosses the $s+id$ region. This result shows that the possibility to observe the BTRS state in bulk superconductors with dominant d-wave and minor s-wave pairing interactions can be greatly enhanced by the nonmagnetic impurity scattering. Moreover, the boundary line AC between s-wave phase and

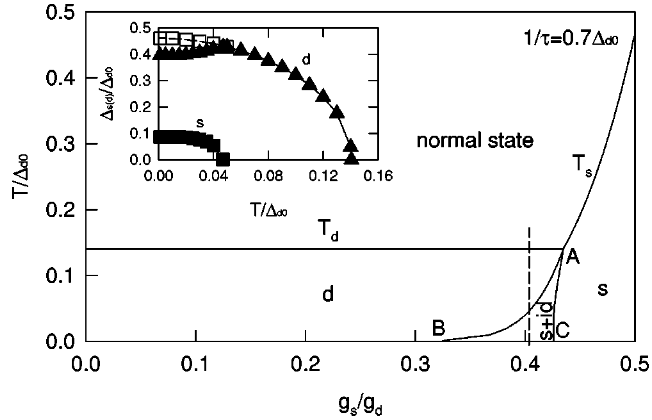

FIG. 2. Phase diagram for mixed s- and d-wave symmetry superconductors with nonmagnetic impurity scattering rate $\tau^{-1}=0.7\Delta_{d0}$. The values of g_s/g_d at points A, B, and C are, respectively, 0.435, 0.325, and 0.426. The inset shows the temperature dependence of the d-wave (filled triangle) and s-wave (filled square) components with $g_s/g_d=0.404$. The pure d-wave OP with $g_s=0$ (open square) is shown for comparison.

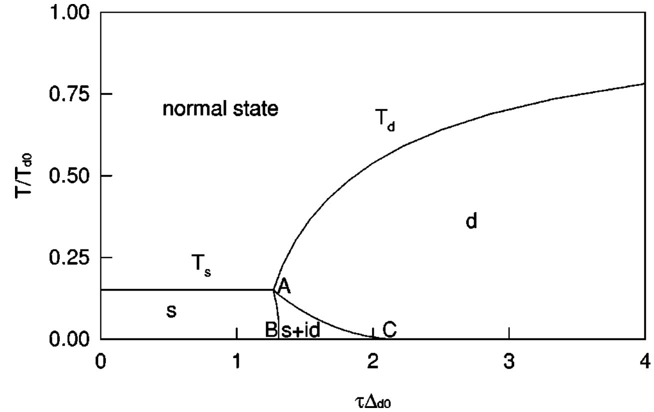

FIG. 3. Phase diagram in the T-τ parameter space with $g_s/g_d=0.404$.

the $s+id$ phase is a little declined. These results are completely due to the fact that the nonmagnetic scattering only influences the d-wave superconductivity. In the inset of Fig. 2, we plot the temperature dependence of the OP in the mixed region by taking $g_s/g_d=0.404$, which shows further that in the $s+id$ phase, the d-wave component OP decreases when the temperature is lowered. The effect of nonmagnetic impurity scatterings can be seen more clearly in Fig. 3, where the phase diagram is given in the T-τ parameter space with g_s/g_d fixed at 0.404. At low temperatures, with the increase of nonmagnetic impurity concentration, the system can start with a pure d-wave phase, cross the $s+id$ state, and finally enter into the pure s-wave phase. These behaviors are expected to be experimentally observable.

Finally we would like to point out that an attractive subdominant s-channel interaction is a prerequisite[4] for the realization of the surface BTRS $s+id$ state. It has been shown based on the Ginzburg-Landau theory[9] that if the s-channel interaction is repulsive, the OP near the surface is locked into a real combination of s- and d-wave components by the mixed gradient term in the free-energy functional, which means that a surface BTRS state could not be induced by the proximity effect. We argue further that for the case of repulsive s-channel interaction, even the angle between the crystalline a axis and the surface normal vector is $\pi/4$ so that the mixed gradient term vanishes, there is no possibility to realize a BTRS state near the surface. Actually, even for the case of attractive s-channel interaction, a surface BTRS state is stable only in certain regions of interaction and at very low temperatures.[4]

In summary, the phase diagram of superconductors with mixed s- and d-wave symmetry has been studied by considering the nonmagnetic impurity scattering effect. We predict that it is possible to observe the $s+id$ state by introducing the nonmagnetic impurity scattering since it affects the d-wave superconductivity but has no influence on the s-wave superconductivity. Moreover, by taking the ratio of two interaction strengths such that the system could go into the $s+id$ state, we find that the amplitude of d-wave component decreases with the lowered temperature.

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