IMPURITY SCATTERING IN A D-WAVE SUPERCONDUCTOR

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The influence of (non-magnetic and magnetic) impurities on the transition temperature of a d-wave superconductor is studied anew within the framework of BCS theory. Pairing interaction decreases linearly with the impurity concentration. Accordingly T_c suppression is proportional to the (potential or exchange) scattering rate, $1/\tau$, due to impurities. The initial slope versus $1/\tau$ is found to depend on the superconductor contrary to Abrikosov-Gor'kov type theory. Near the critical impurity concentration T_c drops abruptly to zero. Because the potential scattering rate is generally much larger than the exchange scattering rate, magnetic impurities will also act as non-magnetic impurities as far as the T_c decrease is concerned. The implication for the impurity doping effect in high T_c superconductors is also discussed.

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1. Introduction

Recently there has been much attention on the d-wave pairing state in connection with high-temperature superconductors.[1,2,3] The impurity effect on the d-wave pairing is particularly interesting because it may give a clue to the symmetry of the superconducting state of the high T_c cuprates. There are already many theoretical works on this issue.[4−12] For examples, the impurity effects on the penetration depth,[4] the superfluid density,[4] the transition temperature,[5] the quasiparticle states,[6] the density of states,[7,10−12] the nuclear spin relaxation rate,[7] the spin susceptibility,[8] and the infrared conductivity,[9] have been investigated.

The above theoretical works were essentially based on the Abrikosov-Gorkov's (AG) pair breaking theory[13] for the s-wave superconductors. However, Kim and Overhauser[14] proposed a new theory with different predictions: (i) The initial slope of T_c decrease depends on the superconductor and is not the universal constant suggested by AG. (ii) The T_c reduction by exchange scattering is partially suppressed by potential scattering when the mean free path is smaller than the coherence length, which has been confirmed in several experiments.[15−17] Kim[18] also showed that the failure of AG theory comes from the intrinsic pairing problem in Gor'kov's formalism, which can be cured by incorporating the pairing constraint. The purpose of this paper is to reconsider the T_c suppression due to (non-magnetic and magnetic) impurities in a d-wave superconductor within the framework of BCS theory.

It is shown that the pairing interaction decreases linearly with the (non-magnetic or magnetic) impurity concentration. The ratio of the average correlation length, $\xi_o = 0.18\frac{v_F}{T_c}$, to the mean free path, ξ_o/ℓ, determines the weakening of the pairing interaction. Consequently T_c suppression and the initial slope depend strongly on the superconductor contrary to Abrikosov-Gor'kov type theory. For the magnetic impurities, because the cross section of the potential scattering is generally much larger than that of the exchange scattering, the T_c decrease is also determined by the potential scattering of the magnetic impurities.[13,19]

The interpretation of the high T_c data[20,21] by the present study is not clear, though. The observed T_c decrease due to impurity scattering is much slower than the theory predicts. The discrepancy seems to come from the neglect of the strong Coulomb interaction effect in calculating the impurity response of the superconducting state. In other words, the impurity responses are different in Fermi liquids and strongly correlated systems. Note that it was pointed out[22] the T_c decrease caused by impurity doping and ion-beam-induced damage in high T_c superconductors is related with the proximity to a metal-insulator transition.

2. D-Wave Superconductor

For a d-wave superconductor, the pairing interaction $V_{\vec{k},\vec{k}'}$ for the plane states is taken to be[23]

$$V_{\vec{k},\vec{k}'} = \int e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} V(\mathbf{r}) d^3r = -5V_2 \ \frac{1}{2}[3(\hat{k}\cdot\hat{k}')^2 - 1], \tag{1}$$

where $\hat{k}$ is the unit vector parallel to $\vec{k}$. Substituting Eq. (1) into the BCS gap equation, one finds

$$\Delta_{\vec{k}} = 5V_2 \sum_{\vec{k}'} \frac{1}{2}[3(\hat{k}\cdot\hat{k}')^2 - 1] \frac{\Delta_{\vec{k}'}}{2E_{\vec{k}'}} tanh \frac{E_{\vec{k}'}}{2T}, \tag{2}$$

where

$$E_{\vec{k}'} = \sqrt{\epsilon^2_{\vec{k}'} + |\Delta_{\vec{k}'}|^2}, \tag{3}$$

and $\epsilon_{\vec{k}}$ is the electron energy. Among the possible solutions, we consider

$$\Delta_{\vec{k}} = \Delta_o(\hat{k}^2_x - \hat{k}^2_y). \tag{4}$$

This solution has the same symmetry property as $d_{x^2-y^2} = \Delta_o(cosk_x - cosk_y)$ which is believed to describe the gap structure of the cuprate high T_c superconductors. Upon substitution in Eq. (2), one obtains the T_c equation

$$T_c = 1.13\epsilon_c e^{-1/N_o V_2}, \tag{5}$$

where ϵ_c is the cutoff energy and N_o is the electronic density of states at the Fermi level.

In the presence of impurities, the scattered states ψ_n may be expanded in terms of plane waves, such as[24]

$$\psi_n = \sum_{\vec{k}} e^{i\vec{k}\cdot\mathbf{r}} < \vec{k}|n> . \tag{6}$$

Now the pairing interaction $V_{nn'}$ between scattered basis pairs $(\psi_n, \psi_{\bar{n}})$ and $(\psi_{n'}, \psi_{\bar{n}'})$ is given by

$$V_{nn'} = \int\int d\mathbf{r}_1 d\mathbf{r}_2 \psi^*_{n'}(\mathbf{r}_1)\psi^*_{\bar{n}'}(\mathbf{r}_2)V(|\mathbf{r}_1 - \mathbf{r}_2|)\psi_{\bar{n}}(\mathbf{r}_2)\psi_n(\mathbf{r}_1). \tag{7}$$

Here $\psi_{\bar{n}}$ denotes the time-reversed state of ψ_n. ¿From Eqs. (1), (6) and (7) we can calculate $V_{nn'}$.

3. Non-Magnetic Impurity Effect

The non-magnetic impurities will be examined first. The scattering potential from the impurities is given

$$U(\mathbf{r}) = \sum_i u\delta(\mathbf{r} - \mathbf{R}_i). \tag{8}$$

$\{\mathbf{R}_i\}$ is the impurity sites. We consider the impurity effect using the 2-nd order perturbation theory. Then, the scattered state which carries the label $\vec{k}\alpha$ is

$$\psi_{\vec{k}\alpha} = N_{\vec{k}}[e^{i\vec{k}\cdot\mathbf{r}} + \sum_{i,\vec{q}} \frac{u}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{q}}} e^{-i\vec{q}\cdot\mathbf{R}_i} e^{i(\vec{k}+\vec{q})\cdot\mathbf{r}}]\alpha, \tag{9}$$

where $N_{\vec{k}}$ is the normalizing factor. The time-reversed degenerate partner of Eq. (9) is

$$\psi_{-\vec{k}\beta} = N_{\vec{k}}[e^{-i\vec{k}\cdot\mathbf{r}} + \sum_{i,\vec{q}} \frac{u}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{q}}} e^{i\vec{q}\cdot\mathbf{R}_i} e^{-i(\vec{k}+\vec{q})\cdot\mathbf{r}}]\beta. \tag{10}$$

The matrix elements which cause Cooper pairing are between scattered basis pairs $(\psi_{\vec{k}\alpha}, \psi_{-\vec{k}\beta})$ and $(\psi_{\vec{k}'\alpha}, \psi_{-\vec{k}'\beta})$.[14,24] Each basis pair is a 2×2 Slater determinant. The matrix element $V_{\vec{k},\vec{k}'}$ between the two scattered basis determinants is

$$V_{\vec{k},\vec{k}'} = < \mathcal{D}_{\vec{k}'}(\vec{r}_1, \vec{r}_2) \big| V(|\vec{r}_1 - \vec{r}_2|) \big| \mathcal{D}_{\vec{k}}(\vec{r}_1, \vec{r}_2) >, \tag{11}$$

where

$$\mathcal{D}_{\vec{k}}(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_{\vec{k}\alpha}(\mathbf{r}_1) & \psi_{\vec{k}\alpha}(\mathbf{r}_2) \\ \psi_{-\vec{k}\beta}(\mathbf{r}_1) & \psi_{-\vec{k}\beta}(\mathbf{r}_2) \end{vmatrix}. \tag{12}$$

Upon employing Eqs. (1), (11), and (12), we find

$$V_{\vec{k},\vec{k}'} = -5V_2 \, \frac{1}{2}[3(\hat{k} \cdot \hat{k}')^2 - 1] N_{\vec{k}}^2 N_{\vec{k}'}^2. \tag{13}$$

The normalizing factor $N_{\vec{k}}^2$ is given

$$N_{\vec{k}}^2 = \frac{1}{1 + |W_{\vec{k}}|^2}, \tag{14}$$

where $|W_{\vec{k}}|^2$ is the relative probability contained in the virtual spherical waves surrounding the impurities (compared to the plane wave part). As in s-wave superconductor case, in computing $|W_{\vec{k}}|^2$, we cut off the radial integral at $R = 3.5\xi_o/2$, because the pair-correlation amplitude falls exponentially as $exp(-r/3.5\xi_o)$ near T_c.[23] The average correlation length ξ_o is defined by

$$\xi_o = 0.18 \frac{v_F}{T_c}. \tag{15}$$

With Eqs. (13), (14) and (15), one readily finds

$$N_{\vec{k}}^2 = \frac{1}{1 + \frac{3.5\xi_o}{4\ell}}, \tag{16}$$

where ℓ is the mean free path.

Therefore the pairing interaction is reduced:

$$V_{\vec{k},\vec{k}'} = -5V_2 \, \frac{1}{2}[3(\hat{k} \cdot \hat{k}')^2 - 1][1 + \frac{3.5\xi_o}{4\ell}]^{-2}. \tag{17}$$

Notice that in dilute limit the reduction is proportional to the ratio of the average correlation length to the mean free path, ξ_o/ℓ and the pairing interaction decreases linearly with the impurity concentration. The T_c equation is now,

$$T_c = 1.13\epsilon_c e^{-1/N_o V_2[1+\frac{3.5\xi_o}{4\ell}]^{-2}}. \tag{18}$$

Figure 1 shows T_c versus $1/\tau$ for $T_{co} = 40K$ and 80K respectively. T_{co} denotes the transition temperature without impurities. We used $\epsilon_c = 500K$. For a metal with $v_F = 2\times 10^7 cm/sec$, the superconductivity is completely suppressed when the mean free paths are about $1000\mathring{A}$ and $350\mathring{A}$ for $T_{co} = 40K$ and 80K, respectively. As in magnetic impurity effect on s-wave superconductors,[14] we find a sudden drop of T_c near the critical impurity concentration. This effect was much weakened by potential scattering in s-wave case. In this case, this effect may be real. Note that Porto and Parpia[25] found a sudden drop of T_c in p-wave superfluid He^3 caused by aerogel. On the other hand, the inelastic scattering may decrease the effect in high T_c superconductors.

The change in T_c relative to T_{co} can be calculated to first order in the impurity concentration. ¿From Eqs. (15) - (18)

$$\Delta T_c \approx -\frac{0.32}{\lambda\tau}, \tag{19}$$

where τ is the collision time due to impurities. The factor $1/\lambda$ shows that the initial slope (versus $1/\tau$) depends on the superconductor and, consequently, is not a universal constant. Weak superconductors lose their T_c more rapidly than strong ones.

4. Magnetic Impurity Effect

The magnetic impurities give rise to both potential and magnetic scattering. For the potential scattering, the result of the previous section is applicable. In this section, we consider the effect of magnetic scattering. The magnetic interaction between a conduction electron at $\mathbf{r}$ and a magnetic solute (having spin $\mathbf{S}$), located at $\mathbf{R}_i$, is

$$H_m = J\mathbf{s}\cdot\mathbf{S}_i v_o \delta(\mathbf{r}-\mathbf{R}_i), \tag{20}$$

where $\mathbf{s} = \frac{1}{2}\sigma$ and v_o is the atomic volume. The three components of σ are the Pauli matrices. As in Sec. 3, we consider the magnetic impurity effect up to the second order of J. Then, the scattered state which carries the label, $\vec{k}\alpha$, is

$$\Psi_{\vec{k}\alpha} = \mathcal{N}_{\vec{k}}\Omega^{-\frac{1}{2}}[e^{i\vec{k}\cdot\vec{r}}\alpha + \sum_{\vec{q}} e^{i(\vec{k}+\vec{q})\cdot\vec{r}}(W_{\vec{k}\vec{q}}\beta + W'_{\vec{k}\vec{q}}\alpha)], \tag{21}$$

where,

$$W_{\vec{k}\vec{q}} = \frac{\frac{1}{2}J\overline{S}v_o\Omega^{-1}}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{q}}}\sum_j sin\chi_j e^{i\phi_j - i\vec{q}\cdot\mathbf{R}_j}, \tag{22}$$

and,

$$W'_{\vec{k}\vec{q}} = \frac{\frac{1}{2}J\overline{S}v_o\Omega^{-1}}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{q}}}\sum_j cos\chi_j e^{-i\vec{q}\cdot\mathbf{R}_j}. \tag{23}$$

χ_j and ϕ_j are the polar and azimuthal angles of the spin $\vec{S}_j$ at $\mathbf{R}_j$, and $\overline{S} = \sqrt{S(S+1)}$. The degenerate partner of Eq. (21) is:

$$\Psi_{-\vec{k}\beta} = \mathcal{N}_{\vec{k}}\Omega^{-\frac{1}{2}}[e^{-i\vec{k}\cdot\vec{r}}\beta + \sum_{\vec{q}} e^{-i(\vec{k}+\vec{q})\cdot\vec{r}}(W^*_{\vec{k}\vec{q}}\alpha - W'^*_{\vec{k}\vec{q}}\beta)]. \tag{24}$$

In this case, we pair $\Psi_{\vec{k}\alpha}$ and $\Psi_{-\vec{k}\beta}$.

Accordingly, the matrix element $V_{\vec{k},\vec{k}'}$ is given

$$V_{\vec{k},\vec{k}'} = < \mathcal{D}_{\vec{k}'}(\vec{r}_1, \vec{r}_2)\big|V(|\vec{r}_1 - \vec{r}_2|)\big|\mathcal{D}_{\vec{k}}(\vec{r}_1, \vec{r}_2) >, \tag{25}$$

where

$$\mathcal{D}_{\vec{k}}(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}\begin{vmatrix} \Psi_{\vec{k}\alpha}(\mathbf{r}_1) & \Psi_{\vec{k}\alpha}(\mathbf{r}_2) \\ \Psi_{-\vec{k}\beta}(\mathbf{r}_1) & \Psi_{-\vec{k}\beta}(\mathbf{r}_2) \end{vmatrix}. \tag{26}$$

Using Eqs. (1) and (26), we find

$$V_{\vec{k},\vec{k}'} = -5V_2\ \frac{1}{2}[3(\hat{k}\cdot\hat{k}')^2 - 1]\mathcal{N}^2_{\vec{k}}\mathcal{N}^2_{\vec{k}'}. \tag{27}$$

Note that Eq. (27) is the same form as Eq. (13) in Sec. II. As a result, the T_c reduction caused by the magnetic impurities can be calculated by the same formulas, Eqs. (17) - (19). The only difference is using ℓ_s and τ_s instead of ℓ and τ. ℓ_s is the mean free path for the spin disorder scattering and τ_s is the spin-disorder scattering time. However, because the cross section for the potential scattering of the magnetic impurities is generally much larger than that for exchange scattering, we only need to consider the potential scattering due to magnetic impurities as far as T_c change is concerned.

5. Discussions

This study has been done in the framework of the BCS theory. But the same result can be obtained from the Gor'kov's Green's function theory if we impose a pairing constraint on the self-consistency equation. Near T_c, the d-wave self-consistency equation with degenerate pairing constraint is given by[26]

$$\Delta^*(\mathbf{r},\mathbf{l}) = V(\mathbf{r}-\mathbf{l})T\sum_{\omega}\int\int d\mathbf{r}'d\mathbf{l}'\{G_N(\mathbf{r}',\mathbf{r},-\omega)G_N(\mathbf{l}',\mathbf{l},\omega)\}^P\Delta^*(\mathbf{r}',\mathbf{l}'). \tag{28}$$

The superscript P denotes the pairing constraint and G_N is the normal state Green's function in the presence of ordinary impurities. Using the relation between Δ_n and $\Delta^*(\mathbf{r},\mathbf{l})$,

$$\Delta_n = \int\int d\mathbf{r}d\mathbf{l}\Delta^*(\mathbf{r},\mathbf{l})\psi_{\bar{n}}(\mathbf{l})\psi_n(\mathbf{r}), \tag{29}$$

it can be shown that Eq. (28) is the nothing but another form of the BCS gap equation. We can also show that the physical constraint of the Anomalous Green's function $F^\dagger(\mathbf{r},\mathbf{l},\omega)$, (i.e.),

$$\overline{F^\dagger(\mathbf{r},\mathbf{l},\omega)}^{imp} = \overline{F^\dagger(\mathbf{r}-\mathbf{l},\omega)}^{imp}, \tag{30}$$

gives rise to the degenerate pairing constraint. The superscript $^{-imp}$ means an average over the impurity positions.

In high T_c superconductors, the impurity doping and ion-beam induced damage[27] suppress strongly T_c. But the T_c reduction is not fast enough to be explained by this study. The experimental data show that T_c reduction is closely related with the proximity to a metal-insulator transition caused by the impurity doping and the ion-beam-induced damage.[20,21,27] We believe that the impurity response of the strongly correlated systems like high T_c cuprates may be understood only when we consider the impurity scattering and the strong correlation on equal footing. Because both non-magnetic and magnetic impurities suppress T_c almost equally, anisotropic pairing may be plausible.

6. Conclusion

In conclusion, we considered the effects of the (non-magnetic and magnetic) impurities on T_c in a d-wave superconductor. The pairing interaction decreases linearly with the impurity concentration. The initial slope of the T_c suppression depends on the superconductor and therefore is not a universal constant. Because the cross section of the potential scattering is much larger than that of the exchange scattering, T_c suppression is determined entirely by the potential scattering of the magnetic impurities. We also discussed the implications of this study for the impurity doping effect in high T_c superconductors.

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Figure Captions

Fig. 1 Variation of T_c with impurity concentration (measured in terms of the scattering rate, $\frac{1}{\tau}$) for $T_{co} = 40K$ and $80K$, respectively. The cutoff energy ϵ_c is $500K$.