Weak Localization Effect in Superconductors

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Abstract

We study the effect of weak localization on the transition temperatures of superconductors using time-reversed scattered state pairs, and find that the weak localization effect weakens electron-phonon interactions. With solving the BCS $T_c$ equation, the calculated values for $T_c$ are in good agreement with experimental data for various two- and three-dimensional disordered superconductors. We also find that the critical sheet resistance for the suppression of superconductivity in thin films does not satisfy the universal behavior but depends on sample, in good agreement with experiments.

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I. INTRODUCTION

Since the scaling theory of Anderson localization,\(^1\) our understanding of the electronic properties of disordered conductors has been advanced considerably.\(^2\,^3\) However, the effect of localization on superconductivity is still not well understood.\(^4\,^5\,^6\) A unified picture for the disorder effects on the superconducting temperature \((T_c)\) and the critical field \((H_{c2})\) is still lacking. In the presence of disorder, it was even claimed that the Eliashberg theory breaks down for two-dimensional superconductors.\(^8\) There have been many experimental studies to explain a competition between localization and superconductivity in two- and three-dimensional systems.\(^8\,^9\,^10\,^11\,^12\,^13\,^14\,^15\,^16\) In homogeneous amorphous thin films, an empirical formula\(^5\) showed that the reduction of \(T_c\) is proportional to the sheet resistance \(R_{\square}\). For bulk amorphous InO\(_x\), Fiory and Hebard\(^13\) found that both the normal-state conductivity \(\sigma\) and the critical temperature vary as \((k_F\ell)^{-2}\) due to the localization effect, where \(k_F\) and \(\ell\) are the Fermi wave vector and the elastic mean free path, respectively. In A15 superconductors such as Nb\(_2\)Sn, V\(_3\)Si, and V\(_3\)Ga, the universal degradation of \(T_c\) with impurities was also found,\(^17\) following the variation of \(\rho^2 \propto (k_F\ell)^{-2}\),\(^18\,^19\,^20\) where \(\rho\) is the normal-state resistivity. Previously, the decrease of \(T_c\) with increasing of disorder was attributed to the enhanced Coulomb repulsion \(\mu^*\).\(^4\,^17\,^21\,^22\) However, tunneling experiments\(^8\,^23\,^24\,^25\) did not support such an argument and indicated instead a decrease of the electron-phonon coupling \(\lambda\).\(^8\,^23\,^24\,^25\) As an alternative explanation, a singularity of the density of states at the Fermi level caused by long-range Coulomb interactions was suggested to change \(T_c\)’s for Pb and Sn thin films.\(^27\) However, it was pointed out that the singularity of the density of states does not affect thermodynamic quantities such as \(T_c\).\(^28\) In addition, it was shown experimentally that the effect of the Coulomb gap is minor in superconductors.\(^29\,^30\)

In this paper we present the results of theoretical studies on the weak localization effect on the superconducting temperatures of disordered superconductors. Using time-reversed scattered state pairs, we are able to explain available experimental data, based on a unified picture that the electron-phonon coupling decreases with increasing of disorder. Our
theory also explains other experimental results that in disordered superconductors $T_c$ can be enhanced by spin-orbit scatterings,\textsuperscript{12,31–33} which results from the anti-localization effect. In thin films, we suggest that the critical sheet resistance for the suppression of superconductivity is not a universal constant but a sample-dependent quantity. Some preliminary results were reported elsewhere.\textsuperscript{34}

II. THEORY

It has been recently realized that there exist localization corrections in electron-phonon interactions. To find these correction terms,\textsuperscript{35–38} it is a prerequisite to understand the limitation of Anderson’s theorem and the pairing problem in Gor’kov’s formalism and Bogoliubov-de Gennes equations. The Anderson’s theory in dirty superconductors\textsuperscript{39} is based on the fact that the exact eigenstates in the presence of impurities consist of time-reversed degenerate pairs; the scattered state $\psi_n$ of an electron with spin up is paired with the other electron with spin down in the time-reversed state $\psi_{\bar{n}}$. Then, the reduced Hamiltonian in scattered-state representation is written as

$$H'_{\text{red}} = \sum_{nn'} V_{nn'} c_{n'}^\dagger c_n^\dagger c_{\bar{n}} c_{\bar{n}}^\dagger,$$

where $c_n^\dagger$ and $c_n$ are creation and annihilation operators, respectively, for an electron in the state $\psi_n$. Assuming a point coupling $-V \delta(\mathbf{r}_1 - \mathbf{r}_2)$ for phonon-mediated electron-electron interactions, the matrix elements $V_{nn'}$ are expressed as\textsuperscript{40}

$$V_{nn'} = -V \int \psi_{n'}^\dagger(\mathbf{r}) \psi_{\bar{n}}^\dagger(\mathbf{r}) \psi_{\bar{n}}(\mathbf{r}) \psi_n(\mathbf{r}) d\mathbf{r}.$$  \hspace{8cm} (2)

If the scattered state $\psi_{n\sigma}$ is expanded in terms of plane waves $\phi_{\mathbf{k}\sigma}$,

$$\psi_{n\sigma} = \sum_{\mathbf{k}} \phi_{\mathbf{k}\sigma} \langle \mathbf{k} | n \rangle,$$

$V_{nn'}$ is rewritten as\textsuperscript{41}

$$V_{nn'} = -V (1 + \sum_{\mathbf{k} \neq \mathbf{k}', \mathbf{q}} \langle \mathbf{k} | n \rangle^\dagger \langle \mathbf{k} | n \rangle^* \langle -\mathbf{k} - \mathbf{q} | n' \rangle^\dagger \langle -\mathbf{k} - \mathbf{q} | n' \rangle^* \langle \mathbf{k}' - \mathbf{q} | n' \rangle^*).$$  \hspace{8cm} (4)
The second term in Eq. (4) is negligible in dirty limit, where the mean free path $\ell$ is in the range of 100 Å, while its contribution is meaningful in weak localization limit, where $\ell$ is of the order of 10 Å. Consequently, the Anderson’s theorem is only valid in the dirty limit.

In order to calculate the correction term in Eq. (4), we need information on the weakly localized scattered states. Kaveh and Mott\textsuperscript{42} derived these scattered states in the form of power-law and extended wavefunctions for both two and three dimensional systems. Haydock\textsuperscript{43} also showed that the asymptotic form of the scattered states is power-law like in weakly disordered two-dimensional systems. Here we use the scattered states of Kaveh and Mott\textsuperscript{42} to calculate the matrix elements $V_{nn'}$. In this case, since we are dealing with the bound state of a Cooper pair in a BCS condensate, only the power-law wavefunctions within the BCS coherence length $\xi_o$ are relevant.\textsuperscript{44} In weak localization limit, the effective coherence length is reduced to $\xi_{eff} \approx \sqrt{\ell \xi_o}$. It is important to take into account the size of the Cooper pairs for self-consistent calculations of the matrix elements. A similar situation also occurs for the localized states, which are not very sensitive to the change of the boundary conditions.\textsuperscript{45} Because of the power-law-like wavefunctions, the correction term due to weak localization represents physically the decrease of the amplitudes of the plane waves. Thus, the Cooper-pair wavefunctions basically consist of the plane waves with reduced amplitudes. Including the weak localization effect, the resulting matrix elements $V_{nn'}$ for two-and three-dimensional systems are written as

\begin{equation}
V^{2d}_{nn'} \approx -V[1 - \frac{2}{\pi k_F \ell} \ln(L/\ell)],
\end{equation}

\begin{equation}
V^{3d}_{nn'} \approx -V[1 - \frac{3}{(k_F \ell)^2}(1 - \frac{\ell}{L})].
\end{equation}

Because of the impurity effect, the electron-phonon interactions are weakened, as clearly seen in Eqs. (5) and (6).
III. RESULTS AND DISCUSSION

If we assume that the electron-phonon coupling constant is modified by the weak localization effect, the effective coupling constant $\lambda_{\text{eff}}$ from Eq. (5) for three-dimensional systems can be written as

$$\lambda_{\text{eff}} = \lambda[1 - \frac{3}{(k_F\ell)^2}(1 - \frac{\ell}{L})].$$  \hspace{1cm} (7)

Then, using the modified BCS $T_c$ equation,

$$k_B T_c = 1.13\hbar \omega_D \exp(-1/\lambda_{\text{eff}}),$$ \hspace{1cm} (8)

the change of $T_c$ relative to $T_{co}$ (for a pure metal) can be easily estimated to first order in the weak localization correction term of the coupling constant;

$$\frac{T_{co} - T_c}{T_{co}} \cong \frac{1}{\lambda} \frac{3}{(k_F\ell)^2}(1 - \frac{\ell}{L}).$$ \hspace{1cm} (9)

For a metal with $\omega_D = 300$ K, $k_F = 1$ Å$^{-1}$, and $L = 1000$ Å/$T$, the variations of $T_c$ are plotted as a function of $1/k_F\ell$ in Fig. 1, assuming $T_{co} = 4$ and 12 K. The inelastic mean free path results from electron-electron scatterings, and the correction term in Eq. (9) is negligible for $L \gg \ell$. We find that $T_c$ changes slowly with increasing of $1/k_F\ell$ until $1/k_F\ell$ equals to 0.1, in good agreement with experimental results.\textsuperscript{13,18–20} This behavior which satisfies the Anderson’s theorem is attributed to the fact that the change of $T_c$ is proportional to $\rho^2$, i.e., the square of impurity concentration. However, for $1/k_F\ell > 0.1$, $T_c$ decreases more significantly due to the weak localization effect caused by ordinary impurities. In this weak localization limit, the Anderson’s theorem is not valid. Our theoretical results are also compared with experimental data\textsuperscript{46} for A15 superconducting materials in Fig. 2. Using the same values of $k_F = 0.87$ Å$^{-1}$ and $L = 1000$ Å/$T$ for Nb$_3$Ge and V$_3$Si with $\omega_D = 302$ and 330 K and $T_{co} = 23$ and 17 K, respectively, we find good agreements between theory and experiment. In this case, since it is difficult to evaluate $k_F\ell$ up to a factor of 2,\textsuperscript{47} we assume that $\rho = 100\mu\Omega cm$ corresponds to $k_F\ell = 3.3$ and 3.75 for Nb$_3$Ge and V$_3$Si, respectively.
Similarly, we can write down the effective electron-phonon coupling constant for two-dimensional systems such as

$$\lambda_{\text{eff}} = \lambda [1 - \frac{2}{\pi k_F \ell} \ln(L/\ell)].$$

Since $1/k_F \ell$ is related to $R_\square$ by the Drude formula, the change of $T_c$ is expressed as,

$$\frac{T_{co} - T_c}{T_{co}} \approx \frac{1}{\lambda} \frac{e^2}{\pi^2 \hbar} R_\square \ln(L/\ell),$$

and this formula well satisfies the empirical relationship between $T_c$ and $R_\square$ for two-dimensional superconductors. In Fig. 3, the variations of $T_c$ with $1/k_F \ell$ are drawn for two superconductors with $T_{co} = 4$ and 8 K, assuming the same values of $\omega_D = 300$ K, $\ell = 4$ Å, and $L = 1000$ Å$\sqrt{T}$. The inelastic mean free path obtained from disordered two-dimensional systems are employed, with the $1/\sqrt{\ln T}$ dependence removed. In contrast to the 3-dimensional case, $T_c$ varies linearly with increasing of impurity concentration, and the initial slope of $T_c$ depends on superconductor because of the prefactor $1/\lambda$ in Eq. (12). Thus, the critical sheet resistances for the suppression of superconductivity in thin films do not provide the universal behavior, in good agreement with experiments.

Since the inelastic mean free path depends on temperature, the effective electron-phonon coupling also varies with temperature. Including the temperature effect on $\lambda_{\text{eff}}$, the variation of the gap parameter with temperature is plotted for two different values of $1/k_F \ell = 0.039$ and 0.078 in Fig. 4. The gap parameters are found to be lower than those obtained using the $T$-independent $\lambda_{\text{eff}}$'s. Experimentally, this behavior may be observable for lower $T_c$ superconductors, while strongly-coupled superconductors such as Pb and Nb may not be appropriate because the BCS model is not applicable for these systems.

For Mo-C and a-MoGe thin films, our calculated $T_c$'s are plotted as a function of $1/k_F \ell$ and compared with experimental data in Fig. 5. Here we employ the Drude formula to represent the decrease of $\ell$ when the sheet resistance $R_\square$ increases. As in the 3-dimensional case, because of the difficulty in evaluating $1/k_F \ell$ up to a factor of 2 from experimental data, we assume $\ell = 3.5$ Å and $L = 2000$ Å$\sqrt{T}$ for best fit in the Mo-C sample. For the a-MoGe
film, the use of $\ell = 4.0$ Å and $L = 1000$ Å$\sqrt{\mathcal{T}}$ is found to give the best agreement with experiment. In this case, the Drude formula is slightly adjusted by the relation $1/k_F\ell = 1.6667 (e^2/2\pi\hbar)R_c$. Similarly to the three-dimensional case, we find that the critical sheet resistance for the suppression of superconductivity does not follow the universal behavior.

We can also examine the effect of weak localization on superconductivity, using the strong or weak coupling Green’s function theory. In previous approaches, because the Anderson’s time-reversed scattered-state pairs were not employed, the correction term due to weak localization was missing in the electron-phonon interaction. The Green’s function formalism leads to the pairing states formed by a linear combination of the scattered states. Since these are still extended states, we do not expect the weak localization effect. Using the Anderson’s pairing condition for the strong coupling equation and the Einstein model for the phonon spectrum, the gap equation can be written as,

$$\Delta(n,\omega) = \sum_{\omega'} \lambda(\omega - \omega') \sum_{n'} V_{nn'} \frac{\Delta(n',\omega')}{\omega'^2 + \epsilon_{n'}^2},$$  \hspace{1cm} (12)

where

$$V_{nn'} = -V \int |\psi_n(r)|^2 |\psi_{n'}(r)|^2 dr,$$  \hspace{1cm} (13)

$$\lambda(\omega - \omega') = \frac{\omega_p^2}{\omega_p^2 + (\omega - \omega')^2}. $$  \hspace{1cm} (14)



In this case, the use of $V_{nn'}$ in Eq. (2) can also give rise to a modification of the electron-phonon interaction due to impurities in the strong coupling theory. In previous theories, however, the electron-phonon interaction remains unchanged, even if the wavefunctions are localized.

It is interesting to see the superconductor-to-insulator transitions in ultrathin films, which usually occur by changing film thickness or applying magnetic fields. Previously, a dirty boson theory was used to explain this experimental feature, implying that the critical sheet resistance for the suppression of superconductivity is a universal constant, $\hbar/4e^2 = 6.45$ KΩ. However, although it is difficult to determine experimentally a well-defined value for the critical sheet resistance $R_c^\square$ because the transitions do not occur sharply,
the measured values for $R_c$ were shown to depend on sample.\textsuperscript{49,53,54} We point out that the weak localization effect considered here is still a dominant contribution to the suppression of superconductivity over other higher order terms beyond the weak localization regime.\textsuperscript{2,3} In fact, Fig. 3 shows that $T_c$ is completely suppressed in the region of $k_F\ell \approx 6$ or 7, which is still in the weak localization regime. Thus, our results indicate that the superconductor-insulator transition is not a sharp phase transition but a crossover phenomena from quasi-two dimensional to two-dimensional.

Finally, we suggest that if the decrease of $T_c$ is caused by weak localization in disordered superconductors, adding impurities with large spin-orbit couplings will compensate for this decrease. In fact, such behavior was observed for several 3-dimensional samples,\textsuperscript{12,31–33} while it needs to be tested for 2-dimensional case. We expect that the critical sheet resistance is increased by enhancing the spin-orbit scattering. It is known that magnetic fields suppresses the weak localization effect. In this case, however, since the magnetic field decreases $T_c$, the $T_c$ decrease in a pure sample should be compared with that of a weakly disordered one. If the difference would exist, it is suggested to result from the weak localization effect, then, the critical sheet resistance will also change with increasing of magnetic field.

**IV. CONCLUSIONS**

In conclusion, we have studied the effect of weak localization on superconductors within the BCS theory. We find that the weak localization decreases the electron-phonon coupling constant, thereby, suppressing $T_c$. The calculated variations of $T_c$ with increasing of impurity concentration are found to be in good agreement with experiments for both 2- and 3-dimensional systems. The recovery of $T_c$ with impurities having large spin-orbit scatterings supports strongly our theory. We suggest that the critical sheet resistance for the suppression of superconductivity in thin films is not a universal constant, but a sample-dependent quantity, in good agreement with experiments.
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FIGURES

FIG. 1. Variation of $T_c$ with disorder parameter $1/k_F\ell$ (which represents ordinary impurity concentration) for 3-dimensional superconductors with $T_{co} = 4$ and 12 K.

FIG. 2. Calculated $T_c$’s versus resistivity $\rho$ for 3-dimensional Nb$_3$Ge (dotted line) and V$_3$Si (solid line). Experimental data are from Ref. 46.

FIG. 3. Variation of $T_c$ with disorder parameter $1/k_F\ell$ for 2-dimensional superconductors with $T_{co} = 4$ and 8 K.

FIG. 4. Temperature dependence of the gap parameter for 2-dimensional superconductors. The values of $1/k_F\ell = 0.039$ and $R_\square = 2000 \Omega$ are chosen for the upper curves, while $1/k_F\ell = 0.078$ and $R_\square = 3000 \Omega$ for the lower curves, with $T_{co} = 4$ K fixed. The $T$-independent ($T$-dependent) effective electron-phonon coupling is used for the solid (dotted) lines.

FIG. 5. Calculated $T_c$’s versus sheet resistance $R_\square$ for a-MoGe (solid line) and Mo-C (dotted line) thin films. Experimental data for a-MoGe and Mo-C are from Refs. 12 and 49, respectively.
FIG. 1

\[ T_c(K) \]

\[ 1/k_F l \]

3-D

FIG. 1
FIG. 2

\[ T_c (K) \]

\[ \rho (\mu \Omega \text{cm}) \]
FIG. 3

2-D

$T_c(K)$ vs $1/k_F l$
FIG. 4

![Graph of 2-D system with temperature (T(K)) on the x-axis and a parameter (Δ) on the y-axis. The graph shows two curves, one solid and one dashed, indicating a phase transition or critical point.](image)
