Effect of Spinless Impurities on Reduction of $T_c$ in High $T_c$ Superconductors

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The notion of a finite pairing interaction energy range suggested by Nam, results in some states at the Fermi level not participating in pairings when there are scattering centers such as impurities. The fact that not all states at the Fermi level participate in pairing is shown to suppress $T_c$ in an isotropic superconductor and destroy superconductivity. We have presented quantitative calculations of $T_c$ reduced via spinless impurities, in good agreements with data of Zn-doped YBCO and LSCO, respectively. Moreover, the incomplete condensation results in the picture of multiconnected superconductors$^1$ which can account for the $\pi$-phase shift in the Pb-YBCO SQUID$^2$ and magnetic fluxoid quantum observed in the YBCO ring with three grain boundary junctions$^3$.

One of intriguing experiments in high $T_c$ superconductors (HTS) is that the non-magnetic impurity Zn reduces $T_c$ and destroy superconductivity in Zn-doped YBCO$^1$, respectively.

The spinless impurity scattering, according to Anderson$^4$, would not change thermodynamical properties of superconductor, such as $T_c$, providing the order parameter being a uniform function, that is, a constant. He argued that the pairing of the state and its time reversal state in the scattering quantum space, would yield the same order parameter as that in the unscattered case, since the states in the former space can be mapped via the unitary transformation from those in the latter. In practice, one of crucial parameters to determine $T_c$ is the BCS coupling parameter

$$g = \langle N(0) V_{BCS} \rangle \quad (1)$$

with the density of states at the Fermi level $N(0)$ and the BCS pairing interaction $V_{BCS}$ averaged. We expect, thus, that the anisotropic pairing interaction would affect $T_c$. In fact, Markowitz and Kadanoff$^5$ have examined the anisotropic effect on $T_c$ and obtained good agreements between calculations and data for low concentrations of non-magnetic impurities in low $T_c$ superconductors (LTS).

On the other hand, Abrikosov and Gor’kov (AG)$^6$ have shown that the spin-flip scatterings suppress $T_c$ and destroy superconductivity. Also, when the order parameter has nodes, say $p$- or $d$-wave pairing states, Hirschfeld, Wölfle, and Einzel$^7$ argued that the resonance impurity scattering causes $T_c$ be reduced in the way of AG formula. In essence, the anisotropic effects and pair breaking scatterings, such as, spin-flip scattering, are known to be, up to now, the causes for destruction of superconductivity. We will show shortly a new chapter of destruction of superconductivity via non-magnetic impurity scatterings in an isotropic superconductor.

The notion of a finite pairing interaction energy range $T_d$$^8$ results in the incomplete condensation in which not all states participate in pairings. The states not participating in pairings yield low energy states responsible for the linear $T$ dependence of superelectron density at low $T$ in an isotropic superconductor$^9$. The quantitative calculations of magnetic penetration depth length in all $T$ ranges based on a finite $T_d$ are in good agreements with data of YBCO$^{12,13}$, BSCCO$^{14}$, HBCCO$^{15}$, LSCO$^{16}$, and Sr214$^{17}$, respectively. Moreover, the magnetic fluxoid quantum observed in the YBCO ring with three grain boundary junctions$^{20}$.

First we recapitulate the pertinent results of a finite $T_d$$^8$. To see the phase transition, $T_c$ should have a finite value, that is, neither zero nor infinite. To have a finite value $T_c$, $T_d$ should be finite, since $T_c$ is scaled with $T_d$ within the pairing theory. In other words, we may write the order parameter $\Delta(k, \omega)$ as$^9$

$$\Delta(k, \omega) = \begin{cases} \Delta & \text{for } |e_k| < T_d \\ 0 & \text{for } |e_k| > T_d \end{cases} \quad (2)$$

for all dynamical energies $\omega$. Here $e_k$ is the usual normal state excitation energy of wave number $k$, measured with respect to the Fermi energy. Hereafter units of $h = c = k_B = 1$ are used. And later $\Delta(T)$ for $\Delta$ may be used as well. The $\Delta$ is a solution of BCS like equation

$$\frac{1}{g} = \int_0^{T_d} \frac{d\epsilon}{E} \tanh \left( \frac{E}{2T} \right). \quad (3)$$

with $E = (\epsilon^2 + \Delta^2)^{1/2}$. For $\Delta(T_{c0}) = 0$, we get$^8$

$$1/g = (2/\pi) \sum_j (2/j) \tan^{-1}((y/j)). \quad (4)$$

where $y = T_d/(\pi T_{c0})$ with the transition temperature $T_{c0}$ for a pure system, and sum is over the positive odd integers $j$. The factor of arc tangent function makes the sum converge. For large $y$, Eq. (4) yields the BCS result $T_{c0}(BCS)$. The quantitative calculations of $T_{c0}$ and $\Delta$ vs $g$ and $T$ are given in Ref. $^1$. The $T_{c0}$ from Eq. (4) is always greater than $T_{c0}(BCS)$ and does not have
any upper limit. The fact is that for large $g > 2.32$,
$T_{c0}$ increases with increasing $g$ as $T_{c0} \approx gT_d/2$. One
interesting value of $g = 0.657$ yields $T_{c0} \approx 100$ K with
$T_d = 400$ K which is of the order of Debye temperature
in HTS. This value of $g$ may be realized in YBCO by
considering the electron-phonon interaction of the order of
$\lambda_p = 1.3 \sim 2.3$ [21].

The key idea of this letter is a novel one. When
there are scattering centers such as impurities in a Fermi
system, the spectral weight distribution function at the
Fermi level, that is, the imaginary part of the Green’s
function at $\omega = 0$, may be considered as a Lorentzian
form. The sum of spectral weights outside $T_d < |\epsilon_k|$, that is, the integral of the imaginary part of the Green’s
function with $\epsilon_k$ in the ranges of $|\epsilon_k| > T_d$, is given as

$$N(0)R = N(0)(2/\pi)\tan^{-1}(T/T_d), \quad (5)$$

where $\Gamma$ is the imaginary part of self-energy due to the
impurity scatterings, or the half impurity scattering rate
$1/(2\tau)$. The states of $N(0)R$ do not participate in pairings,
and are predicted [22] to be responsible for the linear $T$
dependence of the specific heat at low $T$ in Zn-
doped YBCO [23,24] and also for the $T^2$ term in the
magnetic penetration depth length at low $T$ in the
imperfect HTS such as Sr214 [17]. The effective density
of states at the Fermi level participating in pairings,
becomes $N(0)(1-R)$ less than the usual one $N(0)$, and
results in the reduced $T_c$. For simplicity, we assumed here
the effective BCS coupling parameter $g$ be not changed
via impurity scatterings. Also the Born approximation is used for calculations of impurity scatterings.

To incorporate the above key idea into the calculation of $T_c$, we use the Green’s function formalism [25]. In
the thermal Green’s function scheme, i.e., replacing $\omega$
by $i(2n + 1)\pi T$ with integer $n$, we may, taking into account the order parameter of Eq. (6) consistently, rewrite Eqs. (3.5a, b, c) of Ref. [25] as

$$Z_n\omega_n = \omega_n + (\Gamma + \Gamma_s)[\Phi_1(\omega_n) + \Phi_2(\omega_n)], \quad (6)$$

$$Z_n\Delta_n = \Delta + (\Gamma - \Gamma_s)\Phi_3(\omega_n), \quad (7)$$

$$\Delta = gT\sum_n \Phi_3(\omega_n), \quad (8)$$

$$\Phi_1(\omega_n) = (\omega_n/E_n)(2/\pi)\tan^{-1}(T_d/(Z_nE_n)), \quad (9)$$

$$\Phi_2(\omega_n) = (2/\pi)\tan^{-1}(Z_n\omega_n/T_d), \quad (10)$$

$$\Phi_3(\omega_n) = (\Delta_n/\omega_n)\Phi_1(\omega_n), \quad (11)$$

$$E_n = (\omega_n^2 + \Delta^2)^{1/2}. \quad (12)$$

Here $\Gamma$ and $\Gamma_s$ are the imaginary parts of self-energy via
non-magnetic and magnetic impurity scatterings, respectively. When $\Gamma = 0 = \Gamma_s$, $Z_n = 1$, and $\Delta_n = \Delta$, Eq. (8) becomes Eq. (11) of the BCS like equation, as it should.

For $T \rightarrow T_c$, $\Delta \rightarrow 0$, from Eqs. (8), (7), and (6), we, after simple algebras, get the equation for $T_c$ as

$$1/g = \sum_n 2\pi T_c \epsilon_n/\omega_n + D_n, \quad (9)$$

$$D_n = (1 - r_n)\Gamma + (1 + r_n)\Gamma_s, \quad (10)$$

$$r_n = (2/\pi)\tan^{-1}[T_d/(\omega_n + \Gamma + \Gamma_s)], \quad (11)$$

$$\omega_n = (2n + 1)\pi T_c. \quad (12)$$

The sum is over integers $n \geq 0$. For $\Gamma = 0 = \Gamma_s$, Eq. (9) becomes Eq. (11) for a pure superconductor. In the
infinite $T_d$ limit, equivalently small $g$ limit, that is, LTS
case, combining Eq. (3) and Eq. (4), yields the AG result, with $r_n = 1$ and $D_n = 2\Gamma_s$, as [22,23]

$$\ln(T_c/T_{c0}) = \sum_n \left(\frac{2}{2n + 1 + d} - \frac{2}{2n + 1}\right), \quad (13)$$

where the depairing parameter $d = 2\Gamma_s/(\pi T_c)$. Furthermore, $T_c$ becomes independent of $\Gamma$, and the Anderson
theorem [3] follows with $\Gamma_s = 0$. In general cases, combining Eq. (12) and Eq. (11), we calculate easily $T_c/T_{c0}$ and $T_c/T_d$ vs $\Gamma$, $\Gamma_s$, and $g$, respectively. The calculations for $g = 0.3, 0.45, 0.657, 1$, and $2$, have been carried out, and some results are presented here.

In Fig. 1 is shown $T_c/T_d$ vs $2\Gamma/T_d$ and $2\Gamma_s/T_d$ for $g = 0.657$ for example. The general shape of $T_c/T_d$
appears to be similar in any direction of $\Gamma$ and $\Gamma_s$.
To see somewhat in detail, in Fig. 2 are shown $T_c/T_d$ vs $2\Gamma/T_d$ for $\Gamma_s = 0$ and $T_c/T_d$ vs $2\Gamma_s/T_d$ for $\Gamma = 0$, for $g = 0.3, 0.45, 0.657, 1, \text{ and } 2$, respectively.

The reductions of $T_c$ via $\Gamma$ are slow for small $g$, and the steepness increases with increasing $g$. On the other hand, the reductions of $T_c$ via $\Gamma_s$ are almost the same shape for all $g$ values.

To see some more differences between non-magnetic and magnetic impurity scatterings, we have changed the scales of $2\Gamma/T_d$ and $2\Gamma_s/T_d$ by $2\Gamma/\Delta_0$ and $2\Gamma_s/\Delta_0$, with $\Delta_0 = \Delta(0)$ the order parameter in a pure superconductor, at $T = 0$, and a function of $g$. In Fig. 3 are shown $T_c/T_d$ vs $2\Gamma/\Delta_0$ and $T_c/T_d$ vs $2\Gamma_s/\Delta_0$.

The insets in Fig. 3 contain the normalized $T_c/T_{c0}$ vs $2\Gamma/\Delta_0$ and $T_c/T_{c0}$ vs $2\Gamma_s/\Delta_0$, respectively. The normalized $T_c/T_{c0}$ for all cases have almost the same shape.

In the $T_c = 0$ limit, we may rewrite Eq. (11) as

$$
\frac{1}{g} = \int_0^\infty dx \frac{r_c(x)}{x + D_c(x)}.
$$

$$
r_c(x) = (2/\pi) \tan^{-1}\left[ (T_d/\Delta_0)/(x + x_1 + x_2) \right],
$$

$$
D_c(x) = [1 - r_c(x)]x_1 + [1 + r_c(x)]x_2,
$$

$$
x_1 = \Gamma_c/\Delta_0,
$$

$$
x_2 = \Gamma_{sc}/\Delta_0.
$$

The phase diagram for $T_c = 0$ is shown in Fig. 4.

In the inset in Fig. 4, the critical values of $2\Gamma_c/\Delta_0$ decrease with increasing $g$, contrast to those of $2\Gamma_c/T_d$ in Fig. 2 increase with increasing $g$, since $T_c$ increases with increasing $g$. However, both $2\Gamma_{sc}/\Delta_0$ and $2\Gamma_{sc}/T_d$ increase with increasing $g$. For small $g$ limit, LTS case, the AG result $2\Gamma_{sc}/\Delta_0 = 0.5$ is obtained. In the large $g$ limit, HTS case, we get from Eq. (11) as

$$
2\Gamma_c/\Delta_0 + 2\Gamma_{sc}/\Delta_0 = 4/\pi.
$$

This can be realized from Eq. (11) as well by observing $r_n = 0$ and $D_n = 1 + \Gamma_s$ for large $g$ or small $T_d$ limit. This implies the effects of non-magnetic and magnetic scatterings on $T_c$ are the same in HTS. Data in HTS indeed indicated such as shown in Fig. 5. To compare calculations with data, we used $T_c/T_{c0}$ vs $\Gamma/\Gamma_c$ in Fig. 5. In addition to data of Zn-doped HTS, those of
Ni-doped YBCO and LSCO also are included to demonstrate both non-magnetic and magnetic scatterings affect $T_c$ in the same way for large $g$, that is, HTS case.

The data of YBCO [1] are poor but that of YBCO [2,3] are in good agreements with our calculations. The data of YBCO [1] are poor but that of YBCO [2,3] are in good agreements with our calculations.

In summary, even though the model of the order parameter of Eq. (3) is ideal, and the Born approximation of impurity scatterings in an isotropic superconductor is used, the calculations of $T_c$ vs non-magnetic and magnetic impurity scatterings, are in good agreements with data of YBCO and LSCO, respectively. The notable results are the normalized $T_c/T_{c0}$ vs $\Gamma/\Gamma_c$ are almost the same each other for all $g$ values, and $T_c/T_{c0}$ vs $\Gamma_s/\Gamma_{c\nu}$ yields the AG result. For improvement, one may use the $T$ matrix formulation for impurity scatterings, and take into account the retardation effect on the order parameter. However, we expect the $T_c/T_{c0}$ would not be changed much from that discussed here. The spinless impurity scatterings can destroy superconductivity in an isotropic superconductor as well. The notion of a finite $T_d$ is sound theoretically. We hope it would account for other unsolved problems in HTS.

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