Extended Gapless Regions in Disordered $d_{x^2−y^2}$-Wave Superconductors

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A generalization of the Abrikosov-Gorkov equations for non-magnetic impurities in unconventional superconductors is proposed, including higher harmonics in the expansion of the momentum dependent gap function and a momentum dependent impurity scattering potential. This model is treated within a self-consistent calculation to obtain the electronic density of states, the optical conductivity, and the gap function in a two-dimensional $d_{x^2−y^2}$-wave superconductor. It is argued that momentum dependent scattering from the impurities may lead to extended gapless regions in the gap function centered around the nodes of the pure $d_{x^2−y^2}$-wave superconductor. The associated enhancement of the residual density of states may be responsible for the rapid decrease of $T_c$ and the increase of the London penetration depth with hole doping observed in overdoped cuprate superconductors.

The pair-breaking role of impurities in d-wave superconductors in the weak coupling limit is well known. Recently the evidence that such weak coupling descriptions apply in the overdoped region of the high-$T_c$ cuprates has been growing. However, the experiments that track the behavior of the gap function have come to divergent conclusions. This raises the question of the evolution of the gap function in a d-wave superconductor as a function of the pairing interaction strength and the impurity concentration. In this letter we examine this question, allowing for angular dependent impurity scattering potentials. Our conclusion is that the evolution of the gap function depends on the character of the impurity scattering potential. In particular, we find that extended gapless regions grow as the critical point is reached when the impurity scattering potential is weighted towards forward scattering. In this case the scattering processes near the gap nodes, which connect regions of opposite sign pairing amplitude, are of increasing importance and reduce the gap in this region. This contrasts with the regions around the gap maxima, where the impurity scattering is less effective. The resulting evolution of the gap function is sketched in Fig. 1.

In conventional Abrikosov-Gorkov (AG) theory, the interaction of electrons with non-magnetic impurities is governed by a momentum independent scattering potential. Here we generalize this approach to the momentum dependent case, with a scattering potential $u_{k,k'}$. The contribution to the self-energy of electrons scattering from this static potential is given by the self-consistent T-matrix equation,

$$\hat{T}_{k,k'}(i\omega_n) = u_{k,k'}\hat{\sigma}_3 + \sum_q u_{k,q}\hat{\sigma}_3\hat{G}_q(i\omega_n)\hat{T}_{q,k'}(i\omega_n),$$  \hspace{1cm} (1)

where $\hat{G}_q(i\omega_n)$ is the Nambu single particle Green’s function in a superconductor.

and the Pauli matrices $\hat{\sigma}_i$ ($\hat{\sigma}_0 = 1$) form a complete basis in Nambu space. The renormalization of the bare Green’s function is given by the self energy $\hat{\Sigma}_{k}(i\omega_n) = \Gamma \hat{T}_{k,k}(i\omega_n)$, where $\Gamma$ is the concentration of impurities. In the limits $|u_{k,k'}| \to 0$ (Born limit) and $|u_{k,k'}| \to \infty$ (unitary limit) the T-matrix is simplified considerably. Hence, these limiting cases have been studied extensively in the literature. However, the strength of the scattering potential is not known from first principles, and only comparison with experiments indicates that some impurities in high-$T_c$ cuprates, such as Zn, are closer to the unitary limit.

FIG. 1. Schematic illustration of the momentum dependence of the gap function in a $d_{x^2−y^2}$ superconductor (a) without disorder ($\Gamma = 0$), and (b) in the presence of non-magnetic impurities ($\Gamma \neq 0$).

For computational simplicity, the Fermi surface is assumed to have a cylindrical shape as shown in Fig. 1, neglecting effects of the more complicated material-dependent band structure observed in high-$T_c$ com-
Here the wave vector \( k \) at the Fermi surface can be simply expressed as an azimuthal angle, \( \phi \). This simplifying assumption of a large and approximately cylindrical Fermi surface is in qualitative agreement with photoemission and Hall angle experiments on overdoped and even optimally doped cuprate samples.\[2\]

The equations for the single particle Green’s function, \( \hat{G}_k^{-1}(i\omega_n) = \hat{G}_k^{-1}(i\omega_n) - \Sigma_k(i\omega_n) \), have to be solved simultaneously with the zero-temperature gap equation,

\[
\Delta_{k'} = 2 \int_0^{\infty} d\omega_n \sum_k V_{k,k'} \Delta_k / \sqrt{\omega_n^2 + \Delta_k^2},
\]

yield to both the amplitude of the gap function and the components of the renormalized Green’s function at a given impurity concentration \( \Gamma \). Here, \( V_{k,k'} \) is the effective pairing potential in the d-wave channel of the same functional form as \( \Delta_k \). To describe the angular evolution of the gap function, we allow for a higher harmonic, \( \Delta_k = \Delta_0 \cos(2\phi) + \Delta_1 \cos(6\phi) \), and simultaneously include such higher harmonics in \( V_{k,k'} \), which we parametrize in factorized form, 

\[
V_{k,k'} = V(\cos(2\phi) + \alpha \cos(6\phi))(\cos(2\phi') + \alpha \cos(6\phi')) \]

where \( \alpha \) is the parameter which determines the gap shape in the absence of impurities.

In the following, we analyze how the renormalization due to electron-impurity scattering affects the amplitude and the in particular the shape of the gap function, \( \Delta_0 = \Delta_0 \cos(2\phi) + \Delta_1 \cos(6\phi) \). Let us examine the Born limit. For the choice of the impurity scattering potential, \( u_{k,k'} = \sigma_3[u_0 + u_1 \cos(\phi - \phi')] \), the AG equations take the form

\[
\tilde{\omega}_n = \omega_n + \Gamma(\tilde{\omega}_n(u_0^2 + u_1^2 \cos^2(\phi))) / \sqrt{\omega_n^2 + \Delta_0^2},
\]

\[
\tilde{\Delta}_{\phi'} = \Delta_{\phi'} - \Gamma(\tilde{\Delta}_{\phi' \cos(2\phi)}) \cos(2\phi').
\]

Here \( \langle \ldots \rangle \) denotes the angular average over the Fermi surface, and constants arising from the radial momentum integration are absorbed in \( \Gamma \). Note that \( \Delta_{\phi} \) depends on \( \tilde{\omega}_n \) (r.h.s. of Eq. (4)), and hence the actual shape of the renormalized gap can be defined only by analyzing the corresponding angular dependent density of states (DOS).

There is a gap equation for each of the two components of \( \Delta_\phi \). However, due to our particular choice of the impurity scattering potential only \( \Delta_0 \) is renormalized,

\[
\Delta_0 = 2N_0 V \int_0^{\infty} d\omega_n \langle \cos(2\phi) + \alpha \cos(6\phi) \rangle \tilde{\Delta}_{\phi' \cos(2\phi)} / \sqrt{\omega_n^2 + \Delta_0^2},
\]

while the gap equation for the second harmonic gives \( \Delta_1 = \alpha \Delta_0 \). Thus the renormalized gap function is of the form:

\[
\Delta_{\phi}(i\omega_n) = \Delta_0(\omega_n) \cos(2\phi) + \alpha \Delta_0 \cos(6\phi).
\]

Since only the first component of the gap function is reduced by impurity scattering, Eq. (4), it is evident that the node region widens with increasing impurity concentration (\( \Delta_1/\Delta_0 \rightarrow 1/4 \)).

In Fig. 2(a) the gap amplitude \( \Delta_0 \) obtained from the numerical solution of Eqs. (3-5) is shown as a function of impurity concentration and of the strength of the pairing interaction. Here we have chosen \( \alpha=0.2 \), \( u_0 = 1 \), and \( u_1 = 1 \), i.e. the case favoring forward scattering. The superconducting gap can be destroyed both by increasing the impurity concentration beyond a critical value, \( \Gamma_c \), or by reducing the pairing potential \( V \) below a critical \( V_c \). While the first case naturally occurs when introducing disorder into samples by impurity doping, the latter case may be realized by introducing additional holes into overdoped cuprate superconductors.\[10\]

From an expansion of Eqs. (3-5) about \( \Gamma_c \) we find that for large impurity concentrations the amplitude of the gap function vanishes as \( \Delta_0 \propto \sqrt{1 - \Gamma/\Gamma_c} \). Similarly, if one drives the system critical by reducing \( V/V_c \), we find \( \Delta_0 \propto \sqrt{V/V_c - 1} \), in agreement with the full numerical solution of these equations.

From an analytic continuation of Eqs. (3) and (4) onto the real frequency axis, the electronic DOS can be evaluated as \( N(\omega) = -\frac{1}{\pi} \sum_\delta \text{Im}[\tilde{G}_k(i\omega_n)][i\omega_n - \omega - i\delta] \). In Fig. 2(b) the DOS is shown at \( \Gamma/\Gamma_c = 0.15 \) (indicated by the dashed line in Fig. 2(a)). As the strength of the pairing potential is lowered, the system approaches the critical region where the gap is small, and hence the residual DOS increases with decreasing \( V \). As will be discussed.
in the following, this increase in $N(0)$ is enhanced by the occurrence of flat regions around the nodes.

The above results were obtained in the Born limit. In the unitary limit, the AG equations do not reduce to simple expressions like Eqs. (3-5) if the impurity scattering potential is taken to be momentum dependent. Hence, instead of attempting to solve the AG equations for the general $u_{kk'}$ used above, we restrict ourselves here to the case $u_0 = 1$, $u_1 = 0$, i.e. only isotropic impurity scattering. The results are shown in Fig. 2(c) and (d). It is obvious that in the limit of strong scattering the gap amplitude is reduced more rapidly by the introduction of impurities than in the Born limit (comparing Fig. 2(a) and (c)). When approaching the critical regime by decreasing $V/V_c$, a reduction of the gap amplitude (position of the peak in $N(\omega)$) and an increase in the residual DOS is observed, similar to the Born limit treated above. However, since only isotropic impurity scattering was considered in the latter case there is no widening of the node regions in the gap function and hence no additional enhancement of $N(0)$. While from the experimental side it has not been settled what the strength of the effective scattering potential, $|u_{kk'}|$, should be, a comparison of the two extreme limits suggests that no dramatic differences are to be expected within AG calculations. Qualitative differences between these two limits do appear for the single impurity problem, where anisotropic impurity resonances appear in the unitary limit.

Let us now turn to the qualitative changes in the shape of the gap function in the presence of a momentum dependent impurity scattering potential. In the clean case, there are four nodes located at $\phi = (2n-1)\pi/4$ ($n=1,...,4$) (Fig. 1(a)). The first of these nodes is shown in Figs. 3(a) and (b) for a fixed impurity concentration ($\Gamma/\Gamma_0 = 0.15$) and various values of $V$. In Fig. 3(a) only isotropic impurity scattering was considered ($u_0 = 1$, $u_1 = 0$) while in Fig. 3(c) the case favoring forward scattering is shown ($u_0 = u_1 = 1$). In the latter case the gap function was extracted by analyzing the angle resolved DOS: $\Delta(\phi)$ was defined as the position of the inflection point in $N(\phi, \omega)$ (maximum in $\partial N(\phi, \omega)/\partial \omega$). In both cases the gap amplitude decreases with decreasing $V$. (A similar behavior occurs when $V$ is kept fixed and $\Gamma$ is increased.) In the case of forward scattering, however, a flattening of the gap function around the nodes is observed. To quantify this behavior, we plot the extension, $d_\phi$, of the “flat” part of $\Delta(\phi)$ in the insets. With $d_\phi$ we denote those segments of $\Delta(\phi)$ where the magnitude of $\Delta(\phi)$ has fallen below half of its maximum value, $d_\phi = \pi/2 - 2\phi(\Delta_{\text{max}}/2)$. Note that as long as only a finite number of harmonics in the expansion of $\Delta(\phi)$ is considered, only extended saddle points can occur. However, it is obvious from the above discussion that there is a clear tendency towards gapless (“normal”) areas in the presence of momentum dependence in the impurity scattering potential coexisting with gapped regions (as depicted schematically in Fig. 1(b)). This prediction may be verified in overdoped cuprate superconductors by tunneling experiments, and by angle resolved photoemission spectroscopy (ARPES) if an adequate energy resolution (of order 1 meV) can be achieved.

![FIG. 3. (a) Angular dependence of the magnitude of the gap function in the Born limit at $\Gamma/\Gamma_0 = 0.15$, $u_0 = 1$, $u_1 = 0$, and $\alpha = 0.2$. The inset shows the length of the segment of the gap function where $|\Delta(\phi)/\Delta(0)| \leq 0.5$. (b) Optical conductivity corresponding to the parameters chosen in (a). $\sigma_{\text{00}}$ is the normal state value of the optical conductivity. (c) As (a), but with $u_1 = 1$. (d) As (b), but with $u_1 = 1$.](image-url)
In Fig. 4(a) and (c) the residual DOS is shown for the Born limit at \( u_0 = 1, u_1 = 1, \) and \( \alpha = 0.2 \), and for the unitary limit at \( u_0 = 1, u_1 = 0, \) and \( \alpha = 0 \). By expanding about the clean limit, it is seen that in the Born limit, the zero-frequency DOS vanishes exponentially slowly, \( N(0) \propto \exp(-\text{const}/R) \), for small impurity concentrations. On the other hand, in the unitary limit an infinitesimal amount of impurities is sufficient to yield a finite residual DOS, \( N(0) \propto \sqrt{R} \). Hence an enhancement of the residual DOS can be induced both by increasing the strength of the scattering potential and by introducing angular dependence in it. However, only the latter case leads to extended flat regions in the gap function.

As a consequence of the finite residual DOS, the low-temperature London penetration depth has the form \( \lambda(\Gamma, T) = \lambda(0,0) + N(\Gamma, 0)/2 + O(T^2) \). As the effective electron-electron interaction strength is decreased, i.e. when introducing additional holes into optimally doped or overdoped cuprate superconductors, \( \lambda \) grows rapidly. This behavior, illustrated in Figs. 4(b) and (d), is in agreement with recent measurements by Locquet et al.\( \cite{16} \)

![FIG. 4. (a) Residual DOS as a function of impurity concentration in the Born limit. Here \( u_0 = 1, u_1 = 1, \) and \( \alpha = 0.2 \). (b) Low-temperature London penetration depth as a function of the \( e^- - e^- \) pairing potential. The parameters are chosen as in (a). (c) As in (a), but in the unitary limit, and with \( u_0 = 1, u_1 = 0, \) and \( \alpha = 0 \). (d) Low-temperature London penetration depth for the parameters chosen in (c).](image)

In our results the maximum value of the gap is reduced consistently as either \( \Gamma \) is increased or \( V \) is reduced. This agrees with the results of ARPES and tunneling experiments. It disagrees with the conclusion from studies of the optical conductivity. However, there is an increase in the gapless region in the case of forward weighted impurity scattering which goes some way towards explaining the optical experiments. Our conclusion is that variations in impurity character may be at least partly responsible for the divergence of the experimental results, although an explanation for the absence of renormalization of the gap maximum is not possible within this weak coupling scheme.

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