Enhanced Coherence of Antinodal Quasiparticles in a Dirty d-wave Superconductor

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Recent ARPES experiments show a narrow quasiparticle peak at the gap edge along the antinodal [0,0]-direction for the overdoped cuprate superconductors. We show that within weak coupling BCS theory for a d-wave superconductor the s-wave single-impurity scattering cross section vanishes for energies \( \omega = \Delta \) (gap edge). This coherence effect occurs through multiple scattering off the impurity. For small impurity concentrations the spectral function has a pronounced increase of the (scattering) lifetime for antinodal quasiparticles but shows a very broad peak in the nodal direction, in qualitative agreement with experiment and in strong contrast to the behavior observed in underdoped cuprates.

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It is well known that non-magnetic impurities have little influence on the thermodynamic properties of the conventional s-wave superconductors in zero magnetic field. Non-magnetic impurities are, however, detrimental to unconventional superconductors with higher angular momentum such as d-wave superconductors. For such superconductors momentum conservation is essential, due to the anisotropic structure of the pair wavefunctions. Impurities although they used a self-consistent Born approximation which does not reproduce the suppression by multiple scattering off a single impurity. Because of the coherence effect a quasiparticle peak appears at the Fermi wavevector in a dirty d-wave superconductor in the antinodal direction but not at the Fermi wavevector in the nodal direction. Such behavior was reported recently in angle resolved photoemission spectra (ARPES) on strongly overdoped Tl-cuprates by Platé et. al. who commented on the striking contrast to underdoped cuprates where coherence is observed in the nodal direction.

We discuss briefly the single-impurity problem in a d-wave superconductor. The scattering off the impurity is described by the Hamiltonian

\[
H_{imp} = \sum_{k,k',\sigma} V c_{k,\sigma}^\dagger c_{k',\sigma},
\]

where \( V \) is the coupling strength of the impurity located at \( r = 0 \), and \( c_{k,\sigma} (c_{k,\sigma}^\dagger) \) is the creation (annihilation) operator for electron with wave vector \( k \) and spin \( \sigma \). We restrict ourselves here to s-wave scattering. The effect of the impurity scattering is described by the T-matrix, \( T(\omega) \). The Green’s function in the presence of an impurity is

\[
\hat{G}_{k,k'}(\omega) = \hat{G}_{k,k'}^{(0)}(\omega) + \hat{G}_{k,k'}^{(0)}(\omega) \hat{T}(\omega) \hat{G}_{k',k}^{(0)}(\omega),
\]

where both \( \hat{G}_{k,k'}^{(0)}(\omega) \) and \( \hat{T}(\omega) \) are matrices in the Nambu particle-hole space. \( \hat{G}_{k,k'}^{(0)}(\omega) \) is the Green’s function in the absence of impurities, written as

\[
\hat{G}_{k,k'}^{(0)}(\omega) = (\omega - i\epsilon_k - \xi_k)^{-1},
\]

where \( \xi_k \) is the quasi-particle energy, \( \Delta_k = \Delta \cos(2\phi_k) \) is the gap function with \( d_{x^2-y^2} \) symmetry and \( \phi_k \) is the angle of the wave vector \( k \) with respect to the \( k_x \)-axis. The matrices \( \hat{\rho}_i \) are the Pauli matrices and \( \hat{\rho}_0 \) is unit matrix in the particle-hole space.

The T-matrix for the s-wave scattering is expressed by

\[
\hat{T} = T_0 \hat{\rho}_0 + T_3 \hat{\rho}_3 \quad \text{with}
\]

\[
T_0 = \frac{G_0}{c^2 - G_0^2}, \quad T_3 = \frac{-c}{c^2 - G_0^2}.
\]

The parameter \( c = \cot \delta_0 \) introduces the scattering phase shift \( \delta_0 \), with \( c = 0 \) in the unitarity limit, and \( c \gg 1 \) in the weak scattering limit. \( G_0(\omega) = 1/(2\pi N_0) \sum_k \text{Tr} \hat{G}_k^{(0)}(\omega) \hat{\rho}_0 \), where \( N_0 \) is the density of states (DOS) per spin at the Fermi energy in the normal state. Explicitly, we can rewrite \( G_0 \) as

\[
G_0(\omega) = -\left( \frac{\omega}{\sqrt{\Delta_k^2 - \omega^2}} \right) = -\frac{2}{\pi} \frac{\omega}{\sqrt{1 - \omega^2}} K \left( \frac{1}{1 - \omega^2} \right).
\]

Here \( \langle \cdots \rangle \) means the average over the angle \( \phi_k \), and \( K(x) \) is the complete elliptic integral of the first kind. Note that the quasiparticle DOS in the d-wave superconductor is given by \( N(\omega) = -\text{Im}(G_0(\omega)) \). It diverges logarithmically at \( \omega / \Delta = 1 \) (see the case of \( \Gamma = 0 \) in Fig.1). The divergence of \( G_0(\omega) \) at the gap edge \( (\omega / \Delta = 1) \) implies that both \( T_0 \) and \( T_3 \) vanish. The scattering cross section which is proportional to the square of the modulus of the T-matrix \( T_0 \), vanishes at the quasiparticle energy \( \omega = \Delta \). This remarkable result is a coherence effect as it only appears with multiple scattering, but not for the Born limit, i.e. \( c \rightarrow \infty \).
We proceed to discuss this interference feature in the presence of a finite small concentration of impurities. After averaging over all impurity configurations, the translational symmetry in the system is effectively restored, and we can rewrite the Green’s function,

\[ \hat{G}_\omega = \left( \omega - \Delta_k \hat{\rho}_1 - \xi_k \hat{\rho}_3 - \hat{\Sigma} \right)^{-1}, \]

(6)

\[ = \left( \omega - \Delta_k \hat{\rho}_1 - \xi_k \hat{\rho}_3 \right)^{-1}. \]

(7)

The self-energy \( \hat{\Sigma} \) includes the effects of impurity scattering, and \( \omega \) and \( \Delta_k \) are the renormalized frequency and gap function, respectively. We decompose the self-energy into \( \hat{\Sigma} = \Sigma_0 \hat{\rho}_0 + \Sigma_1 \hat{\rho}_1 + \Sigma_2 \hat{\rho}_2 \), and obtain

\[ \hat{\omega} = \omega - \Sigma_0, \quad \Delta_k = \Delta_k - \Sigma_1, \quad \xi_k = \xi_k - \Sigma_3. \]

(8)

Under particle-hole symmetry \( \Sigma_3 \) vanishes. In a conventional s-wave superconductor without magnetic impurities, both \( \hat{\omega} \) and \( \Delta \) are renormalized in the same way, resulting in the absence of pair breaking. However, in an unconventional superconductor, there is no renormalization in \( \Delta \), i.e. \( \Delta_k = \Delta_k \), because \( \Sigma_1 \) is zero. The self-energy for various cases is summarized in the table I.

Next we compare the two scattering limits, the Born and the unitarity limit. The former yields the renormalized frequency \( \hat{\omega} \), given by

\[ \hat{\omega} = \omega + \Gamma \left( \frac{\hat{\omega}}{\sqrt{\Delta_k^2 - \omega^2}} \right), \]

(9)

Here \( \Delta_k = \Delta \cos(2\phi_k) \), \( \Gamma = n_i / \pi N_0 \) and \( n_i \) is the impurity concentration. Note that \( \Gamma^{-1} \) corresponds to the quasiparticle lifetime close to the Fermi energy in the normal metal state. The DOS is obtained by

\[ \frac{N(\omega)}{N_0} = \text{Im} \left( \frac{\hat{\omega}}{\sqrt{\Delta_k^2 - \omega^2}} \right), \]

(10)

\[ \text{TABLE I}: \text{ The self-energy term for the Born limit. “Imp.” indicates the type of impurities, i.e. N(M) is non-magnetic (magnetic) impurities. The min(\tau^{-1}) means the value of \omega which gives minimum value of the inverse lifetime \tau^{-1}. Here 1/\tau_1 and 1/\tau_2 are the parameter which represents pair-breaking caused by non-magnetic and magnetic impurity, respectively. } u = \omega/\Delta. \]

\[ \begin{array}{ccc}
\text{Imp.} & \Sigma_0 & \Sigma_1 \\
\text{d-wave} & N & \Gamma \left( \frac{\hat{\omega}}{\sqrt{\Delta_k^2 - \omega^2}} \right) \quad 0 & 0 \\
\text{s-wave}^1 & N & -\frac{1}{2\tau_1} \frac{1}{\sqrt{1-u^2}} + \frac{1}{2\tau_1} \frac{1}{\sqrt{1-u^2}} \Delta \\
\text{s-wave}^2 & M & -\frac{1}{2\tau_2} \frac{1}{\sqrt{1-u^2}} - \frac{1}{2\tau_2} \frac{1}{\sqrt{1-u^2}} 0 \\
\end{array} \]

where \( \hat{\omega} \) is self-consistently determined by Eq. (9) for given \( \omega/\Delta \) and \( \Gamma/\Delta \). In the upper panel of Fig.1 (a), the DOS is shown for several values of \( \Gamma \). For pure samples (\( \Gamma = 0 \)) the DOS logarithmically diverges at the gap edge (\( \omega/\Delta = 1 \)). This singularity is removed, however, by the presence of potential scattering, and the progressively weaker maximum moves toward lower energy with increasing \( \Gamma \).

The lifetime of the quasi-particle, \( \tau \), is deduced from the imaginary part of the self-energy

\[ 1/\tau = \text{Im}[\hat{\omega}] = \text{Im}[\Sigma_0]. \]

(11)

at the pole \( \hat{\omega}_p \) of the Green’s function given by the zero of the denominator:

\[ \hat{\omega}_p^2 - \Delta_k^2 - \xi_k^2 = 0. \]

(12)

In the lower panel of the Fig.1(a), the inverse lifetime as a function of \( \omega \) is depicted in the Born limit. Note that the \( 1/\tau \propto -N(\omega) \) and the lifetime increases towards lower frequencies \( \omega \) in this limit. Towards \( \omega \rightarrow \Delta \) and \( n_i \rightarrow 0 \) the lifetime vanishes due to the divergence in the DOS.

Now we turn to the unitarity limit\[11\]\[12\]\[13\] where the renormalized frequency is obtained as

\[ \hat{\omega} = \omega + \Gamma \left( \frac{\hat{\omega}}{\sqrt{\Delta_k^2 - \omega^2}} \right)^{-1}. \]

(13)

The DOS in the unitarity limit is determined through the Eq. (13) for given \( \omega/\Delta \) and \( \Gamma/\Delta \). Similar to the Born limit impurity scattering removes the logarithmic singularity in the DOS of the pure system (Fig.1 (b)). In contrast to the Born limit the maximum moves toward higher energies with increasing \( \Gamma \).

In the lower panel of the Fig.1(b), the lifetime as a function of \( \omega \) is shown for the unitarity limit, where \( 1/\tau \propto -1/N(\omega) \). As anticipated from the single-impurity discussion the quasiparticle lifetime increases at \( \omega/\Delta = 1 \) compared to the normal state value. While in the single-impurity case at \( \omega = \Delta \) scattering is completely absent, the effect on the quasiparticle life time becomes...
less pronounced with increasing impurity concentration. The reason lies in the broadening of the quasiparticle spectrum, such that the condition of \( \omega = \Delta \) cannot be perfectly satisfied by a quasiparticle state. Clearly this effect is most significant in the low impurity concentration regime where the spectral width of the quasiparticle narrows. It is also interesting to see that the lifetime behaves very differently for the two scattering limits for energies much lower than \( \Delta \). The dramatic decrease of the lifetime towards \( \omega = 0 \) in the unitarity limit is connected with the presence of a zero-energy bound state at the impurity which gives rise to resonant scattering. Again the broadening of the quasiparticle spectrum with increasing impurity concentration makes this feature less pronounced. In the Born limit obviously this feature is absent, as the Born limit does not capture the boundstate which is a result of multiple scattering at the impurity. In this case actually the opposite happens, the lifetime increases as the quasiparticle energy goes towards zero.

A possibility to observe this enhanced coherence lies in ARPES measurements of the quasiparticle spectrum. We consider the spectral function \( A(\xi_k, \omega) \) given by

\[
A(\xi_k, \omega) = -\frac{1}{\pi} \text{Im} G_{11}(\xi_k, \omega).
\]

There are two distinct directions, nodal and anti-nodal momentum directions. In Fig. 2, the spectral densities of the (a) anti-nodal (\( \phi_k = 0 \)) and (b) nodal (\( \phi_k = \pi/4 \)) direction are shown for \( \Gamma/\Delta = 0.1 \). The longer lifetime gives rise to sharper peaks in the spectral density, which we see as peak narrowing and rising around \( \omega/\Delta = 1 \) for both directions. In addition for the nodal direction the lower energy states become considerably broadened. In Fig. 2 (c) and (d), the dependence of the spectral density on the pair breaking parameter at the Fermi wavevector \( (k_F) \), i.e. \( \xi_k = 0 \) is shown. The increase of the impurity concentration strongly suppresses these peak structure as shown.

Finally we would like to interpolate between the Born and unitarity limits by a varying coupling strength \[15\]. The selfenergy \( \Sigma_0 \) is given by

\[
\Sigma_0 = \Gamma \frac{G_0(\omega)}{\cos^2 \delta_0 - \sin^2 \delta_0 G_0^2(\omega)},
\]

where \( \delta_0 \) is the (s-wave) scattering phase shift. In Fig. 3 (a) and (b), the phase shift dependence of lifetime for various values of \( \Gamma \) is shown at \( \omega/\Delta = 0 \) and \( \omega/\Delta = 1 \), respectively. At \( \omega/\Delta = 1 \), the enhancement of the lifetime grows with increasing the phase shift, in the low impurity concentration regime. On the other hand, at \( \omega/\Delta = 0 \), the lifetime rapidly shrinks with increasing phase shift. This is the effect of the bound state whose energy is determined by the condition \( G_0(\omega) = \cot \delta_0 \) and which approaches zero for \( \delta_0 \to \pi/2 \).

Finally, we shall discuss the s-wave superconductor with non-magnetic or magnetic impurities in both Born and unitarity limit \[16\]. In order to discuss the magnetic impurities we introduce the 4×4 Green’s function including spin degrees of freedom \[8 \[16\]. The magnetic impuri-
ties in the superconductor are classical, and interact with electrons through the s-d Hamiltonian

$$H_{sd} = -\frac{J}{2N} \sum_{k,k'} C_k^{\dagger} \alpha C_{k'} \cdot \mathbf{S},$$

(16)

where $C_k = (c_{k\uparrow}^{\dagger}, c_{k\downarrow}^{\dagger}, -c_{-k\uparrow}, -c_{-k\downarrow})$, and the electron spin operator

$$\alpha = \frac{1}{2} \sigma + \frac{1}{2} \sigma_2 \sigma_2,$$

(17)

with $\delta_i (i=1,2,3)$ as the Pauli matrices in spin space. Then we obtain the renormalized frequency and gap function as

$$\tilde{\omega} = \omega - \Sigma_0, \quad \tilde{\Delta}_k = \Delta_k - \Sigma_1.$$  

(18)

The expression of $\Sigma_0$ and $\Sigma_1$ are shown in table I, II for both Born and unitarity limits. Since both frequency and order parameter are renormalized, the lifetime is given as

$$1/\tau = \text{Im}[\tilde{\omega}] = \text{Im}[\Sigma_0 \pm \sqrt{\xi^2 + (\Delta + \Sigma_1)^2}].$$

(19)

The values of $\omega$ which gives the enhancement of the quasiparticle lifetime are summarized in tables I and II. In the unitarity limit, again the enhancement of the quasiparticle lifetime is observed at the gap edge, i.e. $\omega/\Delta = 1$. On the other hand, in the Born limit, the analogous effect occurs at $\omega/\Delta = 0$. In the case of the s-wave superconductor with non-magnetic impurities, the frequency and gap function renormalize in the same way irrespective to the phase shift $(\omega/\Delta = \tilde{\omega}/\Delta)$. In zero field thermodynamic properties remain unchanged by non-magnetic impurities according to Anderson's theorem.[11]

In conclusion, we have investigated the lifetime of the quasiparticles in d-wave superconductor by using the Green’s function techniques with $T-$matrix approximation. A quasiparticle with energy $\omega/\Delta = 1$ does not suffer scattering from a single non-magnetic impurity. This peculiar feature, which is the manifestation of the superconducting coherence of the quasiparticle, leads to a long lifetime of the quasiparticle in the regime of diluted density of impurities and a spectral function which shows a peak narrowing in the antinodal direction. The best case to look for this effect in the cuprate superconductors is in the strongly overdoped region. These are the most metallic samples so the condition of s-wave scattering is best fulfilled. Simultaneously the superconductivity approaches a weak coupling d-wave limit. Very recently Platé et al.[2] reported an ARPES study of an overdoped Tl-cuprate. Their Fig.4(b) shows a quasiparticle peak in the antinodal but not in the nodal directions in contrast to the observations in the underdoped samples but in agreement with the analysis presented here.

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