Local density of states induced by anisotropic impurity scattering in a d-wave superconductor

P. Pisarski and G. Harań
Institute of Physics, Politechnika Wrocławska, Wybrowe Wyspiańskiego 27, 50-370 Wrocław, Poland

We study a single impurity effect on the local density of states in a d-wave superconductor accounting for the momentum-dependent impurity potential. We show that the anisotropy of the scattering potential can alter significantly the spatial dependence of the quasiparticle density of states in the vicinity of the impurity.

A search for the symmetry of the cuprate superconducting state involves among others theoretical studies of the disordered systems [1, 2, 3]. The most direct probe of a simple defect impact on superconductivity is provided by the scanning tunneling microscopy (STM) measurement of the position-dependent quasiparticle density of states. The STM images of Zn and Ni substitutions at the planar Cu sites in Bi$_2$Sr$_2$CaCu$_2$O$_8$+δ reveal a distinct four-fold symmetry of the local density of states (LDOS) [4, 5] predicted for the d-wave superconductor response to disorder [6, 7]. In addition to providing detailed information on the superconducting state, this kind of experiment may shed light on the nature of the quasiparticle scattering centers. Although the main feature of the four-fold symmetry of the tunneling currents is captured by the model of isotropic impurity scattering, the observed spatial dependence of the quasiparticle density of states is far more complex, and may originate from a non trivial structure of the impurity potential. This aspect of the quasiparticle scattering process has been raised in the discussion of macroscopic measurements in these compounds [8, 9, 10, 11]. It has been shown that the unexpected for the d-wave superconductivity weak impurity-induced suppression of the critical temperature can be understood within a scenario of a momentum-dependent (anisotropic) impurity scattering potential [12, 13, 14, 15]. In the present paper we discuss the effect of anisotropic impurity potential on the local density of states in the vicinity of a single impurity and verify to what extend this scenario can reproduce the STM maps of Bi$_2$Sr$_2$CaCu$_2$O$_8$+δ. There are studies of the momentum-dependent impurity scattering which indicate the existence of the impurity-bound states even for the potential strength far from resonant [16]. Therefore, we focus here on the symmetry of the LDOS and its spatial dependence. For this purpose and for analytical simplicity we consider scattering in the Born approximation. Hereafter we show that the anisotropy of the scattering potential alters the local density of states in the d-wave superconductor but preserves its tetragonal symmetry. Compared to the effect of the isotropic impurity potential it enhances the spatial variation of the quasiparticle density of states and can lead to a long-range spatial modulation of the LDOS spectra. We note that the anisotropy of the impurity potential, if the same as the anisotropy of the superconducting order parameter, enhances the relative magnitude of oscillations in the LDOS for the direction of a gap maximum, especially in the vicinity of the impurity, whereas the impurity potential with maxima in the nodal region inverts this tendency and leads to a larger quasiparticle density of states along the gap node direction.

We consider the momentum-dependent impurity potential [12, 13, 14, 15, 16]

\[ \hat{v}(\mathbf{k}, \mathbf{k}') = [v_i + v_a f(k) f(k')] \hat{r}_3 \]

(1)

where \(v_i, v_a\) are isotropic and anisotropic scattering amplitudes, respectively, \(f(k)\) is the anisotropy function, and \(\hat{r}_i\) (\(i = 1, 2, 3\)) are Pauli matrices. We assume \(f(k) = \pm 1\) such as its Fermi surface (FS) average vanishes, i.e., \(\langle f \rangle = \int_{FS} d\mathbf{S} n(k) f(k) = 0\), where \(n(k)\) is the normalized angle resolved FS density of states, \(\int_{FS} d\mathbf{S} n(k) = 1\). Potential determined by \(f(k) = sgn(k_x^2 - k_y^2) = sgn(\cos 2\phi)\), which is in phase with the d-wave superconducting order parameter leads to a particularly moderate suppression of the critical temperature [12, 13, 16]. In the above \(\phi\) is a polar angle.

We study the effect of the impurity potential on the quasiparticle states using the one particle Green’s function of the \(d_{x^2-y^2}\)-wave superconducting state in the particle-hole notation

\[ \hat{G}_0(\mathbf{k}, \omega_n) = [i\omega_n \hat{r}_0 - \xi_k \hat{r}_3 - \Delta(\mathbf{k}) \hat{r}_1]^{-1} \]

(2)

where \(\Delta(\mathbf{k}) = \Delta(k_x^2 - k_y^2) = \Delta \cos 2\phi\) represents the superconducting order parameter, \(\omega_n\) is the Matsubara frequency, \(\xi_k = \varepsilon_k - \varepsilon_F\) is the quasiparticle energy in the normal state, \(\varepsilon_F\) is the Fermi energy, and \(\hat{r}_0\) is the identity matrix. For simplicity we assume a parabolic dispersion and a two-dimensional (planar) superconductivity. Neglecting the anisotropy of the Fermi surface we concentrate on the feature of coupled anisotropies of the order parameter and the impurity potential. The impurity effect is studied at zero temperature by the analytic continuation of

\[ \hat{G}_0(\mathbf{k}, \omega) = \hat{G}_0(\mathbf{k}, \omega_n)|_{\omega_n = \omega + i0^+} \]

(3)

In order to discuss the real space distribution of the quasiparticle states we take a two-dimensional Fourier transform of the Green’s function [14], which for the parabolic
band $\varepsilon_k = k^2/2m$ and for positive $\omega$ smaller than the Fermi energy reads

$$
\delta G'(k', k, \omega) = \hat{G}_0(k, \omega) \hat{v}(k, k') \hat{G}_0(k', \omega) \tag{5}
$$

while the quadratic term represents the proper Born correction and takes the finite quasiparticle life-time into account

$$
\delta \hat{G}''(k, k', \omega) = \hat{G}_0(k, \omega) \hat{\Sigma}_B(k, k') \hat{G}_0(k', \omega) \tag{6}
$$

where the self-energy $\hat{\Sigma}_B$ is determined by

$$
\hat{\Sigma}_B(k, k') = \sum_{k''} \hat{v}(k, k'') \hat{G}_0(k'', \omega) \hat{v}(k'', k') \tag{7}
$$

Both corrections are evaluated for a single impurity which means that the self-energy is not determined self-consistently. We have neglected changes to the absolute value of the order parameter in the vicinity of the impurity which will not change the symmetry of LDOS images but their absolute magnitudes. The total correction to the Green’s function reads

$$
\delta \hat{G}(k, k', \omega) = \delta \hat{G}'(k, k', \omega) + \delta \hat{G}''(k, k', \omega) \tag{8}
$$

and its real space transform is given by

$$
\delta \hat{G}(r, \omega) = \sum_{k, k'} e^{i(k' - k) r} \delta \hat{G}(k, k', \omega) \tag{9}
$$

Function $\delta \hat{G}$ determines the position dependent impurity-induced change of the quasiparticle density of states near a single impurity

$$
\delta \hat{G}_0(r, \omega) = \int_{-\infty}^{\infty} \frac{d^2 k}{(2\pi)^2} e^{i k r} \hat{G}_0(k, \omega) = \frac{-i \pi m}{2 (2\pi)^2} \int_0^{2\pi} d\phi_k \left[ \frac{\omega \hat{g}_0 + \Delta(k) \hat{\tau}_1}{\sqrt{\omega^2 - \Delta^2(k)}} \left( e^{i k_x r + e^{-i k_y r}} + \hat{\tau}_3 \left( e^{i k_x r} - e^{-i k_y r} \right) \right) \right]
$$

(4)

where similarly to the three-dimensional case $k_\pm = \sqrt{2m} \left[ \varepsilon_F \pm \sqrt{\omega^2 - \Delta^2(k)} \right]^{1/2}$ and $\text{Im} \sqrt{\omega^2 - \Delta^2(k)} \geq 0$. For negative $\omega$ one must multiply the imaginary part of (4) by $\text{sgn}(\omega)$. Here $\hbar = 1$.

We consider the impurity effect in the Born approximation, that is, proceed with the perturbative expansion of the Green’s function up to the second order term in the scattering potential $\hat{v}$. The linear correction results from the impurity-induced change of the Fermi energy

$$
\delta \hat{G}'(k, k', \omega) = \hat{G}_0(k, \omega) \hat{v}(k, k') \hat{G}_0(k', \omega) \tag{5}
$$

and the quadratic term represents the proper Born correction and takes the finite quasiparticle life-time into account

$$
\delta \hat{G}''(k, k', \omega) = \hat{G}_0(k, \omega) \hat{\Sigma}_B(k, k') \hat{G}_0(k', \omega) \tag{6}
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$$
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$$

(4)

We have evaluated the LDOS for equal impurity scattering strength in isotropic and anisotropic channel $\pi N_0 \bar{v}_i = \pi N_0 v_a = 0.1$, where $N_0$ is the density of states per spin at the Fermi level in the normal state, and for the coherence length $\xi_0 = 12 \pi k_F^{-1}$. The distance scale in the figures is set by $k_F^{-1}$. We observe a pronounced spatial variation of the quasiparticle density of states for anisotropic impurity potential. This feature is in agreement with the result of an enhanced LDOS due to a finite range of the scattering potential $\hat{v}$. In Figs. 1a-c we show the distance dependence of the impurity-induced change to the LDOS at the quasiparticle energy $\omega = 1.1 \Delta$ along the a-axis ($\phi = 0$), i.e., gap maximum, and nodal ($\phi = \pi/4$) direction for isotropic scattering (Fig. 1a) and two representative anisotropic impurity potentials $\hat{v}$: $f(k) = \text{sgn} (k_x^2 - k_y^2) = \text{sgn} (\cos 2\phi)$ which is in phase with the d-wave order parameter (Fig. 1b), and $f(k) = \text{sgn} (k_x k_y) = \text{sgn} (\sin 2\phi)$ (Fig. 1c) scattering out of the order parameter phase. We note that the impurity potential in phase with the order parameter enhances the magnitude of oscillations in the LDOS for the direction of a gap maximum, especially in the vicinity of the impurity, whereas the out of phase impurity potential inverts this tendency and leads to a larger quasiparticle density of states in the nodal regions. Significant is also very weak anisotropy of the LDOS near the isotropic impurity (Fig. 1a) where discernible differences between $\phi = 0$ and $\phi = \pi/4$ directions occur at a distance of about $50 k_F^{-1}$ from impurity $\hat{v}$. It shows that visible spatial distribution of intensity maxima and minima in the STM maps is induced by the anisotropy of defect potential. Therefore, we suggest that the apparent anisotropy of the experimental images $\hat{v}$ may possibly result in part from the presence of the momentum-dependent scattering potential. We have also performed the LDOS calculation for quasiparticles below the gap threshold energy and displayed them for $\omega = 0.1 \Delta$ in Figs. 2a-c. Another interesting feature of the anisotropic scattering is a presence of a long-range spatial modulation of the LDOS for the impurity potential in phase with the d-wave order parameter, i.e., $f(k) = \text{sgn} (k_x^2 - k_y^2)$. Such a modulation is absent for isotropic or out of phase scattering (Fig. 3). We summarize our discussion by showing in Figs. 4-5...
comprehensive pictures of the STM images at the frequencies $\omega = 1.1\Delta$ and $\omega = 0.1\Delta$ around simple defects of isotropic and anisotropic Born potential in the ab plane of the d-wave superconductor. The potential strength, coherence length and distance units have been fixed as in Figs. 1-3. The quasiparticle density of states is given in the units of the FS two-spin density of states $N(0)$, $N(0) = 2N_0$, and varies from the lowest (black) to the highest (white) value according to the scale in each figure. We have checked that similarly to the effect on the critical temperature [13] any other scattering potential which is orthogonal to the order parameter (in the sense of the FS integral as the scalar product) gives qualitatively the same LDOS as the discussed above $f(k) = \text{sgn}(\sin 2\phi)$, i.e., out of phase potential. The effect of potentials in phase with the order parameter like $f(k) = \cos 2\phi$ agrees qualitatively with $f(k) = \text{sgn}(\cos 2\phi)$. Therefore, both studied anisotropies can be considered representative for the impurity potential [14]. Although we have restricted our study to nonmagnetic impurity scattering, as a closing remark we note that inclusion of spin $S = 1/2$, 1 or 3/2 scattering does not contribute any quantitative change to the results for the impurity potential obeying the Born approximation.

Concluding, we have shown that the anisotropy of the impurity potential enhances the quasiparticle LDOS in the vicinity of the impurity and leads to discernible differences of its intensity in horizontal and diagonal direction. Depending on its symmetry the impurity potential can rotate the LDOS maxima and minima by 45° degrees and can induce a long-range spatial modulation of the quasiparticle density of states but cannot change the induced by the d-wave superconductivity four-fold symmetry of the STM images.

Note added in proof: A similar modulation to the one in Fig. 3(b) is seen along the gap nodal direction for the potential out of the order parameter phase.

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FIG. 1: Distance dependence of the impurity-induced change to the LDOS, $\delta N(r)$, at the quasiparticle energy $\omega = 1.1\Delta$ along the a-axis ($\phi = 0$ - solid line) and diagonal direction ($\phi = \pi/4$ - dashed line) away from the impurity located at $r = 0$ for a) isotropic impurity potential; b) potential in phase with the order parameter, $f(k) = \text{sgn}(k_x^2 - k_y^2)$; c) potential out of the order parameter phase, $f(k) = \text{sgn}(k_xk_y)$. $N(0)$ is the FS density of states in the normal state and $k_F$ is the Fermi momentum.
FIG. 2: Distance dependence of the impurity-induced change to the LDOS at the quasiparticle energy $\omega = 0.1\Delta$ along the a-axis ($\phi = 0$ - solid line) and diagonal direction ($\phi = \pi/4$ - dashed line) away from the impurity located at $r = 0$ for a) isotropic impurity potential; b) potential in phase with the order parameter, $f(k) = \text{sgn}(k_x^2 - k_y^2)$; c) potential out of the order parameter phase, $f(k) = \text{sgn}(k_x k_y)$. 
FIG. 3: Long-range distance dependence of the impurity-induced change to the quasiparticle density of states along $\phi = 0$ direction at the frequency $\omega = 1.1\Delta$ for a) isotropic impurity potential and the out of the order parameter phase potential, $f(k) = \text{sgn}(k_x k_y)$; b) potential in phase with the order parameter, $f(k) = \text{sgn}(k_x^2 - k_y^2)$. 
FIG. 4: LDOS-map at the frequency $\omega = 1.1\Delta$ around the Born impurity located at (0,0) in the ab plane of the d-wave superconductor for a) isotropic impurity potential; b) potential in phase with the order parameter, $f(k) = sgn(k_x^2 - k_y^2)$; c) potential out of the order parameter phase, $f(k) = sgn(k_x k_y)$. The density of states is given in the units of $N(0)$ by the scale next to each map and the distance is measured in $k_F^{-1}$ units.
FIG. 5: LDOS-map at the frequency $\omega = 0.1\Delta$ around the Born impurity located at (0,0) in the ab plane of the d-wave superconductor for a) isotropic impurity potential; b) potential in phase with the order parameter, $f(k) = \text{sgn}(k_x^2 - k_y^2)$; c) potential out of the order parameter phase, $f(k) = \text{sgn}(k_x k_y)$. Units as in Fig. 4.