Effects of extended impurity perturbation in d-wave superconductor

Yu.G. Pogorelov and M.C. Santos

CFP/Departamento de Física, Universidade do Porto, 4169-007 Porto, Portugal
(Dated: March 22, 2022)

We describe the effects of electronic perturbation distributed on nearest neighbor sites to the impurity center in a planar d-wave superconductor, in approximation of circular Fermi surface. Alike the behavior previously reported for point-like perturbation and square Fermi surface, the quasiparticle density of states \( \rho(\varepsilon) \) can display a resonance inside the gap (and very weak features from low symmetry representations of non-local perturbation) and asymptotically vanishes at \( \varepsilon \to 0 \) as \( \rho \to \varepsilon/\ln^2 \varepsilon \). The local suppression of SC order parameter in this model is found to be somewhat weaker than for an equivalent point-like (non-magnetic) perturbation and much weaker than for a spin-dependent (extended) perturbation.

PACS numbers: 74.25.Jb, 74.62.Dh, 74.72.-h

INTRODUCTION

The study of the density of states (DOS) in high-\( T_c \) superconducting (SC) metal oxides has motivated many theorists and experimentalists through the last years, because it defines such fundamental physical parameters as the quasiparticle conductivity \( \sigma \), the penetration length \( \lambda \), the electronic specific heat, etc. This study is guided by the facts that i) the charge carriers are practically confined to the CuO\(_2\) planes and characterized by 2D wavevectors \( \mathbf{k} = (k_x, k_y) \) and ii) the SC order parameter has d-wave symmetry with four nodal points \( \mathbf{k}_i = (\pm k_F/\sqrt{2}, \pm k_F/\sqrt{2}) \), where the Fermi surface crosses the nodal directions \( k_z = \pm k_y \), the SC gap function \( \Delta_k \) turns zero, and the quasiparticle dispersion law \( E_k = \sqrt{\xi^2_k + \Delta^2_k} \) coincides with that of normal metal, \( \xi_k \). Another important factor is that the high-\( T_c \) materials are the so-called doped metals, where the Fermi energy \( \varepsilon_F \) is defined by the density of charge carriers, introduced by the doping process. This very process creates the scattering centers for quasiparticles, due to random Coulomb fields from ionized dopants. Other scatterers, not related to the density of carriers, can be additionally introduced into the system, and all them can produce considerable effects on its physical properties.

In particular, some resonances can emerge in the quasiparticle spectrum with d-wave gap symmetry, even at low concentrations of impurities. Such resonance manifests itself in a maximum of DOS at a certain energy \( \varepsilon_{res} < \Delta = \max_k |\Delta_k| \), as well as in logarithmic suppression of DOS at \( \varepsilon \ll \varepsilon_{res} \) (the energies being referred to \( \varepsilon_F \)). These conclusions can be directly compared to experimental results, as those obtained in the scanning tunnelling microscopy experiments.

The perturbation that impurities introduce into the electronic subsystem of crystal, depend either on their positions with respect to the lattice and on the potential they produce on nearest matrix sites. Within the simplest possible model, where an impurity only disturbs a single site in the lattice \( \mathbf{k} \in \mathbb{Z} \), the potential is characterized by a single perturbation parameter. This point-like perturbation model allows one to obtain a simple solution for the quasiparticle DOS in terms of their Green functions, leading to the above mentioned possibility of low energy resonances. However, in reality, the impurity perturbations in high-\( T_c \) materials are not exactly point-like but rather extended to a finite number of nearest neighbor lattice sites to the impurity center. This raises an important question on how robust are the results of point-like approximation to the spatial extent and geometry of impurity perturbation. The opposite limit to the point-like perturbation, when the defect is much bigger of the Fermi wavelength and can be treated quasiclassically, hardly applies to real atomic substitutes in high-\( T_c \) systems where the perturbation extends to few nearest neighbors of the impurity site. Recently, an example of such extended impurity center was considered for a specific type of spin-dependent perturbation. Here we use a similar approach to get comparison of the point-like and extended perturbations within the same type of perturbation operator, impossible for the above mentioned case.

Usually, the treatment of low energy excitations in d-wave systems involves a certain parametrization of the spectrum in the vicinity of nodal points. Thus, in the popular approach proposed by P. Lee, one expands the difference \( \mathbf{k} - \mathbf{k}_i \) in the local axes, \( \mathbf{e}_{i,1} = \mathbf{k}_i/k_F \) and \( \mathbf{e}_{i,2} = (\mathbf{e}_{i+1,1} - \mathbf{e}_{i-1,1})/2 \), and then approximates the spectrum components as:

\[
\xi_k = \hbar v_F k_1, \quad \Delta_k = \hbar v_2 k_2,
\]

with two characteristic velocities \( v_2 \ll v_F \). However, this implies a "square" geometry of Fermi surface and, strictly speaking, it only holds close enough to the half-filling condition \( \varepsilon_F/W \approx 1/2 \) (where \( W \) is the bandwidth). Instead, in many high-\( T_c \) compounds we have \( \varepsilon_F/W \ll 1 \) and the geometry of Fermi surface is closer to circular (Fig. 1b). In this case, a more adequate parametrization of spectrum is obtained with \( \xi_k = \hbar v_F (k - k_F) \) and \( \Delta_k = \Delta \cos 2\varphi_k \theta (\varepsilon^2_D - \xi^2_k) \) where \( \varphi_k = \arctan(k_y/k_x) \) and
the theta-function factor restricts SC pairing to the BCS shell of width $\varepsilon_D$ (Debye energy) around $\varepsilon_F$.

Most of the known treatments of impurity effects in doped and disordered $d$-wave SC systems, including a self-consistent T-matrix analysis of DOS, were developed within point-like perturbation model and “square” geometry of Fermi surface \[4, 7\]. The present paper is aimed to extend those studies, in order to include a more realistic features, either of the impurity perturbation (which can affect several equivalent neighbor sites to the impurity ion) and of the Fermi surface geometry (in a more adequate circular approximation).

**PHYSICAL DESCRIPTION OF THE SYSTEM**

We use the Nambu spinors $\Psi_k = (\alpha^\dagger_k \uparrow, a_{-k,\downarrow})$ where $\alpha^\dagger_{k,\sigma}$ and $a_{k,\sigma}$ are the Fermi operators for quasiparticles with wave vector $k$ and spin $\sigma$ and the model Hamiltonian for disordered $d$-wave superconductor:

$$
H = H_0 + H_{imp},
$$
$$
H_0 = \sum_k \Psi_k^\dagger (\xi_k \tilde{\tau}_3 - \Delta_k \tilde{\tau}_1) \Psi_k,
$$
$$
H_{imp} = -\frac{1}{N} \sum_{k,k',p} e^{i(k-k'p)} \sum_{\delta} e^{i(k-k')\delta} \Psi_{k'}^\dagger \tilde{V} \Psi_k.
$$

In what follows we denote by hats the matrices in Nambu indices, e.g., the Pauli matrices $\tilde{\tau}_i$ and the matrix $\tilde{V} = V_{imp} \tilde{\tau}_3$ which describes the quasiparticle scattering by extended (attractive) perturbation $V_{imp}$ around an impurity center $p$, over its near neighbors $\delta$ (Fig. 2). Formally, this perturbation only differs by the presence of $\tilde{\tau}_3$ factor from that considered in Ref. \[14\]. The concentration of randomly distributed centers $c = N^{-1} \sum_p 1$ (where $N$ is the number of cells) is supposed small, $c \ll 1$.

We define the Green function (GF) matrices as:

$$
\hat{G}_{k,k'}(\varepsilon) = \langle \langle \hat{\Psi}_k | \hat{\Psi}_{k'}^\dagger \rangle \rangle = \int_{-\infty}^{0} e^{i(\varepsilon - it)\tau} \langle \langle \hat{\Psi}_k(t) | \hat{\Psi}_{k'}^\dagger(0) \rangle \rangle dt,
$$

where $\langle \langle \ldots \rangle \rangle$ is the quantum-statistical average with Hamiltonian. Eq. 4 and $\{a(t),b(0)|$ the anticommutator of Heisenberg operators. The energy $\varepsilon$ is referred to the chemical potential $\mu$ (identified in what follows with the Fermi energy $\varepsilon_F$). The observable characteristics follow from the averages of products of these operators (at given inverse temperature $\beta$), expressed through the corresponding GF’s by the spectral theorem:

$$
\langle ab \rangle = \int_{-\infty}^{\infty} \frac{d\varepsilon}{e^{\beta \varepsilon} + 1} \text{Im} \langle \langle \hat{\Psi}_k | \hat{\Psi}_{k'}^\dagger \rangle \rangle \varepsilon.
$$

For the disordered system with the Hamiltonian, Eq. 1 we calculate GF’s from the basic equation of motion:

$$
\hat{G}_{k,k'} = \hat{G}_{k,0} \delta_{k,k'} - \frac{1}{N} \sum_{k',p,j} e^{i(k-k'p)} \alpha_{jk} \alpha_{jk'} \hat{G}_{k,0} \tilde{V} \hat{G}_{k',k'}.
$$

Here $\hat{G}_{k,0} = (\varepsilon - \xi_k \tilde{\tau}_3 - \Delta_k \tilde{\tau}_1)^{-1}$, and we expanded the structural functional for impurity scattering in Eq. 4 as: $\sum_{\delta} e^{i(k-k')\delta} = \sum_{j=1}^{4} \alpha_{jk} \alpha_{jk'}$. The functions

$$
\alpha_{1,k} = 2 \cos \frac{k_x}{2} \cos \frac{k_y}{2}, \quad \alpha_{2,k} = 2 \cos \frac{k_x}{2} \sin \frac{k_y}{2},
$$
$$
\alpha_{3,k} = 2 \sin \frac{k_x}{2} \cos \frac{k_y}{2}, \quad \alpha_{4,k} = 2 \sin \frac{k_x}{2} \sin \frac{k_y}{2},
$$

realize irreducible representations of the $C_4$ point group ($j = 1$ being related to $A_-, j = 2, 3$ to $E_-$, and $j = 4$ to
B-representations \(13\) and thus satisfy the orthogonality condition
\[
\frac{1}{N} \sum_{\mathbf{k}} \alpha_{j,k} \alpha_{j',k} = \delta_{jj'}.
\]
The impurity effects on quasiparticle spectrum are then naturally classified along these representations, alike the known results for magnetic impurities in ferro- and antiferromagnetic crystals \(16\) \(17\).

**T-MATRIX SOLUTIONS FOR THE GREEN FUNCTIONS**

The orthogonality of the \(\alpha_{j,k}\) functions implies that in the general solution to Eq. 4
\[
\tilde{G}_k = \left[\left(\tilde{G}_k^0\right)^{-1} - \tilde{\Sigma}_k\right]^{-1},
\]
the self-energy matrix turns additive in these representations: \(\tilde{\Sigma}_k = \sum_{j} \tilde{\Sigma}_{jk}\). Each partial term in the latter sum can be given by a specific group expansion (GE), like those known for point-like impurity perturbations in normal \(18\) or superconducting \(4\) \(14\) systems and also for extended perturbations in magnetic systems \(17\),
\[
\tilde{\Sigma}_{jk} = -c\tilde{T}_j \left[1 - c\tilde{A}_j - c\tilde{A}_j^2 + \right. \\
+ c \sum_{n \neq 0} \left( \tilde{A}_j(n) e^{-i\mathbf{k} \cdot \mathbf{n}} + \tilde{A}_j^4(n) \right) \\
\left. \times \left(1 - \tilde{A}_j^2(n)\right)^{-1} + \ldots \right].
\]
(Eq. 7)

Here \(\tilde{T}_j = \tilde{V}(1 + \tilde{G}_j)^{-1}\) is the (renormalized) partial T-matrix, and the matrices \(\tilde{A}_j(n)\) represent indirect interactions (in \(j\) symmetry channel) between scatterers at sites 0 and \(n\):
\[
\tilde{A}_j(n) = -\tilde{G}_j(n) \tilde{T}_j, \quad \tilde{G}_j(n) = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{n}} \alpha_{j,k} \tilde{G}_k,
\]
\[
\tilde{A}_j = \tilde{G}_j \tilde{T}_j, \quad \tilde{G}_j = \tilde{G}_j(0).
\]
(Eq. 6)

The sum \(\sum_{n \neq 0}\) in Eq. 6 describes all the processes involving pairs of impurities, it implies averaging in random impurity configurations and hence runs over all the lattice sites \(n\), the omitted terms are for triples and more of impurities. This defines a generalization of the GE approach for extended impurity centers in superconductors. If the series in the brackets is restricted to its first term, the self-energy matrix \(\tilde{\Sigma}_k\) becomes independent of \(\mathbf{k}\):
\[
\tilde{\Sigma}_k \rightarrow \tilde{\Sigma} = -c \sum_{j} \tilde{T}_j.
\]
(Eq. 8)

Then, for small enough concentration of impurities, the renormalization of T-matrices can be neglected and we arrive at
\[
\tilde{T}_j \rightarrow \tilde{T}_j^0 = \tilde{V}(1 + \tilde{G}_j^0)^{-1}, \quad \tilde{G}_j^0 = \frac{1}{N} \sum_{\mathbf{k}} \alpha_{j,k} \tilde{G}_k^0.
\]
(Eq. 9)
The matrix functions \(\tilde{G}_j^0\) can be expanded in the basis of Pauli matrices
\[
\tilde{G}_j = \rho_2 (g_{j0} + g_{j1} \tau_1 - g_{j3} \tau_3)
\]
(Eq. 10)
where \(\rho_2 = 4/(\pi W)\) is the constant DOS in 2D normal system (the absence of \(\tau_2\) component in Eq. 10 is related to the fact that the gap function \(\Delta_k\) is chosen real). Passing in Eq. 4 from summation in \(\mathbf{k}\) to integration in "polar" coordinates \(\xi_k = \xi\) and \(\varphi_k = \varphi\) (Fig. 1b) accordingly to the rule:
\[
\frac{1}{N} \sum_{\mathbf{k}} f_k \approx \rho_0 \frac{\alpha_2}{4\pi} \int_{-\mu}^{2/\rho_0 - \mu} d\xi \int_0^{2\pi} d\varphi f(\xi, \varphi),
\]
we calculate the dimensionless coefficient functions \(g_{ji}\).
Some of them are zero by the symmetry reasons: \(g_{11} = g_{41} = 0\), the rest can be approximated as:
\[
g_{j0} \approx \alpha_{2j} g_{0}, \quad g_{j3} \approx \alpha_{2j} g_{1}, \quad g_{21} = -g_{31} \approx \alpha_{2j} g_{1}.
\]
(Eq. 11)

Here \(\alpha_{2j}\) are the average values of \(\alpha_{j,k}^2\) over the Fermi surface: \(\alpha_{11}^2 \approx 4(1 - \omega)\), \(\alpha_{2,3}^2 \approx 4\omega\), \(\alpha_3^2 \approx 2\omega^2\), where the band occupation parameter \(\omega = \mu/W\) is supposed small, in concordance with the chosen circular geometry. The functions \(g_{0}\) and \(g_{1}\) are known from the studies of point-like perturbations \(20\), \(21\).

\[
g_0(\epsilon) = \frac{\epsilon}{4\pi} \int_{-\mu}^{2/\rho_0 - \mu} d\xi \int_0^{2\pi} \frac{d\varphi}{\epsilon^2 - \xi^2 - \Delta^2 \cos^2 2\varphi} \\
\approx \epsilon \left[1/\tilde{\mu} - F_1(1 - \epsilon^2/\Delta^2)/\Delta\right],
\]
(Eq. 12)

\[
g_1(\epsilon) = \Delta \frac{2\pi}{\rho_0} \int_0^{\epsilon_D} d\xi \int_0^{2\pi} \frac{\cos^2 2\varphi d\varphi}{\epsilon^2 - \xi^2 - \Delta^2 \cos^2 2\varphi} \\
\approx \Delta/\epsilon_D + 2 \left[F_2(1 - \epsilon^2/\Delta^2) + \epsilon^2/\Delta^2 F_1(1 - \epsilon^2/\Delta^2)\right],
\]
(Eq. 13)

they include \(\tilde{\mu} = \mu(1 - 2\omega/\pi) \approx \mu\) and the functions
\(F_1(z) = K(1/z)/\sqrt{z}\) and \(F_2(z) = \sqrt{2E(1/z)}\) with full elliptic integrals of 1st and 2nd kind \(K\) and \(E\), having similar behavior with the elementary functions obtained within square geometry \(3\). In the same similarity, the function
\(g_3 = (4\pi)^{-1} \int_{-\mu}^{2/\rho_0 - \mu} d\xi \int_0^{2\pi} d\varphi (\epsilon^2 - \xi^2 - \Delta^2 \cos^2 2\varphi)\) is practically constant: \(g_3 \approx \ln(\sqrt{2}/2\omega) - 1\), within the relevant energy range \(|\epsilon| \ll W, \mu\).

Using these results, we readily calculate the partial T-matrices, Eq. 10. The most important contribution to \(\tilde{\Sigma}\) comes from the \(j = 1\) term (\(A\)-representation):
\[
\tilde{F}_1^0 = \frac{\rho_0}{\alpha_{1j}^2 \rho_0} \frac{v_A v_{Ag} - \tilde{\tau}_3}{D_A},
\]
(Eq. 14)
where \( v_{A} = \alpha_{A}^{2}V_{imp}\rho_{0}/(1 - \alpha_{A}^{2}V_{imp}\rho_{0}g_{3}) \) is the dimensionless perturbation parameter in the A-channel, and
\[ D_{A}(\varepsilon) = 1 - v_{E}^{2}g_{0}^{2}(\varepsilon) \]
is the energy dependent denominator. In particular, it can produce a low energy resonance at \( \varepsilon = \varepsilon_{res} \) such that \( \text{Re}D_{A}(\varepsilon_{res}) = 0 \), analogous to the above mentioned resonance from point-like impurity center. This requires that \( v_{A} \) exceeds some critical value \( \approx 2/\pi \).

The contributions from \( j = 2, 3 \) (E-representation) are:
\[ \tilde{T}^{0}_{2,3} = \frac{\nu E}{\alpha_{A}^{2}\rho_{0}} \left( \frac{\varepsilon}{D_{E}} \right), \]
with the respective perturbation parameter \( \nu_{E} = \alpha_{E}^{2}V_{imp}\rho_{0}/(1 - \alpha_{E}^{2}V_{imp}\rho_{0}g_{3}) \) and denominator \( D_{E} = 1 - v_{E}^{2}(g_{0}^{2} - g_{1}^{2}) \). It is less probable to have a resonance effect in this channel at low occupation \( \omega \ll 1 \), since i) the parameter \( \nu_{E} \) is reduced vs the A-channel value, and ii) there is a competition between \( \text{Re}g_{0}^{2} \) and \( \text{Re}g_{1}^{2} \) in the denominator \( D_{E} \).

The B-channel contribution \( (j = 4) \) has the same structure as the A-channel term, Eq. 14 but with \( v_{A} \) replaced by a strongly reduced value \( v_{B} = \alpha_{4}^{2}V_{imp}\rho_{0}/(1 - \alpha_{4}^{2}V_{imp}\rho_{0}g_{3}) \), hence it turns even less important than the E-channel terms.

**PERTURBATION OF OBSERVABLE VALUES**

Now we are in a position to describe the perturbation of basic observable characteristics of SC system by extended impurity centers. Thus, the global DOS is defined by the momentum diagonal GF’s, \( \rho(\varepsilon) = (\pi N)^{-1}\sum_{k} \text{Im Tr} \hat{G}_{k} \), and, using Eqs. 8, 14, 15 in Eq. 6 it is obtained as
\[ \rho(\varepsilon) = \frac{\rho_{0}}{\pi} \text{Im} g_{0}(\varepsilon - \Sigma_{0}). \]

Here the scalar self-energy
\[ \Sigma_{0} = \frac{cg_{0}(\varepsilon)}{\rho_{0}} \left( \frac{\nu_{A}^{2}D_{A}}{\alpha_{A}^{2}D_{A}} + \frac{\nu_{E}^{2}D_{0}}{\alpha_{E}^{2}D_{E}} + \frac{\nu_{B}^{2}D_{0}}{\alpha_{B}^{2}D_{B}} \right) \]
includes the effects of extended impurity centers in all three channels. The result of direct calculation from Eq. 10 with use of Eq. 17 for the characteristic choice of parameters, \( W = 2 \text{ eV}, \mu = 0.3 \text{ eV}, \varepsilon_{D} = 0.15 \text{ eV}, V_{imp} = 0.2 \text{ eV} \) (giving for particular channels: \( v_{A} \approx 0.934, v_{E} \approx 0.888, \) and \( v_{B} \approx 0.006 \)), and \( c = 0.15 \), is shown in Fig. 3. It is quite similar to the known results for point-like impurities [2, 4], showing a reduction of the sharp coherence peak at \( \varepsilon = \Delta \) and emergence of a relatively broad low-energy resonance at \( \varepsilon_{res} \) (shown by the arrow), mainly due to the A-channel effect. But, additionally, there are small “antiresonance” effects from the E-channel (insets to Fig. 3) at \( \varepsilon \approx \Delta \) and at some high enough energy \( \sim 70\Delta \) in this case. Clearly, these E-channel features shouldn’t have any practical effect on the system thermodynamics.

The local density of states (LDOS) on \( n^{th} \) site is expressed in terms of GF’s as \( \rho_{n}(\varepsilon) = (\pi N)^{-1} \sum_{k,k'} \text{Im Tr} e^{i(k-k')\varepsilon} \hat{G}_{k,k'} \). Its variation \( \delta \rho_{n}(\varepsilon) = \rho_{n}(\varepsilon) - \rho(\varepsilon) \), compared to the mean value \( \rho(\varepsilon) = N^{-1} \sum_{n} \rho_{n}(\varepsilon) \) (identical to the global DOS), is only given by the momentum-nondiagonal GF’s:
\[ \delta \rho_{n}(\varepsilon) = \frac{1}{\pi N} \sum_{k,k' \neq k} \text{Im Tr} e^{i(k-k')\varepsilon} \hat{G}_{k,k'}. \]

These functions are easily calculated for the simplest case of a single impurity center at \( p = 0 \):
\[ \hat{G}_{k,k'} = \frac{1}{N} \sum_{j} \alpha_{j,k} \hat{G}_{j}^{0} \hat{T}_{j}^{0} G_{k',\alpha_{j,k}^{0}}, \]
describing a finite effect on the local characteristics near the impurity. Thus, the quantity \( \delta \rho_{n} \) attains its maximum value at \( n = \delta \), the nearest neighbor sites to the impurity. Using Eq. 14 and the orthogonality relations,
we expand this value in a sum:
\[
\delta \rho_n(\varepsilon) = \frac{1}{N^2} \times \sum_{k,k'} \text{Im} \sum_{j,j'} \text{Tr} \left( e^{ik-\delta} \alpha_{j,k} \tilde{G}_k^{\alpha} \tilde{G}_j^{\alpha} \right) e^{-ik'-\delta} = \frac{1}{\pi} \sum_{j} \text{Im} \text{Tr} \tilde{G}_j \tilde{G}_j^{\alpha} \tilde{G}_j^{\alpha},
\]
and present the overall maximum LDOS as:
\[
\rho_{n=\delta}(\varepsilon) = \left( 2g_{\delta}\varepsilon + \frac{v_A N_A}{\alpha_d^2 D_A} + \frac{v_E N_E}{\alpha_d^2 D_E} + \frac{v_B N_B}{\alpha_d^2 D_B} \right) \]
Alike Eq. (17) for global DOS and the case of Ref. [14] for LDOS, the resonance contribution to Eq. (20) comes from the A-channel with the numerator \( N_A = 2g_3 + v_A (g_0^2 + g_3^2) \), while other channels with \( N_E = 2g_3 + v_E (g_0^2 - g_3^2) \) and \( N_B = 2g_3 + v_B (g_0^2 + g_3^2) \) mainly contribute to renormalization of the pure d-wave DOS \( \rho_d(\varepsilon) = 2/\pi \text{Im} g_0(\varepsilon) \). The calculated from Eq. (20) behavior of LDOS on nearest neighbor sites to the impurity is shown by solid line in Fig. 3. It displays a low energy resonance (the arrow), much more pronounced than that in the global DOS, Fig. 2 and the overall enhancement compared to the LDOS curve for remote sites from impurity \( \rho_{n=\infty} = \rho_d \) (the dashed line). This picture can be compared with the direct experimental measurements of differential conductance through the STM tip positioned close to and far from an impurity center [8].

In a quite similar manner, the local perturbation of SC order parameter can be considered. The local d-wave SC order in the unit cell containing the impurity (Fig. 2) is given by the average \( \Delta_{32} = 2V\langle a_{\delta_3,\downarrow} a_{\delta_2,\uparrow} \rangle \) [14], where \( V \) is the SC coupling constant and site operators \( a_{n,\sigma} \) are expressed through band operators: \( a_{n,\sigma} = \lambda^{-1/2} \sum_k e^{ik\cdot n} \phi_{k,\sigma} \). For \( V_{\text{imp}} = 0 \), this average coincides with the uniform gap parameter:
\[
\Delta = \frac{2V}{N^2} \sum_{k} e^{ik(\delta_2-\delta_3)} \langle a_{-k,\downarrow} a_{k,\uparrow} \rangle = \frac{4\lambda\Delta}{\pi} \int_0^{\varepsilon_D/\Delta} \left[ F_2(1+x^2) - F_1(1+x^2) \right] dx, \tag{21}
\]
the latter expression (with the dimensionless d-wave coupling constant \( \lambda = V\rho_0(\omega) \) being obtained from Eqs. 9 and 13). The integral in Eq. (21) behaves as a logarithm: \( \varepsilon_D/\Delta \int_0^\infty \left[ F_2(1+x^2) - F_1(1+x^2) \right] dx \approx (\pi/4) \ln(2.428a) \) at \( a \gg 1 \), thus providing \( \Delta \approx 2.428a \exp(-1/\lambda) \).

But for \( V_{\text{imp}} \neq 0 \) this value is locally suppressed. The suppression is characterized by the dimensionless parameter \( \eta_{\text{sup}} = 1 - \Delta_{32}/\Delta \), confined between 0 (pure SC) and 1 (complete local suppression of SC order) [14], and it only results from non-diagonal GF’s:
\[
\eta_{\text{sup}} = \frac{2V}{N^2} \sum_{k,k'} (-1)^j \sum_{\delta_2} \text{Tr} \tilde{G}_j \tilde{G}_k^{\alpha} \tilde{G}_j^{\alpha} \tilde{G}_k^{\alpha} \tag{22}
\]

Using here Eqs. (19) and (20) leads to the expression:
\[
\eta_{\text{sup}} = \frac{4\lambda\Delta}{\pi} \int_0^{\varepsilon_D/\Delta} F(x) dx, \tag{23}
\]
where only the E-channel terms contribute to the dimensionless function
\[
F(x) = \frac{-2v_E}{v_A} \text{Im} g_1(x\Delta) N_E \]
(compared in Fig. 5 with the integrand for the uniform gap equation, Eq. 21). Numeric analysis of this expression for the above chosen perturbation parameters results in \( \eta_{\text{sup}} \approx 0.47 \). This is somewhat smaller than the respective value for point-like impurity in d-wave system [6]: \( \eta_{\text{sup}} = 1/(1+v^2) \) (assuming \( v \) equal to \( v_A \)), and more than twice weaker than almost complete suppression in the case of spin-dependent perturbation of the same dimensionless magnitude [14]. Those relations confirm the general Abrikosov-Gor’kov conclusion [22] on the pair-breaking effects by impurities in superconductors, irrespectively of their spatial extension.

FIG. 4: Local density of states on the nearest neighbor site to an extended impurity center, for the same choice of parameters as in Fig. 3 (but supposing \( c \to 0 \)). Note an overall enhancement of electronic density compared to remote sites from impurity (dashed line) and a much stronger effect of the low-energy resonance (the arrow).
The above given analysis corresponds to the simplest restriction of the group series, Eq. 4, for self-energy to its first, single-impurity term with use of unperturbed GF’s. The resulting linear approximation in impurity concentration: $\Sigma = - c \sum_j T_j^0$, is only justified when this concentration is low enough $c \ll c_0$, where $c_0 \sim \rho_0 \varepsilon_0$ is related to the characteristic energy scale $\varepsilon_0$ for impurity perturbation (in this case $\varepsilon_0 \sim \varepsilon_{\text{rel}}$). At higher concentrations, $c > c_0$, when perturbations from different impurity centers effectively overlap, a simplest way to take account of these collective impurity effects is provided by replacement of $\Sigma$ by its self-consistent analogue $\Sigma^{(sc)} = -c \sum_j T_j^{(sc)}$, in the spirit of well-known self-consistent T-matrix approximation \[11\]. It was shown for the case of point-like impurity perturbation \[11\], that effects of such self-consistency are most essential at the lowest excitation energies, $\varepsilon \ll \Delta$. In view of the similarity in the system response to point-like and extended perturbations and of the predominant role of the $A$-channel at low energies, we can restrict the self-consistency of T-matrix only to its $A$-channel term. Then Eqs. (6) and (8) are modified to:

$$\tilde{G}^{(sc)}_k = \left[ \left( G^0_k \right)^{-1} + c \sum_{j=2}^4 \tilde{T}_j + c \tilde{T}_1^{(sc)} \right]^{-1} \tag{24}$$

including the self-consistent $A$-channel T-matrix:

$$\tilde{T}_1^{(sc)} = \tilde{V}[1 + \tilde{G}_1^{(sc)} \tilde{V}]^{-1}.$$  

Alike Eq. 10 the self-consistent GF matrix $\tilde{G}_1^{(sc)} = N^{-1} \sum_k \alpha_{1k}^2 \tilde{G}_k^{(sc)}$ can be parametrized in Pauli matrices:

$$\tilde{G}_1^{(sc)} = \rho_0 \alpha_1^2 \left(g - g_3 \tilde{r}_3\right).$$

Then, using Eq. 15 in Eq. 24, we readily conclude that $\Sigma^{(sc)}$ is diagonal in Nambu indices that is, within the considered self-consistent $T$-matrix approximation for extended impurity centers, the scattering by dopants does not influence the $d$-wave order parameter, the same as for point-like centers \[4\]. Hence, the self-consistency should be achieved only for the scalar function $g = (2N)^{-1} \sum \text{Tr} \tilde{G}_k^{(sc)}$ through the equation:

$$g(\varepsilon) = g_0(\varepsilon - \Sigma_0^{(sc)}(\varepsilon)), \tag{25}$$

where the scalar self-consistent self-energy:

$$\Sigma_0^{(sc)}(\varepsilon) = \frac{c g(\varepsilon)}{\rho_0} \left( \frac{v_A^2}{\alpha_1^2 D_A} + \frac{2 v_E^2}{\alpha_2^2 D_E} + \frac{v_B^2}{\alpha_2^2 D_B} \right), \tag{26}$$

includes the self-consistent denominator: $D^{(sc)}(\varepsilon) = 1 - v_A^2 g^2(\varepsilon)$. Then, passing to dimensionless energy $x = \varepsilon/\Delta$ and denoting

$$\frac{\Sigma_0^{(sc)}}{\Delta} = \sigma(g) = \alpha g \left( \frac{\beta}{1 - \alpha^2 g^2 + \beta^2} \right) \tag{27}$$

with $\alpha = v_A$, $\beta = cv_A/(\alpha_1 \rho_0 \Delta)$, $\beta' = c[2v_E^2/(\alpha_2^2 D_E) + v_B^2/(\alpha_1^2 D_B)]/(v_A \rho_0 \Delta)$ and $\gamma = \Delta/\mu (1 - 2\omega/\pi)$, we arrive at the self-consistency equation for $g = g(x)$ as:

$$g = (x - \sigma) \left\{ \gamma - \frac{1}{\sqrt{1 - (x - \sigma)^2}} K \left[ \frac{1}{1 - (x - \sigma)^2} \right] \right\}, \tag{28}$$

with $\sigma = \sigma(g)$ defined by Eq. 27. This equation is quite similar to that reported for point-like impurity centers and square-like geometry \[11\], \[11\], differing only by the appearance of additional term $\beta'$ in Eq. 27. In the same way, Eq. 28 admits two types of solutions in the energy range of principal interest $x \rightarrow 0$. One of them, $g = g^{(1)}(x)$, tends in this limit to a finite imaginary value: $g^{(1)}(x \rightarrow 0) \rightarrow i \gamma_0$, defined by the equation

$$1 = -\alpha f(\gamma_0) \left\{ \gamma - \frac{1}{\sqrt{1 + \alpha^2 g_0^2}} \times \right.$$  

$$\times K \left[ \frac{1}{1 + \alpha^2 g_0^2} \right] \right\}, \tag{29}$$

with $f(\gamma_0) = \beta' + \beta/(1 + \alpha^2 \gamma_0^2)$. Another solution, $g = g^{(2)}(x)$, is vanishing in this limit: $g^{(2)}(x \rightarrow 0) \rightarrow 0$, so
that all the denominators \( D \) in Eq. 26 can be safely put equal unity, simplifying Eq. 28 to:

\[
g = (x - \alpha' g) \left\{ \frac{1}{\left[ 1 - (x - \alpha' g)^2 \right]} \right\},
\]

with \( \alpha' = \alpha (\beta + \beta') \). Its solution has the same logarithmic asymptotics at \( x \to 0 \):

\[
g(x) \approx x \left[ 1 - \frac{1}{\pi \alpha' \ln(2 \pi \alpha' / x)} \right],
\]

as found in Refs. 4, 7. Also the conclusion on the validity range for each of the two solutions, \( g^{(1)} \) far enough from and \( g^{(2)} \) close to the Fermi level 20, remains true in the present situation. Thus the DOS \( \rho(\varepsilon) \) at \( \varepsilon \ll \varepsilon_{\text{res}} \) should be suppressed as:

\[
\rho(\varepsilon) \approx \frac{\rho_0 \varepsilon}{2 \pi \Delta \left[ \alpha' \ln(2 \pi \alpha' / \varepsilon) \right]^2}
\]

compared to its linear asymptotics \( \rho \sim \rho_0 \varepsilon / \Delta \) resulting from the linear in \( c \) approximation, seen in Fig. 3.

**CONCLUSION**

The Green function analysis is developed for the quasiparticle spectrum in a planar \( d \)-wave superconductor with finite concentration of impurity centers which perturb atomic energy levels on nearest neighbor lattice sites. A generalization of the method of group expansions for quasiparticle self-energy is obtained for such extended impurity centers. The general picture of spectrum restructuring is found quite similar to that previously established for point-like impurity perturbation, though some new specific features due to extended nature of the perturbation are also indicated. In particular, it is found that the effects on the quasiparticle DOS and on the SC order parameter result from different irreducible representations of the point symmetry group of the impurity center. The self-consistent procedure is proposed for higher concentration of extended impurities, generalizing the known formulations for point-like centers, and a qualitative similarity with that case is demonstrated.

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