Nodal quasiparticles in doped d-wave superconductors: self-consistent T-matrix approach

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A comparative analysis has been done of the formerly established two self-consistent solutions for the density of quasiparticle states in doped d-wave superconductors, having strikingly different and disputed behavior near the Fermi energy. One of them (1) remains finite in this limit, while the other (2) tends to zero. To resolve this discrepancy, the known Ioffe-Regel criterion for band states, widely used for doped semiconductors, was applied to these solutions. It is shown that both them are valid in limited and different energy regions, where the corresponding quasiparticles are weakly damped. In particular, density of states of nodal quasiparticles near the Fermi level is provided by the (2) solution, while the (1) only applies far enough from this level.

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The self-consistent T-matrix approximation (SCTMA [1], or FLEX method [2]) is extensively used for description of quasiparticles and their density of states (DOS) in disordered crystals, in particular, in the doped high-Tc superconducting cuprates. Its advantage consists in relative simplicity and transparency for numeric calculations. In fact, a number of controversies emerge when the tailed substantiation of the method. Perhaps the central ambiguity motivates us to reconsider this situation in a more general context of the theory of elementary excitations in disordered systems [11].

There is a consensus on that the single-particle excitations in disordered sysytems can be either of band (extended) type or localized type [12], both types forming certain continuous regions of spectrum separated by the so-called mobility edges $\varepsilon_c$ (Fig. 1). The extended states can be approximately described by the wavevector $k$, through a dispersion law $E_k$ and a broadening $\Gamma_k$, as far as the Ioffe-Regel criterion (IRC) [13] for the mean free path $\ell$ and the wavelength $\lambda$ holds:

$$\ell \gg \lambda, \quad k |\partial E_k/\partial k| \gg \Gamma_k. \quad (1)$$

Then the real and imaginary parts of self-energy $\Sigma_k$ in the disorder averaged Green function (GF) $G_k = (\varepsilon - \varepsilon_k - \Sigma_k)^{-1}$ permit to define: $E_k = \varepsilon_k - \Re \Sigma_k(E_k)$, $\Gamma_k = \Im \Sigma_k(E_k)$ [14], and the modified DOS $\rho(\varepsilon) = \pi^{-1} \Im G(\varepsilon) \approx \rho_0(\varepsilon) / (\partial E_k/\partial \varepsilon_k)_{E_k=\varepsilon}$ ($\varepsilon_k$ and $\rho_0(\varepsilon)$ being respectively the dispersion law and DOS in pure crystal). The condition $\ell \sim \lambda$ is reached when $E_k$ approaches the mobility edges, then the very notion of self-energy correction to the initial band spectrum $\varepsilon_k$ ceases to make sense and the averaged properties of localized states are only described by their DOS $\rho(\varepsilon)$.

In the case of disorder due to fixed impurity perturbation $V_p$ at random sites $p$ (Lifshitz model) for the normal metal quasiparticles, the modification of band spectrum can involve new specific features like local or resonance levels [13], and there are various ways to expand the self-energy in groups of interacting impurity centers [16], analogous to the classical Ursell-Mayer group expansions (GE) for statistical sum [17]. For instance, the so-called fully renormalized GE [18] reads:

$$\Sigma_k = \sum_p \frac{V_p}{1 - GV_p} \left[ 1 + \frac{A_{p,p'} e^{i(k' - p)} - A_{p,p'} A_{p',p}}{1 - A_{p,p'} A_{p',p}} + \ldots \right],$$

where $A_{p,p'} = V_p G_{p,p'}/(1 - GV_p)$ includes $G_{p,p'} = N^{-1} \sum_{k \neq k'} e^{i(p' - p)k'} G_k$ and $G = G_{p,p}$. Other types

FIG. 1: General Mott picture of spectrum of elementary excitations in a disordered system.
of GE can differ from Eq.\ref{eq:2} either in the structure of next to unity terms and in the degree of renormalization of $G$ and $A$ functions present in them. The relevant expansion parameter is not simply the impurity concentration $c = \sum_p N^{-1}$ (supposedly small, $c \ll 1$) but the "gas parameter" $c\sum_{n\neq 0}^{\infty} A_{0,n}^2$ for the "non-ideal gas" of impurities with effective interaction described by the (energy dependent) functions $A_{p,p'}$. Hence the convergence of the series \cite{22} turns also energy dependent, reflecting the division between the above referred types of states. It can be shown that this convergence is equivalent to validity of the IRC \cite{10}. Within the energy domain of convergence, the self-energy can be approximated by Eq.\ref{eq:2} with only unity term retained in the brackets: $\Sigma_k \approx \Sigma = cV_L/(1 - GV_L)$, the momentum-independent SCTMA form. But beyond this domain, the SCTMA does not make sense and a better description of DOS is obtained with GE's, different from Eq.\ref{eq:2}. Below we check the fulfillment of IRC for nodal quasiparticle states in a d-wave superconductor with dopants and conclude on the validity of the SCTMA solutions.

Let us start from the most common model Hamiltonian for this problem:

$$H = \sum_k \psi_k^\dagger (\xi_k \tilde{c}_k + \Delta_k \tilde{c}_k^\dagger) \psi_k - \frac{V_L}{N} \sum_{k,k',p} e^{i(k-k')_p} \psi_k^\dagger \tilde{c}_k \tilde{c}_k \psi_{k'}.$$ \hspace{1cm} (3)

Here the Nambu spinors $\psi_k^\dagger = \left( c_{k\uparrow}^\dagger, c_{-k \downarrow} \right)$ include Fermi operators of normal quasiparticles with the simplest 2D dispersion law $\xi_k = 2t (2 - \cos ak_x - \cos ak_y) - \mu$ in square lattice, approximately constant DOS $\rho(\varepsilon) \approx \rho_0 = 4/(\pi W)$ where $W = 8t$ is the bandwidth, and chemical potential $\mu$; $\tilde{c}_k$ are the Pauli matrices. The d-wave gap function is $\Delta_k = \Delta \theta (\varepsilon_F^2 - \xi_k^2)$, where the "Debye" energy $\varepsilon_D \gg \Delta$, and $\varphi_k = \arctan k_x/k_y$ defines the nodal lines $k_x = \pm k_y$. The Lifshitz perturbation term in Eq.\ref{eq:3} produces scattering of quasiparticles, modelling the impurity effect of dopants.

The relevant GF is a Nambu matrix $\tilde{G}_k = \left\langle \langle \psi_k^\dagger \mid \psi_k^\dagger \right\rangle \right.$ with matrix elements being Fourier transformed two-time GF's:

$$\left\langle \langle a \mid b \right\rangle \rangle_\varepsilon = i \int_0^{\infty} e^{i(\varepsilon + \mu)t} \left\langle \{ a(t), b(0) \} \right\rangle dt$$

where $\langle \ldots \rangle$ is the quantum statistical average with the Hamiltonian\cite{22} and $\{ \ldots \}$ is the anticommutator of Heisenberg operators. In analogy with the above scalar GF $G_k$ for normal quasiparticles, the general solution for this matrix is

$$\tilde{G}_k = (\varepsilon - \mu - \xi_k \tilde{c}_k - \Delta_k \tilde{c}_k^\dagger - \tilde{\Sigma}_k)^{-1}.$$ \hspace{1cm} (4)

All the impurity effects are now accounted for by a GE for the self-energy matrix $\tilde{\Sigma}_k$ \cite{20} (cf. Eq.\ref{eq:2}):

$$\tilde{\Sigma}_k = \frac{1}{N} \sum_p \tilde{V} \left( 1 - \tilde{G} \tilde{V} \right)^{-1} \left\{ 1 + \sum_{p' \neq p} [\tilde{A}_{p,p'} e^{ik(p-p')} - \tilde{A}_{p,p'} \tilde{A}_{p',p}] \times \left[ 1 - \tilde{A}_{p,p'} \tilde{A}_{p',p} \right]^{-1} + \ldots \right\}.$$ \hspace{1cm} (5)

Here the matrices: $\tilde{V} = V_L \tilde{c}_k$, $\tilde{G} = N^{-1} \sum_k \tilde{G}_k$, and $$\tilde{A}_{p,p'} = N^{-1} \sum_{k^\prime \neq k} e^{ik'(p-p')} \tilde{G}_{k'} \left( 1 - \tilde{G} \tilde{V} \right)^{-1},$$ and some additional restrictions are imposed on summation in momenta in the products like $\tilde{A}_{p,p'} \tilde{A}_{p',p}$, resulting from a specific procedure of consecutive elimination of GF's in the infinite chain of coupled Dyson equations. There are possible different such procedures and, respectively, different types of GE \cite{10}. Generally, GE’s are only asymptotically convergent and the best choice between them is determined by their convergence range with respect to energy $\varepsilon$.

The conditions for convergence of different GE’s were studied in detail for a number of types of elementary excitations in crystals with impurities \cite{22, 7}, and this permitted to establish certain general criteria for the corresponding characteristic regions of spectrum. In particular, the region of band states is best described by the so-called fully renormalized GE which ceases to converge at approaching the mobility edges where IRC, Eq.\ref{eq:11} fails. For the GE, this is expressed by the tendency of all its terms, next to the unity in curled brackets in Eq.\ref{eq:3} to become $\sim 1$.

Alike the above mentioned scalar case, the SCTMA just corresponds to the fully renormalized GE, restricted to only its first term. Hence it is only justified when IRC holds. Bearing this in mind, let us analyze the SCTMA solutions in the vicinity of the Fermi energy for the system, described by the Hamiltonian\cite{9}.

Then, using the $k$-independent SCTMA self-energy $\Sigma = \tilde{V} \left( 1 - \tilde{G} \tilde{V} \right)^{-1}$ and following the procedure of Refs. \cite{24, 7}, one can arrive at the explicit average local GF:

$$G = \frac{1}{2} \left[ \tilde{\Sigma} \tilde{G} \right] = \tilde{G}_0 \left[ \frac{1}{\mu} + \frac{2}{\sqrt{\varepsilon^2 - \mu^2}} K \left( \frac{\Delta^2}{\Delta^2 - \varepsilon^2} \right) \right].$$ \hspace{1cm} (6)

In Eq.\ref{eq:6} the renormalized energy $\varepsilon = \varepsilon - \Sigma (\varepsilon)$ includes the scalar value $\Sigma = \tilde{V} \tilde{\Sigma} / 2$, the parameter $\mu = \mu(1 - \mu \rho_0 / 2)$, and $K$ is the 1st kind full elliptic integral. Having the explicit relation \cite{9} $\Sigma = e^{V^2 G/(1 - V^2 G^2)}$ between the self-energy and GF, where the renormalized perturbation parameter $\tilde{V} = V_L / [1 + V_L \rho_0 \ln(1 - \tilde{\mu} / \mu)]$, one obtains the self-consistent equation for $G$ which can
be solved in principle numerically. Since the analytic structure of Eq. involves singular points in the complex $G$ plane (including essential singularity of the $K$-function), it possesses multiple solutions. The physical solutions among them should be then selected by IRC, as a necessary condition for SCTMA validity.

The analysis turns most transparent in the important limit $\varepsilon \to 0$ (related to the Fermi energy). There are two characteristic solutions [21] of Eq. in this limit. One of them, $G(\varepsilon) = G^{(1)}(\varepsilon)$, tending to a constant imaginary value, $G^{(1)}(\varepsilon \to 0) \to i \cdot \text{const}$, was first obtained by Gor’kov and Kalugin in the Born scattering limit [8] and then by P.A. Lee in the unitary scattering limit [9]. Later on, it was repeatedly reproduced by various numerical techniques [8] and hence believed to be the unique SCTMA solution. Nevertheless, it was shown recently by the authors [7] that another solution exists, $G(\varepsilon) = G^{(2)}(\varepsilon)$, with low energy asymptotics:

$$G^{(2)}(\varepsilon) \approx \frac{\varepsilon}{cV^2} \left[ 1 - \frac{\Delta}{\pi eV^2 \rho_0 \ln \left( 2\pi eV^2 \rho_0 / \varepsilon \right)} \right], \quad (7)$$

which tends to zero with $\varepsilon$. The behavior of real and imaginary parts of the two solutions in function of energy for a particular choice of parameters: $c = 10\%$, $V_L = 0.3$ eV, $W = 2$ eV, and $\Delta = 30$ meV, is shown in Fig.2. Notice that at low energies, $\varepsilon \ll \Delta$, the solution $G^{(1)}$ is dominated by the above mentioned imaginary constant, presented as $i\pi e\rho_0 g_0$ where $g_0 \lesssim 1$ is a root of a certain transcendental equation [7]. In contrary, the tendency of $G^{(2)}$ to zero is characterized by the progressive domination of its real part. The renormalized dispersion law $\tilde{E}_k$ (as far as the condition [11] holds) is given by the common equation [14]

$$\tilde{E}_k - \text{Re}\Sigma \left( \tilde{E}_k \right) = E_k, \quad (8)$$

where $E_k = \sqrt{\xi^2 + \Delta^2}$ is the non-perturbed superconducting dispersion law and $\Sigma$ is specified for particular $G^{(j)}$, $j = 1, 2$. Then the IRC is written down as:

$$(k - k_0) \cdot \nabla_k \tilde{E}_k \gg \Gamma_k,$$

near a nodal point $k_0$ where a nodal line crosses the Fermi surface.

The low energy asymptotics of Eq. corresponding to the $G^{(2)}$ solution, Eq. is: $\tilde{E}_k^{(2)} \approx (\pi eV^2 \rho_0 / \Delta)E_k \ln(2\Delta / E_k)$, and with the related damping $\Gamma_k^{(2)} = \text{Im}\Sigma^{(2)} \left( \tilde{E}_k^{(2)} \right) \approx E_k / \ln(2\Delta / E_k)$, we arrive at the condition:

$$E_k \ll \Delta \exp \left( - \frac{\Delta}{\pi eV^2 \rho_0} \right), \quad (9)$$

which defines a narrow enough vicinity of the Fermi energy where this solution makes sense.

Applying the same treatment to the $G^{(1)}$ solution, which formally defines the low energy dispersion law $\tilde{E}_k^{(1)} \approx E_k$ and the damping $\Gamma_k^{(1)} = \text{Im}\Sigma^{(1)} \left( \tilde{E}_k^{(1)} \right) \approx \pi eV^2 \rho_0 g_0$, we obtain the condition

$$E_k \gg \pi eV^2 \rho_0 g_0, \quad (10)$$

so that this solution is valid far enough from the nodal points, where it provides also a correct limit of pure d-wave DOS. However, this solution is clearly eliminated near the nodal point. Thus we come to the conclusion that the only SCTMA solution, valid in the close vicinity of the Fermi energy, is that given by Eq. A physical consequence of vanishing DOS at $\varepsilon \to 0$ for this solution is that the much disputed conjecture of universal electric and thermal conductivity [3], [22] turns impossible. Nevertheless, if the validity range for the $G^{(2)}$ solution, Eq. is very narrow, these conductivities, as far as being defined by the $G^{(1)}$ solution, can display an apparent tendency to those universal values.

Notably, the two estimates, Eqs. do not necessarily assure the overlap between the two validity regions, so that for $\pi eV^2 \rho_0 \gg \Delta$ there can exist some intermediate energy range where neither of SCTMA solutions applies. This range roughly corresponds to the broad linewidth of the known impurity resonance $\varepsilon_{res}$ [7] where DOS cannot be rigorously obtained even with use of the next terms from GE, Eq. though some plausible interpolation is possible between the two SCTMA asymptotics.

Finally it is worthwhile to notice that other known non-perturbative solutions for d-wave disordered systems with DOS vanishing at $\varepsilon \to 0$ as a certain power law:
\( \rho(\varepsilon) \sim \varepsilon^\alpha \) [4,6], also have to satisfy IRC since they use field theoretic approach, only compatible with band-like states. But it can be easily shown that this criterion can be only fulfilled for such DOS if the power is \( \alpha > 1 \), while the reported values are \( \alpha = 1/7 \) [4] and \( \alpha = 1 \) [6].

In fact, let the renormalized radial dispersion law (in the low energy limit) behave as \( \tilde{\xi}_k \sim (k - k_F)^\nu \propto \xi^\nu \) with certain \( \nu > 0 \), then the simplest estimate for d-wave DOS is

\[
\rho(\varepsilon) \propto \varepsilon \int_0^\Delta d\eta \int d\xi \delta(\varepsilon^2 - \tilde{\xi}^2 - \eta^2) \propto \varepsilon \int_0^\varepsilon \frac{d\eta}{(\varepsilon^2 - \eta^2)^{\nu-1/2}} = \frac{\sqrt{\pi} \Gamma(3/2 - \nu)}{4\nu \Gamma(2 - \nu)} \varepsilon^{3-2\nu},
\]

that is \( \alpha = 3 - 2\nu \). In the considered field models, DOS defines the quasiparticle broadening \( \Gamma_k = u^2 \rho\left( \tilde{\xi}_k \right) \), with a disorder parameter \( u \). Then the criterion, Eq.1 is reformulated as

\[
\xi \frac{d\tilde{\xi}}{d\xi} \gg u^2 \rho\left( \tilde{\xi}_k \right),
\]

leading to the condition \( \xi^\nu \gg \text{const.} \nu^{3-2\nu} \), and in the limit \( \xi \to 0 \) this is only possible if \( 3 - 2\nu > 1 \), that is \( \alpha > 1 \).

So, the above considerations essentially restrict possible candidate solutions for quasiparticle spectrum in the disordered d-wave superconductor and in fact suggest Eq.1 as the only known consistent low energy solution for the problem.

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