Linear response function around a localized impurity in a superconductor

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Abstract

Imaging the effects of an impurity like Zn in high-Tc superconductors [see, e.g., S. H. Pan et al., Nature 61 (2000) 746] has rekindled interest in defect problems in the superconducting phase. This has prompted us here to re-examine the early work of March and Murray [Phys. Rev. 120 (1960) 830] on the linear response function in an initially translationally invariant Fermi gas. In particular, we present corresponding results for a superconductor at zero temperature, both in the s- and in the d-wave case, and mention their direct physical relevance in the case when the impurity potential is highly localized.

Key words: A. Superconductors; D. Electronic structure; D. Defects.

1 Introduction

The unconventional nature of the pairing state in the high-Tc superconductors (HTCS) has been recently provided with further evidence by the observation of the spatial inhomogeneity of the electron distribution around an isolated non-magnetic impurity, such as Zn, in cuprate Bi-2212, imaged by scanning tunneling microscopy (STM) [1,2,3,4]. These experimental studies demonstrated the existence of impurity-induced quasi-bound states (resonances) near the Fermi level. Such results have been naturally interpreted as fingerprints of the momentum-space anisotropy of the order parameter in the HTSC. In particular, the four-lobed structure of the STM differential conductivity observed around an isolated impurity is a clear manifestation of the d-wave symmetry.
of the superconducting gap in these materials. More recently, similar results have been reported for Nd/Ba-substituted YBCO thin films [5,6], thus lending further support to the $d$-wave scenario for the hole-doped high-$T_c$ cuprates.

The idea that an anisotropic superconducting gap should give rise to directly observable spatial features in the tunneling conductance near an impurity was suggested by Byers et al. [7], whereas earlier studies [8] had considered perturbations of the order parameter in unconventional superconductors to occur within a distance of the order of the coherence length $\xi$ around an impurity. Later, it was shown that an isolated impurity in a $d$-wave superconductor produces virtual bound states close to the Fermi level, in the nearly unitary limit [9]. Such a quasi-bound state should appear as a pronounced peak near the Fermi level in the local density of states (LDOS) corresponding to an impurity site [10], as is indeed observed in Bi-2212 [1] and YBCO [5].

The location and number of such low-energy peaks in the LDOS around an impurity could also provide important new insights into the nature of the pseudogap state in the underdoped cuprates above the critical temperature $T_c$ [11,12]. Within the preformed pairs scenario, a pseudogap in the normal state is related to the presence of fluctuating pairs, still lacking phase coherence, characterized by a much shorter coherence length and lifetime than superconducting pairs below $T_c$ [13]. On the other hand, the $d$-density wave (DDW) scenario has been recently proposed [14], in which the normal state is characterized by an actual gap in the quasiparticle spectrum, due to a hidden broken symmetry of $d_{x^2−y^2}$-type. In the presence of a pseudogap depleting the DOS at the Fermi level, an impurity-induced resonant state should survive above $T_c$, although broadened in energy. However, if preformed pairs above $T_c$ have a superconducting origin, they would be composed of a superposition of hole as well as electron states, like Bogoliubov quasiparticles below $T_c$. Therefore, impurity-induced resonances in the LDOS probed by STM spectroscopy would be expected at both signs of the applied bias. On the other hand, if the normal state (pseudo)gap has no direct connection with the superconducting gap, as in the DDW scenario, then only a definite kind of peaks, either of electron or of hole kind, should appear.

The spatial inhomogeneity of the local electronic structure around an isolated impurity in an unconventional superconductor has been already studied via the solution of the Bogoliubov-De Gennes equations for a disordered system [15,16,17,18], and within a self-consistent approach, taking into account the changes in the order parameter induced by the impurity potential [19]. Here, we follow a different approach, and address the problem of finding the change in the local electron density around an isolated impurity in an anisotropic superconductor, within linear response theory.

The outline of the paper is then as follows. After reviewing the expression of
the linear response function $F$ in real space for a uniform electron gas [20], in Sect. 2 we calculate the first-order Dirac density matrix, both for an isotropic, $s$-wave superconductor in three dimensions (3D), and for an anisotropic, $d$-wave superconductor in two dimensions (2D). In Sect. 3 we then generalize the above expression for $F$ to the superconducting case, but now in momentum space, where it is directly related to the Fourier transform of the electron density change in a superconductor around a highly localized impurity. A numerical analysis then demonstrates that a $d$-wave order parameter gives rise to an azimuthal modulation in the momentum dependence of $F$, which is responsible of the four-lobed pattern observed in the density change around an impurity. Later in Sect. 4 we summarize and give directions for future work.

2 Linear response theory for normal and superconducting state

The linear response function $F(r, r', E_F)$ for a one-body potential $V(r)$ introduced into an initially uniform Fermi gas provides the density change $\delta \rho(r)$ in that gas due to the ‘impurity’ generating $V(r)$. This quantity $F$ is given in the early work of March and Murray [20] and is translationally invariant and spherically symmetric, namely

$$F(r, r', E_F) \equiv F(|r - r'|, E_F) = -\frac{k_F^2}{2\pi^3} \frac{j_1(2k_F|r - r'|)}{|r - r'|^2},$$

where $j_1(x) = (\sin x - x \cos x)/x^2$ is the spherical Bessel function of order one, $k_F$ the modulus of the Fermi momentum, and $E_F = \frac{1}{2}k_F^2$ the Fermi energy (in units such that $\hbar = m = 1$, to be used throughout the present work). Here, prompted by the rekindling of interest in defect problems in superconductors [1,2,3,4], the analogous response function is calculated within the BCS model of the superconducting phase [21], for both isotropic and anisotropic superconductors. Due to the ‘rounding off’ of the Fermi momentum distribution $n(p)$, which at $T = 0$ in the normal state is the usual step function terminating at Fermi momentum $p_F = \hbar k_F$, the superconducting ($S$) response function $F_S(r - r', E_F)$ has more pronounced ‘damped’ oscillations at large separations $|r - r'|$, as compared to the normal state case, the damping factor of the oscillations measuring the ‘blurring’ of the ‘edge’ at $n(p_F)$ due to Cooper pair formation. In addition to that, for an anisotropic superconducting state, as is the case for a $d$-wave order parameter, the superconducting response function $F_S(r - r', E_F)$ is expected to lose spherical symmetry.

Returning to the study of March and Murray [20], these authors obtained the displaced charge $\delta \rho(r)$ due to a perturbation $V(r)$ introduced into an initially
uniform Fermi gas having electron density $\rho_0 = \frac{k_F^3}{3\pi^2}$ as

$$\delta \rho(r) = \int V(r') F(|r - r'|, E_F) \, d^3r'.$$  \hspace{1cm} (2)

Here, our interest is to generalize Eq. (2) in order to treat the effect of a given perturbation $V(r)$ introduced into the superconducting phase as described by the BCS model [21]. Then we can write the analogue of Eq. (2) in the form

$$\delta \rho_S(r) = \int V(r') F_S(r - r', E_F) \, d^3r'.$$  \hspace{1cm} (3)

To proceed to calculate $F_S$ below, we note next the result of Stoddart, March, and Stott [22] (see also Ref. [23]) that

$$\frac{\partial F(r, r', E)}{\partial E} = 2 \text{Re} \left[ G(r, r', E^+) \frac{\partial \gamma(r, r', E)}{\partial E} \right],$$  \hspace{1cm} (4)

where $E^+ = E + i\delta$. Inserting the Green function for an outgoing spherical wave

$$G(r, r', E^+) = \frac{\exp(ik|r - r'|)}{4\pi|r - r'|},$$  \hspace{1cm} (5)

where $E = \frac{1}{2}k^2$, and the first-order Dirac density matrix

$$\gamma(r, r', E_F) = 2 \sum_{|k| < k_F} \exp[ik \cdot (r - r')] = \frac{k_F^3}{\pi^2} \frac{j_1(k_F|r - r'|)}{k_F|r - r'|}$$  \hspace{1cm} (6)

into Eq. (4), one regains the response function, Eq. (1), after some manipulation. We also remind that Eq. (4) can be equivalently cast in the integral form [24]:

$$F(r, r', E_F) = i \int G(r, r', E)G(r', r, E) \, dE.$$  \hspace{1cm} (7)

In the superconducting state, the upper branch of the Bogoliubov excitations is characterized by a dispersion relation $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$, where $\xi_k = \frac{1}{2}(k^2 - k_F^2)$ is the free particle dispersion, measured with respect to the Fermi level, and $\Delta_k$ is the superconducting gap at $T = 0$ (in general, a function of momentum $k$). Eq. (6) is immediately generalized then to read in the superconducting phase

$$\gamma_S(r, r', E_F) = 2 \sum_k n_S(k) \exp[ik \cdot (r - r')],$$  \hspace{1cm} (8)
where $n_S(k)$ denotes the momentum distribution in the superconducting phase at $T = 0$, which coincides with the coherence factor $v^2_k = \frac{1}{2}(1 - \xi_k/E_k)$ of BCS theory [21]. In the s-wave case, corresponding to having a constant gap $\Delta_k = \Delta_0$ over momentum space, $v^2_k$ is characterized by an inflection point at $k_F$ of width $\sim 2\Delta_0$ (see Fig. 2.4 in Ref. [21], or Fig. 7.12 in Ref. [25]), and $\gamma_S(r,r',E_F) \equiv \gamma_S(|r - r'|,E_F)$. We have plotted Eq. (8) for $\gamma_S(|r - r'|, E_F)/\gamma_S(0, E_F)$ as a function of separation $|r - r'|$ for three instances of the ratio $\Delta_0/E_F$ in Fig. 1, where these three curves are compared with the normal state result, Eq. (6). The ‘damping’ of the oscillations in the normal state response function on going to the superconducting phase is evident from the plots in Fig. 1.

The above derivation can be readily generalized to an anisotropic superconductor. In the case of the high-$T_c$ cuprates, we assume a $d$-wave gap $\Delta_k = \Delta_0 \cos \theta$, with $k$ now a two-dimensional (2D) wavevector, $\theta$ being the angle it forms with the $x$ direction. Such an order parameter is characterized by nodes for $\theta = \pm \pi/2$, corresponding to the directions $y = \pm x$. In the normal case, but now in 2D, we find the translationally invariant, spherically
symmetric first-order Dirac density matrix:

$$\gamma(r, r', E_F) = \frac{k_F^2}{\pi} \frac{J_1(k_F|r - r'|)}{k_F|r - r'|},$$  \hspace{1cm} (9)

with \(J_1(x)\) here denoting the Bessel function of the first kind and order one, which again displays oscillations as Eq. (6), but now with a weaker asymptotic decay in the limit \(k_F|r - r'| \gg 1\) (see Fig. 2, upper left panel). In the superconducting case, taking into account the \(d\)-wave symmetry of the order parameter, \(\gamma_S(r - r', E_F)\), Eq. (8), loses its spherical symmetry. We plot \(\gamma_S(r - r', E_F) / \gamma_S(0, E_F)\) in Fig. 2 as a function of the 2D vector \(r - r'\). As in the isotropic, 3D case, we recover a ‘damping’ of the oscillations in the normal state response function in going into the superconducting phase, which is now more pronounced in the fully gapped \(x\) and \(y\) directions, than in the gapless directions \(y = \pm x\).

3 Linear response function for an anisotropic superconductor

We now turn to the problem of explicitly evaluating the linear response function for a 2D superconductor, both in the \(s\)- and in the \(d\)-wave case. We start by noting that Eqs. (2–3) express the relation between the density change \(\delta \rho\) and the impurity potential \(V\) as a convolution in real space, the convolution kernel being the linear response function \(F\). Such a convolution naturally translates into a simple product in momentum space, \(\delta \rho(q) = V(q)F_S(q, E_F)\). Moreover, in the case of a highly localized impurity, as is the case of a \(\delta\)-function-like impurity potential in real space [7], one has \(V(q) = V_0\), so that the Fourier transform of the linear response function \(F_S(q, E_F)\) practically coincides with the Fourier transform of the density change. In the normal state, the latter quantity is readily obtained by Fourier transforming Eq. (7) as a convolution of Green’s functions in momentum space. In the superconducting state, such an expression is generalized by the static limit \((\omega = 0)\) of the polarization function, which for a 2D superconductor reads [26]

$$F_S(q, E_F) = \frac{i}{2\pi} \text{Tr} \int dE \int \frac{d^2k}{(2\pi)^2} \tau_3 G(k, E) \tau_3 G(k - q, E)$$
$$= 2 \int \frac{d^2k}{(2\pi)^2} \frac{(u_{k+q}v_k + u_k v_{k+q})^2}{E_{k+q} + E_k},$$  \hspace{1cm} (10)

where again \(u_k^2\) and \(u_k^2 = 1 - v_k^2\) are the coherence factors of BCS theory [21], but now in general depending on an anisotropic gap \(\Delta_k\). In Eq. (10), \(G\) denotes the matrix Green’s function in Nambu notation [21], and \(\tau_3\) is a Pauli matrix.
Fig. 2. Shows ratio of first-order density matrix to its diagonal value for three different values of the ratio $\Delta_0/E_F = 0$ (normal case), 0.1, 0.3, 0.5 (left to right, bottom to top), but now for the 2D, $d$-wave case. As in Fig. 1, all contour plots are against $k_F(r - r')$ (now a 2D vector). Damping of the normal-state oscillations is more pronounced in the fully gapped $x$ and $y$ directions than in the gapless $y = \pm x$ directions.

In the normal state ($\Delta_0 \to 0$), the integration in Eq. (10) is feasible analytically, and we find:

$$F(q, E_F) \equiv F_S(q, E_F; \Delta_0 = 0) = \begin{cases} 
\frac{1}{\pi}, & \text{if } q \leq 2k_F, \\
\frac{1}{\pi} \frac{q - \sqrt{q^2 - 4}}{q}, & \text{if } q > 2k_F.
\end{cases}$$

(11)

Therefore, we find that the linear response function for a 2D system in the normal state is characterized by a step discontinuity at $q = 2k_F$ (Fig. 3), which is responsible of damped Friedel-like oscillations of period $\sim \pi/k_F$ for $F(r, E_F)$ in real space.

In the superconducting state, for an $s$-wave, isotropic order parameter in 2D, such a discontinuity is smoothed over a width of $\sim 2\Delta_0$ around $q = 2k_F$, as
Fig. 3. Linear response function in momentum space, $F_S(q, E_F)$, Eq. (10), in the case of a translationally invariant, isotropic 2D system. Dashed line shows the normal state analytical result, Eq. (11). Continuous lines show our numerical results for the superconducting state, when an $s$-wave order parameter is assumed, for the same values of $\Delta_0/E_F$ as in Fig. 1. Notice the step discontinuity at $q = 2k_F$ in the normal state, which gets smoothed over a width $\sim 2\Delta_0$ in the superconducting case.

is shown numerically in Fig. 3. This is again expected to give rise to more pronounced damped oscillations in the $r$-dependence of the linear response function in real space.

In the case of a 2D, $d$-wave superconductor, $F_S(q, E_F)$ must be analyzed as a function of $q$ as a vector. Numerical results are plotted in Fig. 4 for different values of the ratio $\Delta_0/E_F$, and compared to the (isotropic) result for the normal state. As in the isotropic, $s$-wave case, the opening of a superconducting gap at the Fermi level tends to smear out the step discontinuity at $q = 2k_F$ over a width $\sim 2\Delta_0$. However, such an effect is more enhanced in the $q_x$ and $q_y$ directions, corresponding to maxima in the energy gap, than in the $q_y = \pm q_x$ directions (gap nodes), where it is virtually absent. This gives rise to an azimuthal modulation of $F_S(q, E_F)$, of period $\pi/2$, which is ultimately responsible for the clover pattern in the density change around an isolated impurity, as observed in STM imaging experiments.
Motivated by the recent imaging results around an isolated impurity in HTSC [1,2,3,4,5,6], we have analyzed the linear response function in momentum space for a 2D uniform electron gas, both in the normal and in the superconducting state. The opening of an energy gap at the Fermi level manifests itself already in the radial dependence of the first-order Dirac density matrix. In the $s$-wave case, its diagonal element $\gamma_S(|r - r'|, E_F)$ decays more rapidly with distance from the diagonal than does its normal state counterpart. In the $d$-wave case, fingerprints of the anisotropic momentum dependence of the energy gap are already present in the angular dependence of $\gamma_S(r - r', E_F)$, with more pronounced damping of the oscillations in the fully gapped $x$ and $y$ directions than in the gapless $y = \pm x$ directions. Such a behaviour is confirmed by
the momentum dependence of the linear response function $F_S(q, E_F)$. In the normal, isotropic state, the latter function is characterized by a step discontinuity at $q = 2k_F$, giving rise to (damped) Friedel-like oscillations in its real space counterpart. The discontinuity at $q = 2k_F$ gets smoothed over a width $\sim 2\Delta_0$ in going into the superconducting state. For a $d$-wave superconductor, however, such an effect is more pronounced in the fully gapped $q_x$ and $q_y$ directions, than along the $q_y = \pm q_x$ nodes. This gives rise to an azimuthal modulation of $F_S(q, E_F)$, which is ultimately responsible of the four-lobed pattern in the density change, observed in STM imaging experiments around an impurity. Before a direct comparison could be made with such experimental results, however, we believe that a more accurate band dispersion relation should be considered (see, e.g., Ref. [27]), as well as a more realistic choice for the impurity potential, which we reserve to future work.

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