

Resonant states and order-parameter suppression near pointlike impurities in d -wave superconductors

Alexander Shnirman, İnanç Adagideli, Paul M. Goldbart, and Ali Yazdani

Department of Physics and Material Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

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We examine the role of order-parameter suppression in the development of low-energy peaks (i.e., resonances) in the tunneling density of states near a nonmagnetic impurity in a d -wave superconductor. Without order-parameter suppression, the zero-energy resonance appears only in the unitary (i.e., strong impurity) limit. However, suppression makes the resonance appear even when the impurity is much weaker. To model this situation, we make the physical hypothesis that the order parameter is reduced whenever one electron of a Cooper pair encounters the impurity, a hypothesis that retains the exact solvability of the problem. In this way, we determine that suppression of the order parameter drives the effective strength of the impurity towards the unitary limit. We determine the order-parameter reduction variationally, and show that the ratios between the main energy scales—the bandwidth and superconducting gap—strongly affect this reduction and, in consequence, the position and width of the resonance. [S0163-1829(99)11033-6]

I. INTRODUCTION

The role played by nonmagnetic impurities in high-temperature superconductors (HTSC's) represents an important element of the subject of high-temperature superconductivity. In contrast with the case of conventional superconductors, in which the s -wave symmetry of the order parameter tends to weaken the effect of such impurities (cf. Anderson's theorem¹), the HTSC materials display rich and interesting sensitivity to the amount of disorder, even at low disorder-concentrations. Indeed, many physical properties are affected at low temperatures and frequencies, the most direct example being the appearance of a nonzero density of states (DOS) at the Fermi level.² One of the reasons for this sensitivity lies in the properties of *individual* nonmagnetic impurities in a d -wave superconducting host, such impurities giving rise to resonant quasiparticle states at subgap energies. The occurrence of these states was predicted theoretically by Balatsky, Salkola, and co-workers,^{3,4} and is consistent with recent experimental observations by Yazdani *et al.*⁵ These states are localized near impurity sites, and have finite lifetimes, due to the existence of bulk quasiparticle states into which they may decay. Upon neglecting the changes in the order parameter induced by an impurity, it was found that, as the strength of the impurity increases, the resonances move towards the Fermi level and their widths decrease; only in the unitary (i.e., infinitely-strong impurity) limit do the resonances reach the Fermi level and become infinitely sharp. The role of the order-parameter changes (i.e., suppression) has been analyzed by several groups (see, e.g., Refs. 6–10). In the present paper we focus on one particular effect of order-parameter suppression which has not been reported previously: we show that the suppression of the order parameter drives (i.e., renormalizes) the effective strength of the impurity towards the unitary limit. Further, we argue that this renormalization may be appreciable in the HTSC materials, and may be important for the development of a more complete understanding of the low-temperature behavior of the

cuprates. Indeed, as was argued in Ref. 11, the observed low-temperature behavior of cuprates is inconsistent with the relatively small suppression of the critical temperature, unless the impurities are (or at least behave as if they are) in the unitary limit.

II. MODEL OF ORDER-PARAMETER SUPPRESSION NEAR AN IMPURITY

Consider a pointlike impurity in a two-dimensional d -wave superconductor. As a fully self-consistent treatment of the order-parameter suppression is out of reach, we shall proceed by exploring a physically motivated hypothesis for the functional form of this suppression. It is commonly assumed^{7,8} that this suppression takes the form

$$\delta\Delta(r, r') \propto f\left(\frac{r+r'}{2}\right)\Delta_0(r-r'), \quad (1)$$

where f gives the spatial shape of the suppression, $\Delta_0(r-r')$ is the bulk value of the d -wave order parameter, and the impurity is located at the origin. This form includes only the d -wave pairing channel, and therefore is very convenient. We show, however, that Eq. (1) is meaningful only for smooth f (varying on length scales much longer than the Fermi wave length k_F^{-1}), and does not describe the physical situation at short distances from the impurity. This short-distance behavior is important, as it affects the formation of the scattering resonances. As an extreme example, consider the setting of tight-binding electrons moving on a two-dimensional square lattice with on-site repulsion and nearest-neighbor attraction (i.e., the simplest situation for d -wave superconductivity). If we locate an impurity at the origin and wish to suppress the order parameter in the four bonds connecting the origin to its nearest neighbors, we arrive at the following functional form of the suppression:

$$\delta\Delta(r, r') = \alpha[\delta(r) + \delta(r')]\Delta_0(r-r'), \quad (2)$$

where α is the amplitude of the suppression which has the dimensionality of a volume. This form may also be used for other cases, inasmuch as it encodes the idea that the order parameter is altered whenever one of the electrons in the Cooper pair encounters the impurity. The Fourier transform of Eq. (2) reads

$$\begin{aligned}\delta\Delta(k,k') &\equiv \int dr dr' \delta\Delta(r,r') \exp(ikr + ik'r') \\ &= \alpha[\Delta_0(k) + \Delta_0(-k')].\end{aligned}\quad (3)$$

As usual for superconductivity, the most important regime is the one in which both k and k' are close to the Fermi surface. Thus the assumption (2) may be relaxed in favor of Eq. (3) near the Fermi surface. The form (3) includes pairing channels other than d -wave. Let us, e.g., adopt the tight-binding shape of the order parameter: $\Delta_0(k) = \Delta \phi_d(k)$, where

$$\phi_{d/s}(k) \equiv \cos(ap_x) \mp \cos(ap_y), \quad (4)$$

in which a is the lattice constant, and the subscripts d/s stand for the d and extended- s channels. By introducing the total [$q \equiv k + k'$] and the relative [$p \equiv (k - k')/2$] momenta of a Cooper pair we arrive at

$$\delta\Delta_{p,q} = \alpha\Delta[\phi_d(p)\phi_s(q/2) + \phi_s(p)\phi_d(q/2)]. \quad (5)$$

Recent numerical self-consistent simulations⁶ yield an order-parameter suppression having a form similar to Eq. (5), with the d -wave contribution having the form factor of the s -wave symmetry and vice versa. Note that at small values of q only the d -wave contribution survives, which reconciles Eqs. (3) and (1). Further support for the choice of the functional form (3) may be provided by examining the imbalance in the self-consistent equation for the order parameter with the impurity present and the order parameter unchanged (i.e., the model considered in Ref. 4). The imbalance means that the gradient of the free energy in the function space of $\Delta(k,k')$ is non-zero and the ‘‘direction’’ of this gradient gives the functional form of the linear response of the order parameter $\delta\Delta$ to the presence of the impurity. We find that the ‘‘direction’’ of the imbalance is close to Eq. (3), and also has the same symmetry as Eq. (3).

III. DENSITY OF STATES NEAR THE IMPURITY

First, we investigate the local DOS near the impurity. We employ the standard T -matrix technique. The system is governed by the Hamiltonian

$$\begin{aligned}\hat{H}(r,r') &= \hat{H}_0(r,r') + \hat{\Sigma}(r,r') \\ &= \hat{H}_0(r,r') + U\delta(r)\delta(r')\hat{\sigma}_z - \delta\Delta(r,r')\hat{\sigma}_x,\end{aligned}\quad (6)$$

where \hat{H}_0 is the Bogolubov–de Gennes kernel, which describes the unperturbed d -wave superconductor, and the term with the coefficient U represents the potential scatterer (i.e., impurity), hats denote 2×2 matrices in the Nambu space.

The Dyson equation for the full Matsubara Green’s function $\hat{G}(r,r',i\omega_n) \equiv [i\omega_n - H(r,r')]^{-1}$ reads

$$\begin{aligned}\hat{G}(r,r') &= \hat{G}_0(r,r') \\ &+ \int dx_1 dx_2 \hat{G}_0(r,x_1) \hat{\Sigma}(x_1,x_2) \hat{G}(x_2,r')\end{aligned}\quad (7a)$$

$$= \hat{G}_0(r,r') + \int dx_1 dx_2 \hat{G}_0(r,x_1) \hat{T}(x_1,x_2) \hat{G}_0(x_2,r'). \quad (7b)$$

Our aim is to find the T matrix $\hat{T}(x_1,x_2)$, which would allow us to calculate, via Eq. (7b), the full Green’s function and therefore the DOS. The Dyson equation for the T matrix reads

$$\begin{aligned}\hat{T}(x_1,x_2) &= \hat{\Sigma}(x_1,x_2) \\ &+ \int dy_1 dy_2 \hat{\Sigma}(x_1,y_1) \hat{G}_0(y_1,y_2) \hat{T}(y_2,x_2).\end{aligned}\quad (8)$$

This model is exactly solvable, owing to the fact that the Fourier transform of the self-energy $\hat{\Sigma}(k,k')$ is a degenerate kernel (i.e., a sum of factorized functions of k and k'):

$$\hat{\Sigma}(k,k') = U\hat{\sigma}_z - \alpha[\Delta_0(k) + \Delta_0(-k')]\hat{\sigma}_x. \quad (9)$$

By using this degeneracy property we may rewrite Eq. (8) as

$$\begin{aligned}\hat{T}(k,k') &= U\hat{\sigma}_z - \alpha[\Delta_0(k) + \Delta_0(k')]\hat{\sigma}_x + U\hat{\sigma}_z \hat{F}(k') \\ &- \alpha\hat{\sigma}_x \hat{H}(k') - \alpha\Delta_0(k)\hat{\sigma}_x \hat{F}(k'),\end{aligned}\quad (10a)$$

$$\hat{F}(k') \equiv V^{-1} \sum_{k''} \hat{G}_0(k'') \hat{T}(k'',k'), \quad (10b)$$

$$\hat{H}(k') \equiv V^{-1} \sum_{k''} \Delta_0(k'') \hat{G}_0(k'') \hat{T}(k'',k'), \quad (10c)$$

the remaining task being to determine the as-yet unknown matrix-valued functions F and H . Here and subsequently, we use the symmetry $\Delta_0(-k) = \Delta_0(k)$. By multiplying Eq. (10a) first by $\hat{G}_0(k)$ and then by $\Delta_0(k)\hat{G}_0(k)$ from the left, and integrating over k , we obtain a system of linear equations for \hat{F} and \hat{H} :

$$\begin{aligned}(U\hat{P}\hat{\sigma}_z - \alpha\hat{L}\hat{\sigma}_x - \hat{1})\hat{F}(k) - \alpha\hat{P}\hat{\sigma}_x \hat{H}(k) \\ = -U\hat{P}\hat{\sigma}_z + \alpha\hat{L}\hat{\sigma}_x + \alpha\hat{P}\Delta_0(k)\hat{\sigma}_x,\end{aligned}\quad (11a)$$

$$\begin{aligned}(U\hat{L}\hat{\sigma}_z - \alpha\hat{M}\hat{\sigma}_x)\hat{F}(k) - (\alpha\hat{L}\hat{\sigma}_x + \hat{1})\hat{H}(k) \\ = -U\hat{L}\hat{\sigma}_z + \alpha\hat{M}\hat{\sigma}_x + \alpha\hat{L}\Delta_0(k)\hat{\sigma}_x,\end{aligned}\quad (11b)$$

where $\hat{P} \equiv V^{-1} \sum_k \hat{G}_0(k)$, $\hat{L} \equiv V^{-1} \sum_k \Delta_0(k) \hat{G}_0(k)$, and $\hat{M} \equiv V^{-1} \sum_k \Delta_0^2(k) \hat{G}_0(k)$.

Thus far, we have not made use of the d -wave symmetry of the order parameter, and we have not made any approximation beyond the mean-field (Bogolubov–de Gennes) approximation. To determine the matrices \hat{P} , \hat{L} , and \hat{M} we use

the d -wave character of the order parameter to eliminate integrals of the odd powers of $\Delta_0(k)$, and we assume the presence of particle-hole symmetry to eliminate integrals of odd powers of the single-electron energy $\epsilon(k)$. Taking for the unperturbed Green's function

$$\hat{G}_0(k) = \frac{1}{\Delta_0^2(k) + \epsilon^2(k) + \omega_n^2} \begin{pmatrix} -i\omega_n - \epsilon(k) & -\Delta_0(k) \\ -\Delta_0(k) & -i\omega_n + \epsilon(k) \end{pmatrix} \quad (12)$$

we obtain $\hat{P}(i\omega_n) = P(i\omega_n)(-\hat{1})$, $\hat{L}(i\omega_n) = L(i\omega_n)(-\hat{\sigma}_x)$, and $\hat{M}(i\omega_n) = i\omega_n L(i\omega_n)(-\hat{1})$, where

$$P(i\omega_n) \equiv V^{-1} \sum_k \frac{i\omega_n}{\Delta_0^2(k) + \epsilon^2(k) + \omega_n^2}, \quad (13a)$$

$$L(i\omega_n) \equiv V^{-1} \sum_k \frac{\Delta_0^2(k)}{\Delta_0^2(k) + \epsilon^2(k) + \omega_n^2}. \quad (13b)$$

The system (11a) and (11b) consists of a pair of four-dimensional systems of linear equations having common coefficient matrices and distinct inhomogeneous terms. These two systems may be analytically solved, and thus the exact T matrix may be rebuilt using Eq. (10a). Then the exact Green's function can be built by using Eq. (7b), and hence the local DOS may be calculated via

$$\nu(r, E) = -\frac{1}{\pi} \text{Im} \hat{G}_{1,1}(r, r, E + i\delta) \Big|_{\delta \rightarrow 0}. \quad (14)$$

Before we present exact results for the DOS, it may be noted that the singular behavior (i.e., resonances) of the T matrix at subgap energies (for $E < \Delta$) originate only from zeros of the determinant $D(E)$ of the system (11a) and (11b). This is so because the right-hand side of Eqs. (11a) and (11b) has at most branch cuts at the subgap energies. Thus it is instructive to write down this determinant:

$$D(E) = D_1(E)D_2(E),$$

$$D_{1,2}(E) \equiv 1 - 2\alpha L(E) + \alpha^2 L^2(E) - \alpha^2 E L(E) P(E) \pm U P(E). \quad (15)$$

If $\alpha = 0$ (i.e., no order-parameter suppression) the characteristic equation $D(E) = 0$ is identical to the equation for the poles of the T matrix obtained in Ref. 4. Thus we may conclude that the role of the order-parameter suppression in the present model is to modify (i.e., shift) the resonance found in Ref. 4, rather than to add a new resonance (as results from the model proposed in Ref. 7).

We now calculate the DOS precisely *at* the impurity. We obtain

$$\begin{aligned} \nu(r, E) \Big|_{r=0} &= \nu_0(E) - \frac{1}{\pi} \text{Im} \left[\frac{P(E)(D_1(E) - 1)}{D_1(E)} \right] \\ &= \frac{1}{\pi} \text{Im} \left[\frac{P(E)}{D_1(E)} \right], \end{aligned} \quad (16)$$

where $\nu_0(E) = (\pi^{-1}) \text{Im} P(E)$ is the unperturbed DOS in the d -wave superconductor. For $\alpha = 0$, the behavior of $\nu(r, E)$ for $r = 0$ was described in Ref. 4. There it was shown that a resonant peak appears at negative energies when $\tilde{U} \equiv U\nu_F$ becomes comparable to 1 (ν_F being the DOS at the Fermi surface in the normal state). The peak moves toward zero energy and becomes narrower and weaker as \tilde{U} grows. In the unitary limit (i.e., for $\tilde{U} \rightarrow \infty$) the peak disappears. This disappearance simply means that an infinitely strong impurity repels all the electronic density from itself. The resonance is still there, and to analyze it, one should calculate the tunneling density of states in the vicinity of the impurity (see Ref. 4). There, four maxima appear along the lobes of the d -wave order parameter at a distance of the order of the Fermi wave length λ_F from the impurity site. Moreover, a second resonance, corresponding to a singularity of the subdeterminant D_2 , shows up in the vicinity of the impurity. The width of this second resonance is exactly equal to the width of the first, and the positions of the two are symmetric with respect to the Fermi energy. However, the spatial density distributions of the two resonances differ from one another.

The effect that we report here is that if one fixes the impurity potential \tilde{U} and allows the order-parameter suppression α to grow instead, the DOS behaves similarly to the scenario outlined above. Specifically, the resonances move toward zero energy, become sharper, and a maximum in the DOS is found along the lobes of $\Delta_0(k)$ at a distance of the order of λ_F from the impurity. Indeed, for $E \rightarrow 0$, we obtain from Eq. (13b) that $L(E) \rightarrow 2\Delta\nu_F$ [we have taken $\Delta_0(k) = \Delta \cos(2\phi_k)$]. In this regime we can approximate $D_{1,2}(E)$ as $(1 - 2\tilde{\alpha})^2 \pm U P(E)$, where $\tilde{\alpha} \equiv \alpha\Delta\nu_F$. We find that the positions ($\pm\Omega_0$) and the width (Γ) of the resonances may be now determined using the formulas of Ref. 4:

$$\Omega_0 = \frac{\Delta}{2\tilde{U}_{\text{eff}} \ln(8\tilde{U}_{\text{eff}})}, \quad \Gamma = \frac{\pi\Omega_0}{2\ln(8\tilde{U}_{\text{eff}})}, \quad (17)$$

in which the original strength of the impurity is substituted by a renormalized one, viz., $\tilde{U}_{\text{eff}} \equiv \tilde{U}/(1 - 2\tilde{\alpha})^2$. Now, unitary behavior is achieved if $\tilde{U}_{\text{eff}} \gg 1$, and a strong renormalization of the bare strength of the impurity occurs if it is possible for $\tilde{\alpha}$ to be close to 1/2. In the next section we will argue that such a regime may be realistic in the HTSC materials. In the meantime, let us assume that strong renormalization has occurred, i.e., that the bare strength of the impurity \tilde{U} was not large enough to cause the unitary behavior but that U_{eff} is. Then we may ask the question: Is there any difference in the spatial distribution of the resonant-state density between this case and the case when $\tilde{U} \gg 1$? We find that the only difference is precisely *at* the impurity site: there, the electrons “know” that the impurity is not so strong, and therefore the DOS is less suppressed than in the “true” unitary limit (i.e., $\tilde{U} \gg 1$). Farther from the impurity, however, the two cases are indistinguishable. The scaling relation between these two cases may be expressed as

$$\nu(r, E, \tilde{U}, \tilde{\alpha}) \approx \begin{cases} \frac{\nu(r, E, \tilde{U}_{\text{eff}}, \tilde{\alpha})|_{\tilde{\alpha}=0}}{(1-2\tilde{\alpha})^2}, & \text{for } r=0, E \approx 0; \\ \nu(r, E, \tilde{U}_{\text{eff}}, \tilde{\alpha})|_{\tilde{\alpha}=0}, & \text{for } |r| > \lambda_F, E \approx 0. \end{cases} \quad (18)$$

It is not clear that such a behavior could be detectable experimentally because even when STM tips are precisely above impurities tunneling occurs over some neighborhood of the impurity. However, this is at least consistent with the experimental results reported in Ref. 5.

IV. AMPLITUDE OF THE ORDER-PARAMETER SUPPRESSION

Our next step is to estimate the amplitude of the order parameter suppression α . In principle, one may envision two different scenarios. In the first, the electron-electron interaction is unchanged by the presence of the impurity, and, in the d -wave case, the suppression of the order-parameter is only due to the pair breaking effect of the impurity. In the second scenario, the electron-electron interaction is itself suppressed near the impurity, thus furthering the suppression of $\Delta(r, r')$. Let us make a very crude estimate for the second scenario. We again exploit the tight-binding model, and assume that the order parameter is zero in the four bonds connecting the impurity to its neighbors but unchanged elsewhere. This regime would be reasonable for purely electronic mechanisms of superconductivity, as the local electronic structure is completely altered by the impurity. Then $\alpha \approx a^d$ and $\tilde{\alpha} = \alpha \Delta \nu \approx \Delta/2t$, where $2t$ is the bandwidth and we have used as an estimate for the density of states $\nu \approx 1/2ta^d$. If we take into account the fact that in the definition of $\tilde{\alpha}$ the DOS at the Fermi level ν_F should be used, whereas the lattice constant a is naturally connected to the DOS averaged over the whole band (i.e., $\bar{\nu}$), we arrive at a more refined estimate: $\tilde{\alpha} \approx (\Delta/2t)(\nu_F/\bar{\nu})$. We see that in conventional superconductors $\tilde{\alpha}$ is always small, and thus essentially no renormalization can happen. In the HTSC materials, however, $\Delta/2t$ can be of the order 0.1, and the proximity of the Van Hove singularity makes the factor $\nu_F/\bar{\nu}$ important. Thus in this case a strong renormalization situation cannot be ruled out.

Next, we show that, even if the electron-electron interaction is unchanged near the impurity, the pair breaking process creates a suppression of the order parameter to the value estimated above [$\tilde{\alpha} \approx (\Delta/2t)(\nu_F/\bar{\nu})$] when $\tilde{U} \approx 1$. We establish this variationally, i.e., we minimize the free energy of the system with respect to α . To calculate this free energy one has to know the form of the electron-electron interaction responsible for the superconductivity of the system.

The most general form of the pairing interaction may be written as

$$H_{\text{int}} = \frac{1}{V^3} \sum_{p, p', q, q'} g(p, p'; q) \times \delta_{q, q'} c_{p+q/2, \uparrow}^\dagger c_{-p+q/2, \downarrow}^\dagger c_{-p'+q'/2, \downarrow} c_{p'+q'/2, \uparrow}. \quad (19)$$

Note that we have introduced the Kronecker symbol $\delta_{q, q'}$, corresponding to the conservation of the total momentum, in order to emphasize the matrix structure of this interaction. This matrix has a twofold index (p, q) corresponding to the relative and the total momenta of the electrons in a Cooper pair, respectively. To avoid confusion, we shall use the letters p and q for the relative and the total momenta of the electrons in a Cooper pair, reserving the letter k for momenta of individual electrons. The standard Hubbard-Stratonovich decoupling procedure¹² yields the following effective action for the order parameter:

$$S = S_1 + S_2 \equiv \int_0^\beta d\tau \left[-\frac{1}{V^3} \sum_{p, p', q, q'} \bar{g}(p, p'; q) \delta_{q, q'} \Delta_{p, q} \Delta_{p', q'}^* \right] - \text{Tr} \ln \hat{G}^{-1}, \quad (20)$$

where $\hat{G}^{-1}(r, t; r', t') \equiv \hat{1} \delta(t-t') \delta(r-r') i \partial / \partial t' - \delta(t-t') \hat{H}(r, r')$, and $\bar{g}(p, p'; q)$ stands for the inverse of the $g(p, p'; q)$ matrix in p space [the inversion in q space is trivially performed in Eq. (20)]:

$$\frac{1}{V} \sum_{p'} g(p, p'; q) \bar{g}(p', p''; q) = V \delta_{p, p''}. \quad (21)$$

The electronic free energy F in the mean-field approximation is thus given by

$$F[\Delta_{p, q}] = \frac{S}{\beta} = F_1 + F_2 = -\frac{1}{V^3} \sum_{p, p', q} \bar{g}(p, p'; q) \Delta_{p, q} \Delta_{p', q}^* - \frac{1}{\beta} \text{Tr} \ln G^{-1}. \quad (22)$$

We now minimize Eq. (22) with respect to α . The second term of Eq. (22) is treated readily; indeed,

$$\begin{aligned} \frac{\partial}{\partial \alpha} F_2 &= -\frac{\partial}{\partial \alpha} \left(\frac{1}{\beta} \text{Tr} \ln \hat{G}^{-1} \right) \\ &= -\frac{1}{\beta} \text{Tr} \hat{G} \frac{\partial}{\partial \alpha} \hat{G}^{-1} \\ &= -\frac{1}{\beta V^2} \sum_{k, k', \omega_n} \text{tr} [\hat{G}(k, k', i\omega_n) (\Delta_0(k) + \Delta_0(k')) \hat{\sigma}_x], \end{aligned} \quad (23)$$

where the symbol tr stands for the trace in the Nambu space only. The Green's function \hat{G} is known exactly: $\hat{G}(k, k') = V \delta_{k, -k'} \hat{G}_0(k) + \hat{G}_0(k) \hat{T}(k, k') \hat{G}_0(k')$. Therefore we can rewrite Eq. (23) as

$$\begin{aligned} \frac{\partial}{\partial \alpha} F_2 = & -\frac{2}{\beta V} \sum_{k, \omega_n} \Delta_0(k) \operatorname{tr}[\hat{G}_0(k, i\omega_n) \hat{\sigma}_x] \\ & -\frac{1}{\beta V^2} \sum_{k, k', \omega_n} [\Delta_0(k) + \Delta_0(k')] \operatorname{tr}[\hat{G}_0(k, i\omega_n) \\ & \times \hat{T}(k, k', i\omega_n) \hat{G}_0(k', i\omega_n) \hat{\sigma}_x]. \end{aligned} \quad (24)$$

As for the first term of Eq. (22), we recall that

$$\Delta_{p,q} = V \delta_{q,0} \Delta_0(p) - \alpha [\Delta_0(p+q/2) + \Delta_0(p-q/2)], \quad (25)$$

and therefore F_1 is a quadratic polynomial in α . The derivative of F_1 with respect to α contains a term independent of α and a term linear in α . It is straightforward to verify that the term independent of α in $\partial F_1 / \partial \alpha$, when combined with the first term in Eq. (24), cancel, as together they constitute the BCS self-consistency equation for the unperturbed order parameter. (The appearance of this equation was to be expected as it emerges from the condition that the free energy be minimal when no impurity is present.) We denote the parts of F_1 and F_2 remaining after the cancellation as $F_1^{(2)}$ and $F_2^{(2)}$, respectively, and the variational condition for α now reads

$$\frac{\partial F}{\partial \alpha} = \frac{\partial}{\partial \alpha} F_1^{(2)} - \frac{\partial}{\partial \alpha} F_2^{(2)} = 0, \quad (26a)$$

$$\begin{aligned} \frac{\partial}{\partial \alpha} F_2^{(2)} \equiv & \frac{1}{\beta V^2} \sum_{k, k', \omega_n} 2\Delta_0(k) \operatorname{tr}[\hat{G}_0(k, i\omega_n) \\ & \times \hat{T}(k, k', i\omega_n) \hat{G}_0(k', i\omega_n) \hat{\sigma}_x], \end{aligned} \quad (26b)$$

$$F_1^{(2)} \equiv -\frac{1}{V^3} \sum_{p, p', q} \bar{g}(p, p'; q) \delta \Delta_{p,q} \delta \Delta_{p',q}^*. \quad (26c)$$

To estimate $F_1^{(2)}$, we choose the standard form of the interaction, which has no q dependence:

$$g(p, p'; q) = -g_d \phi_d(p) \phi_d(p') - g_s \phi_s(p) \phi_s(p'). \quad (27)$$

We include here both d - and s -channel interactions. The part of F_1 quadratic in α reads

$$\begin{aligned} F_1^{(2)} = & \frac{1}{V^3} \sum_{p, p', q} \left(\frac{1}{g_d} \frac{\phi_d(p) \phi_d(p')}{N_d^2} \right. \\ & \left. + \frac{1}{g_s} \frac{\phi_s(p) \phi_s(p')}{N_s^2} \right) \delta \Delta_{p,q} \delta \Delta_{p',q}^*, \end{aligned} \quad (28)$$

where $N_{s,d} \equiv V^{-1} \sum_p \phi_{s/d}^2(p)$.

To proceed further we need to assume some particular form of the wave functions $\phi_{d/s}$. The simplest choice is the tight-binding one [Eqs. (4) and (5)], for which $F_1^{(2)}$ is readily calculated:

$$F_1^{(2)} = \frac{\alpha^2 \Delta^2}{a^d} (g_d^{-1} + g_s^{-1}), \quad (29)$$

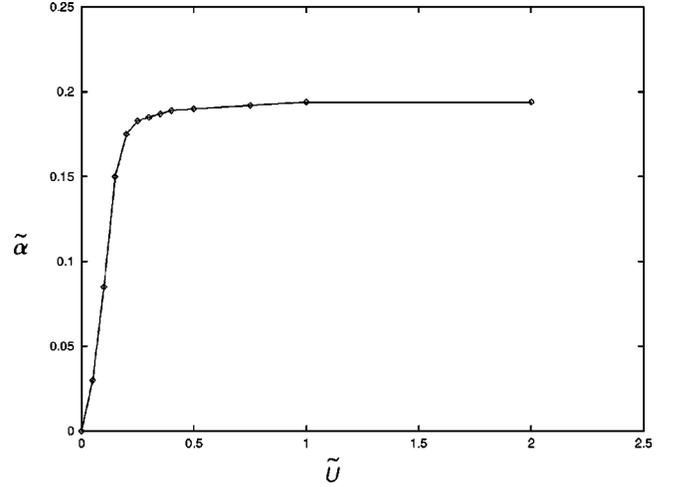


FIG. 1. Results of the numerical simulations for $\tilde{\alpha}(\tilde{U})$. $\Delta/2t = 0.1$, $\nu_F/\bar{\nu} = 1$, the coupling constant $\tilde{g}_d \approx 0.8$ is determined self-consistently, and it is assumed that $\tilde{d}_s = \tilde{d}_d$.

where we have used the identity $V^{-1} \sum_q \phi_{d/s}^2(q/2) = 1/a^d$. The appearance of the volume of the lattice cell a^d in Eq. (29) introduces the bandwidth energy scale $2t$, via $\bar{\nu} \approx 1/2ta^d$. Defining, as usual, the pair of dimensionless coupling constants $\tilde{g}_{d/s} \equiv \nu_F g_{d/s}$, and differentiating Eq. (29) with respect to α , we obtain

$$\frac{\partial}{\partial \alpha} F_1^{(2)} = \frac{2\alpha \Delta^2}{a^d} (g_d^{-1} + g_s^{-1}) = 2\tilde{\alpha} (\tilde{g}_d^{-1} + \tilde{g}_s^{-1}) \left(\frac{2t\bar{\nu}}{\Delta \nu_F} \right) \Delta^2 \nu_F. \quad (30)$$

Finally, to find $\tilde{\alpha}$ we must evaluate $\partial F_2^{(2)} / \partial \alpha$, as given by Eq. (26b). Although all the components of (26b) are known analytically and the integrals over k and k' can be expressed via the functions $P(i\omega_n)$ and $L(i\omega_n)$ defined by Eqs. (13a) and (13b), the remaining sum over the Matsubara frequencies must be carried out numerically. An analytical result is obtained only in the ‘‘true’’ unitary limit $\tilde{U} \rightarrow \infty$:

$$\frac{\partial}{\partial \alpha} F_2^{(2)} \rightarrow \frac{1}{\beta} \sum_{\omega_n} 4L(i\omega_n) = 4\tilde{g}_d^{-1} \Delta^2 \nu_F, \quad (31)$$

where the last equation is obtained from the self-consistency condition for the unperturbed order parameter (without impurities). From Eqs. (30) and (31) we obtain

$$\tilde{\alpha}(\tilde{U})|_{\tilde{U} \rightarrow \infty} = \frac{2\tilde{g}_d^{-1}}{\tilde{g}_d^{-1} + \tilde{g}_s^{-1}} \frac{\Delta}{2t} \frac{\nu_F}{\bar{\nu}} \approx \frac{\Delta}{2t} \frac{\nu_F}{\bar{\nu}}. \quad (32)$$

This result would still be meaningless if the asymptotic value (32) were achieved only for $\tilde{U} \rightarrow \infty$, as the renormalization has no effect in the ‘‘true’’ unitary limit. To check how fast this asymptotic value is achieved, we have solved Eq. (26a) numerically for different choices of the system parameters. We observe that the asymptotic value is always reached already for $\tilde{U} \approx 1$ (see, e.g., Fig. 1). Thus impurities having ‘‘mild’’ values of \tilde{U} may be renormalized to the unitary

limit. We were unable, however, to approach numerically the regime $\tilde{\alpha} \approx 1/2$ without employing the Van Hove singularity (i.e., for $v_F/\bar{v} \approx 1$). This is because the ratio $\Delta/2t$ would have to become of order 1, which is inconsistent with the BCS approximation. On the other hand, exploring the Van Hove scenario would demand calculations with realistic band structures (see, e.g., Ref. 9), the task we leave for the future.

V. CONCLUSIONS

To conclude, we have investigated the role of the order-parameter suppression in the development of resonant scattering states around impurities in d -wave superconductors. We show that the suppression of the order parameter drives the effective strength of the impurity towards the unitary limit. This effect may be relevant in the HTSC materials, due to the relatively large value of the ratio between the superconducting gap Δ and the bandwidth and due to the possi-

bility of a Van Hove singularity in the DOS. The electronic DOS around a renormalized impurity is indistinguishable from the DOS around a “truly” unitary impurity, except precisely at the impurity site. Further calculations involving the strong-coupling regime and the effects of the real band structures are needed to establish the feasibility of the strong renormalization of the strength of impurities.

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