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Quantum interference phenomena between impurity states in d-wave superconductors

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Abstract

We investigate the mutual influence of impurities in two-dimensional d-wave superconductors involving self-consistent solutions of the Bogoliubov–de Gennes equations. The local order parameter suppression, the local density of states as well as the interference of impurity-induced structures are analyzed. We employ an impurity position averaging scheme for the density of states that does not neglect these interference effects, as the commonly used *T*-matrix approaches do.

Keywords: A. Superconductors; D. Electronic structure

In recent years scanning tunneling microscopy (STM) has become an excellent high resolution probe of the electronic structure near defects. In particular it has been used to investigate the effects of individual Zn and Ni atoms in the d-wave superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) [1–3]. These experiments show the appearance of a quasiparticle bound state with a fourfold symmetry around each impurity, reflecting directly the anisotropic $d_{x^2-y^2}$ pairing symmetry [1–3].

The existence of impurity-induced bound states and their characteristics were studied early on by Balatsky et al. using the *T*-matrix approximation [4,5]. Often, local variations in the local order parameter (LOP) dynamically generated by the impurity potential were neglected. Since the LOP varies only on a coherence length scale, which is very short ($\xi \approx 20$ Å) in high-T_c superconductors, the overall effect of this variation was argued to be negligible. Recent calculations, however, indicate otherwise [7–9] showing that the inclusion of the order parameter relaxation allows to achieve a better agreement with microwave conductivity data.

In pure $d_{x^2-y^2}$ superconductors the averaged density of states (DOS) $\rho(E)$ vanishes linearly for $|E| \to 0$. With impurities the self-consistent *T*-matrix approximation [10] leads to a finite DOS at $E = 0$, non-perturbative approaches have variously predicted that $\rho(E)$ vanishes [11] or that it diverges [12]. These issues are still controversial and some efforts are needed to settle the low energy DOS issue in the presence of a finite concentration of impurities.

In this paper we include the local gap suppression of the order parameter and examine the local density of states (LDOS) for two nearby non-magnetic impurities and for a finite impurity concentration to explore how impurity induced structures can interfere with each other, and to what extent this influences the impurity position averaged DOS.

We start from a pairing Hamiltonian for electrons hopping on a square lattice with nearest neighbor hopping matrix element t, and a super-conducting bond order parameter $\Delta_{i,j}$:

$$H = -t \sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \sum_{\{l\},\sigma} U_l c^{\dagger}_{l,\sigma} c_{l,\sigma} + \sum_{\langle i,j\rangle} \{\Delta_{i,j} c^{\dagger}_{i,\uparrow} c^{\dagger}_{j,\downarrow} + \text{h.c.}\} - \mu \sum_{i,\sigma} c^{\dagger}_{i,\sigma} c_{i,\sigma}. \quad (1)$$

The non-magnetic impurity potential is summed over impurity positions ($\{l\}$) and U_l is the local potential at the impurity site l. Energies will be measured in units of t and lengths in units of the lattice constant a. In what follows we set $\mu = 0$ corresponding to half-filling since the variation of the filling does not change our conclusions. Note however that, even for $\mu = 0$, H is not particle–hole (PH) symmetric due to the presence of U_l.

We first consider a single impurity located at site $\hat{1}$, and

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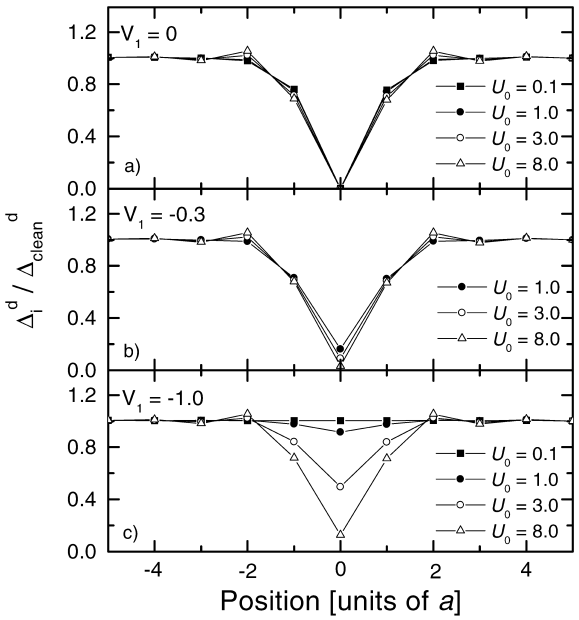

Fig. 1. Normalized d-wave component of the order parameter along the (1,0) direction for different impurity potential strengths U_0.The pairing interaction is set to $V_0 = -1$. Panels *a*, *b*, *c* correspond to different values of $V_1$to account for the suppression of the pairing interaction near the impurity. The position is measured with respect to the impurity site.

we choose $U_{\hat{1}} = U_0$. We perform the unitary transformation [13].

$$c_{i,\sigma} = \sum_n \left(\gamma_{n,\sigma} u_{i,n} + (-1)^{\sigma} \gamma^{\dagger}_{n,-\sigma} v^{*}_{i,n}\right), \tag{2}$$

and by imposing the condition that the transformation (2) diagonalizes the Hamiltonian (1) we obtain the Bogoliubov–de Gennes (BdG) equations [13]

$$\sum_j \begin{pmatrix} H_{i,j} & \Delta_{i,j} \\ \Delta^{*}_{i,j} & H^{*}_{i,j} \end{pmatrix} \begin{pmatrix} u^n_j \\ v^n_j \end{pmatrix} = E_n \begin{pmatrix} u^n_i \\ v^n_i \end{pmatrix}. \tag{3}$$

Here $\Delta_{i,j}$ is the self-consistent mean field solution for the order parameter

$$\Delta_{i,j} = V_{i,j} \langle c_{i,\uparrow} c_{j,\downarrow} \rangle, \tag{4}$$

and $V_{i,j}$ is the attractive pairing interaction.

We solve numerically the self-consistent BdG Eqs. (3) and (4) on lattices of 20×20 sites and with open boundary conditions. For the pairing interaction we choose

$$V_{i,j} = V_0 \hat{\delta}_{i,j} + V_1 (1 - \hat{\delta}_{i,j}), \tag{5}$$

where $\hat{\delta}_{i,j} = 1$ when $i,j \neq \hat{1}$ and i,j nearest neighbors. This form is motivated by the assumption that the pairing interaction is reduced around the impurity, and we therefore consider parameters with $|V_1| < |V_0|$. Note that for $V_1 = V_0 < 0$ this form of the pairing leads to a $d_{x^2-y^2}$ structure of the order parameter. The local d-wave component of $\Delta_{i,j}$ is obtained from:

$$\Delta^d_i = \tfrac{1}{2}(\Delta_{i,i+x} + \Delta_{i,i-x} - \Delta_{i,i+y} - \Delta_{i,i-y}). \tag{6}$$

In the clean case Δ^d_i is uniform in space and has a value of $\Delta^d_i \approx 0.48$ for $V_0 = -1$. Modifications due to impurities or due to the border extend in space on a length scale of the order of the coherence length ξ. For our set of parameters we estimate $\xi \approx 4$ using $\xi = v_F/\Delta_0$, where v_F is the Fermi velocity and Δ_0 is the maximum of LOP. The value of V_0 and consequently the value of Δ^d_i are chosen to render ξ small enough on a 20×20 system so that a sizeable portion of the lattice can still be considered as representative of the bulk of the system. Fig. 1 shows Δ^d_i near the impurity site along the (1,0) direction for various values of V_1 and U_0. A common feature is a strong suppression of the d-wave component of the order parameter around the impurity site on a range of roughly three lattice constants, in agreement with the estimated coherence length ξ. The LOP along the (1,1) direction is modified on the same length scale. Note that in the case of $V_1 = 0$ we have $\Delta^d_{\hat{1}} = 0$ since $\Delta_{\hat{1},\hat{1}\pm x} = \Delta_{\hat{1},\hat{1}\pm y} = 0$.

The LDOS as obtained from

$$\rho_i(E) = \sum_n \left\{ |u^n_i|^2 \delta(E - E_n) + |v^n_i|^2 \delta(E + E_n) \right\} \tag{7}$$

near the impurity is seen in Fig. 2 as the continuous line. In Eq. (7) the sum is over the eigenstates n of the Hamiltonian (1) and E_n denote the corresponding eigenenergies. In the numerical calculation the delta functions present in Eq. (7) are approximated by Lorentzians with a width Γ. Typically we use $\Gamma/t = 0.1$. On the impurity site the LDOS is strongly reduced while on the nearest neighbor sites we find two peaks around zero energy in the LDOS, associated with two resonant quasiparticle bound states with energies $\pm\omega_R$ (see Fig. 3 where the DOS is calculated with $\Gamma = 0.001$). The two peaks are not resolved in Fig. 2 due to the large broadening $\Gamma = 0.1$, and only one peak is observed around zero energy. This peak is, also if not evident from the figure, asymmetric revealing the underlying double peak structure at $\pm\omega_R$. Measuring the distance variation of the LDOS around the impurity at the resonance energy reveals also the well known fourfold symmetric structure characteristic for a $d_{x^2-y^2}$ superconductor [1–3].

In the next step we add a second impurity and explore the mutual influence of the two impurities. The resulting LDOS at a selected site between the two impurities is shown in Fig. 2 (dashed line), for different impurity distances along the (1,0) direction. With one impurity we observe a resonance peak at very low energy ω_R corresponding to the lowest positive eigenvalues of the system that has an energy of $E_0 = \omega_R \approx 0.04$. When a second impurity is added at a distance $d = 2$ from the first, the peak is strongly enhanced by a factor of roughly 2.5. Its asymmetry is again reflecting the underlying resonant impurity states at positive and negative energies (see Fig. 3). When the second impurity is moved one site further away, the peak disappears leaving a

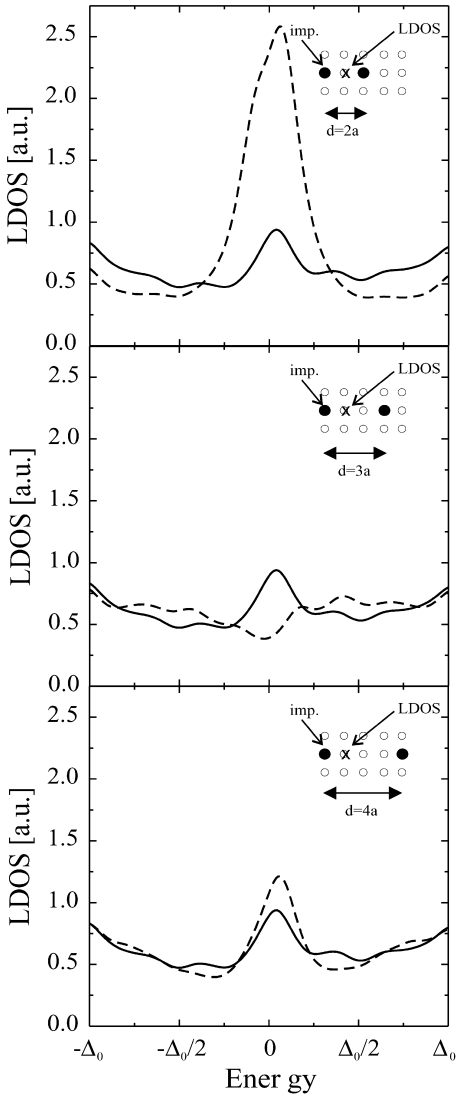

Fig. 2. Local density of states in the presence of two impurities measured near one impurity site. The continuous lines are the calculated densities of states with only one impurity, the dashed ones when the second impurity is added. The LDOS is always measured immediately on the adjacent site of the first impurity. The parameters used are: $\Gamma = 0.1$, $V_0 = -1$, $V_1 = 0$, $U_0 = 8$.

dip around zero energy. The peak is again recovered when the distance is increased further ($d = 4$). This alternating variation is naturally explained as an interference phenomenon due to the overlap of the bound state wave functions near each impurity. In order to demonstrate in detail what is happening at low energies when one or more impurities are added to the system we see in Fig. 3 the DOS for $\Gamma = 10^{-3}$. In Fig. 3(a) we show the clean case as a reference; the spikes at $|E| \approx 0.1$ are the lowest energy eigenvalues for a 20×20 system with open boundary conditions; note the symmetry of the LDOS in the clean case: for $U_0 = 0$ the Hamiltonian

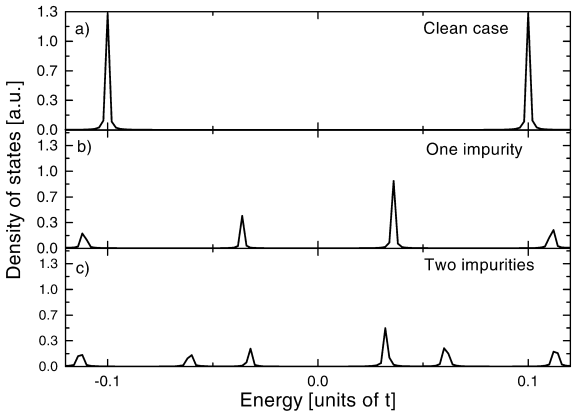

Fig. 3. Plot of the DOS with $\Gamma = 0.001$ in the region $|E| < 0.1$. (a) Clean case result; (b) with one impurity; (c) with two impurities located three sites away one from each other in the (1,0) direction, for $U_0 = 8$, $V_0 = -1$, $V_1 = 0$.

is particle–hole symmetric for $\mu = 0$. When we add an impurity at the center of the system we observe the appearance of two additional eigenvalues with asymmetric weights at energies $|E| \approx 0.04$. The asymmetry results from the broken particle–hole symmetry due to the presence of the impurity. When we add a second impurity near the first one (see Fig. 3(c)) the number of eigenvalues in the region $|E| < 0.1$ is doubled. Thus, by adding impurities one by one an impurity band of finite width is formed due to the overlaps of individual impurity induced quasiparticle bound states [14,15].

When a self-consistent T-matrix approach is used to calculate the impurity position averaged DOS the interaction effects between impurities are neglected due to the selection of non-crossing diagrams for impurity scattering in the standard T-matrix approximation. Therefore, the mutual influence of impurities as observed earlier is missed in the conventional T-matrix approach. An obvious question to ask is to what extent the interference effects and the impurity band formation may survive an appropriate impurity position averaging scheme. In order to answer this question we introduce in the system a fixed number of impurities in random positions and calculate the LDOS in the center of the lattice $\rho^{(1)}(E)$. We keep the site for the measurement of the LDOS fixed for all impurity configurations with the same impurity concentration. The averaged DOS is calculated according to:

$$\rho_{\mathrm{av}}(E) = \frac{1}{N_{\mathrm{c}}} \sum_{m} \rho^{(m)}(E). \tag{8}$$

where m enumerates an impurity configuration and N_{c} is the total number of impurity configurations. Typically we choose $N_{\mathrm{c}} \sim 10^2$, convergence is usually achieved already for $N_{\mathrm{c}} > 50$. In Fig. 4 $\rho_{\mathrm{av}}(E)$ is shown for a large impurity concentration $n_i = 20\%$ to highlight a new low energy structure in the averaged DOS that is not appearing in the

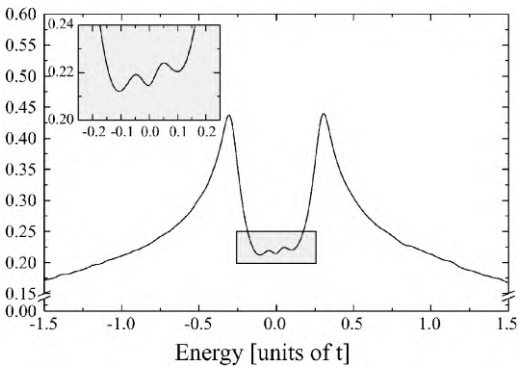

Fig. 4. Averaged DOS for an impurity concentration of $n_i = 20\%$. The inset is a zoom of the low energy part of the calculated DOS.

usual T-matrix calculation, that leads to a flat and finite DOS around zero energy. The new feature that we find consists of an asymmetric structure centered around zero energy. This previously unresolved feature in the DOS survives also when n_i decreases to a few percent although it becomes less pronounced; its origin is clearly related to the overlap of the impurities induced bound states and the accompanying impurity band formation. The above discussed evolution of the impurity band naturally suggests furthermore that the DOS at zero energy will remain zero even for a finite impurity concentration.

In conclusion, we have outlined an extension of the BdG formalism to two dimensional superconductors with a finite concentration of impurities. We have shown how impurities interact between each other giving rise to interference phenomena and leading eventually to an impurity band formation due to the finite overlap of quasiparticle bound states. These phenomena survive for an appropriately chosen impurity position averaging scheme leading to a double peak structure in the averaged DOS at low energies, which may be resolvable in STM measurements.

Acknowledgments

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