Temperature dependence of impurity bound states in $d_{x^2-y^2}$-wave superconductors

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Abstract

We study the evolution with temperature of quasiparticle bound states around non-magnetic impurities in $d_{x^2-y^2}$-wave superconductors. The associated local density of states has a fourfold symmetry which has recently been observed in Zn-doped Bi2212 using scanning tunneling microscopy (STM). From the corresponding Bogoliubov-de Gennes equation we find that with increasing temperature the magnitude of the bound state energy increases and the amplitude of the fourfold contribution to the spinor wave functions decreases. In the pseudogap regime above $T_c$ the fourfold angular dependence of the local tunneling conductance persists as long as the superconducting fluctuations are sufficiently strong to support a finite local order parameter. Once the gap function vanishes completely, the angular structure of the bound state wave function becomes featureless. These effects should be observable in STM studies of impurity doped high-temperature superconductors.
Introduction: It is well known that impurity doping, such as Zn or Ni substitution in the high-temperature superconductors LSCO, YBCO, and BSCCO, is a useful tool in demonstrating the underlying nodal structure of their order parameter. It also provides a semi-quantitative test of the BCS theory for \( d_{x^2-y^2} \)-wave superconductors. [1–4] In particular, an examination of the thermodynamic and transport properties in these compounds suggests that Zn impurities can be modeled with a scattering potential in the unitary limit. [3,4] On the other hand, little is known experimentally about the local structure of the impurity bound states around the Zn sites despite numerous theoretical studies on this question. [3,4] Recently, Pan et al. have provided the first scanning tunneling microscope (STM) images of the local tunneling conductance around Zn impurities in Bi2212 at low temperatures, \( T \approx 4.3 \) K, and fixed at \( \pm E \), where \( E \approx \Delta/30 \) is the binding energy of the impurity bound state. [7] The corresponding wave function was shown to exhibit a fourfold angular symmetry associated with the underlying \( d_{x^2-y^2} \)-wave order parameter. We have found that this quasiparticle bound state wave function around impurity sites can be described within the formalism of the Bogoliubov - de Gennes (BdG) equations for \( d_{x^2-y^2} \)-wave superconductors. [6] Within this framework, the main features of these observations, in particular the characteristic angular patterns seen in the STM images of Zn-doped BSCCO, were reproduced.

While this previous work was based on an analysis of the BdG equations at zero temperature, the thermal evolution of the properties of the impurity bound state is of particular interest. Here we will study how the angular STM patterns around impurities may provide valuable information regarding the nature of the pseudogap in the temperature regime above \( T_c \). We will assume that the origin of the pseudogap is dominated by standard superconducting fluctuations. [8–11] This assumption is motivated by recent angle-resolved photoemission spectroscopy (ARPES) measurements on underdoped BSCCO which have clearly indicated an angular dependence of the pseudogap feature proportional to \( \cos^2 (2\phi) \), analogous to \( |\Delta(k)|^2 \) in the \( d_{x^2-y^2} \)-wave superconducting phase of this compound. [12] In the following, we will address the consequences of the pseudogap phenomenon on the bound state wave function in a semi-phenomenological manner. In particular, we will investigate
how the characteristic fourfold symmetry pattern in the wave function gradually disappears as the temperature is increased.

**Bogoliubov - de Gennes equations:** Let us start our analysis by examining the BdG equations for the spinor wave functions in a \( d_{x^2-y^2} \)-wave superconductor, given by

\[
Eu(r) = \left( -\frac{\nabla^2}{2m} - \mu - V(\mathbf{r}) \right) u(\mathbf{r}) + \frac{1}{p_F^2} \Delta (\partial_x^2 - \partial_y^2)v(\mathbf{r}), \tag{1}
\]

\[
Ev(r) = -\left( -\frac{\nabla^2}{2m} - \mu - V(\mathbf{r}) \right) v(\mathbf{r}) + \frac{1}{p_F^2} \Delta (\partial_x^2 - \partial_y^2)u(\mathbf{r}), \tag{2}
\]

where \( \mu \) is the chemical potential, \( p_F \) is the Fermi momentum, and \( V(r) = V_0 \delta^2(r) > 0 \) is an isotropic impurity scattering potential, centered at \( r = 0 \). In previous work it was shown that the spinor wave functions \( u(\mathbf{r}) \) and \( v(\mathbf{r}) \) can be expanded in terms of Bessel functions of the first kind, leading to the Ansatz

\[
u(r) = A \exp (-\gamma r) \left( J_0(p_F r) + \sqrt{2} \beta J_2(p_F r) \cos (4\phi) \right), \tag{3}
\]

\[
v(r) = \sqrt{2} A \alpha \exp (-\gamma r) J_2(p_F r) \cos (2\phi), \tag{4}
\]

where \( J_l(p_F r) \) are Bessel functions of the first kind, \( \alpha, \beta, \) and \( \gamma \) are variational parameters, and \( A \) is a global normalization factor. In this expansion, only the leading-order angle-dependent terms have been retained.

Since the spinor wave function \( v(\mathbf{r}) \) does not contain an s-wave component, it can be eliminated from Eq. (1), yielding

\[
Eu(\mathbf{r}) = \left( K - V + \frac{\Delta^2(1 + \cos (4\phi))}{2(K + E)} \right) u(\mathbf{r}), \tag{5}
\]

where the contributions of the kinetic energy and the impurity scattering potential are given by

\[
K \equiv \int_0^\infty drr \left[ (\partial_r \exp (-\gamma r) J_l(p_F r))^2 + \frac{l^2 \exp (-\gamma r) J_l(p_F r)}{l+1} \right] \right) - \mu \approx \frac{\gamma^2}{2m}, \tag{6}
\]

\[
V \equiv \int_0^\infty drr \frac{\exp (-2\gamma r) J_2^2(p_F r) V(\mathbf{r})}{\int_0^\infty drr \exp (-2\gamma r) J_0^2(p_F r)} \approx (2\pi \gamma p_F) \int_0^\infty drr \exp (-2\gamma r) J_0^2(p_F r) \frac{V(\mathbf{r})}{\int_0^\infty drr \exp (-2\gamma r) J_0^2(p_F r)}. \tag{7}
\]

Note that the contribution of the impurity potential \( V \) does not appear in the denominator of the last term in Eq. (5) because the spinor wave function \( v(\mathbf{r}) \) does not have an s-wave component. Furthermore, the kinetic energy contribution reduces to \( \gamma^2 / 2m \) for all
The two parameters of interest which will be determined in the following are the temperature-dependent binding energy $E(T)$ and the coefficient of the fourfold symmetric term $\beta(T)$. Because $u(r)$ contains two orthogonal angular components, and the kinetic energy $K$ is independent of angular momentum, it follows that

$$
\left( E - K + V - \frac{\Delta^2}{2(E + K)} \right) - \frac{\beta \Delta^2}{2\sqrt{2}(E + K)} = 0, \\
\left( E - K - \frac{\Delta^2}{2(E + K)} \right) \beta - \frac{\Delta^2}{2\sqrt{2}(E + K)} = 0.
$$

(8)

(9)

Solving these two equations for $E$ and $\beta$, one obtains

$$
\beta = \frac{\Delta^2}{2\sqrt{2}(E^2 - K^2 - \Delta^2/2)},
$$

(10)

$$
\Delta^4/8 = \left( E^2 - K^2 + V(K + E) - \Delta^2/2 \right) \left( E^2 - K^2 - \Delta^2/2 \right).
$$

(11)

The quartic equation for $E$ contains one root which will determine the bound state energy.

To make further progress, we will assume that (i) the impurity scattering is in the unitary limit, $V_0 \gtrsim \Delta_0$, leading to a small binding energy $E$ especially at low temperatures, (ii) the energy contributions $K$ and $V$ are independent of temperature in the regime of interest, $T \in [0, 3T_c]$, and (iii) the local amplitude of the superconducting gap function $\Delta(T)$ is small but finite in the pseudogap regime above $T_c$.

Superconducting regime: Let us first consider the zero-temperature limit, assuming that the impurity scattering potential is in the unitary scattering limit. In this case, $E \to 0$, leading to

$$
V \to \frac{1}{K^2 + \Delta_0^2/2} \left[ K(K^2 + \Delta_0^2) + \Delta_0^4/8K \right].
$$

(12)

Following the assumption of temperature-independent energy contributions $K$ and $V$, we can set $K = a\Delta_0$, where $\Delta_0$ is the gap amplitude at $T = 0$, and $a$ is a proportionality constant whose physical range can be inferred from experiments. It then follows that

$$
V \simeq \frac{1 + 8a^2(1 + a^2)}{4a(1 + 2a^2)} \Delta_0.
$$

(13)
Furthermore, it is known that at zero temperature \( \beta < 0 \), leading to the characteristic fourfold symmetric patterns in the local density of states around impurity sites that have been observed in recent STM measurements. It is therefore natural to postulate that \( \beta < 0 \) for all temperatures, imposing the constraint: \( a > 2^{-3/4} = 0.5946 \). Therefore, we will only consider the physical parameter regime \( a > 2^{-3/4} \). For example, we can set \( a = 2/3 \), yielding \( \beta = -9/(17\sqrt{2}) = -0.3743 \) at \( T=0 \). We have verified that the finite-temperature properties of the bound state that will be discussed in the following do not depend strongly on the choice of \( a \).

**Normal state:** In the opposite limit, \( T \gg T_c \), the gap function vanishes \( \Delta^2(T \to \infty) \to 0 \). Assuming that \( K \) and \( V \) are basically unaffected by temperature, this gives

\[
E(T \to \infty) = K - V = -\frac{(1 + 4a^2)}{4a(1 + 2a^2)} \Delta_0. \tag{14}
\]

Hence, the magnitude of the impurity bound state energy \( E \) increases with increasing temperature. The parameter \( \beta \) vanishes in this limit, indicating that the bound state wave function loses its fourfold angular symmetry pattern at high temperatures when \( \Delta^2(T) \to 0 \).

**Pseudogap regime:** In the pseudogap regime the amplitude of the local order parameter, \( |\Delta(T)| \), is assumed to be small but finite, and by perturbing about the limit \( T \to \infty \) one finds to leading order that

\[
E(T > T_c) \approx E(T \to \infty) + \frac{\Delta^2(T)}{2(K + E)} \simeq -\frac{(1 + 4a^2)}{4a(1 + 2a^2)} \Delta_0 + \frac{2a(1 + 2a^2) \Delta^2(T)}{(8a^4 - 1) \Delta_0}, \tag{15}
\]

and

\[
\beta(T > T_c) \approx -\frac{16a^2(1 + 2a^2) \Delta^2(T)}{2\sqrt{2}(64a^6(1 + a^2) - (1 + 8a^2)) \Delta_0^2}. \tag{16}
\]

Hence the magnitude of the binding energy \( E(T) \) decreases as \( T \to 0 \) due to the progressive opening of the energy gap.

Provided that the pseudogap above \( T_c \) arises mainly due to superconducting fluctuations, it is straightforward to incorporate its physical consequences by assuming a small but finite amplitude of the local order parameter above \( T_c \). This can be modeled by
\[ \Delta^2(T) = \frac{1}{2} \left[ \Delta_0^2(1 - (T/T_c)^3)^2 + \sqrt{\Delta_0^4(1 - (T/T_c)^3)^4 + C} \right], \tag{17} \]

where \( C = 0.027572 \). The coefficient \( C \) is obtained from

\[ \frac{C}{4\Delta_0^4((T/T_c)^3 - 1)^2} \approx \frac{2\pi T}{m\xi_0^2 \ln (T/T_c)}, \tag{18} \]

where the right hand side is the spatial average of the fluctuation order parameter, and \( \xi_0 = \frac{73(3)\nu^2}{2(2\pi T)^2} \). The approximate ratio \( T_c/E_F \simeq 0.03 \) in Bi2212 has been deduced from the low-temperature behavior of the thermal conductivity. \[13\] This interpolation formula for \( \Delta^2(T) \) has already proven successful in the analysis of the excess Dingle temperatures in the vortex state of the \( \kappa-(ET) \_2 \) salts. \[14,15\]

In Fig. 1, the temperature-dependent gap amplitude is plotted along with the energy of the bound state and the coefficient of the fourfold symmetry term in the spinor wave function \( u(r) \). The gap amplitude at zero-temperature has been set equal to unity, \( \Delta_0 \equiv 1 \). At very small temperatures, we observe that \( \Delta(T \to 0) \to 1 \), \( E(T \to 0) \to 0 \), and \( \beta(T \to 0) \to -\frac{1}{(\sqrt{2}(a^2 + 1))^{-1}} \), as expected from the discussion of the \( T \to 0 \) limit. In the limit \( T \to \infty \), we find that \( \Delta(T \to 0) \to 0 \), \( E(T \to -1 + 4a^2)(4a + 8a^3)^{-1} \), and \( \beta(T \to 0) \to 0 \), implying that the magnitude of the binding energy increases with temperature, and that the fourfold angular features in the spinor wave function disappear at high temperatures. The intermediate-temperature regime of \( E(T) \) and \( \beta(T) \) in Fig. 1 has been determined by a numerical solution of the coupled equations (10) and (11). In the fluctuation regime around \( T_c \), the coefficient \( \beta(T \approx T_c) \) is found to be appreciable. Therefore, remnants of the characteristic \( \cos^2(2\phi) \) dependence in the square of the bound state spinor wave function \( u(r) \) should be reflected in the local tunneling density of states, measured by STM experiments in the pseudogap regime above \( T_c \). In Fig. 2, the corresponding temperature evolution of \( |u(r)|^2 \) is shown.

**Conclusions:** In summary, we have studied the effect of temperature on the bound state wave function around impurities in d\(_{x^2-y^2}\)-wave superconductors. Within the framework of the BdG equations, the magnitude of the binding energy is found to increase with temperature, but stays on the order of \( \Delta_0 \). On the other hand, the fourfold contribution to the local
density of states disappears gradually with increasing temperature. Therefore it appears to be possible to take a “snapshot” of the pseudogap by STM imaging. The present analysis may also be applicable to other unconventional superconductors, such as the layered organic superconductors $\kappa-(ET)_{2}\text{Cu}[\text{N(CN)}_{2}]\text{Br}$ and $\kappa-(ET)_{2}\text{Cu(}\text{NCS)}_{2}$, and $\text{Sr}_2\text{RuO}_4$.

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FIG. 1. Temperature dependence of the gap amplitude $\Delta$ (solid line), the bound state energy $E$ (dashed line), and the coefficient of the fourfold symmetry term in the bound state wave function $\beta$ (dot-dashed line). The proportionality constant $a$ has been set to $a = 2/3$.

FIG. 2. Temperature dependence of the bound state wave function, $|u(r)|^2$, localized around a strong-scattering impurity in a $d_{x^2-y^2}$-wave superconductor. left: superconducting regime ($T = 0$), center: pseudogap regime ($T > T_c$), right: normal state ($T = \infty$).