Localized Bosonic Modes in Superconductors

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We show that a localized bosonic mode acts as a new type of “defect” in s- and \(d_{x^2−y^2}\)-wave superconductors. The mode induces bound or resonance states, whose spectral signature are peaks in the superconductor’s density of states (DOS). We study the peaks’ shape and energy as a function of temperature and the mode’s frequency and lifetime. We identify several characteristic signatures of the localized mode that qualitatively distinguishes its effects from those of magnetic or non-magnetic impurities.

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The study of local defects or impurities in superconductors has attracted significant experimental \(\cite{1,2}\) and theoretical \(\cite{3,4,5}\) interest over the last few years. These studies have proven particularly important for further elucidating the nature of the superconducting (SC) pairing mechanism in unconventional superconductors. In particular, recent scanning tunnelling microscopy (STM) experiments provided a detailed picture of the frequency and spatial dependence of defect induced resonance states in the high-temperature superconductor (HTSC) \(\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}\) \(\cite{2}\), and the triplet superconductor \(\text{Sr}_2\text{RuO}_4\) \(\cite{6}\). Several theoretical scenarios for the physical origin of these impurity states have been proposed, ranging from electronic scattering off classical impurities \(\text{7, 8, 9}\) to the onset of Kondo-screening \(\text{10}\).

In this Letter we investigate a new type of “defect”, a localized bosonic mode, and study its effect on the local electronic structure in s- and \(d_{x^2−y^2}\)-wave superconductors. The study of localized modes, and in particular phonon modes in normal metals, has been of great interest in the context of molecular spectroscopy \(\text{11, 12, 13}\) (or inelastic electron tunnelling). It was recently argued that a localized magnetic mode could also arise from unscreened magnetic moments in a \(d_{x^2−y^2}\)-wave superconductor \(\text{14}\). The nature of the mode is only relevant for the present study to the extent that it determines the form of its coupling to the electronic degrees of freedom. While theoretical studies \(\text{11, 15}\) have so far only focused on the Born-limit of weak electronic scattering off the localized mode, we show that the strong-scattering, unitary limit gives rise to an abundance of novel phenomena. In particular, we show that the presence of a localized mode leads to the appearance of fermionic bound or resonance states whose spectral signature are peaks in the SC DOS. We study the peaks’ energy and shape as a function of the mode’s characteristic frequency \(\omega_0\), lifetime \(\Gamma\), and temperature. It is of particular interest that the peaks move to higher energies with increasing \(\omega_0\) or \(\Gamma\), but are shifted to lower energies with increasing temperature, \(T\). In addition, the temperature evolution of the peaks differs qualitatively if its frequency is smaller or larger than \(\Delta_0 − \omega_0\), where \(\Delta_0\) is the maximum SC gap. Moreover, we show the mode also induces a “dip” in the DOS at frequencies \(±(\Delta_0 + \omega_0)\). This dip, together with the temperature evolution of the DOS, qualitatively distinguishes the effects of a localized mode from those of non-magnetic or static magnetic impurities \(\text{16, 17}\). These characteristic differences therefore provide an important tool for future experiments to further study and clarify the nature of “defects”.

Starting point for our calculations is the Hamiltonian

\[
H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} + \sum_{\mathbf{k}} \Delta_{\mathbf{k}} c_{\mathbf{k},\uparrow}^\dagger c_{\mathbf{k},\downarrow}^\dagger + h.c.
+ \omega_0 b_0^\dagger b_0 + \sum_{\mathbf{k},\mathbf{q},\sigma} g_\sigma (b_\mathbf{q}^\dagger + b_\mathbf{q}) c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{q},\sigma}.
\]

Here, \(c_{\mathbf{k},\sigma}^\dagger, b_\mathbf{q}^\dagger\) are the fermionic and bosonic creation operators, respectively. We consider a two-dimensional electronic system with normal state dispersion \(\epsilon_{\mathbf{k}}\) and SC gap \(\Delta_{\mathbf{k}}\). The bosonic mode with frequency \(\omega_0\) is localized at \(\mathbf{r} = 0\). We allow for a spin dependence of the scattering vertex, \(g_\sigma\), and for simplicity consider only an on-site interaction. In the following, we study a single bosonic mode with no internal degrees of freedom, i.e., spin \(S = 0\). The extension of our results to \(S \geq 1\), in which case electronic spin-flip scattering is allowed, is straightforward and will be discussed in a future publication \(\text{17}\). The retarded bosonic Greens function \(D_R(\omega)\)
in frequency space is given by

\[ D_R(\omega) = \frac{\alpha}{(\omega + i/2)^2 - \omega_0^2}. \]  

(2)

where \( \alpha \) depends on \( \Gamma \) and \( \omega_0 \), and is determined via

\[ 1 + 2n_b(\omega_0) = -\int_{-\infty}^{\infty} d\omega \pi n_b(\omega) \text{Im} D_R(\omega). \]  

(3)

We assume that \( \omega_0 \) and the mode’s lifetime, \( \Gamma^{-1} \), are determined intrinsically such as in the case of phonon modes \( 7 \). Possible feedback effects on \( \omega_0 \) and \( \Gamma \) due to the fermion-boson coupling are accounted for (to the extent that they do not induce a frequency dependence of \( \Gamma \)) by considering \( \omega_0 \) and \( \Gamma \) to be effective temperature independent input parameters of our theory. The unperturbed (clean) fermionic Greens function is given by \( \hat{G}_0^{-1}(k, \omega_n) = [\omega_n \tau_0 - \epsilon_k \tau_3] \sigma_0 + \Delta_k \tau_2 \sigma_2 \), where \( \sigma_i \) and \( \tau_i \) are the Pauli-matrices in spin and Nambu-space, respectively. Changes in the fermionic Greens function due to the scattering of the localized mode are accounted for by summing the infinite series of diagrams shown in Fig. 1a, which yields

\[
\hat{G}(r, r', \omega_n) = \hat{G}_0(r, r', \omega_n) + \hat{G}_0(r, 0, \omega_n) \hat{S}(\omega_n) \hat{G}_0(0, r', \omega_n). 
\]  

(4)

Here

\[
\hat{S}(\omega_n) = \hat{\Sigma}(\omega_n) \left[ 1 - \hat{G}_0(0, 0, \omega_n) \hat{\Sigma}(\omega_n) \right]^{-1} 
\]  

(5)

and \( \hat{\Sigma} \) is the local fermionic self-energy given by

\[
\hat{\Sigma}(\omega_n) = T \sum_m \tau_3 \hat{g} \hat{G}_0(0, 0, \omega_n - \nu_m) \hat{D}(\nu_m) \tau_3 \hat{g}. 
\]  

(6)

with \( \hat{g} \) being determined by the spin dependence of \( g_0 \). We show later that vertex corrections (see Fig. 1b) are negligible for the range of parameters considered here. Based on earlier studies \( 8, 10 \), we expect that the inclusion of non-crossing diagrams in the calculation of \( \hat{G} \) does not qualitatively change our results and therefore reserve its discussion for a future publication \( 11 \). The DOS, \( N = A_{11} + A_{22} \) with \( A_{ii}(r, \omega) = -2\text{Im} \ G_{ii}(r, \omega + i\delta) \) is obtained numerically from Eqs. 4-6 with \( \delta = 0.2 \text{ meV} \).

As a frame of reference, we first consider a localized mode in an \( s \)-wave superconductor with normal state dispersion \( \epsilon_k = k^2/2m - \mu \), \( m^{-1}/\Delta_0 = 15 \). Fermi momentum \( k_F = \pi/2 \), and a momentum independent SC gap \( \Delta_0 \). For a spin-independent coupling, \( \hat{g} = g \hat{1} \), no bound states are induced, similar to the case of a non-magnetic impurity in an \( s \)-wave superconductor \( 12 \). In contrast, if the coupling is spin-dependent the mode induces a bound state, with poles in the \( \hat{S} \)-matrix leading to two peaks in the DOS. For simplicity we take \( g_\uparrow = g \), and \( g_\downarrow = -g \), i.e., \( \hat{g} = g \sigma_3 \), and in Fig. 2 present the DOS at \( r = 0 \) for \( \Gamma = 0^+ \) as a function of \( \omega_0 \) and temperature. For

\[ T = 0, \omega_0 = 0 \] (see Fig. 2a) the frequencies \( \pm \Omega_b \) of the bound state peaks are given by \( \Omega_b/\Delta_0 = D_-/D_+ \) with \( D_{\pm} = 1 \pm (gm/4)^2 \). This result is similar to the energy of a bound state induced by a static magnetic impurity \( 12 \).

Note that increasing \( g \), i.e., stronger scattering, leads to a decrease of \( \Omega_b \). For \( \omega_0, T \neq 0 \) the bound state frequencies are shifted from \( \Omega_b \), and in the limit \( T \ll \Delta_0 \) are determined by a transcendental equation. It is too cumbersome to be presented here, but can be simplified in the limit \( \Omega_b, \omega_0 \ll \Delta_0 \), where we find to leading order in \( \omega_0/\Delta_0 \) and \( n_B(\omega_0) \)

\[
\Omega_b(T, \omega_0) = \Omega_b + \omega_0/\pi - n_B(\omega_0)\Delta_0. 
\]  

(7)

Note, that the localized mode effectively behaves as an “oscillating vector” with Ising symmetry (for a single bosonic degree of freedom) and frequency \( \omega_0 \). When \( \omega_0 \) increases (and in particular, when it becomes comparable to the rate of electronic scattering, \( \mu/\hbar \)) subsequent scattering events begin to cancel each other; the effective scattering becomes weaker, and the peaks are shifted to higher energies. In particular, for \( \omega_0 \rightarrow \infty \) the bound state vanishes and the DOS becomes that of the unperturbed systems \( 11 \). This picture provides an explanation for our analytical results in Eq. 7 and fully agrees
with the numerically obtained DOS shown in Fig. 2 for $T = 0$ and several values of $\omega_0$. A non-zero $\omega_0$ also leads to a "dip" in the DOS at $|\Omega| = \Delta_0 + \omega_0$, as shown in the inset of Fig. 2. This dip is a characteristic signature of the localized mode, which distinguishes it from a static magnetic impurity. The origin of the dip lies in the poles of the retarded self-energy, $\Sigma_{\text{loc}}(k, \Omega)$ at $|\Omega| = E_k + \omega_0$. The imaginary part of the retarded local self-energy, $\Im \Sigma_{\text{loc}}$, then possesses a threshold energy, $\Omega_0^+ = \Delta_0 + \omega_0$, with $\Im \Sigma_{\text{loc}} \sim 1/|\sqrt{(|\Omega| - \omega_0)^2 - \Delta_0^2}|$ for $|\Omega| \geq \Omega_0^+$, and $\Im \Sigma_{\text{loc}} \equiv 0$ for $|\Omega| < \Omega_0^-$. As a result, $\Re \Sigma_{\text{loc}}$ exhibits a square-root singularity for $|\Omega| \to \Omega_0^+ - \epsilon^+$, which is the denominator of $\hat{S}$ leads to a suppression, i.e., dip, in the DOS. This dip is therefore similar in nature to that observed in angle-resolved photoemission experiments in the HTSC [14]. Finally, we find that the amplitude of the bound state peaks exhibits spatial oscillations described by $\cos(2k_Fr)e^{-r/\xi}/r$, where $\xi = k_F/m\sqrt{\Delta_0^2 - \Omega_0^2}$ [11].

For non-zero temperatures the $\omega = +\omega_0$ branch of the bosonic mode becomes populated, opening a new scattering channel and yielding significant changes in the DOS, as shown in Fig. 2b. We find that the specific temperature evolution of the bound state peaks depends on whether $\Omega_0$ at $T = 0$ is smaller or larger than $\Omega_0^- = \Delta_0 - \omega_0$. This distinction arises since $\Sigma_{\text{loc}}(k, \Omega)$ now not only possesses poles at $|\Omega| = E_k + \omega_0$, with weight $1 + n_B(\omega_0)$ (for $T, \omega_0 \ll \Delta_0$), but also poles at $|\Omega| = E_k - \omega_0$ with weight $n_B(\omega_0)$. Hence, $\Im \Sigma_{\text{loc}} \not\equiv 0$ already for $|\Omega| \geq \Omega_0^-$, in contrast to the case at $T = 0$. Thus, a bound state peak with $\Omega_0^- < \Omega_0 < \Delta_0$ at $T = 0$ becomes damped with increasing temperature, as shown in Fig. 2b, for $T = 0.15\Delta_0$. At the same time, a new peak appears in the DOS at $|\Omega| = \Omega_0^-$, since $\Im \Sigma_{\text{loc}}$ now also possesses square root singularities at $\pm \Omega_0^-$. With increasing temperature the damping of the bound state peak grows ($T = 0.4\Delta_0$) and its amplitude consequently decreases, while the newly emerged peak moves towards lower energies. In contrast, if $\Omega_0 \leq \Omega_0^-$ (not shown) the bound state peak simply moves towards lower energies with increasing temperature, in agreement with our analytical results in Eq (7). This downshift is expected since the population of the mode’s branches grows with increasing temperature, thus leading to stronger scattering. Thus, varying $T$ or $\omega_0$ has an opposite effect on the energies of the bound state peaks in the DOS.

We next consider a localized mode in a $d_{x^2-y^2}$-wave superconductor with SC gap $\Delta_k = \Delta_0(\cos k_x - \cos k_y)/2$ and $\Delta_0 = 25$ meV. To simplify the discussion we consider a particle-hole symmetric dispersion, $\epsilon_k = -2t(\cos k_x + \cos k_y)$, with $t = 300$ meV. A band dispersion with strong particle-hole asymmetry, characteristic of the HTSC, yields qualitatively similar results [11]. In contrast to the s-wave superconductor, a localized mode induces a resonance state even with a spin-independent coupling, $g_\alpha = g$. These resonances are a hallmark of the strong coupling theory, and are not observed in the weak scattering limit.

In Fig. 3 we present the DOS at $r = 0$ as a function of $\omega_0$ and temperature ($\Gamma = 0^+$). For $T, \omega_0 = 0$ (see Fig. 2a), the energy of the resonance peaks, $\Omega_r$, is given by the solution of $\Omega_r = \pm 2\pi \Delta_0 / \{g \log(1/(4\Delta_0))\}$, similar to the energies of resonance states induced by a non-magnetic impurity [2] (this result was also independently obtained by Si [13]). For $|\Omega| \geq \omega_0 \neq 0$,

$$\Im \Sigma_{\text{loc}}(\Omega) = -\frac{1}{\pi} \frac{|\Omega| - \omega_0}{\Delta_0} K \left( \frac{|\Omega| - \omega_0}{\Delta_0} \right)$$

where $K$ is the complete elliptic integral of the first kind, while $\Im \Sigma_{\text{loc}} \equiv 0$ for $|\Omega| < \omega_0$. Thus there exist a real gap in $\Im \Sigma_{\text{loc}}$, in contrast to $\Im G_{\text{loc}}$. Performing a Kramers-Kronig transform, we find for $\Omega_r/\omega_0 \ll 1$, $\Re \Sigma_{\text{loc}} / \omega_0 \approx -A \Omega_r / \omega_0$ where $A = -\frac{1}{2} \int_0^\infty dx \Im \Sigma_{\text{loc}}(x)/x^2$. In the limit $\Omega_r \ll \Delta_0$, the resulting equation for $\Omega_r$ is

$$\Omega_r^2 = \frac{4\pi \Delta_0 \Omega}{g^2} \left[ A \log \left( \frac{4\Delta_0}{|\Omega_r|} \right) \right]^{-1}$$

As expected, increasing $\omega_0$ leads to a shift of $\Omega_r$ to higher energies, in agreement with our numerical results shown in Fig. 3. Moreover, for $\omega_0 \to \infty$ we again recover the
unperturbed DOS (see, e.g., $\omega_0 = 200$ meV). The logarithmic divergence in $\Sigma_{loc}$ at $|\Omega| = |\Delta_0 + \omega_0|$ leads to a dip in the DOS (see arrows in the inset of Fig. 3). A much weaker dip emerges in the weak scattering limit [11].

The specific temperature evolution of the resonance peaks again depends on the relative order of $|\Omega_r|$ at $T = 0$ and $\Omega_c^- = \Delta - \omega_0$, similar to the $s$-wave case. For $|\Omega_r| < \Omega_c^-$ (see Fig. 3b) the resonance peak is shifted to lower energies with increasing temperature. In addition, the opening of a second scattering channel for $T \neq 0$ leads to a logarithmic divergence in $\Sigma_{loc}$, and consequently a dip in the DOS at $|\Omega| = |\Omega_c^-| = 15$ meV, as indicated by the arrows. In contrast, for $\Omega_c^- < |\Omega_r| < \Delta_0$ (see Fig. 3c), the same opening of a second scattering channel leads to an increase in $\text{Im} \Sigma_{loc}$ for $|\Omega| > \omega_0$, which in turn shifts the peaks to higher energies and suppresses their amplitude. The smaller peaks at $|\Omega| = |\Omega_c^-| = 5$ meV (see arrows) arise from the opening of the second scattering channel, and the resulting logarithmic divergence of $\text{Im} \Sigma_{loc}$ at $\Omega_c^-$. Finally, we find that due to the momentum dependence of the SC gap, the spatial dependence of the resonance peaks (not shown) [11] is qualitatively similar to that observed experimentally near impurities in the HTSC [2].

To study the effects of a mode with finite lifetime, $\Gamma \neq 0$, we present in Fig. 4 the DOS in a $d_{x^2-y^2}$-wave and $s$-wave (see inset) superconductor at $T = 0$ and for several values of $\Gamma$. In both superconductors the peaks shift to higher energies with increasing $\Gamma$. Note that a non-zero $\Gamma$ does not directly change the lifetime of the induced state, i.e., the width of the peaks. This is particularly evident for the $s$-wave case (see inset). A non-zero $\Gamma$ lowers the threshold frequency for $\text{Im} \Sigma_{loc} \neq 0$ from $\Omega_{n}^+ = \Delta_0 + \omega_0$, (for $\Gamma = 0^+$) to $\Omega_{n} = \Delta_0$. However, for $|\Omega| < \Delta_0$, we still have $\text{Im} \Sigma_{loc} = 0$ and the width of the bound or resonance peaks remains unaffected by $\Gamma \neq 0$.

Finally, we consider the lowest order vertex correction, shown in Fig. 4. For a quadratic normal state dispersion, the general form of this correction is $\delta g/g = -\Omega^2 F(\Omega_m, \nu_n, \omega_0, \Delta_0)$ where $\Omega_m, \nu_n$ are the bosonic and fermionic Matsubara frequencies, respectively, and $F$ is a bounded function of $O(1)$. In particular, for an $s$-wave superconductor, we have $F = +1$ for $\Omega_m, \nu_n, \omega_0 \gg \Delta_0$, and $F = -1$ for $\Omega_m, \nu_n, \omega_0 \ll \Delta_0$, implying that the bare vertex is enhanced (suppressed) for frequencies smaller (larger) than the SC gap. In contrast, in a $d_{x^2-y^2}$-wave superconductor we obtain $F \rightarrow 0$ for $\Omega_m, \nu_n, \omega_0 \ll \Delta_0$, and vertex corrections become irrelevant. Thus, vertex corrections can in general be neglected for $g m/4 < 1$, which applies to all cases considered above.

In conclusion, we consider the effects of a localized bosonic mode on the electronic structure in $s$- and $d_{x^2-y^2}$-wave superconductors. The mode acts as a new type of “defect”, leading to the emergence of bound or resonance states. We identify several characteristic features, such as a “dip” in the DOS and the temperature dependence of the mode induced peaks, that qualitatively distinguishes the effects of a localized mode from those of static impurities. This result provides further insight into the nature of impurities observed in STM experiments.

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