

Impurity bound-state as a probe of order-parameter symmetry in iron-pnictide superconductors: T -matrix approach

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Abstract. The impurity induced in-gap bound state in multi-orbital superconductors is discussed based on Bogoliubov-de Gennes equation and T -matrix approximation. It is shown that multiple bound states appear depending on the strength of the impurity potential in the case of unconventional s-wave (or s_{+-} -wave) superconductivity. This result can be used to distinguish between the conventional s-wave and unconventional s-wave states. T -matrix approximation using a simplified model supports the numerical results obtained in the Bogoliubov-de Gennes equation. It is shown that the T -matrix can be block diagonalized when we use orbital representation. As a result, each orbital can make the impurity bound state independently, leading to the multiple structure of the bound states. From the analysis of the T -matrix approximation, we understand the reasons why the bound states always appear pair-wise at the positions of $\pm\omega$ and why there is a large asymmetry of the two peaks. We also show that the particle-hole asymmetry of the density of states gives rise to the asymmetry with respect to the strength of the impurity potential. The connection between the obtained results and the iron-pnictide superconductors is also provided.

1. Introduction

The discovery of iron-based superconductors [1] shed light on the high-temperature superconductivity in multi-orbital systems and the possibility of unconventional s-wave superconducting states [2]. Here, unconventional s-wave superconductor means that its gap function changes its sign but has s-wave symmetry. In multi-orbital superconductors, the gap functions are represented by matrices which represent orbital degrees of freedom. It is very interesting to develop a theory to characterize the unconventional s-wave superconductivity in multi-orbital superconductors.

In iron-pnictide superconductors, the order parameter is now controversial, i.e., simple s-wave (s_{++} -wave) or unconventional s_{+-} -wave superconductivity. Usually the latter is believed to be realized next to the magnetic phase [2]. Actually it is supported by the quasi-particle interference experiment [3]. However, the former s_{++} -wave state is claimed based on the fact that the superconductivity is robust against nonmagnetic impurities [4]. For this s_{++} state to be stabilized, the importance of lattice and orbital degrees of freedom has been discussed [5].

Having these in mind, it is necessary to have a theory to distinguish between the two candidates of superconductivity, i.e., s_{+-} -wave or s_{++} -wave. In contrast to the high- T_c cuprate superconductivity with $d_{x^2-y^2}$ -wave, the phase sensitive experiment will be difficult in iron-



pnictide since the s_{+-} - and s_{++} -wave states have the same crystallographic symmetry. However, we noticed that the single impurity problem is suitable for distinguishing between the two states [6]. It is well known that there is no bound state around a nonmagnetic impurity in a simple s-wave state, while a bound state appears in unconventional superconductors, such as $d_{x^2-y^2}$ -wave superconductivity due to the phase change of the order parameter along the quasi-particle trajectory. However, it was not known what happens in the case of s_{+-} -wave state.

In the previous paper [6], we studied a single-impurity problem by solving Bogoliubov-de Gennes equation in real-space with a nonmagnetic impurity using a realistic five-orbital model for iron-pnictides and discussed the impurity bound-states. We found that multiple bound states appear depending on the strength of the impurity potential. Our results can be used to distinguish between the s_{+-} -wave and s_{++} -wave state. Namely, if any bound state around an nonmagnetic impurity is observed, for example, in STS experiments, we can exclude the s_{++} -wave state which should not give any impurity bound state.

In the next section, we summarize the essence of the previous work by pointing out several important numerical results. In section 3, we develop T -matrix approach for the multi-orbital superconductors and study the impurity-induced in-gap bound state in section 4.

2. Impurity bound state obtained in Bogoliubov-de Gennes equations

In the previous paper [6], we studied numerically a single-impurity by solving Bogoliubov-de Gennes equation for five-orbital iron-pnictide model. The model and formalism are as follows.

- (i) For the kinetic energy part, we use five band Hubbard model developed by Kuroki *et al* [7].
- (ii) We construct a simple effective attractive interaction which reproduces the RPA results obtained in the multi-orbital Hubbard model with the above kinetic energy. For this purpose, we notice that using the orbital representation (not the band representation) and using the real-space picture are essential for making a simple effective interaction [8]. Actually, the multi-orbital gap functions obtained in RPA can be reproduced quite well by real-space pairings up to the next-nearest-neighbor sites when we use the orbital representation. Accordingly, our effective attractive interaction is up to the next-nearest-neighbor sites.
- (iii) By using this simple effective interaction, we can study Bogoliubov-de Gennes equation that is basically a real-space mean-field approximation of the BCS theory. Note that the multi-orbital Hubbard model can not be used in the Bogoliubov-de Gennes equation, and it is essential to use the simplified model. We solve Bogoliubov-de Gennes equation in a unit cell with up-to 28×28 lattice sites with a single impurity at the center. We use a super-cell method which was used before for the vortex problem in the t - J model [9].
- (iv) As an impurity potential we assume

$$\mathcal{H}_{\text{imp}} = \sum_{a\sigma} I_a c_{\mathbf{r}_0 a \sigma}^\dagger c_{\mathbf{r}_0 a \sigma}, \quad (1)$$

where a represents the five orbitals and \mathbf{r}_0 is the impurity site. Generally, we can choose orbital-dependent strengths of the impurity potential, I_a . However, in the numerical simulations we assumed $I_a = I$ for simplicity. Even then, there appear many interesting phenomena as shown below.

The obtained results are summarized as follows [6].

- (i) For the s_{+-} -wave state obtained in the RPA in multi-orbital Hubbard model, we found that the impurity-bound states near the Fermi energy become prominent when $I = 1$ -2eV. They give relatively sharp peaks in local density of states around the impurity, which can be directly checked by STS experiments. We also found that bound-states appear near the gap edge when $I = 0.5$ eV, $I = 8$ eV or I is negative. These results indicate that the impurity bound-state is sensitive to the impurity strength, I . This situation is different from the d-wave case in which

the bound state is a resonance state due to the finite density of states inside the gap and it is sometimes difficult to be observed.

(ii) We found multiple bound states for the cases with $I = 1-2\text{eV}$. When we checked the components of these bound states, we can see that the multiplicity comes from the orbital degrees of freedom. In other words, the positions of the bound states are orbital-dependent.

(iii) The bound states always appear pair-wise at the positions of $\pm\omega$, with ω being the energy measured from the Fermi energy. However there is a large asymmetry of these two peaks. Depending on the parameter I and the related orbital, the wights of the two peaks change.

(iv) The impurity bound state is localized around the impurity site. The spatial extension is about up-to the next-nearest-neighbor sites. Also the peak height oscillates as a function of the distance from the impurity.

(v) We checked that there appears no bound state for the s_{++} -wave case.

This kind of variety of bound-state spectra is a new aspect for the unconventional multi-orbital superconductivity. A recent experiment of STS by Hanaguri *et al* [10] supports this phenomenon. To repeat our claim, our results can be used to distinguish between the s_{+-} -wave and s_{++} -wave state. Namely, if any bound state around a nonmagnetic impurity is observed, we can exclude the s_{++} -wave state which does not give any impurity bound states.

3. T -matrix approximation in multi-orbital superconductors

In order to understand the impurity bound states discussed in the previous section, we develop a T -matrix approach for the multi-orbital superconductivity. In particular, we show the reason of the appearance of the orbital-dependent multiple-peaks in the local density of states as well as the characteristic I -dependence observed numerically in the Bogoliubov-de Gennes equation.

For the impurity potential, we use eq. (1) in which the impurity is treated as a simple potential shift, and assume that the potential strength I_a depends on the orbital index a . This on-site potential means that the impurity potential is short-ranged and affects only a single site. Although this assumption is not generally correct, it will capture most of the interesting phenomena. It is also assumed that there are no inter-orbital scatterings. This assumption is not general. However, inter-orbital components will vanish when the impurity scattering is isotropic and the related orbital wave functions are orthogonal to each other. Note that the orbital representation is essential for this argument. As we will see shortly, these assumptions give more benefits than their drawbacks.

Under these assumptions, we obtain Green's function within T -matrix approximation [11] as

$$[\mathcal{G}(\mathbf{k}, \mathbf{k}', i\omega_n)_{\text{imp}}] = \delta_{\mathbf{k}, \mathbf{k}'} [\mathcal{G}(\mathbf{k}, i\omega_n)] + [\mathcal{G}(\mathbf{k}, i\omega_n)] [T(i\omega_n)] [\mathcal{G}(\mathbf{k}', i\omega_n)], \quad (2)$$

where $[\dots]$ represents a $2L \times 2L$ matrix with L being the number of orbitals ($L = 5$ for the model of iron-pnictide), and the Green's function $[\mathcal{G}(\mathbf{k}, i\omega_n)]$ without impurity is expressed as

$$[\mathcal{G}(\mathbf{k}, i\omega_n)] = \begin{pmatrix} G_{ab}(\mathbf{k}, i\omega_n) & F_{ab}(\mathbf{k}, i\omega_n) \\ \bar{F}_{ab}(\mathbf{k}, i\omega_n) & -G_{ab}(-\mathbf{k}, -i\omega_n) \end{pmatrix}. \quad (3)$$

The T -matrix is defined as

$$[T(i\omega_n)] = \left([1] - [I] [\mathcal{G}^{\text{loc}}(i\omega_n)] \right)^{-1} [I]. \quad (4)$$

Here, $[\mathcal{G}^{\text{loc}}(i\omega_n)]$ represents a local Green's function

$$[\mathcal{G}^{\text{loc}}(i\omega_n)] \equiv \frac{1}{N} \sum_{\mathbf{k}} [\mathcal{G}(\mathbf{k}, i\omega_n)], \quad (5)$$

and

$$[I] = \begin{pmatrix} \tilde{I} & 0 \\ 0 & -\tilde{I} \end{pmatrix}, \quad \tilde{I} = \begin{pmatrix} I_1 & & & \\ & I_2 & & \\ & & \ddots & \\ & & & I_L \end{pmatrix}. \quad (6)$$

Although the form of T -matrix is complicated in general, there appears a large simplification when we use the orbital representation. First, we consider the symmetry of Green's function $G_{ab}(\mathbf{k}, i\omega_n)$ in multi-orbital superconductors. It is determined from the symmetries of the wave functions for a and b orbitals together with the symmetry of the lattice. Generally we find

$$\frac{1}{N} \sum_{\mathbf{k}} G_{ab}(\mathbf{k}, i\omega_n) = 0 \quad (\text{for } a \neq b), \quad (7)$$

when the basis wave functions are orthogonal to each other. This is because $\frac{1}{N} \sum_{\mathbf{k}} G_{ab}(\mathbf{k}, i\omega_n)$ represents a kind of on-site hopping between orbital a and b .

For the anomalous Green's function, $F_{ab}(\mathbf{k}, i\omega_n)$, its symmetry is determined as

$$(\text{symm. of } F_{ab}(\mathbf{k}, i\omega_n)) = (\text{symm. of } G_{ab}(\mathbf{k}, i\omega_n)) \times (\text{symm. of } \Delta_{bb}(\mathbf{k})), \quad (8)$$

when the symmetries of the diagonal elements of the gap functions, $\Delta_{bb}(\mathbf{k})$, are specified. This can be understood from the relation

$$F_{ab}(\mathbf{k}, i\omega_n) = G_{ab}(\mathbf{k}, i\omega_n) \Delta_{bb}(\mathbf{k}) G_{bb}(\mathbf{k}, i\omega_n) + (\text{other terms}). \quad (9)$$

When $\Delta_{bb}(\mathbf{k})$ has s-wave-like symmetry, eq. (8) indicates that the symmetry of $F_{ab}(\mathbf{k}, i\omega_n)$ with respect to the direction of \mathbf{k} is same as that of $G_{ab}(\mathbf{k}, i\omega_n)$. As a result, together with eq. (7), we have

$$\frac{1}{N} \sum_{\mathbf{k}} F_{ab}(\mathbf{k}, i\omega_n) = 0 \quad (\text{for } a \neq b), \quad (10)$$

again when the basis wave functions are orthogonal, e.g., in the 3d five orbital model. Actually we confirm this relation in the case of iron-pnictide superconductors.

From eqs. (7) and (10), we find that many components of $[\mathcal{G}^{\text{loc}}(i\omega_n)]$ vanish in multi-orbital superconductors, making the form of the T -matrix very simple. For the s_{+-} and s_{++} -wave cases, we have

$$[\mathcal{G}^{\text{loc}}(i\omega_n)] = \begin{pmatrix} G_{11}(i\omega_n) & 0 & \cdots & F_{11}(i\omega_n) & 0 & \cdots \\ 0 & G_{22}(i\omega_n) & \cdots & 0 & F_{22}(i\omega_n) & \cdots \\ 0 & 0 & \ddots & 0 & 0 & \ddots \\ \bar{F}_{11}(i\omega_n) & 0 & \cdots & -G_{11}(-i\omega_n) & 0 & \cdots \\ 0 & \bar{F}_{22}(i\omega_n) & \cdots & 0 & -G_{22}(-i\omega_n) & \cdots \\ 0 & 0 & \ddots & 0 & 0 & \ddots \end{pmatrix}. \quad (11)$$

After simple exchanges of rows and columns, we can see that the T -matrix is block diagonalized for each orbital, *i.e.*,

$$[T](i\omega_n) = \begin{pmatrix} \hat{T}_1(i\omega_n) & 0 & 0 \\ 0 & \hat{T}_2(i\omega_n) & 0 \\ 0 & 0 & \ddots \end{pmatrix}, \quad \hat{T}_a(i\omega_n) = (\hat{1} - \hat{I}_a \hat{\mathcal{G}}_a^{\text{loc}}(i\omega_n))^{-1} \hat{I}_a \quad (12)$$

where

$$\hat{\mathcal{G}}_a^{\text{loc}}(i\omega_n) = \begin{pmatrix} G_{aa}(i\omega_n) & F_{aa}(i\omega_n) \\ \bar{F}_{aa}(i\omega_n) & -G_{aa}(-i\omega_n) \end{pmatrix}, \quad \hat{I}_a = \begin{pmatrix} I_a & 0 \\ 0 & -I_a \end{pmatrix}. \quad (13)$$

It is remarkable that a multi-orbital problem now becomes as simple as a single-orbital problem. This is due to the assumptions about the impurity potential and due to the symmetry of the Green's functions. Equation (12) also means that the poles of T -matrix, or the impurity bound states are determined independently for each orbital. This is the reason why the multiple bound states (orbital dependent) are obtained numerically [6] as explained in the previous section.

4. Bound State Formation in Some Simple Models

Next question is why we have bound states for the s_{+-} -wave in particular for $I = 1.2\text{eV}$.

Applying the analytic continuation $i\omega_n \rightarrow \omega + i\delta$, T -matrix for each orbital becomes

$$\begin{aligned} \hat{T}_a(\omega) &= \frac{1}{(1 - I_a g_a(\omega))(1 - I_a \bar{g}_a(-\omega)) + I_a^2 \bar{f}_a(\omega) f_a(\omega)} \begin{pmatrix} 1 - I_a \bar{g}_a(-\omega) & I_a f_a(\omega) \\ -I_a \bar{f}_a(\omega) & 1 - I_a g_a(\omega) \end{pmatrix} \\ &= \frac{1}{D_a(\omega)} \begin{pmatrix} c_a - \bar{g}_a(-\omega) & f_a(\omega) \\ -\bar{f}_a(\omega) & c_a - g_a(\omega) \end{pmatrix} \end{aligned} \quad (14)$$

where

$$g_a(\omega) \equiv G_{aa}(\omega + i\delta), \quad \bar{g}_a(\omega) \equiv G_{aa}(-\omega - i\delta) \neq G_{aa}(-\omega + i\delta), \quad (15)$$

$$f_a(\omega) \equiv F_{aa}(\omega), \quad c_a \equiv 1/I_a, \quad (16)$$

$$D_a(\omega) \equiv (c_a - g_a(\omega))(c_a - \bar{g}_a(-\omega)) + \bar{f}_a(\omega) f_a(\omega). \quad (17)$$

Then, the positions of the poles are determined from zeros of $D_a(\omega)$, i.e., $D_a(\omega) = 0$.

In the following, we suppress the orbital index a . $g(\omega)$ and $f(\omega)$ are represented as

$$g(\omega) \equiv \frac{1}{N} \sum_{\mathbf{k}} G(\mathbf{k}, \omega) = \frac{1}{N} \sum_{\mathbf{k}} \frac{\omega + \xi_{\mathbf{k}}}{(\omega + i\delta)^2 - \xi_{\mathbf{k}}^2 - |\Delta_{\mathbf{k}}|^2}, \quad (18)$$

and

$$f(\omega) \equiv \frac{1}{N} \sum_{\mathbf{k}} F(\mathbf{k}, \omega) = \frac{1}{N} \sum_{\mathbf{k}} \frac{\Delta_{\mathbf{k}}}{(\omega + i\delta)^2 - \xi_{\mathbf{k}}^2 - |\Delta_{\mathbf{k}}|^2}. \quad (19)$$

For the simple s-wave case with $\Delta_{\mathbf{k}} = \Delta$ constant, we have

$$g(\omega) = \omega S_1(\omega) + S_2(\omega), \quad (20a)$$

$$f(\omega) = \Delta S_1(\omega), \quad (20b)$$

with

$$S_1(\omega) = \int d\xi N(\xi) \frac{1}{\omega^2 - \xi^2 - \Delta^2}, \quad (21a)$$

$$S_2(\omega) = \int d\xi N(\xi) \frac{\xi}{\omega^2 - \xi^2 - \Delta^2}, \quad (21b)$$

where ω is assumed to be inside the gap ($|\omega| < \Delta$), and $N(\xi)$ is the density of states. Note that the relations $S_1(\omega) = S_1(-\omega)$, $S_2(\omega) = S_2(-\omega)$ hold. [In contrast, for the $d_{x^2-y^2}$ -wave case, we have $f(\omega) = 0$.]

In the s_{+-} -wave case, on the other hand, the gap function $\Delta_{\mathbf{k}}$ has sign reversal between Fermi surfaces, i.e., $\Delta_{\mathbf{k}}$ is positive at some parts on the Fermi surface and negative on other

parts. This kind of gap function should lead to the reduction of $f(\omega)$ compared with the simple s-wave case owing to the cancellation of the positive part and negative part. Thus, we assume

$$f(\omega) = \alpha \Delta S_1(\omega), \quad (0 \leq \alpha < 1), \quad (22)$$

for the s_{+-} -wave case [12]. Although this is a little rough approximation, we think that it captures the essential part of the s_{+-} -wave case.

With this approximation, the denominator of the T -matrix becomes

$$D(\omega) = (c - S_2(\omega))^2 - (\omega^2 - \alpha^2 \Delta^2) S_1(\omega)^2, \quad (23)$$

with c being $c = 1/I$. In a simple estimation, we have

$$S_1(\omega) = -\frac{\pi N(0)}{\sqrt{\Delta^2 - \omega^2}}, \quad (24)$$

for $|\omega| < \Delta$ and $S_2(\omega)$ is nearly constant. In this case, we can see the following features of the positions of poles in the T -matrix. (i) We have a solution at ω_0 satisfying $\alpha \Delta < \omega_0 < \Delta$. (ii) Since eq. (23) is even with respect to ω , we have always solutions at $\pm \omega_0$. This means that the bound states always appear as a pair. (iii) The weights of the poles at $\pm \omega_0$ are different, leading to the asymmetry of the local density of states. These properties are observed numerically as shown in the previous section. Note that, in the d-wave case, only one bound state appears since the weight of one of the poles always vanishes.

Next we discuss the asymmetry with respect to the sign of I which was also observed numerically. For this purpose we consider a special case with $\alpha = 0$. In this case the two solutions are

$$\omega = \pm \frac{\Delta(c - S_2)}{\sqrt{\pi^2 N(0)^2 + (c - S_2)^2}}. \quad (25)$$

However, by checking the numerator of the T -matrix, we find that one of the bound states loses its weight because the numerator vanishes. As a result, we only have a solution at

$$\omega = -\frac{\Delta(c - S_2)}{\sqrt{\pi^2 N(0)^2 + (c - S_2)^2}}, \quad (26)$$

which satisfies a relation $\omega S_1(\omega) = c - S_2$. In this sense, the case with $\alpha = 0$ is rather special, although the following argument becomes simple.

The solution of the pole of T -matrix can be obtained diagrammatically as shown in Fig. 1. Here $\omega S_1(\omega) + S_2$ is plotted as a function of ω for the case with $S_2 > 0$. The pole of the T -matrix is given at the point where this function has a value of c as discussed above. Note that $S_2(\omega)$ vanishes when $N(\xi)$ is an even function of ξ . In other words, $S_2(\omega)$ comes from the asymmetry of the density of states near the Fermi energy. In the iron-pnictide cases, LDA calculations show that the density of states is larger when $\varepsilon < \varepsilon_F$. In such cases, we have $S_2 > 0$ for $|\omega| < \Delta$, which corresponds to the situation in Fig. 1. We can see that, when I is positive (or when c is positive), we have a solution near $\omega = 0$ with a large amplitude. On the other hand, when I is negative (or when c is negative), the solution approaches to $\omega = \Delta$. In this case we can see that the amplitude of the pole is quite small. This is the reason why there is an asymmetry with respect to the impurity strength I .

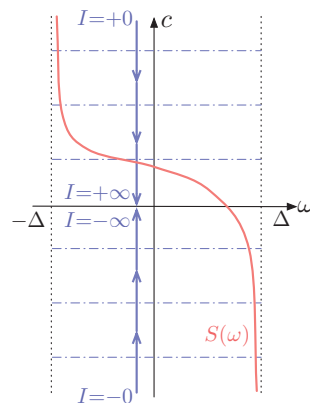


Figure 1. Schematic picture of the search for the solution of $D(\omega) = 0$.

5. Summary and Discussions

In this paper we show that the T -matrix can be block diagonalized in the multi-orbital superconductors when we use orbital representation. This is due to the symmetry of the normal and anomalous Green's functions. This result greatly simplifies the understanding of the bound state formation in multi-orbital superconductors. Since the T -matrix for each orbital can give poles independently, there is a chance to observe the multiple peak structure in the local density of states. In other words, the bound-state energy can take different values for each orbital.

The story becomes more interesting when there is remaining density of state inside the gap, i.e., the case that the gap function has nodes. Actually, the gap function with s-wave symmetry is not necessarily being nodeless, but it is possible to be nodal. In fact, nodal s-wave gap functions are predicted in some kind of iron-pnictide superconductors. In such cases, the bound states usually acquire finite life-time and becomes a virtual bound state. However, when the orbital providing the remaining density of states and that giving the bound state are different, the bound state remains to be sharp even if there is the intrinsic in-gap density of states.

The present analysis of the T -matrix approximation is consistent with the previous numerical study on the single impurity problem [6]. Numerical study shows that the multiple peak structure appears in a certain parameter range with $I > 0$ even if I_a have a common value of I . This is probably because the partial density of states for each orbital are different.

In the s_{+-} -wave case, the bound states can appear because $f(\omega)$ is reduced by a factor $\alpha < 1$, compared with the simple s-wave case. The case with $\alpha = 0$ is special in which only one bound state appears due to the cancellation of the denominator and the numerator of the T -matrix. On the other hand, for the general case with $0 < \alpha < 1$ there appear two bound states at $\omega = \pm\omega_0$ for each orbital. We have also shown that the strong asymmetry with respect to I can be well understood in the present formalism. This is due to the asymmetry of the density of states around the Fermi energy, i.e., S_2 -term. We expect that the effect of S_2 , which is usually neglected for simplicity, plays an important role in iron-pnictide.

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