In-gap bound states induced by nonmagnetic impurities in two-band $s_{\pm}$ superconductors

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(Received 19 June 2009; published 9 September 2009)

The physics of single nonmagnetic impurity immersed in a two-band *s*-wave superconductor with relative phase $\delta \neq 0$ between its two order parameters is studied and elucidated. It is shown that midgap bound states are always induced by nonmagnetic impurities when $\delta = \pi$ ($s_{\pm}$-wave superconductors). These bound states emerge as a consequence of the topological nature of the corresponding Bogoliubov-de Gennes equation.

DOI: 10.1103/PhysRevB.80.104504 PACS number(s): 74.20.−z, 74.25.Jb, 71.10.Fd

I. INTRODUCTION

With the discovery of the iron-based (pnictides) superconductors, the superconductivity characterized by more than one order parameters, i.e., the physics of multigap superconductors, enjoys a revived interest. Band-structure calculations indicate that the pertinent materials have a quasi-two-dimensional electronic structure, with four bands centered around the Γ and M points in the Brillouin zone contributing to the Fermi surface. It has been proposed that the superconducting order parameters in this multiband materials have *s*-wave symmetry, but with opposite sign between bands centered at Γ and M points[1–4] ($s_{\pm}$ superconductors).

The effect of impurities in this class of materials is a focus of experimental and theoretical interest. NMR (Ref. 5) and lower critical field data[6] seem to indicate the existence of nodes in the superconducting order parameter. On the other hand, observations in angle-resolved photoelectron spectroscopy[7,8] favor nodeless gaps. One possible solution to this conundrum is that the order parameters are *s* wavelike, but large number of in-gap states are induced by impurities in the material due to the frustrated sign of order parameters between the various bands. Indeed, such a scenario is supported by self-consistent Born-type calculations with nonmagnetic impurities where in gap states are found to emerge easily.[9–12]

To have a precise understanding of the physical effect of nonmagnetic impurities and the origin of in-gap states, we consider in this paper the effect of a single nonmagnetic impurity on the spectrum of two-band *s*-wave superconductors. The electrons in the two-band superconductor are coupled via Josephson mechanism, which determines the relative sign between the order parameters.[16] The effect of impurities is studied by analyzing the corresponding Bardeen-Schrieffer-Cooper (BCS) theory. The problem of single impurity has also been tackled numerically in certain tight-binding models used to simulate iron pnictides.[13–15] Our analytical work here is independent of the microscopic details of the models and provides results that are complementary to the above numerical works.

II. FORMULATION

The starting point is the path-integral formulation of BCS theory. The system considered here is characterized by the BCS action, $S=S_0+S_I$, where

$$S_0 = -\sum_{i,k} \Psi_i^{+}(k) \begin{pmatrix} i\omega_n - \epsilon_{i\vec{k}} + \mu & \Delta_{0i} \\ \Delta_{0i} & i\omega_n + \epsilon_{i\vec{k}} - \mu \end{pmatrix} \Psi_j(k). \quad (1)$$

$\Psi_i(k) = \left[\begin{smallmatrix} c_{i\uparrow}(k) \\ c_{i\downarrow}^{+}(-k) \end{smallmatrix}\right]$, $i=1,2$ is the band index and $k=(\vec{k}, i\omega_n)$. $\epsilon_{i\vec{k}}$ is the energy dispersion for electrons in band i and $c_\sigma, (c_\sigma^{+})$ are spin-σ electron annihilation(creation) operators.

S_0 is a sum of two bulk BCS mean-field actions describing two superconducting bands coupled only by Josephson interaction. Δ_{0i} is the superconducting gap when impurities are absent. The effect of a single nonmagnetic impurity is represented by S_I, where

$$S_I = \frac{1}{\Omega} \sum_{i,j=1,2,i\omega_n} \Psi_i^{\dagger}(i\omega_n) \begin{pmatrix} U_{ij} & \tilde{\Delta}_{ij} \\ \tilde{\Delta}_{ij}^{*} & -U_{ij} \end{pmatrix} \Psi_j(i\omega_n), \quad (2)$$

where Ω=volume of system and $\Psi_i(i\omega_n)=\Sigma_{\vec{k}}\Psi_i(k)$. S_I describes the effects of an impurity-scattering potential $U(\vec{r}) \sim \delta^d(\vec{r})\Sigma_{(i,j=1,2),\sigma} U_{ij} c_\sigma^{(i)+}(\vec{r}) c_\sigma^{(j)}(\vec{r})$, where U_{ij}'s are the scattering matrix element between bands i and j and $\tilde{\Delta}_{ij} = \delta_{ij}\tilde{\Delta}_i$ is the induced change in local superconducting gap as a result of the impurity-scattering potential. We have approximated the induced change in gap to be of form $\tilde{\Delta}_i(\vec{r}) \sim \delta^d(\vec{r})\tilde{\Delta}_i$ here, consistent with our simplified form of impurity-scattering potential.

The superconducting order parameters are determined by the mean-field equation

$$\Delta_i(\vec{r}) = \Delta_{0i} + \tilde{\Delta}_i(\vec{r}) = -\sum_{j=1,2} V_{ij} \langle c_\uparrow^{(j)}(\vec{r}) c_\downarrow^{(j)}(\vec{r}) \rangle, \quad (3)$$

where $\langle c_\uparrow^{(j)}(\vec{r}) c_\downarrow^{(j)}(\vec{r}) \rangle$ is the pairing amplitude between electrons in jth band, V_{ii} represents the pairing interaction between electrons in band i and $V_{12}=V_{21}$ is the Josephshon coupling between the pairing order parameters in the two bands.

The fermion fields in S can be integrated out to obtain an effective action S_{eff} in terms of U_{ij} and $\tilde{\Delta}_i$, given by

$$S_{eff} = \ln \det(M_0) + \ln \det[1 + G_0 M_1(U, \tilde{\Delta})], \quad (4)$$

where $\ln \det(M_0)$ results from the mean-field BCS action in the absence of impurity and

$$G_0(i\omega_n) = M_0(i\omega_n)^{-1} = \begin{pmatrix} g_{01}(i\omega_n) & 0 \\ 0 & g_{02}(i\omega_n), \end{pmatrix} \quad (5a)$$

where

$$g_{0i}(i\omega_n) = \frac{\pi N_i(0)}{\sqrt{|\Delta_{0i}|^2 - (i\omega_n)^2}} \begin{pmatrix} -i\omega_n & \Delta_{0i} \\ \Delta^*_{0i} & -i\omega_n \end{pmatrix} \theta(\omega_D - |\omega_n|) \quad (5b)$$

is the (on-site) Nambu matrix Green's function for band i electrons in the absence of the impurity. Furthermore, $\omega_D \gg |\Delta_{01}|, |\Delta_{02}|$ is the cut-off energy for attractive interactions (~Debye frequency for phonon superconductors) and $N_i(0) \sim E_F^{-1}$ is the band i density of states at the Fermi level. We have assumed $E_F \gg \omega_D, \Delta_{01(2)}, U_{ij}, \omega_n$, etc., to justify using a constant density of states in Eq. (4). The 4×4 matrix M_1 in Eq. (4) reads,

$$M_1 = \begin{pmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{pmatrix}, \quad W_{ij} = \begin{pmatrix} U_{ij} & \delta_{ij}\tilde{\Delta}_i \\ \delta_{ij}\tilde{\Delta}^*_i & -U_{ij} \end{pmatrix}. \quad (6a)$$

The free energy associated with the impurity is

$$F_I = -\frac{1}{\beta}\sum_{|\omega_n|<\omega_D} \ln \det[1 + G_0 M_1(U,\tilde{\Delta})] + \sum_{ij} (\Delta^*_{0i} + \tilde{\Delta}^*_i)(V^{-1})_{ij}(\Delta_{0j} + \tilde{\Delta}_j) \quad (7)$$

and the mean-field equation for $\tilde{\Delta}_i$ can be obtained by minimizing the free energy with respect to $\tilde{\Delta}_i$, yielding

$$\frac{1}{\beta}\sum_{|\omega_n|,j} V_{ij}\{[1 + G_0(i\omega_n)M_1]^{-1}G_0(i\omega_n)\}_{j_1,j_2} = \tilde{\Delta}_i + \Delta_{0i}, \quad (8)$$

where $(j_1,j_2)=(2j-1,2j)$ for $j=1,2$.

III. SINGLE-BAND CASE

It is helpful to first consider the situation of single-band superconductor. In this case the mean-field equation for $\tilde{\Delta}$ is

$$V'\frac{1}{\beta}\sum_{|\omega_n|<\omega_D} \frac{\pi N(0)\left(\tilde{\Delta}' + \frac{\Delta_0}{\sqrt{|\Delta_0|^2 - (i\omega_n)^2}}\right)}{1 + |U'|^2 + |\tilde{\Delta}'|^2 + \frac{2\,\mathrm{Re}(\Delta^*_0\tilde{\Delta}')}{\sqrt{|\Delta_0|^2 - (i\omega_n)^2}}} = \Delta'_0 + \tilde{\Delta}' \quad (9)$$

with $X' = \pi N(0)X$, where $X = U, V, \tilde{\Delta}, \Delta_0, \omega_D$. The BCS mean-field equation in the absence of impurity is recovered if we set $U' = \tilde{\Delta}' = 0$. Equation (9) can be solved analytically in the limit $V', |U'|, |\Delta'_0|$ and $\omega'_D = \pi N(0)\omega_D \ll 1$, which is the case for weakly coupled BCS superconductors. In this case it is straightforward to show that

$$\tilde{\Delta} \sim -\Delta_0|U'|^2 + O((U',V',\omega'_D)^4),$$

and the effect of impurity is to reduce the gap amplitude at the impurity site. Correspondingly, a bound state is induced at the impurity site which is determined by the equation $1+G_0(\omega)M_1=0$, or

$$\sqrt{|\Delta_0|^2 - \omega^2}(1 + U'|^2 + |\tilde{\Delta}'|^2) + 2\,\mathrm{Re}(\Delta^*_0\tilde{\Delta}') = 0.$$

We see that a solution $\omega < |\Delta_0|$ exists when $\Delta^*_0\tilde{\Delta} < 0$. The solution has energy $\omega \sim \Delta_0(1-2|\Delta'_0|^2|U'|^4) \gg \Delta_0 - |\tilde{\Delta}|$ in the limit $|U'|, V', \omega'_D \ll 1$. The bound-state solution is a direct consequence of local suppression of the superconducting order parameter by the impurity which creates a local "potential well" in the system. The bound state has energy $\omega >$ local gap magnitude $= \Delta_0 - |\tilde{\Delta}|$ and is not a true "in-gap" state.

IV. TWO-BAND SITUATION

Next we consider the two-band situation. To see the physics associated with the appearance of multiple bands we first consider bound states assuming $\tilde{\Delta}_i = 0$. In this case we obtain after some algebra

$$\det(1 + G_0(\omega)M_1) = 1 + \frac{|U'_{12}|^2(|U'_{12}|^2 - 2U'_{11}U'_{22})}{(1 + |U'_{11}|^2)(1 + |U'_{22}|^2)} - \frac{2(\omega^2 - |\Delta_{01}||\Delta_{02}|\cos\,\delta)|U'_{12}|^2}{(1 + |U'_{11}|^2)(1 + |U'_{22}|^2)\sqrt{(|\Delta_{01}|^2 - \omega^2)(|\Delta_{02}|^2 - \omega^2)}}, \quad (10)$$

where $U'_{ij} = \pi\sqrt{N_i(0)N_j(0)}U_{ij}$ and δ is the relative phase between the two order parameters Δ_{01} and Δ_{02}. The solutions to the equation $\det[1+G_0(\omega)M_2]=0$ can be obtained easily since the equation is quadratic in ω^2. We are interested in the bound-state solution with $\omega < \min(|\Delta_{01}|, |\Delta_{02}|)$. Notice that the equation has no solution when $U_{12}=0$, consistent with what is observed in the single-band case.

Assuming that $|\Delta_{02}| > |\Delta_{01}|$, it is easy to see from Eq. (10) that bound-state solution with energy $\omega < |\Delta_{01}|$ exists only when $|\Delta_{01}| > |\Delta_{02}|\cos\,\delta$. In particular, no bound-state solution exists when $\delta=0$. However bound state exists for $\delta=\pi$, when the two superconducting order parameters are out of phase, even when there is no induced local changes in the order parameters. Solving the mean-field equation we obtain

$$\omega^2 = \frac{1}{2(1-4r^2)}(|\Delta_{01}|^2 + |\Delta_{02}|^2 + 8r^2|\Delta_{01}||\Delta_{02}| - (|\Delta_{01}| + |\Delta_{02}|)\sqrt{(|\Delta_{02}| - |\Delta_{01}|)^2 + 16r^2|\Delta_{01}||\Delta_{02}|}), \quad (11)$$

where

$$r=\frac{|U_{12}'|^2}{(1+|U_{11}'|^2)(1+|U_{22}'|^2)-|U_{12}'|^2(|U_{12}'|^2-2U_{11}'U_{22}')}.$$

First we observe that bound-state solutions always exist in the limit of small $|U_{12}'|^2$ (Born limit). The solution has energy

$$\omega-|\Delta_{01}|\sim-2r^2\left|\frac{(|\Delta_{01}|+|\Delta_{02}|)}{(|\Delta_{02}|-|\Delta_{01}|)}\right||\Delta_{01}|+O(r^4), \quad (12a)$$

for $(|\Delta_{02}|-|\Delta_{01}|\gg 4r\sqrt{|\Delta_{01}||\Delta_{02}|})$ and

$$\omega-|\Delta_{01}|\sim-2|\Delta_{01}|r, \quad (12b)$$

for $(|\Delta_{02}|-|\Delta_{01}|\ll 4r\sqrt{|\Delta_{01}||\Delta_{02}|})$. More generally, it is straightforward to show that solutions with $\omega\geq 0$ exists when $r^2\leq 1/4$ and no solution exists at $r^2>1/4$. Therefore there exists an intermediate range of parameters U's where bound-state solution does not exist. At around the critical point $r^2=1/4-\epsilon$ we obtain

$$\omega^2=4\epsilon\frac{|\Delta_{01}|^2|\Delta_{01}|^2}{|\Delta_{01}|^2+|\Delta_{02}|^2}+O(\epsilon^2).$$

Our result indicates that the existence and the bound-state energy of the in-gap state depends on the particular form of impurity-scattering potential which determines the parameters U_{11}, U_{22}, and U_{12}. Assuming the U's are all proportional to each other we find that in the strong scattering (unitary) limit $|U_{ij}'|^2\to\infty$, $r^2\to 0$ and the bound-state energy ω approaches $|\Delta_{01}|$ asymptotically. This result is in qualitative agreement with tight-binding calculations[13–15] where shallow in-gap states are found to exist easily in two-band $s_\pm$ superconductors. Our model-independent result suggests that $\omega\to 0$ bound states are, in general, allowed in two-band superconductors with frustrated sign between order parameters.

To examine whether the in-gap state is robust against changes in the superconducting order parameters we consider the case of symmetric bands with $N_1(0)=N_2(0)$ and $\Delta_{0i}=\Delta_0 e^{i\phi_i}$, i.e., the two bands differ only in the phase of the order parameters. To simplify the problem further we set $U_{11}=U_{22}=0$ and $U_{12}=U_{21}=U$ so that

$$M_1=\begin{pmatrix}0 & \tilde{\Delta}e^{i\theta_1} & U & 0\\ \tilde{\Delta}e^{-i\theta_1} & 0 & 0 & -U\\ U & 0 & 0 & \tilde{\Delta}e^{i\theta_2}\\ 0 & -U & \tilde{\Delta}e^{-i\theta_2} & 0\end{pmatrix}, \quad (13)$$

where $\tilde{\Delta}$ and θ_i are to be solved self-consistently from the mean-field Eq. (8). The determinant $\det(1+G_0M_1)$ can still be computed analytically in this case. We obtain after lengthy algebra

$$\begin{aligned}\det[1+G_0(i\omega)M_1]&=A(i\omega)\\&+B(i\omega)[\cos(\theta_1-\phi_1)+\cos(\theta_2-\phi_2)]\\&+C(i\omega)[\cos(\theta_2-\phi_1)+\cos(\theta_1-\phi_2)]\\&+D(i\omega)\cos(\phi_1-\phi_2)\\&+2|U_{12}'|^2|\tilde{\Delta}'|^2\cos(\theta_1-\theta_2)\\&+E(i\omega)\cos(\theta_1-\phi_1)\cos(\theta_2-\phi_2),\end{aligned} \quad (14)$$

where

$$A(i\omega)=(1+|\tilde{\Delta}'|)^2+|U'|^4+2\frac{(i\omega)^2|U'|^2}{(i\omega)^2-|\Delta_0|^2},$$

$$B(i\omega)=-\frac{2\Delta_0\tilde{\Delta}'\sqrt{|\Delta_0|^2-(i\omega)^2}[1+|\tilde{\Delta}'|^2]}{(i\omega)^2-|\Delta_0|^2},$$

$$C(i\omega)=-\frac{2\Delta_0\tilde{\Delta}'\sqrt{|\Delta_0|^2-(i\omega)^2}|U'|^2}{(i\omega)^2-|\Delta_0|^2},$$

$$D(i\omega)=-\frac{2|\Delta_0|^2|U'|^2}{(i\omega)^2-|\Delta_0|^2}$$

$$E(i\omega)=-\frac{2|\Delta_0|^2|\tilde{\Delta}'|^2}{(i\omega)^2-|\Delta_0|^2},$$

while $X'=\pi N(0)X$ as before.

The mean-field equation can be solved in the weak impurity-scattering limit $|U'|,|\Delta_0'|,|V_{ij}'|,\omega_D'\ll 1$. Keeping only terms to order $|U'|^2$ and $\tilde{\Delta}'$ in the mean-field equation, we obtain $\theta_i=\phi_i(i=1,2)$ and

$$\tilde{\Delta}\sim|U'|^2\Delta_0\cos(\phi_1-\phi_2).$$

Notice that the superconducting order parameter is *enhanced* by scattering between the two bands if $\phi_1=\phi_2$ but is *suppressed* by scattering if $\phi_1-\phi_2=\pm\pi$, suggesting that nonmagnetic impurity induces a local *ferromagnetic* Josephson coupling between the superconducting order parameters which disfavors an $s_\pm$ state.[4,10] We caution here that the model considered here has no intraband scattering and no suppression of pairing interaction V_{ij} by the impurity. For realistic impurities these effects exist and suppress the superconducting order parameter for both pure-s and $s_\pm$ superconductors.

We next examine the solution(s) to the equation $\det[1+G_0(\omega)M_1]=0$ with $\omega^2<|\Delta_0|^2$. Defining $y^2\equiv\Delta_0^2-\omega^2$ we obtain an in-gap solution [with $\theta_i=\phi_i(i=1,2)$]

$$y=(-\beta+\gamma)/\alpha,$$

where

$$\beta=2\Delta_0\tilde{\Delta}'\{1+|\tilde{\Delta}'|^2+|U'|^2\cos(\phi_1-\phi_2)\},$$

$$\alpha = 1 + 2(|U'|^2 + |\tilde{\Delta}'|^2) + [U'^4 + |\tilde{\Delta}'|^4 + 2|U'|^2|\tilde{\Delta}'|^2\cos(\phi_1 - \phi_2)],$$

$$\gamma^2 = 2|U'|^2\Delta_0^2[1 + |U'|^2 + |\tilde{\Delta}'|^2]^2[1 - \cos(\phi_1 - \phi_2)].$$

It is easy to see that

$$y = -\frac{2\Delta_0\tilde{\Delta}'}{1 + |U'|^2 + |\tilde{\Delta}'|^2} \tag{15a}$$

for $\phi_1 = \phi_2$ and a $y > 0$ solution does not exist for small $|U'|^2$, where $\Delta_0\tilde{\Delta}' > 0$. The situation is very different for $\phi_1 - \phi_2 = \pm\pi$. In this case

$$y = 2\Delta_0\frac{|U'|[(1 + |\tilde{\Delta}'|^2 + |U'|^2) - \tilde{\Delta}'(1 + |\tilde{\Delta}'|^2 - |U'|^2)]}{1 + 2(|\tilde{\Delta}'|^2 + |U'|^2) + (|\tilde{\Delta}'|^2 - |U'|^2)^2} \sim 2\Delta_0|U'| \tag{15b}$$

and $\omega \sim \Delta_0 - 2|U'|^2\Delta_0$ in the limit $|U'|, |\tilde{\Delta}'| \ll 1$. Notice that the bound state has energy below the "local" gap magnitude $\Delta_0 + \tilde{\Delta} \sim \Delta_0(1 - |U'|^2)$, indicating that the formation of in-gap bound state is robust to local gap suppression.

V. IMPURITY-AVERAGED SINGLE-PARTICLE DENSITY OF STATES

To have a more quantitative feeling of the effect of impurities we compute the single-particle density of states in our model with $U_{11} = U_{22} = \alpha U_{12} = \alpha U$ and $\tilde{\Delta} = 0$. In this case the matrix Green's function $G(\omega;U) = [1 + G_0(\omega)M_1(U)]^{-1}G_0(\omega)$ can be evaluated exactly and the impurity-averaged Green's function

$$\langle G(\omega)\rangle = \int dU G(\omega;U)P(U) \tag{16}$$

can be evaluated for given impurity potential distribution $P(U)$. Contrary to self-consistent Born-type calculations the calculation here is valid only in the limit of low concentration of impurities where interference effects between different impurity-scattering events are negligible. We find that $\langle G_{12}(\omega)\rangle = \langle G_{21}(\omega)\rangle = 0$ for even distribution $P(U) = P(-U)$ and only the intraband Green's function survives impurity average. (Interband Green's function will contribute when evaluating two-particle correlation functions.) The trace of the total electron Green's function is

$$\text{Tr } G(\omega) = -\frac{2\pi N(0)\omega[1 + U'^2(1 + \alpha^2)][S_1(\omega) + S_2(\omega)]}{a(\omega)U'^4 + b(\omega)U'^2 + c(\omega)}, \tag{17}$$

with $a(\omega) = (1 - \alpha^2)^2 S_1(\omega)S_2(\omega)$, $b(\omega) = -2[\omega^2 - |\Delta_{01}\Delta_{02}|\cos\delta - \alpha^2 S_1(\omega)S_2(\omega)]$, $c(\omega) = S_1(\omega)S_2(\omega)$, where $S_i(\omega) \equiv \sqrt{|\Delta_0^{(i)}|^2 - \omega^2}$.

The single-particle density of states given by $\rho(\omega) = \Im \text{ Tr } G(\omega)$ is evaluated numerically for $s_\pm$ superconductors ($\delta = \pi$) with $P(U') = \sqrt{\frac{a}{\pi}}e^{-aU'^2}$ for different values of $a = 0.5-3$ and $\alpha = 0.4$ with $|\Delta'_{02}| = 1, |\Delta'_{01}| = 0.5$ and $N_1(0) = N_2(0) = N(0)$. $P(U')$ represents a Gaussian distribution of impurity potential strength U' centered at $U' = 0$ with a width of distribution $\sim(\sqrt{a})^{-1}$. The results of the calculation are shown in Fig. 1. The density of states for $a = 1$, $\alpha = 0.95, 1.05$ at $0 \le \omega \le |\Delta_{01}|$ is also shown in Fig. 2 for comparison.

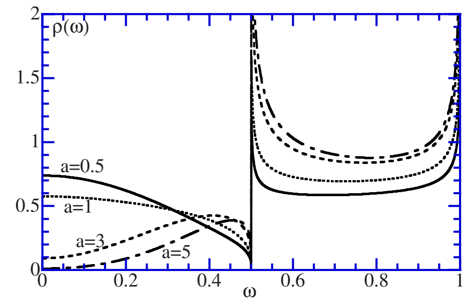

FIG. 1. (Color online) The averaged density of states $\rho(\omega)$ for $a = 0.5, 1, 3, 5$ and $\alpha = 0.4$ with $|\Delta'_{02}| = 1, |\Delta'_{01}| = 0.5$ and $N_1(0) = N_2(0)$.

We find that nonzero in-gap density of states $\rho(\omega)$) is induced when $U_{12} \neq 0$ with $\rho(\omega \to 0) \neq 0$ in general. The precise form of $\rho(\omega)$ depends also on U_{11}, U_{22} and the distribution of impurity-scattering strength $P(U')$. The in-gap spectral weight increases with increasing width of distribution of impurity potentials $\sqrt{a}^{-1}$ and shifts to lower energy with decreasing α, indicating that in-gap states are strengthened by strong interband scattering but suppressed by intraband scattering. Notice also that for $\alpha > 1$, $r < 1/2$ and no $\omega = 0$ bound state exists! The in-gap states have energy $\omega > \omega_c \sim 0.2$ for $\alpha = 1.05$ as shown in Fig. 2. We cautioned that we have not included the induced changes in-gap functions $\tilde{\Delta}$'s in our calculation. The near-gap-edge behavior is expected to be modified by $\tilde{\Delta} \neq 0$ but the deep in-gap behavior should remain qualitatively unchanged.

VI. ORIGIN OF THE IN-GAP STATES

It is important to understand why in-gap bound states are formed rather easily when the relative phase between the two superconducting order parameters is π, independent of the microscopic details of the system. The robustness of the in-gap bound states can be understood if we notice that the approximate mean-field Green's functions (5) employed in

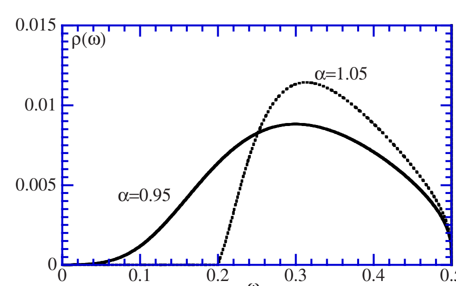

FIG. 2. (Color online) The averaged density of states $\rho(\omega)$ for $a = 1$ and $\alpha = 0.95, 1.05$ with $|\Delta'_{02}| = 1, |\Delta'_{01}| = 0.5$ and $N_1(0) = N_2(0)$.

our calculations is the exact Green's function of a corresponding one-dimensional superconductor problem, if we linearize the fermion spectrum $\epsilon_{i\vec{k}}-\mu\rightarrow\pm v_{fi}(k-k_{Fi})$ in action Eq. (1). In this case the density of states $N_i(\epsilon)\sim dk/d\epsilon$ becomes constant and Eq. (5) becomes exact. In this representation, the impurity introduces finite tunnelling probability between two one-dimensional superconductors, one located on the left of the impurity, and the other one on the right when $U_{12}\neq 0$. This problem has been studied in Refs. 16 and 17, where bound states are found to exist when the phase difference between the two superconductors is $\delta=\pi$.

The existence of in-gap bound states can be understood by noting that the one-dimensional Bogoliubov equation with a linearized electron spectrum around the Fermi surface is essentially a Dirac equation for spinless fermions at one dimension.[16] In particular, the gap function Δ becomes the mass term in the Dirac fermion representation and the problem is mathematically equivalent to a tunnelling problem between two species of Dirac fermions with different masses. For perfect tunnelling, it is known that an $\omega=0$ midgap state exists if the masses of the Dirac fermions have opposite sign at the two sides of the tunnelling barrier because of the topological structure of the problem.[18] The bound states split into two with energies $\pm\omega>0$ when a tunnelling barrier exists[17,19] and eventually merge into the continuum spectrum when the tunnelling barrier is high enough. This is exactly what we have found here when $\tilde{\Delta}_i=0$. In addition, we show that the induced $\tilde{\Delta}_i$ is small and does not affect the in-gap bound states in the limit $|U'_{12}|,|\Delta'_0|,|V'_{ij}|\ll 1$ in the case $|\Delta_{01}|=|\Delta_{02}|$ and $U_{11}=U_{22}=0$.

VII. CONCLUSION

Summarizing, by carefully studying the one-impurity problem, we show in this paper that nonmagnetic impurity is a relevant perturbation to the physics of multiband superconductors with frustrated sign between order parameters. They introduce a "ferromagnetic" Josephson coupling between the two superconducting order parameters which disfavors the $s_\pm$ state and introduce in-gap bound states in the quasiparticle spectrum. The generation of in-gap bound states is a natural phenomena associated with nonmagnetic impurities and should be taken into account carefully in understanding the electronic properties of iron-based superconductors.

ACKNOWLEDGMENTS

T.K.N. acknowledges support by HKUGC through Grant No. CA05/06.Sc04. The research of Y.A. is partially supported by an ISF grant.

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