Impurity Effect as a Probe of the Pairing Symmetry in BiS$_2$-Based Superconductors

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Abstract The impurity effects are studied for the BiS$_2$-layered superconductors based on a two-orbital model with the Bogoliubov-de-Gennes technique. The superconducting critical temperature ($T_c$) is calculated as a function of the impurity concentration. Significant reduction of $T_c$ is found for the spin singlet nearest-neighboring pairing d-wave state and the spin triplet next-nearest-neighboring (NNN) pairing p-wave state, but no depression of $T_c$ for isotropic s-wave state. The single impurity effects for various pairing states are also explored. The impurity resonance peak in the local density of states spectrum is found only for the d-wave state. For the spin triplet NNN pairing p-wave state, two in-gap peaks occur in the case of positive impurity potential and a single in-gap peak is found for the negative impurity potential, and it shifts toward the lower energy with the potential strength decreasing. These results can be used to detect the pairing symmetry of the BiS$_2$-based superconductors.

Keywords BiS$_2$-based superconductor · Pairing symmetry · Impurity effect

Superconductors with layered crystal structures such as cuprates [1], Sr$_2$RuO$_4$ [2], MgB$_2$ [3], Na$_3$Co$_2$O$_2$ [4], and iron pnictides [5] have generated enormous research interest. The low dimensionality can affect the electronic structure and can realize high transition temperatures and/or unconventional superconductivity mechanisms. Quite recently, superconductivity has been observed in the BiS$_2$-based compounds [6], such as Bi$_4$O$_4$S$_3$ [6], LaO$_{1-x}$F$_x$BiS$_2$ [7], NdO$_{1-x}$F$_x$BiS$_2$ [8], CeO$_{1-x}$F$_x$BiS$_2$ [9], and PrO$_{0.5}$F$_{0.5}$BiS$_2$ [10], where the BiS$_2$-layer is a basic unit. Soon after that, considerable efforts have been paid on the investigation of the physical properties in this system [11–25]. The discovery of the new basic superconducting (SC) layers may open new fields in physics and chemistry of low-dimensional superconductors.

The BiS$_2$-based materials are composed of the stacking of BiS$_2$-SC layers and the spacer layers, which resembles those of high-$T_c$ cuprates and the Fe-based superconductors. The first principle band structure calculations [6, 11] predict that the dominating bands for the electron conduction as well as for the superconductivity are derived from the Bi 6$p_z$ and 6$p_y$ orbits. According to the Hall effect and the magnetoresistance measurements [12], an exotic multiband feature is found in the Bi$_2$O$_4$S$_3$ compounds and the SC pairing occurs in the one-dimensional chains. Electrical resistivity measurements under pressure [16] reveal that Bi$_{1-x}$O$_x$S$_3$ and LaO$_{1-x}$F$_x$BiS$_2$ have different $T_c$ versus pressure behavior, and the Fermi surface of LaO$_{1-x}$F$_x$BiS$_2$ may be located in the vicinity of some band edges, which leads to the instability for superconductivity. It is found that the parent phase is a bad metal in the CeO$_{1-x}$F$_x$BiS$_2$ system [9], while a band insulator in the case of Bi$_2$O$_4$S$_3$ compounds [6]. By doping electrons into the system, superconductivity appears together with an insulating normal state [9], which is obviously different from that of the cuprates and the iron pnictides.

The most fundamental issue in this BiS$_2$-based compound is the superconductivity mechanism, which is still unclear. It is predicted that the electron-phonon coupling constant is as large as $\lambda = 0.85$, which indicates that LaO$_{1-x}$F$_x$BiS$_2$ is a strongly coupled electron-phonon superconductor [18, 19]. However, because electron-electron correlation generally is more important in a low dimen-
sional system, the correlation effect might play an important role in driving superconductivity even if the $p$-orbits of Bi are much less localized compared with the $d$-orbits in cuprates and iron-based superconductors [26]. Experimentally, no magnetically ordered phase has been detected so far in the BiS$_2$ compounds. This apparent absence of magnetism in the BiS$_2$ compounds may still locate them in the same category as LiFeAs, FeSe, and possibly Sr$_2$VO$_3$FeAs, which are also nonmagnetic, but their pairing properties are widely believed to still be originated from the short-range magnetic fluctuations [27]. Moreover, a good nesting of the Fermi surface at wave vector $k = (\pi, \pi, 0)$ has been found [11, 18]. It is also proposed that the SC pairing is strong, and it exceeds the limit of the phonon mediated picture [12].

The anharmonic model calculation shows that the vicinity of the charge-density-wave instability is essential for the superconductivity [18]. It is reminiscent to the proximity to spin-density-wave of iron pnictides, which is well established [5]. The correlation effect, therefore, seems to be a good candidate responsible for the SC pairing in these materials. Thus, the spin fluctuation is also proposed to account for the SC pairing in this family [17, 26, 27].

Another puzzle is the SC pairing symmetry of the BiS$_2$-based superconductors. Due to the large electron-phonon coupling constant, the pairing symmetry may usually be a conventional s-wave state with isotropic SC gap. However, the correlation effect is also proposed to account for the SC pairing, which may lead to the pairing symmetry in a complicated situation in these compounds. Moreover, based on the first principle calculation [11], it is found that the Fermi level for the nominal composition is located in the vicinity of the topological change in the Fermi surface. This gives a possibility that the SC symmetry changes depending on the doping level, provided that the superconductivity originates from the electric correlation. Considering various many-body interactions, possible pairing states are proposed, such as sign conserving/reversing s-wave and d-wave states [11, 17]. Furthermore, the first principle calculation indicates the quasi one-dimensional bands [11], which may lead to the spin-triplet pairing. In the CeO$_1$–xF$_x$BiS$_2$ compounds, superconductivity and ferromagnetism (FM) are found to coexist [9], where FM may arise from the Ce moments. The coexistence of superconductivity and FM challenges the spin-singlet pairing mechanism, which reminds us of the Sr$_2$RuO$_4$ material, whose short-range ferromagnetic spin fluctuations give rise to the triplet pairing with $p$-like symmetry [28].

The impurity effect is one of the most important tools for identifying the nature of the pairing state and the microscopic properties, which has been successfully carried out in both conventional superconductors [29] and unconventional ones, such as cuprates [30] and iron pnictides [31–39, 45]. In this paper, we will study theoretically the impurity effect in the BiS$_2$-based materials and look into the pairing symmetry based on the two-orbital model [11] and the Bogoliubov-de-Gennes (BdG) equations. The impurity concentration dependence of the critical temperature is explored. Significant reduction of $T_c$ is found for the spin singlet nearest-neighboring (NN) pairing d-wave state and the spin triplet next-nearest-neighboring (NNN) pairing p-wave state, while no depression of $T_c$ for isotropic s-wave state. The single impurity effects for various pairing states are also calculated. The impurity resonance peak in the local density of states (LDOS) spectrum is found only for the d-wave state. The evolution of the resonance peak with the impurity strength is calculated as well. For the spin triplet NNN pairing p-wave state, two in-gap peaks occur in the case of positive impurity potential and a single in-gap peak is found for the negative impurity potential, and it shifts toward the lower energy with the decreasing of the potential strength. These results can be used to detect the pairing symmetry of the BiS$_2$-based superconductors.

The starting model Hamiltonian with the hopping elements, the pairing terms, and the impurity part is expressed by

$$H = H_t + H_\Delta + H_{\text{imp}}.$$  

In the present work, we use the two-orbital model with the hopping constants from [11]. Thus, the hopping term $H_t$ can be expressed by

$$H_t = - \sum_{i \mu j \nu \sigma} (t_{i \mu j \nu \sigma} c_{i \mu \sigma}^\dagger c_{j \nu \sigma} + \text{H.c.}) - t_0 \sum_{i \mu \sigma} c_{i \mu \sigma}^\dagger c_{i \mu \sigma},$$

where $i, j$ are the site indices, $\mu, \nu = 1, 2$ are the orbital indices, and $t_0$ is the chemical potential. Considering the possibilities of both spin singlet and triplet pairings, the pairing term is written as

$$H_{\Delta} = \sum_{ij} [\Delta_{ij}^{\pm} (c_{i \mu \uparrow} c_{j \nu \downarrow}^{\dagger} \pm c_{i \mu \downarrow} c_{j \nu \uparrow}^{\dagger}) + \text{H.c.}].$$

Here, $\pm$ is for spin-triplet and singlet pairings, respectively, and the pairing potential $\Delta_{ij}^{\pm}$ is defined as $\Delta_{ij}^{\pm} = V_{ij}^{\pm} (c_{i \mu \uparrow} c_{j \nu \downarrow}^{\dagger} \pm c_{i \mu \downarrow} c_{j \nu \uparrow}^{\dagger})$, where $V_{ij}$ is the SC interaction. $H_{\text{imp}}$ is the impurity part of the Hamiltonian, written as

$$H_{\text{imp}} = \sum_{i \mu \sigma} V_{i} c_{i \mu \sigma}^{\dagger} c_{i \mu \sigma}.$$  

In this paper, both single- and multiple-impurity effects are studied, and following [29, 30, 37], only the intraorbital terms, the pairing terms, and the impurity part is expressed by $H_{\text{imp}}$. The impurity concentration dependence of the critical temperature is explored. Significant reduction of $T_c$ is found for the spin singlet nearest-neighboring (NN) pairing d-wave state and the spin triplet next-nearest-neighboring (NNN) pairing p-wave state, while no depression of $T_c$ for isotropic s-wave state. The single impurity effects for various pairing states are also calculated. The impurity resonance peak in the local density of states (LDOS) spectrum is found only for the d-wave state. The evolution of the resonance peak with the impurity strength is calculated as well. For the spin triplet NNN pairing p-wave state, two in-gap peaks occur in the case of positive impurity potential and a single in-gap peak is found for the negative impurity potential, and it shifts toward the lower energy with the decreasing of the potential strength. These results can be used to detect the pairing symmetry of the BiS$_2$-based superconductors.

Then the Hamiltonian can be diagonalized by solving the BdG equations self-consistently,

$$\sum_{\nu} \left( \begin{array}{cc} H_{i \mu j \nu \sigma} & \Delta_{ij}^{\pm} \\ \Delta_{ij}^{\mp} & -H_{i \mu j \nu \sigma} \end{array} \right) \left( \begin{array}{c} u_{i j \nu \sigma}^{\dagger} \\ v_{i j \nu \sigma}^{\dagger} \end{array} \right) = E_{\nu} \left( \begin{array}{c} u_{i \mu j \sigma}^{\dagger} \\ v_{i \mu j \sigma}^{\dagger} \end{array} \right).$$

\[ \text{(5)} \]
where the Hamiltonian $H_{ij,\nu}$ is expressed by

$$
H_{ij,\nu} = -t_{ij} \delta_{\nu} + \sum_{\mu} V_{\mu} \delta_{i,\mu}.
$$

The SC order parameter $\Delta_{ij,\nu}$ and the local electron density $\langle n_{i\mu} \rangle$ are obtained self-consistently:

$$
\Delta_{ij,\nu} = \frac{V_{ij}}{4} \sum_{\kappa} \left( \langle u_{i\mu,\kappa} \rangle^2 + \langle v_{j\nu,\kappa} \rangle^2 \right)
\times \tanh \left( \frac{E_{\kappa}}{2k_B T} \right),
$$

(7)

$$
\langle n_{i\mu} \rangle = \sum_{\kappa} \left[ \langle u_{i\mu,\kappa} \rangle^2 + \langle v_{i\mu,\kappa} \rangle^2 \right] [1 - f(E_{\kappa})].
$$

(8)

Here, $f(x)$ is the Fermi distribution function. The LDOS is expressed by

$$
\rho_i(\omega) = \sum_{n,\nu} \left[ \langle u_{i\mu,\nu} \rangle^2 \delta(E_n - \omega) + \langle v_{i\mu,\nu} \rangle^2 \delta(E_n + \omega) \right],
$$

(9)

where the delta function $\delta(x)$ has been approximated by $\Gamma/\pi(x^2 + \Gamma^2)$ with the quasiparticle damping $\Gamma = 0.002$.

Following [17], we focus our studies on the optimal doped sample with $x = 0.56$, which is used throughout the present work. The pairing strength is chosen to be $V_{ij,\nu} = 0.6$ eV for all pairing states. The numerical calculation is performed on a $24 \times 24$ lattice with the periodic boundary conditions. In this paper, the energy and length are measured in units of eV and the Bi-Bi distance $a$, respectively. To calculate the LDOS, a $80 \times 80$ supercell technique is used.

To search for the possible pairing symmetries, we consider onsite, NN and NNN singlet pairings as well as a NNN triplet pairing. The SC order parameters are calculated self-consistently according to the BdG technique with random initial values. For the onsite singlet pairing, the calculated SC order parameter is isotropic, so it is a conventional s-wave state. For the singlet pairing between the NN sites, the calculated order parameter has amplitude $+\Delta_0$ along the $x$ direction and $-\Delta_0$ along the $y$ direction, resulting in the d-wave state with the $k$-dependent pairing form $\Delta(k) = \Delta_0(\cos k_x - \cos k_y)$. In order to study the impurity effect in the extended s-wave state with the singlet pairing between NN sites, we set the same sign along the $x$ and $y$ directions so that the gap function has the form $\Delta(k) = \Delta_0(\cos k_x + \cos k_y)$. We emphasize that only the d-wave state is the self-consistent result in the case of spin singlet pairing between NN sites. For the singlet pairing between NNN sites, the order parameter has amplitude $+\Delta_1$ along the $x = y$ direction and $-\Delta_2$ along the $x = -y$ direction with $\Delta_1 \neq \Delta_2$ due to the anisotropic hopping. Hence, the gap consists of both s- and d-wave components. For the triplet pairing between NNN sites, the pairing interaction is only considered in the $x = y$ direction of the $p_x$ orbit and in the $x = -y$ direction of the $p_y$ orbit. The calculated amplitude of the order parameter has the form $\Delta_{i,x+y,\nu} = -\Delta_{i,x+y,\nu}$ of the $p_x$ orbit and $\Delta_{i,x+y,\nu} = -\Delta_{i,x-y,\nu}$ of the $p_y$ orbit, resulting in the p-wave state with $k$-dependent pairing form $\Delta(k) = \Delta_0 \sin(k_x \pm k_y)$, where “−,” “+” are for the two orbits respectively.

We first study the multiple-impurity effect for various pairing states. In this case, the impurities are randomly distributed in the $24 \times 24$ lattice. The zinc element has a stable $d^{10}$ configuration in the alloy and can serve as the best nonmagnetic impurity. If the Zn impurity is located in the BiS$_2$ layer, the scattering is quite strong. Hence, only the strong impurity potential $V_z = 10$ eV is considered here. We have considered 20 sets of multiple-impurity configurations and the critical transition temperature is the average value of these configurations. The impurity concentration dependence of the reduced critical transition temperature $T_c/T_{c0}$ is presented in Fig. 1, where $T_{c0}$ is the critical transition temperature without any impurity. As seen, for the onsite pairing s-wave state, the critical temperature $T_c$ does not decrease with the increasing impurity concentration. While it decreases with increasing impurity concentration for the other pairing states, such as spin singlet NN pairing, NNN pairing, and spin triplet NNN pairing states. For the spin singlet NNN pairing state, the critical temperature decreases rapidly in the low impurity concentration region ($\leq 5\%$), then it almost saturates with further increasing the impurity concentration. For the spin singlet NN pairing d-wave state and the spin triplet NNN pairing p-wave state, the critical transition temperature decreases with the increasing impurity concentration monotonically, while the reduction of the critical transition temperature in the p-wave state is faster than that in the d-wave state.

Generally, studying the nonmagnetic impurity effect on superconductors helps greatly to investigate the pairing symmetry. It is well known that superconductivity is robust against small concentrations of nonmagnetic impurities in
conventional s-wave superconductors, according to the Anderson’s theorem [40]. One possible explanation is that since superconductivity is due to the instability of the Fermi surface to pairing of time-reversed quasiparticle states; any perturbation that does not lift the Kramers degeneracy of these states does not affect the mean-field SC transition temperature. However, a magnetic impurity, owing to the effect of breaking the time reversal symmetry, can break Cooper pairs easily. For instance, MgB$_2$ is a BCS-type superconductor with the electron-phonon coupling and its symmetry is a s-wave, revealed by enormous experiments [41], such as the isotope effect by the substitution of $^{11}$B [42] and the observation of a coherent peak in the nuclear magnetic resonance (NMR) experiment [43]. Zn ions have a full d shell and are nominally nonmagnetic. Effect of Zn-substitution on the MgB$_2$ superconductor shows that the critical transition temperature $T_c$ is almost unchanged with small Zn-concentration, while $T_c$ is significantly suppressed by the substitution of magnetic ions [44]. These results are consistent with the Anderson’s theorem. For the BiS$_2$-based superconductor, the density function based calculations shows that this material may be a conventional s-wave superconductor with a large electron-phonon coupling constant [18, 19], but the nonmagnetic impurity effect in the multi-orbital system is subtle. For the iron-based superconductors, theoretical calculations have shown that, in the strong scattering limit, the nonmagnetic impurity effect on the s$\pm$-wave state is severe and similar to the effect on the d-wave SC state [45]. Experimentally, it is found that with the presence of Zn impurity, the SC transition temperature increases in the underdoped regime, remains unchanged in the optimally doped regime, and is severely suppressed in the overdoped regime [46]. The severe suppression of $T_c$ in the overdoped regime may be well explained within the scenario of s$\pm$-wave symmetry. On the other hand, the insensitivity of the impurity effect in the underdoped and optimally doped regimes is not in accordance with the $s_\pm$ pairing, but with the s-wave state corresponding to the same signs of the relative order parameters between the hole and electron Fermi pockets. A very recent theoretical calculation based on a two-orbital model for the iron-based superconductors also indicates that $T_c$ is insensitive to the Zn impurity if the SC order parameter has a large s-wave component with the relatively strong onsite pairing strength [47]. For the BiS$_2$-base superconductor, the symmetry of the order parameter is an isotropic s-wave state if considering the onsite pairing. As revealed by our numerical calculation presented in Fig. 1, $T_c$ is not sensitive to the nonmagnetic impurities in the s-wave state, which is consistent with the results in the iron-based compounds discussed above. Note that there is an enhancement of $T_c$ by the nonmagnetic impurity substitution, which is perhaps due to the enhanced density of state near the Fermi level [48, 49].

In contrast to the isotropic s-wave superconductors, nonmagnetic impurities are pairing breakers in anisotropic superconductors, such as heavy fermion superconductors [50] and cuprates [51]. Based on the second Born approximation and the strong-coupling Eliashberg theory, impurity-induced $T_c$ suppression in d-wave cuprate superconductors has been predicted [51]. Experimentally, Zn substitution for Cu in the high-$T_c$ cuprates dramatically suppresses superconductivity. For instance, it has been shown that an impurity concentration of 2–3 at. % (per Cu) reduces $T_c$ to half or less for unsubstituted systems over a wide region of hole doping level in Zn substituted La$_2$–ySr$_y$CuO$_4$ and YBa$_2$Cu$_3$O$_{6+\delta}$ [52–54]. In our self-consistent calculation, it is found that the pairing symmetry is d-wave in the NN singlet pairing state for BiS$_2$-compounds. The critical transition temperature $T_c$ is suppressed significantly by small concentration of nonmagnetic impurities. This result is similar to that of high $T_c$ cuprate superconductors, indicating the pairing breaking effect in d-wave SC gap. While in the NNN singlet pairing state, $T_c$ is suppressed quickly for small impurity concentration then saturates with further increasing impurities. According to our calculation, the SC gap has both s- and d-wave components. Hence, the suppression of $T_c$ is the consequence of the pairing break effect of the d-wave component in the SC gap, but the saturation of $T_c$ is due to the s-wave component.

In principle, nonmagnetic impurities are pair breakers for higher-orbital momentum states like p-wave state [30]. The reduction of $T_c$ due to nonmagnetic impurity scattering in Sr$_2$RuO$_4$ compound with p-wave like symmetry has been calculated with the conventional Abrikosov–Gorkov formula [28], which has been proved by the substitution of nonmagnetic impurity Ti$^{4+}$ ions [55–57]. For the BiS$_2$-based superconductors, possible spin triplet p-wave pairing state is proposed [11, 17]. From our self-consistent calculation, the rapid depression of $T_c$ by the nonmagnetic impurity substitution can be tested experimentally.

We now turn to study the single impurity effect in the LDOS spectra of various pairing symmetries. The calculated results are presented in Figs. 2(a)–2(e). Shown in Fig. 2(a) is the LDOS spectra around a nonmagnetic impurity for the isotropic s-wave pairing state. As it can be seen, the LDOS spectrum in the bulk has a U-shaped bottom, indicating a full SC gap. Outside the gap, the van Hove singularity peak is clearly seen. At the NN site of the impurity, the LDOS spectrum is almost unchanged compared with that in the bulk, while at the NNN site of the impurity, the SC coherence peaks in the LDOS spectrum are depressed. From the above result, it is found that there is no impurity state in the isotropic s-wave pairing state. In general, the potential scattering impurities are not pair breakers in the s-wave case according to the Anderson theorem [30]. Presented in Fig. 1(b) is the LDOS spectra for the spin singlet NNN pairing state.
Fig. 2 LDOS spectra around a nonmagnetic impurity at various pairing states. The impurity strength is set to be $V_s = 10$ eV. The solid (black) curves are the LDOS spectra in the bulk, the dash–dotted (green) curves are the LDOS spectra at the NN sites of the impurity, and the dashed (red) curves are the LDOS spectra at the NNN sites of the impurity. (a): Spin singlet of onsite pairing state; (b): Spin singlet of NNN pairing state; (c): Spin singlet of NN pairing for d wave state; (d): Spin singlet of NN pairing for extended s wave state; (e): Spin triplet of NNN pairing for the p wave state (Color figure online)

The results are similar to the case of the onsite pairing state, i.e., the LDOS spectrum has a U-shaped bottom and no impurity state occurs inside the SC gap.

The LDOS spectra for the spin singlet NN pairing d-wave state are shown in Fig. 2(c). It is found that the LDOS spectrum has a V-shaped bottom in the bulk, indicating the nodal characteristics. At the NN site of the impurity, there is a sharp resonance peak at $\omega_0 = 9$ meV in the LDOS spectrum. At the NNN site of the impurity, there is also a weak in-gap peak at $\omega_0 = -9$ meV. Note that the SC coherence peaks are also depressed obviously by the impurity at the NNN site. The resonance peak inside the SC gap at the NN site of the impurity is a general feature in a d-wave superconductor, which has already been reported in cuprate superconductors both theoretically [30] and experimentally [58]. The LDOS spectra for the spin singlet NN pairing s-wave state are presented in Fig. 2(d). The LDOS spectrum in the bulk still has a V-shaped bottom. The LDOS spectrum at the NN site of the impurity is almost unchanged compared with that in the bulk. Similar to the spin singlet onsite and NNN pairing states, there is no impurity state in this case. However, at the NNN site of the impurity, the SC coherence peaks are almost flattened, which is quite different from those in the previous cases.

The LDOS spectra for the spin triplet NNN pairing $p$-wave state are shown in Fig. 2(e). As one can see, the LDOS spectrum in the bulk is also V-shaped with nodal characteristics. Previously, a fully nodeless SC gap was
found in the Sr$_2$RuO$_4$ superconductors from the scanning tunnelling microscopy experiments [59], which is quite different from our result. This is most due to its complex pairing symmetry without nodes at the Fermi surface, i.e., sin $p_x + i$ sin $p_y$ wave or sin($p_x + p_y$) + i sin($-p_x + p_y$) wave [60]. At the NN site of the impurity, there is a small in-gap peak at $\omega_0 = 3$ meV in the spectrum. At the NNN site of the impurity, two in-gap peaks are found at $\omega_0 = \pm 3$ meV, where the in-gap peak at the positive energy is much stronger than that at the negative energy. Moreover, the SC coherence peaks are almost flattened by the impurity, similar to that of the spin singlet NN pairing $s$-wave state. From the above discussion, one can conclude that there are impurity resonance peaks only in the spin singlet NN pairing $d$-wave state. The resonance peak is very sharp in the LDOS spectrum at the NN site. However, two in-gap peaks occur in the spectrum at the NNN site for the $p$-wave pairing state and the SC coherence peaks are almost flattened by the impurity. These results can be used to detect the pairing symmetry in the BiS$_2$-based superconductors.

The potential strength response of the impurity state is also calculated. The impurity states at various potential strengths for the $d$-wave pairing state are presented in Figs. 3(a)–3(e). As seen in Figs. 3(a)–3(b), for the positive impurity potential the resonance peak at the NN site of the impurity decreases with the decreasing of the potential strength. At the impurity potential $V_s = 1$ eV, the resonance peak almost disappears and merges into the SC coherence peak. However, the situation is quite different in the case of the negative impurity potential. At the strong impurity potential $V_s = -10$ eV, there is also a sharp resonance peak at the NN site of the impurity located at $\omega_0 = 6$ meV, which is shifted to the lower energy compared with that of the impurity potential $V_s = 10$ eV. With the impurity potential decreasing, as shown in Fig. 3(d), the resonance peak at the NN site of the impurity splits into two peaks located at $\omega_0 = \pm 4.5$ meV, and the peak at the negative energy is much stronger than that at the positive energy. With the impurity potential $V_s = -1$ eV, there are also two in-gap peaks at the NN site of the impurity located at $\omega_0 = \pm 13.5$ meV, and the peak at the positive energy almost disappears.

The potential strength response of the impurity states for the $p$-wave pairing state is presented in Figs. 4(a)–4(c). For the positive impurity strength, the LDOS spectra are similar to that of $V_s = 10$ eV, i.e., two in-gap peaks occurring at the
NNN site of the impurity. These results are not presented for simplicity. Here, we focus on the LDOS spectra of the negative impurity potential for the p-wave pairing state. As it can be seen, at the NN site of the impurity, the LDOS spectra are almost featureless compared with those in the bulk. However, there is an in-gap peak in the LDOS spectra at the NNN site of the impurity, and the SC coherence peaks are almost flattened. Moreover, the location of the in-gap peak shifts from \( \omega_0 = 1.5 \text{ meV} \) at \( V_g = -10 \text{ eV} \) to \( \omega_0 = -4.5 \text{ meV} \) at \( V_g = -1.5 \text{ eV} \).

In summary, the impurity effects are studied for the BiS$_2$-layered superconductors based on a two-orbital model with the BdG technique. From the calculation of the multiple-impurity effect, the significant reduction of \( T_c \) is found for the spin singlet NN pairing d-wave state and the spin triplet NNN pairing p-wave state, while no depression of \( T_c \) for isotropic s-wave state. The single-impurity effects for various pairing states are also calculated. The impurity resonance peak in the LDOS spectrum is found only for the d-wave state. For the spin triplet NNN pairing p-wave state, two in-gap peaks occur in the case of positive impurity potential, while a single in-gap peak is found for the negative impurity potential, and it shifts toward the lower energy with the decreasing of the potential strength. These results can be used to detect the pairing symmetry of the BiS$_2$-based superconductors.

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