Yu–Shiba–Rusinov states of impurities in a triangular lattice of NbSe\textsubscript{2} with spin-orbit coupling

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We study topography of the spin-polarized bound states of magnetic impurities embedded in triangular lattice of a superconducting host. Such states have been observed experimentally in 2H-NbSe\textsubscript{2} crystal [G. C. Ménard \textit{et al.}, \textit{Nat. Phys.} \textbf{11}, 1013 (2015)] and revealed the oscillating particle-hole asymmetry extending to tens of nanometers. Using the Bogoliubov–de Gennes approach we explore the Yu–Shiba–Rusinov states in presence of spin-orbit interaction. We also study the bound states of double impurities for several relative positions in a triangular lattice.

I. INTRODUCTION

Magnetic impurities are detrimental for the Cooper pairs, because they induce the spin-polarized subgap states \cite{1,2,3} and (when impurities are dense enough) partly suppress or completely fill in the energy gap of superconducting sample. Such in-gap quasiparticles, dubbed Yu–Shiba–Rusinov (YSR) states \cite{4,5,6}, have been observed experimentally in various systems \cite{7,8,9,10,11,12,13,14}. They always exist in pairs, appearing symmetrically with respect to the chemical potential (treated here as the ‘zero-energy’ reference level). Their energies can be controlled either electrostatically or magnetically \cite{14}. Another feature is their spin-polarization evidenced by the asymmetric conductance at opposite voltages \cite{15,16}.

The bound states formed at magnetic impurities in 3-dimensional isotropic superconductors are usually characterized by a relatively short spatial extent \cite{17}. Contrary to that, in 2-dimensional (2D) lattices G.C. Ménard \textit{et al.} \cite{11} have reported different behavior, displaying much longer extent of the YSR states with alternating (oscillating) particle-hole spectral weights. Furthermore, the bound states of impurities in superconducting 2H-NbSe\textsubscript{2} \cite{18} with \textit{quasi-2D} triangular lattice structure and strong spin-orbit coupling \cite{19} have revealed the long-range coherent structures of a star-shape, whereas molecular dimers developed more complex spatial features \cite{20}.

Bulk crystals of 2H-NbSe\textsubscript{2} are characterized by centrosymmetric (P6\textsubscript{3}/mmc) structure, formed by the stacking of non-centrosymmetric layers \cite{21,22} (Fig. 1.a). Every layer is arranged in a honeycomb structure, comprising Nb and Se sublattices. Local inversion symmetry breaking \cite{23,24,25} gives rise to the out-of-plane spin polarization \cite{21} in every layer. At $T_{CDW} \approx 33K$ there appears the charge density order \cite{22,26,27}, and below $T_c \approx 7K$ \cite{21} the superconducting state sets in.

The normal state Fermi surface, studied by the angle-resolved photoemission spectroscopy (ARPES) \cite{21,27,28,29,30}, has revealed two pairs of the Nb-derived pockets, which are trigonally-warped around central $\Gamma$ point and at corner of the (hexagonal) first Brillouin zone. \textit{Ab initio} (DFT) calculations indicated that the Fermi surface sheets originate predominantly from Nb 4d-orbitals \cite{21,31,32,33}. In consequence, a triangular lattice formed by Nb atoms plays important role for the superconducting state of this compound \cite{34} and implies further a unique star-like shape of the bound states.

Differently than in bulk systems, the Fermi surface of the single monolayer 2H-NbSe\textsubscript{2} consists of only the pockets around the corner points of the Brillouin zone \cite{21}, whose size depends on the spin polarization (Fig. 1.b). The latter effect originates from the in-plane spin-orbit field \cite{19,30}. Coupling of the spin to the valley distinguishes between non-equivalent parts of the Brillouin zone. Similar behavior has been also observed in other materials with hexagonal lattice structures \cite{36,37,38,39}.

FIG. 1. a. Crystallographic structure of the centrosymmetric NbSe\textsubscript{2} compound and its primitive unit cell (black prism). The image was obtained using VESTA software \cite{35}. b. Schematic view of the Fermi surface in NbSe\textsubscript{2} monolayer, adopted from Ref. [21]. Blue and red colors correspond to different spin (negative/positive) polarizations for each Fermi sheet in the zone-corners.
Motivated by the recent experimental results of G.C. Ménard et al. [11], we study the YSR states of magnetic impurities embedded in a triangular lattice of the 2D superconducting host. The single monolayer of the 2H-NbSe$_2$ can be treated as two dimensional triangular lattice [34] with in-plane spin-orbit field (in the supplementary material we additionally take into account also the out-of-plane spin-orbit component which might be realized in other compounds [40, 41]).

In Sec. II we present the microscopic model and discuss some methodological details. Next, in Sec. III A, we analyze the YSR bound states of single magnetic impurity in a triangular lattice (Fig. 2), focusing on the role of spin-orbit coupling. In Sec. III B we study the bound states of double magnetic impurities (arranged in 3 different configurations) that might be relevant to the experimental data [20] revealing strong interference effects. Finally in Sec. IV we summarize the main results.

II. MODEL AND METHOD

Magnetic impurities embedded in 2D superconducting host with the spin-orbit coupling can be described by the following Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{imp}} + \hat{H}_{\text{int}} + \hat{H}_{\text{SOC}}.$$  \tag{1}

The single particle term

$$\hat{H}_0 = -t \sum_{\langle i,j \rangle \sigma} \hat{c}_{i \sigma}^\dagger \hat{c}_{j \sigma} - \mu \sum_{i \sigma} \hat{c}_{i \sigma}^\dagger \hat{c}_{i \sigma}$$  \tag{2}

describes the kinetic energy of electrons, where $\hat{c}_{i \sigma}^\dagger$ ($\hat{c}_{i \sigma}$) denotes creation (annihilation) of electron with spin $\sigma$ at $i$-th lattice site, $t$ is a hopping integral between the nearest-neighbors, and $\mu$ is the chemical potential. Large spin $S$ of the impurities can be treated classically [1, 2], and in such case the interaction potential can comprise the magnetic $J$ and non-magnetic $K$ parts

$$\hat{H}_{\text{imp}} = -J \left( \hat{c}_{0 \uparrow}^\dagger \hat{c}_{0 \downarrow} - \hat{c}_{0 \downarrow}^\dagger \hat{c}_{0 \uparrow} \right) + K \left( \hat{c}_{0 \uparrow}^\dagger \hat{c}_{0 \uparrow} + \hat{c}_{0 \downarrow}^\dagger \hat{c}_{0 \downarrow} \right).$$  \tag{3}

We describe the superconducting state, imposing the on-site interaction

$$\hat{H}_{\text{int}} = U \sum_i \hat{c}_{i \uparrow}^\dagger \hat{c}_{i \uparrow} \hat{c}_{i \downarrow}^\dagger \hat{c}_{i \downarrow}$$  \tag{4}

with attractive potential $U < 0$. Such effective pairing is assumed to be weak, therefore we can treat it within the standard mean-field decoupling

$$\hat{c}_{i \uparrow}^\dagger \hat{c}_{i \uparrow} \hat{c}_{i \downarrow}^\dagger \hat{c}_{i \downarrow} = \chi_i \hat{c}_{i \uparrow}^\dagger \hat{c}_{i \uparrow} \hat{c}_{i \downarrow}^\dagger \hat{c}_{i \downarrow} + |\chi_i|^2$$

$$+ n_{i \uparrow} \hat{c}_{i \uparrow}^\dagger \hat{c}_{i \uparrow} + n_{i \downarrow} \hat{c}_{i \downarrow}^\dagger \hat{c}_{i \downarrow} - n_{i \uparrow} n_{i \downarrow},$$  \tag{5}

where $\chi_i = \langle \hat{c}_{i \uparrow} \hat{c}_{i \downarrow} \rangle$ is the superconducting order parameter and $n_{i \sigma} = \langle \hat{c}_{i \sigma}^\dagger \hat{c}_{i \sigma} \rangle$ is the average number of spin $\sigma$ particles at $i$-th site. Hartree term can be incorporated into the effective local spin-dependent chemical potential

$$\mu \rightarrow \tilde{\mu}_{i \sigma} = \mu - U n_{i \sigma}.$$  \tag{6}

As we shall see, impurities suppress the local order parameter $\chi_i$ whose magnitude and sign depend on the coupling strength $J$ [42, 43].

The spin-orbit coupling (SOC) can be expressed by [44]

$$\hat{H}_{\text{SOC}} = -i \lambda \sum_{ij\sigma\sigma'} \hat{c}_{i \sigma}^\dagger \hat{c}_{j \sigma'} \left( \hat{d}_j \times \hat{\sigma} \right) \cdot \hat{\omega} \hat{c}_{i \sigma'},$$  \tag{7}

where vector $\hat{d}_j = (d_x^j, d_y^j, 0)$ corresponds to the nearest neighbors of $i$-th site (Fig. 2), and $\hat{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ consists of the Pauli matrices. The unit vector $\hat{\omega}$ shows a direction of the spin orbit field, which in general can be arbitrary, but we restrict our considerations to the in-plane $\hat{\omega} \equiv \hat{x} = (1,0,0)$ and out-of-plane $\hat{\omega} \equiv \hat{z} = (0,0,1)$ polarizations, so formally we have

$$(d_x^j \times \hat{\sigma}) \cdot \hat{\omega} = \begin{cases} \frac{d_y^j}{\sqrt{2}} \sigma_z & \text{for in-plane field,} \\ \frac{d_x^j}{\sqrt{2}} \sigma_y - \frac{d_y^j}{\sqrt{2}} \sigma_z & \text{for out-of-plane field.} \end{cases}$$

Let us notice, that out-of-plane component mixes $\uparrow$ and $\downarrow$ particles, whereas the in plane field corresponds to additional spin-conserving hopping with the spin- and direction-dependent amplitude.

Bogoliubov–de Gennes technique

Magnetic impurities break the translational invariance of the system, therefore the local pairing amplitude $\chi_i$ and occupancy $n_{i \sigma}$ have to be determined for each lattice site individually [45]. One can diagonalize the Hamiltonian (1) via the following unitary transformation

$$c_{i \sigma} = \sum_n \left( u_{i \sigma n} \gamma_n - \sigma v_{i \sigma n}^\dagger \right)$$  \tag{8}

where $\gamma_n$ and $\gamma_n^\dagger$ are quasi-particle fermionic operators, with the eigenvectors $u_{i \sigma n}$ and $v_{i \sigma n}$. This leads to the
Bogoliubov–de Gennes (BdG) equations [46]

\[
\mathcal{E}_n \begin{pmatrix}
    u_{in}^+ \\
    v_{in} \\
    u_{in} \\
    v_{in}^+
\end{pmatrix} = \sum_j \begin{pmatrix}
    H_{ij} & D_{ij}^+ & S_{ij}^+ & S_{ij}^T \\
    D_{ij}^T & -H_{ij} & S_{ij} & 0 \\
    S_{ij}^T & 0 & H_{ij} & D_{ij} \\
    0 & S_{ij}^T & D_{ij} & -H_{ij}^T
\end{pmatrix} \begin{pmatrix}
    u_{jn}^+ \\
    v_{jn} \\
    u_{jn} \\
    v_{jn}^+
\end{pmatrix}
\]

containing the single-particle term \(H_{ij}\sigma = -t\delta_{(i,j)} - (\mu_\sigma + (K - \sigma J)\delta_{0}) \delta_{ij} + S_{ij}^\sigma\) and the spin-orbit coupling term \(S_{ij}^\sigma = -i\lambda \sum_j (\delta l \times \hat{\sigma}^\sigma) \cdot \vec{w} \delta_{j,i+\delta}\). Here, \(S_{ij}^\sigma\) and \(S_{ij}^\sigma\) correspond to in plane and out of plane spin orbit field, respectively, which satisfy \(S_{ij}^\sigma = (S_{ij}^\sigma)^*\) and \(D_{ij} = U\chi_0\delta_{ij}\) describes the on-site pairing. The superconducting order parameter \(\chi_i\) and occupancy \(n_{i\sigma}\) can be computed self-consistently from BdG equations (9)

\[
\chi_i = \sum_n \left[ u_{in}v_{in}^+ f(\mathcal{E}_n) - u_{in}^+v_{in} f(-\mathcal{E}_n) \right],
\]

\[
n_{i\sigma} = \sum_n \left[ u_{in}\sigma^2 f(\mathcal{E}_n) + |v_{in}\sigma|^2 f(-\mathcal{E}_n) \right],
\]

where \(f(\omega) = 1/[1 + \exp(\omega/k_BT)]\) is the Fermi-Dirac distribution. In particular, the spin-resolved local density of states (LDOS) is given by [47]

\[
\rho_{i\sigma}(\omega) = \sum_n \left[ |u_{in}\sigma|^2 \delta(\omega - \mathcal{E}_n) + |v_{in}\sigma|^2 \delta(\omega + \mathcal{E}_n) \right].
\]

For its numerical determination we have replaced the Dirac delta function by Lorentzian \(\delta(\omega) = \zeta/[(\omega^2 + \zeta^2)]\) with a small broadening \(\zeta = 0.025t\).

III. NUMERICAL RESULTS AND DISCUSSION

We now present the BdG results obtained for the single impurity embedded in a triangular lattice (Sec. III A) and for several configurations of two magnetic impurities (Sec. III B). Numerical computations have been done at zero temperature for the finite cluster \(N_a \times N_b = 41 \times 41\), assuming \(U/t = -3\), \(\mu/t = 0\), \(K/t = 0\), and determining the bound states for varying \(J\). In this work we focus on the effect of in-plane spin-orbit field, and additional results for the out-of-plane SOC are shown in the Supplemental Material (SM) [48].

A. Single magnetic impurity

Let us start by discussing the results obtained in absence of the spin-orbit coupling. Typical quasiparticle spectrum is displayed in Fig. 3, where we can recognize the gaped region \(|\omega| \leq \Delta\) of superconducting host (for our set of the model parameters \(\Delta \approx 0.65t\)) and one pair of the bound states, appearing symmetrically around the chemical potential. Energies \(\pm \bar{E}_\alpha\) of these states and spectral weights depend on the coupling \(J\). In particular, at some critical \(J_c\) (indicated by black arrows) they eventually cross each other. This crossing is a hallmark of the quantum phase transition (QPT) [49] in which the ground state undergoes qualitative evolution [15]. When magnetic coupling overcomes the pairing energy (for \(|J| \geq J_c\)) the particle and hole states become degenerate, and the ground state changes from a BCS singlet to a spinful configuration [15, 50–52].

Our BdG dynamic can be confronted with the analytical results of the thermodynamic limit \(N_a \times N_b \to \infty\) [50]:

\[
E_{YSR} = \pm \Delta \frac{1 - \alpha^2}{1 + \alpha^2},
\]

where \(\alpha = \pi \rho_0 J\) is the dimensionless impurity coupling

![FIG. 3. Evolution of the low energy spectrum with respect to the magnetic coupling J. Solid black line shows magnitude of the pairing gap in regions far away from the impurity, black arrows point at the quantum phase transition (i.e. crossing of the subgap YSR states), and thin-dashed lines display the YSR bound states calculated from Eq. (13). Results obtained without the SOC.](image1)

![FIG. 4. Influence of the in-plane SOC on the critical value J_c. Blue/red colors correspond to the discontinuous change of Uχ_0 at the impurity site, and a white line marks the QPT. Black arrows indicate two values of λ, for which the profiles are shown in Fig. 5.](image2)
FIG. 5. The order parameter $\chi_0 = \langle c_{0\downarrow} c_{0\uparrow} \rangle$ obtained at the impurity site $i = 0$ (panel a) for the weak (red line) and strong (blue dotted line) spin-orbit couplings, with $\lambda/t = 0.1$ and 1.0 respectively. Magnetic polarization of the YSR states $\rho_{0\uparrow}(\omega) - \rho_{0\downarrow}(\omega)$ (panel b), obtained for $\lambda/t = 0.1$.

The parameter, $\rho_0$ is the normal state DOS at the Fermi level, and $\Delta$ is the superconducting gap. These quasiparticle energies (13) are displayed in Fig. 3 by a thin-dashed line. In the weak coupling limit $|J| \leq J_c$, the formula (13) matches well with our numerical BdG results. Some differences appear above the QPT (for $|J| \geq J_c$), where the local pairing parameter at magnetic impurity is substantially reduced affecting also the pairing gap of its neighboring sites. With an increasing coupling $\lambda$, the QPT is shifted to higher values (Fig. 4). The critical $J_c$ corresponds to value of $J$ at which the YSR states cross each other. Variation of the critical $J_c$ is caused by influence of the SOC merely on the normal state DOS ($\rho_0$).

Such quantum phase transition is manifested by a sign change of the order parameter $\chi_0$ at the impurity site (Fig. 5.a) and discontinuity of its absolute value is a signature of the first-order phase transition [53–55]. Let us emphasize, that QPT is associated also with a reversal of the YSR polarization (Fig. 5.b) and furthermore the total polarization of the system $P = \frac{1}{2} \sum_i (n_{i\uparrow} - n_{i\downarrow})$ abruptly changes at $J = \pm J_c$ from zero to $\pm 1/2$ [56]. Similar behavior can be observed for multiple impurities [57].

In the weak coupling limit (i.e. for $\lambda \ll t$) we can hardly notice any meaningful influence of SOC on the bulk superconductivity and the YSR states (see Fig. 1 in the SM [48]). Similar conclusion has been previously reported from the $T$-matrix treatment of magnetic impurities for 1D and 2D square lattices by V. Kaladzhyan et al. [52]. Our calculations have been done for $\lambda/t = 0.1$ which could be realistic for NbSe$_2$ compound. Obviously for much stronger values of the spin-orbit coupling, both the superconducting state and the bound YSR states depend on magnitude of $\lambda$ and direction of the magnetic moment [58].

Let us now explore a spatial extent of the YSR states. This can be achieved within the BdG approach by inte-
grating the spectral weights
\[ \rho_{\omega}^{\pm} = \int_{\omega_1}^{\omega_2} \rho_{\omega}(\omega) \, d\omega \] (14)
in the interval \( \omega \in (\omega_1, \omega_2) \) capturing every in-gap quasiparticle below or above the Fermi level [59]. Our numerical calculations have been done for the single impurity in the weak \( J = -1.2t > J_c \) and strong magnetic coupling limits \( J = -2.5t < J_c \), respectively. The results shown in Fig. 6 (notice different scales for each of these panels) reveal the characteristic 6-leg star shape, whose extent spreads on several sites around the magnetic impurity. Spectral weights at the positive and negative energies are quite different, leading to a finite spin polarization of the YSR states (displayed in the bottom panel in Fig. 5).

Upon varying \( J \) we observe, that the star-shape (characterizing \( C_6 \) symmetry of a triangular lattice) is rather robust. Such patterns of YSR states could be probed by the scanning tunneling microscopy, which nowadays has a robust. Such patterns of YSR states could be probed by characterizing in Fig. 8. Profiles of the hole- (blue line) and electron-like (red line) displaced moving average (DMA) \( \bar{\rho}^\pm(r) \) interpreted as an averaged spectral weight contained in a ring of radius \( r \) and its half-width \( \delta r \). It depends only on a radial distance \( r \) from the magnetic impurity \( r_0 \), averaging the angle-dependent fluctuations. Our results are presented in Fig. 8. They clearly show, that functions \( \bar{\rho}^\pm(r) \) of the YSR states are characterized by particle and hole oscillations that are opposite in phase (see the blue and red lines). Such particle-hole oscillations decay exponentially with distance (notice a logarithmic scale in Fig. 8) in agreement with previous studies [11, 56, 64]. In 2D continuum version of this model the wavefunctions of the YSR states have been expressed analytically [11]:

\[ \psi^\pm(r) \propto \frac{1}{\sqrt{k_{FR}}} \sin \left( k_{FR} - \frac{\pi}{4} + \delta^{\pm} \right) \times \exp \left[ -\sin(\delta^{\pm} - \delta^{-}) \frac{r}{\zeta} \right], \] (15)

where \( k_F \) is the Fermi wave vector, \( r \) is the distance from the impurity, whereas \( \zeta \) is the superconducting coherence length. Both functions oscillate with \( k_{FR} \), but with different scattering phase shifts \( \delta^{\pm} = \pm J/\rho_0 \). At short distances the YSR wavefunctions are governed by \( \sin(k_{FR})/\sqrt{k_{FR}} \), whereas for larger \( r \) the exponential envelope function suppresses particle-hole oscillations (dotted line in Fig. 8). Dominant (particle or hole) contributions to the YSR bound states are displayed by an alternating color of the background in Fig. 8. The period of such oscillations is approximately equal to \( 2 \) lattice constants. Out-of-plane spin orbit field leads to a similar behavior (Fig. 5 in [48]).

Quantum phase transition (at \( J_c \) has consequences on a reversal of the magnetization induced near the impurity (see Fig. 9). For \( |J| < J_c \) the impurity is weakly

![FIG. 8. Profiles of the hole- (blue line) and electron-like (red line) displaced moving average (DMA) for the YSR bound states \( \bar{\rho}^\pm(r) \) as a function of distance \( r \) from the impurity (with \( \delta r = 0.5 \)). The left and right panels correspond to \( |J| < J_c \) and \( |J| > J_c \), respectively. Results are obtained for the in-plane spin orbit field \( \lambda/t = 0.1 \). The dashed gray line corresponds to \( \exp(-r) \), which is a guide to eye. The blue/red background color indicates the dominant hole/particle type of YSR state at a given \( r \).](image)

![FIG. 9. Magnetization along z-axis induced near the magnetic impurity for \( |J| < J_c \) (panel a) and \( |J| > J_c \) (panel b).](image)
FIG. 10. Schematic illustration of two magnetic impurities arranged in three different configurations (a) and the subgap spectrum (b) for the nearest neighbors (NN), next nearest neighbors (NNN) and the third nearest neighbors (3NN) as shown by red, blue and green lines, respectively. We assumed the in-plane spin orbit coupling $\lambda/t = 0.1$.

screened, whereas for stronger couplings $|J| > J_c$ the impurity polarizes its neighborhood in the direction of its own magnetic moment. In both cases, this short-range magnetization does not coincide with the six-leg-star shape of the bound states. Differences between the YSR wave-functions and various components of magnetization have been previously discussed for 2D square lattice by V. Kaladzhyan et al. [52].

B. YSR of double impurities

BdG technique has a virtue that it can be easily applied for studying the bound states of more numerous impurities, distributed at arbitrary positions in a crystallographic lattice. In this section we consider the case of double magnetic impurities arranged in three different configurations displayed in Fig. 10.a. Our study of the YSR states is inspired by the results of Ref. [20] for ferromagnetic dimers. Such BdG calculations can be applied to more complex molecules [51, 65–67] and/or multi-impurity structures [68–70]. It is well known [1], that multiple-impurities can develop several quantum phase transitions with some characteristic features. They have been previously studied for 2D lattices, treating the spins classically [57, 71, 72] and taking into account the strong correlation effects within the Anderson-type scenario [73]. Here we explore the YSR states of two classical magnetic impurities embedded in a triangular lattice, assuming the weak in-plane spin orbit interaction $\lambda/t = 0.1$.

Fig. 10 presents the subgap spectrum obtained for different configurations of the double impurities. We notice that coupling between the impurities induces the double-peak structure of YSR states, both at negative and positive energies (panel b). Fig. 11 displays spatial distributions of the YSR states for each configuration of the double magnetic impurities for the weak (left column) and strong (right column) couplings $J$. Although the $C_6$ rotational symmetry is broken, one can clearly see that mirror-symmetry with respect to the axis connecting these double-impurities and the axis perpendicular to it. Novel spatial patterns of the YSR states are due to the constructive/destructive quantum interference between the overlapping subgap states. Obviously, the most significant quantum interference occurs for the quantum impurities either at the nearest neighbor (NN) or next nearest neighbor (NNN) configurations, with clear a bonding-antibonding splitting of the YSR quasiparticle energies. For more distant arrangements of the double impurities (for instance 3NN) their spatial patterns gradually evolve back to the star-like shape. A more in-depth comparison of the results obtained with and without SOC is presented in the SM [48] Fig. 6 and 7. We hope that our theoretical predictions could be empirically verified, using the combined AFM (capable of manipulating the impurities) and STM (suitable for...
probing the subgap spectrum) techniques.

IV. CONCLUSIONS

In summary, we have investigated the energies and spatial extent of the Yu–Shiba–Rusinov (YSR) states induced by the classical magnetic impurities embedded in a 2-dimensional triangular lattice of 2H-NbSe₂ superconducting host. To study this particular crystallographic geometry in presence of local inhomogeneities (in a form of the single or double impurities) and the spin-orbit coupling (SOC) we have adopted the Bogoliubov–de Gennes formalism.

In agreement with the experimental observations [11] we have found that the YSR states acquire the 6-fold rotational symmetry (star-like patterns) whose spectroscopic signatures extend onto about a dozen of intersite distances. Furthermore, their intertwining (π-shifted in phase) particle-hole oscillations are clearly visible. The weak spin orbit coupling (which should be relevant to 2H-NbSe₂ compound) has rather negligible influence on the energies of YSR states, but for relatively stronger SOC their spatial extent eventually increases (beyond 10 lattice constants in some cases). Analysis of the SOC for the single impurity indicates, that the extended range of YSR states reported in [11] stems from the dimensionality and/or the structure of atomic lattice, rather than from the in-plane spin-orbit field of such materials.

We have also studied the subgap quasiparticle spectrum of double magnetic impurities in three different configurations, revealing either the constructive or destructive quantum interference which breaks \( C_6 \) symmetry of the YSR wave-functions. Deviation from the star-like shape (typical for single impurities) depends on the relative distance between such magnetic impurities. When they are close to each other, the YSR states develop a double-peak structure (characteristic for the bonding and antibonding states) whose spatial patterns no longer resemble the star shape. With an increasing distance between the impurities such bonding-antibonding splitting gradually disappears, and the spatial star-like shape of YSR states is gradually restored.

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