Yu Shiba Rusinov physics in 2D s-wave superconductor

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In this article, the effect of an isolated magnetic impurity on a 2D s-wave superconductor is studied using zero temperature Bogoluibov De Gennes mean field theory. The impurity is assumed to be a classical spin interacting with conduction electrons in the lattice. The Local Density of States(LDOS) plot showed the presence of Yu-Shiba-Rusinov(YSR) states within the superconducting gap at nearest neighbours to the impurity. Superconducting pairing amplitude is suppressed at the impurity site, thus pointing towards the pair-breaking effect of the magnetic impurity. In the fourth section, results of an experiment[1] that first observed YSR states in a 2D s-wave superconductor was discussed.

I. INTRODUCTION

Impurities plays an important role in the study of solid state systems. In real materials, these could arise from impurity atoms, dislocations and other forms of imperfections. The study of impurities is rather interesting in the sense that it breaks translational invariance and leads to localized electronic states. The first breakthrough in the field of disordered systems was the celebrated Anderson's theorem[2]. It states that random impurity in a one dimensional or two dimensional non interacting systems cause electronic states to become localized. In the case of three dimensional systems, there exists a critical disorder under which the system is extended, and localized for the strength of disorder above the critical value.

In similar ways, there had been lot of discussions on the effect of impurities in superconductors, by assuming the impurities to be classical spins. Another pioneering work again by Anderson found that, superconducting order is insensitive to disorder, given that the impurity does not break Time Reversal Symmetry[3]. Hence this theorem does not apply for magnetic impurities since they break Time Reversal Symmetry.

A decade later, three independent pioneering theoretical papers[4][5][6] discussed the effect of an isolated magnetic impurity in s-wave superconductors. They predicted the existence of a pair of mid-gap bound states with the energy depending on the exchange coupling strength between classical spin and conduction electrons. These bound states are now called 'Yu Shiba Rusinov States'(YSR). It should be noted that the bound states appear in pairs only because of the particle hole symmetry of Bogoluibov De Gennes Hamiltonian[7]. Qualitatively, this effect can be explained as follows: a magnetic impurity creates a local magnetic field which interacts with the spin of conduction electrons. The cooper pairs in BCS condensate are broken by this local magnetic impurity. Afterwards, one of the electrons forming the pair couples with the impurity while the other forms a subgap bound state.

Eventhough theoretically predicted long ago, it was only recently that researchers could detect the midgap bound states at impurity site, first for 3D isotropic case[8] and latter for a 2D s-wave superconductor[1]. The detection of the bound states were possible due to the development of a novel experimental technique called Scanning Tunnelling Microscopy(STM). The main idea behind this method is to move a conducting tip applied over the surface of a studied material, and to measure the tunnelling conductance that is proportional to the local density of states. In-gap YSR states have now been observed in a variety of systems that could couple superconductivity with magnetic moments in the form of molecules[9], self-assembled[10] and artificial atomic chains[11], magnetic islands[12] [13] and also in proximity induced superconducting molecular break junctions[14].

In this paper, I investigate the physics of Yu Shiba Rusinov physics of a 2D s-wave superconductor in the presence of an isolated magnetic impurity. Here I treat the magnetic impurity as a localised classical spin, which is equivalent to a magnetic field interacting with the conduction electrons in the lattice. The system is studied using zero temperature Bogolyubov de Gennes(BdG) mean field theory on an attractive Hubbard model lattice. The benefit of using BdG method is that we could let pairing amplitude to have spatial variation throughout the lattice, since it is found self-consistently using BdG equations. This is in contrast to the original paper where they assumed the pairing amplitude to be spatially homogeneous[5]. Allowing pairing amplitude to be decided self-consistently has the advantage that it allows us to go to coupling regime where perturbation theory fails. But the mean field approximation off course ignores fluctuations.

In the next section, we discuss the model Hamiltonian which takes into account the necessary interactions required for our problem.

II. MODEL AND METHODOLOGY

Since the presence of impurity breaks the discrete translational symmetry of the 2D material, we chose to work on a real space lattice, with the impurity atom located at the centre. Then we apply periodic boundary

conditions at the edges. In effect, we are investigating the bulk properties of the 2D square lattice since edge effects are not taken into account.

1. Attractive Hubbard Model

We now employ attractive Hubbard model[15], which is a minimal Hamiltonian that takes into account the effects of attractive interaction that leads to superconductivity,

$$H_0 = -t \sum_{<ij>\sigma} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_i c^\dagger_{i\sigma} c_{i\sigma} - U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \quad (1)$$

Here $c^\dagger_{i\sigma}(c_{i\sigma})$ are fermion creation(annihilation) operator which creates(annihilates) an electron of spin $\sigma(\sigma = \uparrow, \downarrow)$ at site 'i'. 't' is the hopping strength. The symbol $\langle ij \rangle$ emphasizes that hopping is allowed only between sites that are adjacent. $\hat{n}_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ is the number operator. Its eigenvalue is either one or zero depending on whether electron of spin σ is present at site i or not. Since a Superconducting system does not conserve the particle number, we consider the system to be a Grand canonical ensemble. Hence we have chemical potential as one of macroscopic parameters of the system. The chemical potential is a free parameter adjusted to produce any desired electron filling. Increasing (decreasing) μ results in a corresponding increase (decrease) in the total number of electrons in the system.

The third term describes effective attractive interaction between electrons which lead to superconductivity. Since the attraction is strongest between electrons at the same site, it is a good approximation to consider only the on-site attraction and ignore the interaction with electrons in the nearest neighbours.

2. Modelling Impurity

As mentioned in the previous section, we assume the magnetic impurity to be a localised classical spin interacting with conduction electrons in the lattice. In the classical limit, this is equivalent to a local magnetic field. Thus a magnetic impurity located at site 'j' results in an energy contribution,

$$H_{imp} = \psi^\dagger_j \vec{\sigma} \cdot \vec{B} \psi_j$$

where $\psi^\dagger_j = \begin{bmatrix} c^\dagger_{j\uparrow} & c^\dagger_{j\downarrow} \end{bmatrix}$ From here, we do the calculations assuming that the classical spin is pointing in z-direction Therefore,

$$H_{imp} = B_z \left(c^\dagger_{j\uparrow} c_{j\uparrow} - c^\dagger_{j\downarrow} c_{j\downarrow} \right) \quad (2)$$

3. Mean Field Treatment

Interaction term is a four fermion operator. Inorder to diagonalise the Hamiltonian, individual terms must be quadratic in creation and annihilation operators. To realise this, we use mean field approximation to decouple the interaction term to an effective single particle Hamiltonian. This is done by ignoring higher order terms in the fluctuation. Since -U < 0, the expectation value of pair creation operator $\left\langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \right\rangle$ will be non-zero[16]. This results in,

$$\begin{aligned} -U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \approx & -U \langle \hat{n}_{i\uparrow} \rangle \hat{n}_{i\downarrow} - U \langle \hat{n}_{i\downarrow} \rangle \hat{n}_{i\uparrow} + U \left\langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \right\rangle c_{i\uparrow} c_{i\downarrow} \\ & + U \langle c_{i\uparrow} c_{i\downarrow} \rangle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} + \frac{|\triangle_i|^2}{U} \end{aligned} \quad (3)$$

Let us define the superconducting order parameter at site i as $\triangle_i = U \langle c_{i\uparrow} c_{i\downarrow} \rangle$. Thus the interaction Hamiltonian can be approximated as,

$$\begin{aligned} H_I = \sum_i & \left(-U \langle \hat{n}_{i\uparrow} \rangle \hat{n}_{i\downarrow} - U \langle \hat{n}_{i\downarrow} \rangle \hat{n}_{i\uparrow} + \triangle^*_i c_{i\uparrow} c_{i\downarrow} \right. \\ & \left. + \triangle_i c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} + \frac{|\triangle_i|^2}{U} \right) \end{aligned} \quad (5)$$

Here $U \langle \hat{n}_{i\uparrow} \rangle \hat{n}_{i\downarrow} + U \langle \hat{n}_{i\downarrow} \rangle \hat{n}_{i\uparrow}$ is the Hartree correction term.

Putting all these together, we get the model Hamiltonian for the 2D lattice as,

$$\begin{aligned} H = & -t \sum_{<ij>\sigma} c^\dagger_{i\sigma} c_{j\sigma} - \sum_i \tilde{\mu}_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma} \\ & + \sum_i \left[\triangle^*_i c_{i\uparrow} c_{i\downarrow} + \triangle_i c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \right] + H_{imp} \end{aligned} \quad (6)$$

where $\tilde{\mu}_{i\sigma}$ is the effective chemical potential given by, $\tilde{\mu}_{i\sigma} = \mu + U \langle n_{i-\sigma} \rangle$, which includes the Hartree shift.

4. Bogoluibov De Gennes Transformation

The Hamiltonian is now diagonalized using the Bogoluibov De Gennes transformation,

$$\begin{aligned} c_{i\uparrow} &= \sum_n u^n_{i\uparrow} \gamma_n - v^{n*}_{i\uparrow} \gamma^\dagger_n \\ c_{i\downarrow} &= \sum_n u^n_{i\downarrow} \gamma_n + v^{n*}_{i\downarrow} \gamma^\dagger_n \end{aligned} \quad (7)$$

where $u_{i\sigma}$ and $v_{i\sigma}$ signifies particle and hole amplitudes respectively. $\gamma^\dagger$ and γ are creation and annihilation operators for non - interacting fermionic quasiparticles. They diagonalise the Hamiltonian, so that

$$H = E_g + \sum_n E_n \gamma^\dagger_n \gamma_n \quad (8)$$

where Eg is the ground state energy. E_n represents positive energies of corresponding quasiparticle states. The detailed derivation of the BdG equation is given in the Appendix. It is evident that the mean field parameters $\triangle_i$, $\langle n_{i\uparrow}\rangle$, $\langle n_{i\downarrow}\rangle$ given by,

$$\begin{aligned}\langle n_{i\uparrow}\rangle &= \sum_n |u^n_{i\uparrow}|^2 f(E_n) + |v^n_{i\uparrow}|^2 f(-E_n)\\ \langle n_{i\downarrow}\rangle &= \sum_n |u^n_{i\downarrow}|^2 f(E_n) + |v^n_{i\downarrow}|^2 f(-E_n)\\ \triangle_i &= U\sum_n u^n_{i\uparrow} v^{n*}_{i\downarrow} f(-E_n) - u^n_{i\downarrow} v^{n*}_{i\uparrow} f(E_n) \end{aligned} \quad (9)$$

have to be found self-consistently. That is some initial guess for the parameters $\triangle_i$, $\langle n_{i\uparrow}\rangle$ and $\langle n_{i\downarrow}\rangle$ are chosen at each site. The guess is inserted into the Hamiltonian matrix and then diagonalized to find the BdG eigenvalues E_n and corresponding eigenvectors $\{u_{n\sigma}, v_{n\sigma}\}$ which is then plugged back to the BdG matrix. This process is continued until self-consistency is achieved upto a tolerance limit. In this paper, I set the tolerance limit to be 10^{-3}. We will also use the lattice averaged order parameter given by $\triangle = \frac{1}{N^2}\sum_i \triangle_i$ in our calculations.

5. *Calculating Local Density of States(LDOS)*

The Local Density of States as a function of energy and site index i at zero temperature can be calculated using the formula :

$$\rho(E,i) = \sum_{\sigma,n} |u^n_{i\sigma}|^2 \delta(E - E_n) + |v^n_{i\sigma}|^2 \delta(E + E_n) \quad (10)$$

where Dirac Delta function can be approximated numerically as,

$$\delta(x) = \frac{1}{\pi}\frac{\Gamma}{\Gamma^2 + x^2}$$

with Γ as a lifetime broadening parameter. LDOS gives the normalised density of states with energy E at site i. It is a very useful quantity to compute because it contains information about spatial distribution of energy states and can be probed very accurately using Scanning Tunnelling Microscopy. For an $N \times N$ lattice, the Hamiltonian would have $4N^2$ discrete energy levels and this spectral resolution is not enough to produce a smooth LDOS. Hence we use a technique known as 'supercell method'. Here we consider identical copies of our 20×20 lattice to be embedded within a bigger $M \times M$ supercell. Effectively, we consider the lattice to be just a unit cell in this giant supercell. Hence the periodic boundary conditions of the BdG eigenvectors changes to Bloch boundary conditions. That is,

$$\begin{aligned} u^n_{i\pm N\sigma} &= u^n_{i\sigma} e^{\pm ikN}\\ v^n_{i\pm N\sigma} &= v^n_{i\sigma} e^{\pm ikN}\end{aligned}$$

where $k_x = \frac{2\pi n_x}{M_x N_x}$ and $k_y = \frac{2\pi n_y}{M_y N_y}$. here $n_x = -M_x/2, -M_x/2 + 1....M_x/2 - 1$ and $n_y = -M_y/2, -M_y/2 + 1....M_y/2 - 1$ The results are averaged over all k values in the first Brillouin zone to get a smooth energy spectrum.

III. RESULTS AND DISCUSSION

For numerical calculation, we choose a lattice of size 20×20, with impurity atom at the centre(10, 10). The electron density is fixed at $\langle n\rangle = 1$ and the hopping strength t is also set to 1 throughout. All the relevant parameters, $\triangle$, U, B_z are all scaled to the hopping strength

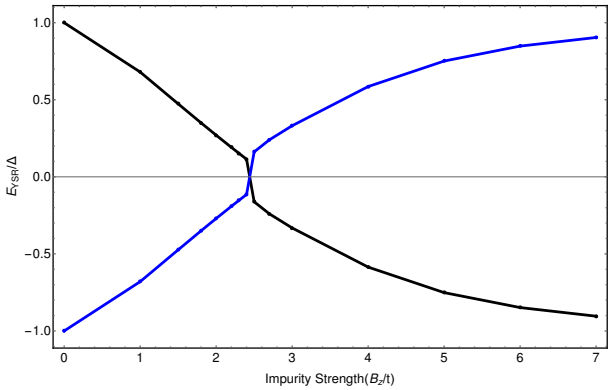

FIG. 1. Plot showing variation of $\frac{E_{YSR}}{\triangle}$ as a function of impurity strength $\frac{B_z}{t}$ Here $\triangle$ is the lattice averaged order parameter. We see that the subgap YSR state moves towards the Fermi energy as impurity strength is increased. At a critical value of Impurity strength, it crosses the Fermi energy . Here we set t = 1, U = 4t, $\langle n\rangle = 1.00$

Figure 1 shows the variation of subgap YSR state energy scaled to lattice averaged pairing amplitude as a function of impurity strength $\frac{B_z}{t}$. Here I set interaction strength $U = 4t$ and the electron filling $\langle n\rangle = 1.00$. We observe here that the energy of subgap YSR state moves towards the Fermi energy as impurity strength is increased. At a critical value of the Impurity strength, it crosses the Fermi energy. Due to particle hole symmetry of the BdG Hamiltonian, we see another bound state crossing the Fermi energy from below. The crossing of the Fermi energy by the YSR state is accompanied by a change in ground state parity. The formula connecting subgap YSR state with impurity strength derived in the original paper by Shiba[6] using perturbation theory is,

$$E_{YSR} = \pm\triangle_0 \frac{1 - ((J/2)S\pi\rho)^2}{1 + ((J/2)S\pi\rho)^2} \quad (11)$$

Here J is the coupling strength and S is the spin of the impurity. In the classical limit $J \to 0$ and $S \to \infty$, JS = finite, which is the impurity strength in our case. ρ is

the density of states at the Fermi level. We could observe that upto a scaling factor, E_{YSR} evolves with impurity strength in a similar manner as the data plot shown in fig. 1 obtained from self-consistent BdG equations.

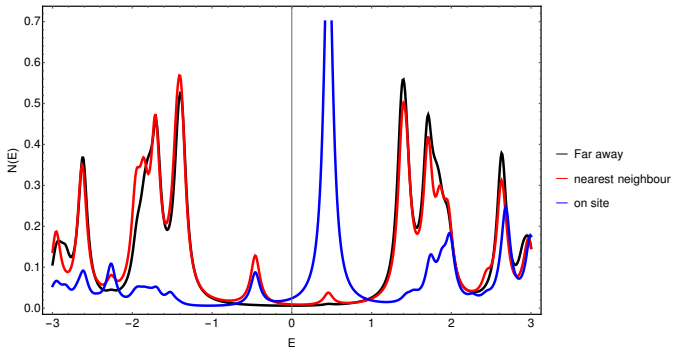

FIG. 2. Plot showing Local Density of States at the impurity site(Blue), nearest neighbour to the impurity(Red) and far away from impurity(Black). Sub-gap quasiparticle state exists as revealed by the resonance peak inside the gap for the nearest neighbours to the impurity. The strength of impurity is kept at $B_z = 3t$. Also we set $U = 4t$ and $\langle n \rangle = 1.0$. I choose $\Gamma = 0.05\triangle$, where $\triangle = 1.38$ is the lattice averaged order parameter

In figure 2, we plot the Local Density of States at three different areas of interest, at the impurity site(Blue), nearest neighbour to the impurity(Red) and far from impurity(Black). All three are plotted for the impurity strength $B_z/t = 3$. The existance of superconducting gap is evident if we look at the LDOS far from impurity(Black), which is followed by a so called 'coherence peak' at the point $E \approx \pm\triangle_i$. The coherence peak appears since the superconducting pairing pushes the states that are near the Fermi level to the gap edge. Also evident is the sub-gap quasiparticle state, as revealed by the peak in the LDOS inside the gap. This sub-gap peak is not seen in the LDOS far away from impurity site implying that the Shiba state is localised around the impurity.

It is also interesting to look at the spatial dependence of the sub-gap bound state. It is shown in the figure 3 for the impurity strength $B_z = 5t$. We could observe that the density of states spreads in space like a circular wave with centre at the impurity. This oscillatory behaviour of the density of states is observed even when superconducting states interact with a non-magnetic impurity which is commonly known as Friedel oscillations([17]).

As we saw in the previous section, pairing amplitude on each site is a self-consistent parameter in Bogoluibov De Gennes(BdG) theory[eq. 9]. Hence we could know how the Cooper pairing strength is affected by the presence of magnetic impurity. Fig. 4 plots the pairing amplitude $\triangle_i$ as a function of lattice site index 'i'. Here we see that superconducting order is suppressed at the

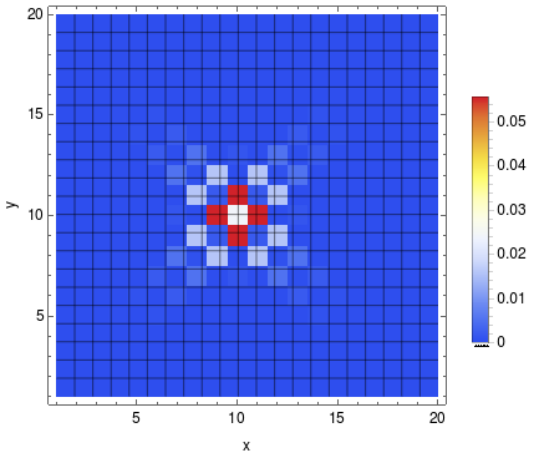

FIG. 3. Density plot showing the spatial dependence of the sub-gap bound state. The impurity strength is kept at $B_z = 5t$.

impurity site. This result go well with our qualitative description(discussed in the 'Introduction' section) that magnetic impurity breaks the Cooper pair resulting in formation of bound states that are localised at the impurity site.

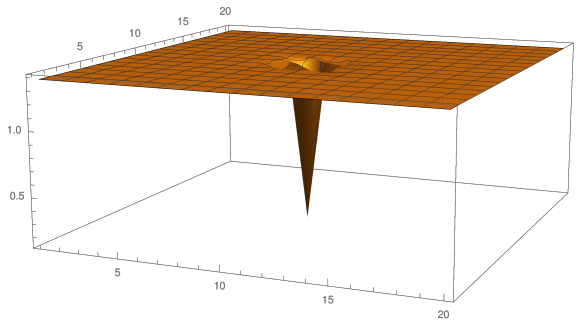

FIG. 4. 3D plot showing spatial variation of pairing amplitude $\triangle_i$ at impurity strength $B_z = 3$. We could see that the superconducting order is suppressed at the impurity site. Here too, we set $U = 4t$ and $\langle n \rangle = 1.00$

IV. EXPERIMENTAL EVIDENCE

Yu Shiba Rusinov states were first observed experimentally for a 2D isotropic superconductor only in 2015[1] even though they were observed for a 3D isotropic one, nearly two decades before[8]. The results of the experiment[1] are shown in fig. 5. In this experiment, they studied single crystals of 2H-NbSe2 containing a few tens of ppm of magnetic impurities. The scanning tunnelling spectroscopy studies performed at

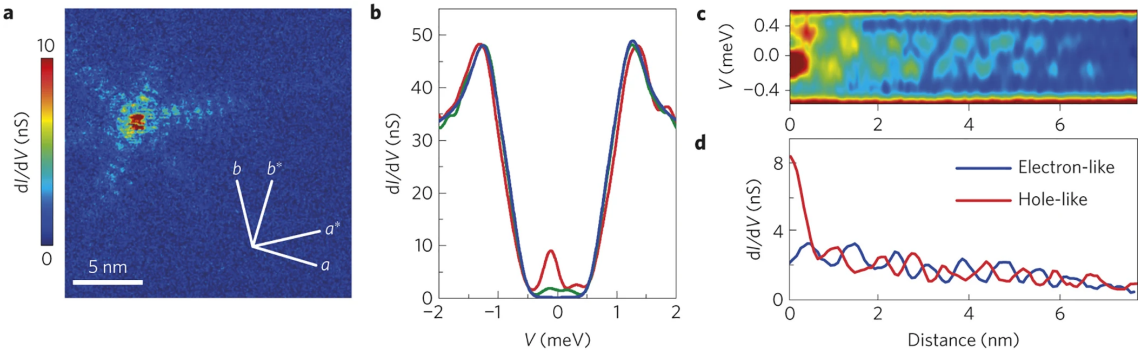

FIG. 5. **a**. Spatial dependence of Sub-gap bound state measured around the Fe impurity. The a and b lines indicate crystollagraphic axes of 2H-NbSe2.**b**Local Density of States on the impurity site(red), nearest neighbour to the impurity(green), and far from the impurity (blue).**c**. Spatial and energy evolution of the Local Density of States, (dI/dV) along one direction from the impurity site. **d** Density of States profiles of the electron- and hole-like YSR states as a function of the distance to the impurity along the same line as for **c**. Image taken from ref [1]

320mK, well below the critical temperature of 7.2K, reveal YSR bound states around the randomly dispersed magnetic iron impurities in 2H–NbSe2. The tunnelling spectra acquired over a chosen Fe impurity(see spectroscopic map in fig.5a) show a YSR bound state which takes the form of two peaks at positive and negative energies ($E_{shiba} \approx \pm 0.2\triangle$) inside the superconducting gap of 2H–NbSe2 (red curve in Fig.5b). Apart from the YSR state, the characteristic superconducting spectrum is perfectly preserved.

We could see that our theoretical calculations using Bogoluibov De Gennes method on an attractive Hubbard lattice matches well with the experimental data. This is apparent if we compare the figures 2 and 3 with their experimental counterparts 5b and 5a respectively. It should be noted that the lattice geometry of 2H-NbSe2 is radically different from a square geometry. Hence the results won't be exact. But we could capture the essential physics of Yu-Shiba-Rusinov states. That is, the formation of bound states inside the superconducting gap.

V. CONCLUSION

In this paper, I studied the Yu-Shiba-Rusinov physics of an s-wave superconductor with isolated magnetic impurity using the Bogolyubov de Gennes mean field theory on an attractive Hubbard model lattice. Using the self-consistent solutions to the BdG equations, I found the evolution of YSR bound state energy as a function of impurity strength. It is also seen that my results match well with the formula derived by Shiba in his paper[6] using Perturbation theory. The LDOS calculated at various distances from the impurity site (see fig. 2) showed the peak inside the superconducting gap at nearest neighbours to the impurity but at the same time, without altering the shape superconducting energy spectrum much. No peak is seen for the LDOS far from the impurity, which implies that the YSR state is localised at the impurity state. This is evident from the spatial distribution of Shiba states as shown in fig. 3. We could also observe the suppression of the superconducting pairing amplitude at the impurity site(see fig. 4) which verifies our qualitative description that the presence of magnetic impurity could result in pair breaking.

In the last section, a brief review of an experiment that first observed YSR state in a 2D isotropic superconductor is conducted. Using STM techniques, they could probe the localised state inside the superconducting gap. The results of the experiment verified the theoretical predictions on the impurity physics put forward by Yu[5], Shiba[6] and Rusinov[4]

Appendix A: Bogolyubov de Gennes Method

The Bogolyubov de Gennes Transormations are defined as

$$c_{i\uparrow} = \sum_n u^n_{i\uparrow}\gamma_n - v^{n*}_{i\uparrow}\gamma^\dagger_n \tag{A1}$$

$$c_{i\downarrow} = \sum_n u^n_{i\downarrow}\gamma_n + v^{n*}_{i\downarrow}\gamma^\dagger_n \tag{A2}$$

The operators $\gamma^\dagger_n(\gamma_n)$ describes creation(annihilation) operators of Bogoluibov quasiparticles at state n. Now we demand the quasiparticles to be Fermions which implies that the quasiparticle operators must follow the anti-commutation rules:

$$\{\gamma_n, \gamma^\dagger_m\} = \delta_{nm}$$
$$\{\gamma_n, \gamma_m\} = 0$$

with these canonical transformations, the Hamiltonian is diagonalized as,

$$H = \sum_n E_n\gamma^\dagger_n\gamma_n + GS \tag{A3}$$

Following the well established technique used by De Gennes[7], we work out the commutation of electron creation and annihilation operators with the Hamiltonian given in eqn 6. After computation, we get,

$$[H, c_{i\uparrow}] = t\sum_{\langle k\rangle} c_{k\uparrow} + (\mu - \epsilon_{i\uparrow} - \delta_{i,m}B_z + U\langle n_{i\downarrow}\rangle)c_{i\uparrow} - \triangle_i c^\dagger_{i\downarrow} \tag{A4}$$

$$[H, c_{i\downarrow}] = t\sum_{\langle k\rangle} c_{k\downarrow} + (\mu - \epsilon_{i\downarrow} + \delta_{i,m}B_z + U\langle n_{i\uparrow}\rangle)c_{i\downarrow} + \triangle_i c^\dagger_{i\uparrow} \tag{A5}$$

where $m = (N/2, N/2)$, that is, we demand impurity atom to be at the centre of the lattice. Here $\langle k\rangle$ represent summing over nearest neighbours to the site i. Now we replace the electron creation and annihilation operators with corresponding Bogolyubov transformation relations given in eq. A2. In the LHS of equations A4 and A5 we use the expression of Hamiltonian in terms of quasiparticle operators to get,

$$\begin{aligned}[H, c_{i\uparrow}] &= [H, \sum_n u^n_{i\uparrow}\gamma_n - v^{n*}_{i\uparrow}\gamma^\dagger_n] \\ &= \sum_n u^n_{i\uparrow}[H, \gamma_n] - v^{n*}_{i\uparrow}[H, \gamma^\dagger_n] \\ &= \sum_n -u^n_{i\uparrow}E_n\gamma_n - v^{n*}_{i\uparrow}E_n\gamma^\dagger_n \end{aligned} \tag{A6}$$

$$\begin{aligned}[H, c_{i\downarrow}] &= [H, \sum_n u^n_{i\downarrow}\gamma_n + v^{n*}_{i\downarrow}\gamma^\dagger_n] \\ &= \sum_n u^n_{i\downarrow}[H, \gamma_n] + v^{n*}_{i\downarrow}[H, \gamma^\dagger_n] \\ &= \sum_n -u^n_{i\downarrow}E_n\gamma_n + v^{n*}_{i\downarrow}E_n\gamma^\dagger_n \end{aligned} \tag{A7}$$

Thereafter, by comparing the coefficients of the quasiparticle operators we arrive at the Bogolyubov de Gennes equations,

$$\begin{aligned} E_n u^n_{i\uparrow} &= -t\sum_{\langle k\rangle} u^n_{k\uparrow} - (\mu - \epsilon_{i\uparrow} - \delta_{i,m}B_z + U\langle n_{i\downarrow}\rangle)u^n_{i\uparrow} \\ &\quad + \triangle_i v^n_{i\downarrow} \\ E_n u^n_{i\downarrow} &= -t\sum_{\langle k\rangle} u^n_{k\downarrow} - (\mu - \epsilon_{i\downarrow} + \delta_{i,m}B_z + U\langle n_{i\uparrow}\rangle)u^n_{i\downarrow} \\ &\quad + \triangle_i v^n_{i\uparrow} \\ E_n v^n_{i\uparrow} &= t\sum_{\langle k\rangle} v^n_{k\uparrow} + (\mu - \epsilon_{i\uparrow} - \delta_{i,m}B_z + U\langle n_{i\downarrow}\rangle)v^n_{i\uparrow} \\ &\quad + \triangle_i u^n_{i\downarrow} \\ E_n v^n_{i\downarrow} &= t\sum_{\langle k\rangle} v^n_{k\downarrow} + (\mu - \epsilon_{i\downarrow} + \delta_{i,m}B_z + U\langle n_{i\uparrow}\rangle)v^n_{i\downarrow} \\ &\quad + \triangle_i u^n_{i\uparrow} \end{aligned} \tag{A8}$$

where $\langle k\rangle$ denotes nearest neighbours of the site i. Now let us derive the expressions for the self-consistent parameters $\langle n_{i\sigma}\rangle$, $\langle \triangle_i\rangle$

$$\begin{aligned}\langle n_{i\uparrow}\rangle &= \left\langle c^\dagger_{i\uparrow}c_{i\uparrow}\right\rangle \\ &= \sum_{n,m}\left\langle \left(u^{n*}_{i\uparrow}\gamma^\dagger_n - v^n_{i\uparrow}\gamma_n\right)\left(u^n_{i\uparrow}\gamma_n - v^{n*}_{i\uparrow}\gamma^\dagger_n\right)\right\rangle \end{aligned} \tag{A9}$$

Since the quasiparticles are non-interacting, we have $\langle\gamma_n\gamma_n\rangle = 0$, $\langle\gamma^\dagger_n\gamma^\dagger_n\rangle = 0$,

$$\left\langle\gamma^\dagger_n\gamma_m\right\rangle = f(E_n)\delta_{nm}$$

and

$$\left\langle\gamma_n\gamma^\dagger_m\right\rangle = \delta_{nm}f(-E_n)$$

Using the above relations we get,

$$\langle n_{i\uparrow}\rangle = \sum_n |u^n_{i\uparrow}|^2 f(E_n) + |v^n_{i\uparrow}|^2 f(-E_n) \tag{A10}$$

Following similar steps for $\langle n_{i\downarrow}\rangle$, we get,

$$\langle n_{i\downarrow}\rangle = \sum_n |u^n_{i\downarrow}|^2 f(E_n) + |v^n_{i\downarrow}|^2 f(-E_n) \tag{A11}$$

The expression for order parameter is,

$$\begin{aligned}\triangle_i &= U\langle c_{i\uparrow}c_{i\downarrow}\rangle \\ &= \sum_{n,m}\left\langle (u^n_{i\uparrow}\gamma_n - v^{n*}_{i\uparrow}\gamma^\dagger_n)(u^m_{i\downarrow}\gamma_m + v^{m*}_{i\downarrow}\gamma^\dagger_m)\right\rangle \end{aligned}$$

Using the properties of quasiparticle operators as discussed above, we arrive at,

$$\triangle_i = U\sum_n u^n_{i\uparrow}v^{n*}_{i\downarrow}f(-E_n) - u^n_{i\downarrow}v^{n*}_{i\uparrow}f(E_n) \tag{A12}$$

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