Impurity states in a family of antiferromagnetic iron arsenides

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\textbf{Abstract.} In this paper, we explore theoretically the impurity states in antiferromagnetic spin-density wave states of iron arsenide. Two types of impurity models are employed: one has only intraband scattering, while the other has both intraband and interband scatterings with equal strength. Interestingly, the impurity bound state is revealed around the impurity site in the energy gap for both models. However, the impurity state is doubly degenerate with respect to spin for the first case, whereas the single-impurity state is observed in either the spin-up or spin-down channel for the second case. The impurity-induced variations of the local density of states are also examined. We propose scanning tunnelling microscopy (STM) measurements of the impurity state with the bound energy and spatial distribution of the wavefunction, which may shed light on the mechanism of the magnetically ordered phase.

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1. Introduction

The recent discovery of iron-based superconductors [1] has triggered intensive efforts to unveil the nature of and interplay between magnetism and superconductivity in this family of materials. A series of iron arsenides have been synthesized, which possess many similar features of the normal and superconducting states. Experimental measurements have reported that the undoped ReFeAsO (where Re = rare-earth metals) and AFe$_2$As$_2$ (where A = divalent metals such as Ba, Ca or Sr) compounds exhibit long-range antiferromagnetic spin-density-wave (SDW) order [2]–[9]. Upon electron/hole doping, the SDW phase is suppressed and superconductivity emerges with $T_c$ above 50 K [10]–[14].

At present, there is likely a certain controversy on the understanding of the SDW state of the undoped FeAs-based parent compounds. Two kinds of theories have been put forward: (i) itinerant antiferromagnetism, which takes advantage of proper Fermi surface (FS) ‘nesting’ (or strong scattering) between different FS sheets [15]–[19]; and (ii) the frustrated Heisenberg exchange model of coupled magnetic moments of the localized d-orbital electrons around the Fe atoms [20]–[23]. As for the itinerant electronic behavior, first principle band structure calculations [24]–[30] based on the density functional theory (DFT) indicate up to five small Fermi pockets with three hole-like pockets centered around the $\Gamma$ point and two electron-like ones centered around the $M$ point of the folded Brillouin zone of the FeAs layers, which have been partially supported by the angle-resolved photoemission spectroscopy (ARPES) from different groups [31]–[36]. Motivated by the DFT calculations and experimental measurements, a kind of excitonic mechanism [37] of itinerant carriers was employed to understand the SDW phase as a condensate of triplet excitonic electron–hole pairs in [17, 19], taking into account the FS ‘nesting’ between electron and hole pockets.

2. Model and method

In this paper, we explore theoretically the effect of a single impurity on the local electronic structure of an Fe-based antiferromagnet in the triplet excitonic phase. It is shown that impurity bound states are formed inside the SDW gap, which may be observed experimentally by local probes. Before introducing the impurity, we first propose an effective model Hamiltonian to...
Figure 1. Schematic diagram of (a) the FSs and (b) the band dispersions of the valence (hole) band and conductance (electron) bands in the unfolded Brillouin zone for the undoped parent compound. See text for details.

address the triplet excitonic state

\[ \hat{H}_{\text{MF}} = \sum_{i,k,\sigma} \varepsilon_{\Gamma_1}^{i} \langle \text{k} \rangle d_{i \text{k} \sigma}^\dagger d_{i \text{k} \sigma} + \sum_{\text{k},\sigma} \varepsilon_{X}^{\text{k} + \text{X}} \langle \text{k} + \text{X} \rangle c_{\text{k} + \text{X} \sigma}^\dagger c_{\text{k} + \text{X} \sigma} + \sum_{i,\text{k},\sigma,\sigma'} [ \Delta_{\Gamma_1 \sigma \sigma'}^{i} \langle \text{k} \rangle d_{i \text{k} \sigma}^\dagger c_{\text{X} \sigma'} + \text{H.c.} ], \]  

(1)

where \( \Gamma = (0,0) \) and \( X = (\pi, 0) \). We use the index \( i \) to label different valence bands around the \( \Gamma \) point. Around the \( X \) and \( Y \) points, there are two conduction bands. \( d_{\text{i k} \sigma} \) and \( c_{\text{k} + \text{X} \sigma} \) are the annihilation operators of electrons in the \( \Gamma_{1} \) and \( X \) bands. Theoretically, \( X \) and \( Y \) are two equivalent nesting directions. Note that the structural phase transition occurring just above/on the SDW transition breaks this equivalence. Without loss of generality, it is assumed that only the conduction band around the \( X \) point couples with the valence bands around the \( \Gamma \) point, which is characterized by the mean-field order parameters \( \Delta_{\Gamma_1 \sigma \sigma'} \). For the triplet excitonic phase (SDW), we have real order parameters satisfying \( \Delta_{\Gamma_1 \uparrow \downarrow} = -\Delta_{\Gamma_1 \downarrow \uparrow} \) and \( \Delta_{\Gamma_1 \uparrow \uparrow} = \Delta_{\Gamma_1 \downarrow \downarrow} = 0 \) [37].

\( \varepsilon_{\Gamma_1}^{i} \langle \text{k} \rangle \) and \( \varepsilon_{X}^{\text{k} + \text{X}} \langle \text{k} + \text{X} \rangle \) are used to denote the band dispersions of the nonmagnetic normal state. For \( \text{k} \) in the vicinity of the \( \Gamma \) point (therefore, \( \text{k} + \text{X} \) in the vicinity of the \( X \) point), the normal-state energy dispersions have approximately the two-dimensional (2D) parabolic forms

\[ \varepsilon_{\Gamma_1}^{i} \langle \text{k} \rangle = -\frac{\hbar^2 (k_x^2 + k_y^2)}{2m_{\Gamma_1}^{i}} + \varepsilon_{0}^{\Gamma_1}, \]  

(2)

\[ \varepsilon_{X}^{\text{k} + \text{X}} \langle \text{k} + \text{X} \rangle = \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_{X}} - \varepsilon_{0}^{X}, \]  

(3)

as schematically shown in figure 1. Here \( m_{\Gamma_1} \) and \( m_{X} \) are the corresponding effective masses. In describing the \( X \) band, the elliptic FS is approximated by the circular one for simplicity. \( \varepsilon_{0}^{\Gamma_1} \) (\( \varepsilon_{0}^{X} \)) denotes the top (bottom) of the hole (electron) bands. According to the ARPES measurement [31], two hole-like Fermi pockets are revealed around the \( \Gamma \) point for undoped BaFe\(_2\)As\(_2\). The band parameters extracted from the experimental data are as follows: \( m_{\Gamma_1} \approx 2.8m_{e} \), \( m_{\Gamma_2} \approx 7.4m_{e} \) and \( m_{X} \approx 6.5m_{e} \), where \( m_{e} \) is the mass of the bare electron.
\[ \varepsilon_0^{\Gamma} \approx 4 \text{ meV}, \quad \varepsilon_0^{T} \approx 16 \text{ meV} \quad \text{and} \quad \varepsilon_0^{X} \approx 24 \text{ meV}. \] These parameters indicate that the nesting between the \( \Gamma 2 \) band and the \( X \) band is much better than that of the \( \Gamma 1 \) band. Therefore it is natural to assume a larger order parameter \( \Delta_2 \) and a vanishingly small parameter \( \Delta_1 \). Let \( E_g = (\varepsilon_0^{\Gamma} + \varepsilon_0^{X})/2 \) and \( \mu_0 = (\varepsilon_0^{T} - \varepsilon_0^{X})/2 \). Here \( E_G = -2E_g \) denotes the indirect gap between the top of the \( \Gamma \) band and the bottom of the \( X \) band. Therefore \( E_g > 0 \) describes a semiconductor and \( E_g < 0 \) a semiconductor. With the help of \( E_g \) and \( \mu_0 \) and a further assumption of \( m_{\Gamma 2} = m_X = m \approx 7m_e \), we can re-express the energy dispersions as

\[ \varepsilon_{\Gamma 2}(k) = -\varepsilon(k) - \mu_0, \]

\[ \varepsilon_X(k + X) = \varepsilon(k) - \mu_0, \]

\[ \varepsilon(k) = \frac{\hbar^2}{2m} k^2 - E_g. \]

Note that for \( \mu_0 = 0 \), the hole and electron bands are perfectly nested since \( \varepsilon_{\Gamma 2}(k) = -\varepsilon_X(k + X) \) and the system is unstable with respect to infinitesimal Coulomb interaction, while for nonzero \( \mu_0 \) finite strength of Coulomb repulsion is needed.

For the reason that the order parameter \( \Delta_1 \) is set to zero, there is no coupling between the \( \Gamma 1 \) band and the \( X \) band. The Hamiltonian of equation (1) is reduced to a model of two bands with one valence band (\( \Gamma 2 \) band) and one conduction band (\( X \) band). Introducing the two-component Nambu operator, \( \hat{\psi}_{k\sigma} = (\hat{c}_{k\sigma}, \hat{c}_{-k\sigma}^\dagger) \), the model Hamiltonian can be simplified as

\[ \hat{H}_{\text{MF}} = \sum_{k\sigma} \hat{\psi}_{k\sigma}^\dagger \begin{pmatrix} \varepsilon_{\Gamma}(k) & \Delta_\sigma \\ \Delta_\sigma & \varepsilon_X(k) \end{pmatrix} \hat{\psi}_{k\sigma} + H_{\text{imp}} \]

with an impurity term taking the form

\[ \hat{H}_{\text{imp}} = \sum_{k,k',\sigma} \hat{\psi}_{k\sigma}^\dagger \hat{U}_{k,k'} \hat{\psi}_{k'\sigma}, \]

where \( \hat{U}_{k,k'} \) represents a \( 2 \times 2 \) matrix of the scattering potential associated with nonmagnetic impurities. Here, we use \( \Delta_\sigma \) to denote \( \Delta_{\sigma\sigma} \) for short. The Green’s function method is applied to study the single-impurity effect. The matrix Green’s functions are defined as

\[ \hat{G}_{\sigma\sigma}(k, \tau; k', \tau') = -\langle T_\tau [\hat{c}_{k\sigma}(\tau) \hat{c}_{k'\sigma}^\dagger(\tau')] \rangle. \]

\[ \hat{G}_{\sigma\sigma}(k, k', i\omega_n) = \int_0^\beta d\tau \hat{G}_{\sigma\sigma}(k, \tau; k', 0) e^{i\omega_n \tau}, \]

\[ \hat{G}_{\sigma\sigma}(k, k', \omega) = \hat{G}_{\sigma\sigma}(k, k', i\omega_n \rightarrow \omega + i0^+). \]

From the Hamiltonian defined in equation (7), we can derive the bare Green’s function

\[ \hat{G}_{\sigma\sigma}^{0}(k, \omega) = \begin{pmatrix} \omega - \varepsilon_{\Gamma}(k) & -\Delta_\sigma \\ -\Delta_\sigma & \omega - \varepsilon_X(k) \end{pmatrix}^{-1} = \frac{\tilde{\omega} \tilde{\tau}_0 + \Delta_\sigma \tilde{\tau}_1 - \varepsilon(k) \tilde{\tau}_3}{\tilde{\omega}^2 - \varepsilon(k)^2 - \Delta_\sigma^2}, \]

where \( \tilde{\omega} = \omega + \mu_0 \). \( \tilde{\tau}_0 \) is the \( 2 \times 2 \) unit matrix and \( \tilde{\tau}_{1,3} \) are the Pauli matrices. The T-matrix approximation is employed to compute the Green’s function in the presence of impurities. For a single impurity, the T-matrix exactly accounts for the multiple scattering off the impurity. The single-particle Green’s function \( \hat{G} \) can be obtained from the following Dyson’s equation:

\[ \hat{G}_{\sigma\sigma}(k, k', \omega) = \hat{G}_{\sigma\sigma}^{0}(k, \omega) \delta_{k,k'} + \hat{G}_{\sigma\sigma}^{0}(k, \omega) \hat{T}_{\sigma\sigma}(k, k', \omega) \hat{G}_{\sigma\sigma}^{0}(k', \omega), \]

\[ \hat{T}_{\sigma\sigma}(k, k', \omega) = \frac{\tilde{\omega} \tilde{\tau}_0 + \Delta_\sigma \tilde{\tau}_1 - \varepsilon(k) \tilde{\tau}_3}{\tilde{\omega}^2 - \varepsilon(k)^2 - \Delta_\sigma^2}, \]

\[ \hat{G}_{\sigma\sigma}^{0}(k, \omega) = \begin{pmatrix} \omega - \varepsilon_{\Gamma}(k) & -\Delta_\sigma \\ -\Delta_\sigma & \omega - \varepsilon_X(k) \end{pmatrix}^{-1} = \frac{\tilde{\omega} \tilde{\tau}_0 + \Delta_\sigma \tilde{\tau}_1 - \varepsilon(k) \tilde{\tau}_3}{\tilde{\omega}^2 - \varepsilon(k)^2 - \Delta_\sigma^2}, \]
where the T-matrix is given by

$$\hat{T}_{\sigma\sigma}(k, k', \omega) = \hat{U}_{k,k'} + \sum_{k''} \hat{U}_{k,k''} \hat{G}^0_{\sigma\sigma}(k'', \omega) \hat{T}_{\sigma\sigma}(k'', k', \omega).$$  \hspace{1cm} (14)

For a point-like scattering potential interacting with itinerant carriers just on the impurity site, the scattering matrix is isotropic, \(\hat{U}_{k,k'} = \hat{U}\). The above equation is greatly simplified to

$$\hat{T}_{\sigma\sigma}(\omega) = \hat{U} + \hat{U} \hat{G}^0_{\sigma\sigma}(\omega) \hat{T}_{\sigma\sigma}(\omega),$$  \hspace{1cm} (15)

where \(\hat{G}^0_{\sigma\sigma}(\omega) = \sum_k \hat{G}^0_{\sigma\sigma}(k, \omega)\). After some derivation we obtain

$$\hat{G}^0_{\sigma\sigma}(\omega) = -\pi N_0 \left[ \frac{\alpha(\tilde{\omega})}{\sqrt{\Delta^2 - \tilde{\omega}^2}} (\tilde{\omega} \tilde{\tau}_0 + \Delta_\sigma \tilde{\tau}_1) + \gamma(\tilde{\omega}) \tilde{\tau}_3 \right],$$  \hspace{1cm} (16)

where

$$\alpha(\tilde{\omega}) = \pi^{-1} \left[ \arctan \left( \frac{E_c}{\sqrt{\Delta^2 - \tilde{\omega}^2}} \right) + \arctan \left( \frac{E_g}{\sqrt{\Delta^2 - \tilde{\omega}^2}} \right) \right],$$  \hspace{1cm} (17)

$$\gamma(\tilde{\omega}) = (2\pi)^{-1} \ln \left( \frac{E_c^2 + \Delta^2 - \tilde{\omega}^2}{E_g^2 + \Delta^2 - \tilde{\omega}^2} \right),$$  \hspace{1cm} (18)

with \(E_c\) denoting the high-energy cutoff and \(N_0 = ma^2/(2\pi \hbar^2)\) the density of states per band per spin. Note that \(\alpha(\tilde{\omega})\) and \(\gamma(\tilde{\omega})\) are independent of the spin index \(\sigma\).

3. Results

3.1. Single-impurity model I

The first impurity model we study is the scattering-potential matrix with only intraband scattering terms, i.e. \(\hat{U} = V_{\text{imp}} \hat{\tau}_0\), which was adopted in [38] to study the effect of many impurities. From equation (15), we obtain

$$\hat{T}_{\sigma\sigma}(\omega) = [\hat{\tau}_0 - \hat{U} \hat{G}^0_{\sigma\sigma}(\omega)]^{-1} \hat{U} = [V_{\text{imp}} - \hat{G}^0_{\sigma\sigma}(\omega)]^{-1}. \hspace{1cm} (19)$$

The energy of the impurity bound state is determined by the pole of \(\hat{T}_{\sigma\sigma}(\omega)\) and by \(\text{det}[V_{\text{imp}} - \hat{G}^0_{\sigma\sigma}(\Omega)] = 0\). Setting \(c \equiv (\pi N_0 V_{\text{imp}})^{-1}\), we have the equation for the energy of impurity bound state

$$c^2 + 2c \frac{\alpha(\Omega) \tilde{\Omega}}{\sqrt{\Delta^2 - \tilde{\Omega}^2}} - \alpha(\tilde{\Omega})^2 - \gamma(\tilde{\Omega})^2 = 0. \hspace{1cm} (20)$$

For the spin triplet excitonic phase \(\Delta^\uparrow = -\Delta^\downarrow\), the above equation gives rise to impurity states with the same bound energy, i.e. the impurity states are doubly degenerate. Generally, the above equation has to be solved numerically to obtain the bound energy \(\tilde{\Omega}\). However, we can get some analytic results under certain approximations. Under the wide-band approximation \(E_c, E_g \gg |\Delta|\), \(\alpha(\tilde{\Omega}) \approx 1\) and \(\gamma(\tilde{\Omega}) \approx \gamma_0 = \pi^{-1} \ln(E_c/E_g)\), so we have

$$\frac{\tilde{\Omega}}{|\Delta|} = \text{sgn}(c) \frac{1 - c^2 + \gamma_0^2}{\sqrt{(1 - c^2 + \gamma_0^2)^2 + 4c^2}}, \hspace{1cm} (21)$$

and furthermore if the system has approximately the particle–hole symmetry \(E_c \approx E_g\), then \(\gamma_0 \approx 0\) and \(\tilde{\Omega}/|\Delta| = \text{sgn}(c)(1 - c^2)/(1 + c^2)|\) from the above equation.
3.2. Single-impurity model II

For the second impurity model, the four matrix elements of $\hat{U}$ are assumed to be the same, i.e. the intra- and interband scattering terms are the same\footnote{The impurity Hamiltonian is expressed as $H_{\text{imp}} = \int U_{\text{imp}}(r)\phi^*(r)\phi(r)\,dr = \sum_{k,k'} \hat{\varphi}^\dagger(k)\hat{U}_{k,k'}\hat{\psi}(k)$, where $\hat{\varphi}^\dagger(k) = (\hat{d}^\dagger_k, \hat{c}^\dagger_{kN})$ and $\hat{\psi}^\dagger(r) = 2^{-1/2} \sum_{k} \varphi_{kN}(r)\hat{d}_k + \varphi_{k}(r)\hat{c}_{kN}$, with $\varphi_{kN}(r)$ and $\varphi_{k}(r)$ the Bloch functions of quasimomentum $k$. In this paper, the scattering potential is assumed to be point-like, $U_{\text{imp}} = V_{\text{imp}}\delta(r)$. With further simplification of the Bloch functions of the form $\exp(ik\cdot r)$, $\hat{U}_{k,k'}$ is $k$ independent and equal to $V_{\text{imp}}(\hat{\xi}_0 + \hat{\xi}_1)/2$.} with $\hat{U} = V_{\text{imp}}(\hat{\xi}_0 + \hat{\xi}_1)/2$. Then the T-matrix according to equation (15) is

$$\hat{T}_{\sigma\sigma}(\omega) = [2V_{\text{imp}}^{-1} - \hat{\xi}'\hat{G}_0^{\sigma\sigma}(\omega)]^{-1}\hat{\xi}'$$

with $\hat{\xi}' = \hat{\xi}_0 + \hat{\xi}_1$. The energy of the impurity bound state is again determined by the pole of $\hat{T}_{\sigma\sigma}(\omega)$. From the above equation, we find that $\hat{\Omega} = \Delta^2_\sigma$, $\vec{\Omega} + \Delta_\sigma$ has the same sign as that of $\Delta_\sigma$. Therefore, the solution of equation (23) exists only if the sign of $c$ is opposite to that of $\Delta_\sigma$. For the SDW state, i.e. the triplet excitonic phase, we have $\Delta_\uparrow = -\Delta_\downarrow$ and so there is exactly one impurity bound state in either the spin-up or the spin-down channel. We may assume $\Delta_\uparrow = -\Delta_\downarrow = \Delta > 0$, then for an attractive scattering $V_{\text{imp}} < 0$, the impurity bound state only exists in the spin-up channel and its energy is given by $\hat{\Omega}/\Delta = -(1 - c^2)/(1 + c^2)$ under the wide-band approximation. If $V_{\text{imp}} > 0$, however, the impurity state will be in the spin-down channel, and $\hat{\Omega}/\Delta = (1 - c^2)/(1 + c^2)$. In general, the impurity bound-state energy is given by

$$\frac{\hat{\Omega}}{\Delta_\sigma} = \text{sgn}(c) \frac{1 - c^2}{1 + c^2}$$

in the valid regime of the wide-band approximation.

3.3. Local density of states (LDOS)

To apply the theoretical results to iron arsenide, we try to pin down the parameters of our model by extracting them from the available experimental data for BaFe$_2$As$_2$ \cite{31}. $\epsilon_{\text{g}}^r \approx 16$ meV and $\epsilon_{\text{g}}^i \approx 24$ meV so that $E_\text{g} \approx 20$ meV. $m_\text{r} \approx m_\text{X} \approx 7.0 m_\text{e}$ and therefore $N_0 \approx 1.2$ eV$^{-1}$. $\Delta_\uparrow = -\Delta_\downarrow = \Delta \approx 20$ meV. The high-energy cutoff is set as $E_\text{c} = 500$ meV, which is of the same order of magnitude as the bandwidth. Note that $E_\text{g}$ extracted from experimental data is very small, which is of the same order of magnitude as the order parameter $\Delta$. Therefore, neither the wide-band approximation nor the particle–hole symmetry can be applied to the present case. Equations (20) and (23) have to be numerically solved.

Now, we examine the local characteristics induced by the impurity by looking into the variation of the LDOS, which can be probed by scanning tunneling microscopy (STM). The LDOS is defined as

$$N(r, \omega) = -\frac{1}{\pi} \sum_{\sigma} \text{Im}[\text{Tr} \hat{G}_{\sigma\sigma}(r, r', \omega)]$$

where $\hat{G} = (\hat{d}^\dagger, \hat{c}^\dagger_{kN})\hat{\psi}^\dagger(r)\hat{\varphi}(r)$ and $\hat{G}_{\sigma\sigma} = \hat{G}_{\sigma\sigma}^\dagger$. The T-matrix according to equation (15) is

$$\hat{T}_{\sigma\sigma}(\omega) = [2V_{\text{imp}}^{-1} - \hat{\xi}'\hat{G}_0^{\sigma\sigma}(\omega)]^{-1}\hat{\xi}'$$

with $\hat{\xi}' = \hat{\xi}_0 + \hat{\xi}_1$. The energy of the impurity bound state is again determined by the pole of $\hat{T}_{\sigma\sigma}(\omega)$. From the above equation, we find that $\hat{\Omega} = \Delta^2_\sigma$, $\vec{\Omega} + \Delta_\sigma$ has the same sign as that of $\Delta_\sigma$. Therefore, the solution of equation (23) exists only if the sign of $c$ is opposite to that of $\Delta_\sigma$. For the SDW state, i.e. the triplet excitonic phase, we have $\Delta_\uparrow = -\Delta_\downarrow$ and so there is exactly one impurity bound state in either the spin-up or the spin-down channel. We may assume $\Delta_\uparrow = -\Delta_\downarrow = \Delta > 0$, then for an attractive scattering $V_{\text{imp}} < 0$, the impurity bound state only exists in the spin-up channel and its energy is given by $\hat{\Omega}/\Delta = -(1 - c^2)/(1 + c^2)$ under the wide-band approximation. If $V_{\text{imp}} > 0$, however, the impurity state will be in the spin-down channel, and $\hat{\Omega}/\Delta = (1 - c^2)/(1 + c^2)$. In general, the impurity bound-state energy is given by

$$\frac{\hat{\Omega}}{\Delta_\sigma} = \text{sgn}(c) \frac{1 - c^2}{1 + c^2}$$

in the valid regime of the wide-band approximation.
where \( \hat{G}_{\sigma\sigma}(\mathbf{r}, \mathbf{r}', \omega) \) is Green’s function in the real space. Applying the T-matrix approximation, we have

\[
\hat{G}_{\sigma\sigma}(\mathbf{r}, \mathbf{r}', \omega) = \hat{G}^0_{\sigma\sigma}(\mathbf{r}, \mathbf{r}', \omega) + \hat{G}^0_{\sigma\sigma}(\mathbf{r}, 0, \omega) \hat{T}(\omega) \hat{G}^0_{\sigma\sigma}(0, \mathbf{r}', \omega).
\]  

(26)

Substituting equation (26) into equation (25), we may single out the variation of LDOS due to the presence of the impurity potential,

\[
N_{\text{imp}}(\mathbf{r}, \omega) = -\frac{1}{\pi} \sum_{\sigma} \text{Im}[\text{Tr}[\hat{\hat{G}}^0_{\sigma\sigma}(\mathbf{r}, 0, \omega) \hat{T}_{\sigma\sigma}(\omega) \hat{G}^0_{\sigma\sigma}(0, \mathbf{r}, \omega)]].
\]  

(27)

For the second impurity model, figure 2(a) shows the LDOS as a function of energy \( \tilde{\omega} \) on the impurity site, namely \( N(0, \tilde{\omega}) \), whereas figure 2(b) shows the impurity-induced LDOS at the bound energy as a function of radial distance \( r \) off the impurity site, i.e. \( N(\mathbf{r}, \tilde{\Omega}) \). \( V_{\text{imp}} \) has been set as \(-0.36, -0.6 \) and \(-4 \) eV, giving rise to the impurity bound states seen as the sharp peaks located, respectively, at the energies \( \tilde{\Omega}/\Delta = 0, -0.5 \) and \(-0.99 \) in figure 2(a). The probability densities of these bound states exhibit a kind of exponential decay with the Friedel oscillation, as seen in figure 2(b). Introducing two length scales, \( \xi_1 \) and \( \xi_2 \), to characterize the oscillation and decay, we obtain the asymptotic behavior of \( N_{\text{imp}}(\mathbf{r}, \tilde{\Omega}) \) for large \( r \),

\[
N_{\text{imp}}(\mathbf{r}, \tilde{\Omega}) \propto r^{-1} \cos^2(\pi r/\xi_1) \exp(-r/\xi_2).
\]  

(28)

\( \xi_1/a = \pi/\sqrt{4\pi N_0 E_g} \), which is approximately 5.7, consistent with the numerical results shown in figure 2(b). \( \xi_2/\xi_1 = E_g/(\pi \sqrt{\Delta^2 - \tilde{\Omega}^2}) = 0.32, 0.37 \) and 2.3 for the three cases of impurity

\[^5\] The following conclusions are also qualitatively correct for the first impurity model.
states. This explains why we see clear Friedel oscillation for impurity states with the bound energy near the gap edge.

4. Discussion and conclusion

In conclusion, we have examined the effect of a single impurity on the antiferromagnetic SDW state of iron arsenide. We have revealed the intriguing impurity bound state around the impurity site in the energy gap. The degeneracy of the impurity state has been investigated for two impurity models. The impurity-induced variations of the LDOS have also been examined with apparent Friedel oscillation for impurity states with energy near the gap edge.

The formation of the bound state induced by a single impurity in the parent iron-based compound can be examined by STM/scanning tunneling spectroscopy (STS), which has been widely used [39] in studying localized impurity resonances in d-wave superconducting cuprites. The high spatial (atomic scale) and energy (∼meV) resolution of STM/STS allows one to investigate the bound energy and the spatial structure of the wavefunction associated with the impurity state localized around the point-like nonmagnetic scatterer. Furthermore, the spin-polarized impurity state, which is (anti)parallel to the underlying magnetic structure as revealed by our second impurity model, may be observed by the spin-polarized STM [40] around native defects such as Fe vacancies or intentionally doped divalent atoms replacing Fe atoms in the FeAs layer. The STM/STS measurements of the impurity states associated with the triplet excitonic phase may shed light on the mechanism of the antiferromagnetic SDW order in the undoped iron arsenide.

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