Nesting-induced local electronic patterns around a single As (Te, Se) vacancy in iron-based superconductors

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Abstract

The local electronic states around a single As (Te, Se) vacancy are investigated in order to shed light on the role of ligands in a series of iron-based superconductors. Such a vacancy can produce a local hopping correction ranging from −0.22 to 0.12 eV and always induce two in-gap resonance peaks in the local density of states (LDOS) at the fixed symmetrical bias voltages, which are rather robust and irrelevant to the phase of superconducting order parameter. The LDOS images near the defect predominantly possess 0° and 45° stripes. These energy-dependent charge modulations created by quasiparticle interference are originated in the nesting effect between the inner (outer) hole Fermi surface around Γ point and the inner (outer) electron Fermi surface around M point.

The mechanism of high temperature superconductivity has been one of the great challenges in the condensed matter physics community since the discovery of the cuprates in 1986 [1]. A series of high Tc cuprate superconductors commonly possesses layered crystal structures consisting of the conducting CuO2 planes separated by the other elements and oxygen layers. The ligand O ions in the CuO2 planes just locate on the Cu–Cu bonds and are believed to play an important role in forming superconductivity. The surface effects of the cuprates can be neglected due to the positions of the O ions. However, it is difficult to evaluate the impact of the O ions on the electronic states in the CuO2 planes due to the lattice distortion or in-plane disorders. Fortunately, new family of high Tc superconductors, i.e. iron-based superconductors, was found in 2008 [2–7]. The iron-based superconductors also have a layer crystal structure and each unit cell contains two Fe ions (A and B) and two As (Te, Se) ions (A and B) (see figure 1). The high temperature superconductivity is originated in the electron pairing in the Fe–Fe plane by doping electrons or holes. The ligand As (Te, Se) ions A and B are located just below and above the center of each face of the Fe square lattice, respectively, rather than in the conducting plane. Such a crystal structure provides us an excellent platform for exploring the ligand effects on the electronic states, which can easily distinguish from the disorders in the conducting plane. Obviously, the impacts of As (Te, Se) ions A and B in the surface layer of the iron-based superconductors on the local density of states (LDOS) are inequivalent due to their different environments. It is known that the experimental results observed by both angle resolved photoemission spectroscopy (ARPES) and scanning tunneling microscopy (STM) contain unavoidably this kind of surface effect.

In order to figure out the origin of high temperature superconductivity in iron-based superconductors, we first understand the role of the ligand As (Te, Se) ions. Recently, Li and Yin investigated the As vacancies on the surface of optimally electron-doped BaFe2–xCo,xAs2 by performing STM observations and found a pair of LDOS peaks within superconducting energy gap [8, 9]. In [10, 11], the dI/dV curves were measured around the Se vacancies in monolayer and crystalline FeSe superconductors. In this work, motivated by the interesting STM experiments, we study the influence of a single As (Te, Se) vacancy on the LDOS in the Fe–Fe plane by employing a two-orbit four-band tight binding model [12], which takes the asymmetric effect of the ligand As (Te, Se) ions.
in the surface Fe–As (Te, Se) layer into account. Such an empirical model can fit excellently the energy band structure of iron-based superconductors and its evolution with electron or hole doping measured by ARPES experiments [13–22]. This model also explained successful a series of STM experiments in iron-based superconductors, e.g. in-gap impurity bound states [12, 23], the negative energy resonance peak in the vortex core [24, 25], the 90° domain walls and anti-phase domain walls [26–29], the zero energy bound state induced by the interstitial excess Fe ions [30–32], etc, and especially repeated the phase diagram observed by nuclear magnetic resonance and neutron scattering experiments [33–35].

The Hamiltonian describing a single As (Te, Se) vacancy located at point \((0,\ 1\ 2)\) in Fe sublattice A (see figure 1) can be written as \(H = H_0 + H_{BCS} + H_V\), where \(H_0\) is the two-orbit four-band tight binding model proposed in [12], \(H_{BCS}\) is the mean field BCS pairing Hamiltonian in the Fe–Fe plane, \(H_V = \sum_{\sigma} \left[ g_{\alpha,\alpha-0,0,0,\sigma} \phi_{\alpha-0,0,0,\sigma} + g_{\alpha,\alpha-1,0,0,\sigma} \phi_{\alpha-1,0,0,\sigma} + h.c. \right] + \sum_{\sigma} \left[ g_{\alpha,\alpha-0,0,0,\sigma} \phi_{\alpha-0,0,0,\sigma} - g_{\alpha,\alpha-1,0,0,\sigma} \phi_{\alpha-1,0,0,\sigma} + h.c. \right] \alpha = 0\ and 1\ represent the degenerate orbitals \(d_{xz}\) and \(d_{yz}\) respectively, \(g_{\alpha,\alpha-0,0,0,\sigma} \phi_{\alpha-0,0,0,\sigma}\) creates (destroys) an \(\alpha\) electron with spin \(\sigma = (\uparrow\ or \) \(\downarrow)\) in the unit cell (\(i, j)\) of the Fe sublattice A (B), and \(U (W)\) is the local hopping correction between the same (different) orbitals due to the As (Te, Se) vacancy. Because a vacancy cannot mix \(d_{xz}\) orbital and \(d_{yz}\) orbital, we always have \(W = -t_4\).

After introducing first the Fourier transformations \(g_{\alpha,\alpha-0,0,0,\sigma} = \frac{1}{N} \sum_k g_{\alpha,\alpha-0,0,0,\sigma} e^{i(k_i x + k_j y)}\) with \(N\) the number of unit cells and the canonical transformations for \(\xi_{\alpha,0,k,\sigma}\) and \(\phi_{\alpha,0,k,\sigma}\), and then taking the Bogoliubov transformations for new fermion operators, we can solve exactly the Hamiltonian \(H\) for a single ligand vacancy in iron-based superconductors by using the T-matrix approach [12, 31, 36]. The analytic formulas for the Green’s functions in momentum space have been derived. The LDOS on the Fe sites at different bias voltages and the Fourier component of LDOS (FCLDOS) can be obtained through the Green’s functions. Here we have calculated a square Fe lattice with \(N = 500 \times 500\) unit cells, which is enough to ensure the accuracy of theoretical results. We have also employed the energy band parameters: \(t_1 = -0.5\ eV, t_2 = -0.2\ eV, t_3 = 1.0\ eV,\ and t_4 = -0.02\ eV\), which are same with the previous works [12, 25, 28, 29, 31, 32, 35]. We note that the electron-doped BaFe$_{2-x}$Co$_x$As$_2$ has a superconducting energy gap \(\Delta_0 = 5.8\ meV\) observed by the STM experiments [10, 11, 37]. After a lots of numerical calculations, we found that when \(U \geq 0.12\ eV\) or \(U < -0.22\ eV\), the LDOS is negative at some bias voltages, which is unphysical. In other words, An As (Te, Se) vacancy can produce a local modification in the interval \([-0.22, 0.12]\ eV\). This manifests that the ligand ions play an important role in forming high temperature superconductivity in iron-based superconductors.

We plot the LDOS on the point (0,0) or (0,1) in the Fe sublattice B as a function of the bias voltage \(\omega\) under different \(U\) and the optimal electron doping (15%) for the \(s_{\pm}\) pairing symmetry \(\Delta_{s_{\pm}} = \frac{1}{2} \Delta_0 (\cos k_x + \cos k_y)\) in figures 2(a) and (b) and the \(s_{\pm}\) pairing symmetry \(\Delta_{s_{\pm}} = \frac{1}{2} \Delta_0 \cos k_x + \cos k_y\) in figures 2(c) and (d), respectively. Here, \(\nu = 0\) (1) represents the Fermi surfaces around M (Γ) point while \(\nu = 0\) (1) denotes the outer
modulation wave vectors shift with the bias voltage, and their change trends along 0° quasiparticle interference phenomenon is different from that in the cuprate superconductors, where the charge modulation wave vectors have

Two resonance peaks exhibit in the LDOS at 4.8 meV and their locations do not move with increasing U. These results agree well the recent STM observations. However, even if U = 0, two resonance peaks still stand there. This means that the hybridization among Fe d and As (Te, Se) p orbitals cannot be neglected. When U < 0, with decreasing U, the superconducting coherence peaks and the resonance peaks are suppressed, and their heights at positive bias voltages become lower than those at negative bias voltages. It is quite obvious that the resonance peak is higher than the coherence peak at the positive energy side for enough small U (see figure 2(a)). If U > 0, with increasing U, the superconducting coherence peaks grow up, but the resonance peaks first become higher, then become lower. However, the coherence peaks and the resonance peaks are symmetric with respect to the bias voltage in figure 2(b). We note that the in-gap resonance peaks is irrelevant to the phase of the superconducting order parameter, similar to those induced by interstitial excess Fe impurities in iron-based superconductor Fe(Te, Se) [30–32]. Therefore, very different from nonmagnetic impurities on the Fe sites [12], such a ligand vacancy cannot be used to distinguish the s±± and s++ pairing symmetries.

Figure 3 shows the LDOS images at different U and ω under optimal electron doping for the s++ pairing symmetry in the Fe sublattice B with 31 × 31 sites due to quasiparticle interference. The As (Te, Se) vacancy is located at the point (0, 1/3). Because up As (Te, Se) and down As (Te, Se) are inequivalent in the surface layer, all the LDOS images have a C2 symmetry. Obviously, the LDOS on the points (0, 0) and (0, 1) has a maximum (minimum) value for U > 0 (<0). Hence we can judge that the As (Te, Se) vacancy is attractive or repulsive according to the extreme value of the LDOS on the nearest neighboring Fe sites around it. When U = −30.0 meV, the LDOS has 0° modulation at ω = 2.0 meV in figure 3(a). With increasing ω, both 0° and 45° stripes show up in figure 3(b). If U = 30.0 meV, the real space LDOS also possesses energy-dependent modulations along both 0° and 45° directions at ω = 2.0 and 4.8 meV (see figures 3(c) and 3(d)).

To understand the origin of the LDOS modulations produced by quasiparticle interference and the modulation periods, we have obtained the FCLDOS at different U and ω. Figures 4(a)–(d) and (e)–(h) exhibit the modulation wave vectors and their intensities along 0° and 45° directions, respectively, corresponding to the real space LDOS images in figure 3. It is very interesting that all the modulation wave vectors are independent of U and ω. Therefore, the energy-dependent charge modulations are due to the variations of the FCLDOS intensities at the modulation wave vectors with energy. Comparing carefully figures 4(e)–(h) with figures 4(a)–(d), we can see clearly that the modulation wave vectors along 0° direction are nothing but the x components of those along 45° direction. The magnitudes of the modulation wave vectors along 45° direction mainly distribute in the range of 0.84 √ 2π ~ 0.97 √ 2π. Because the single vacancy is not located at the center of the Fe sublattice B, the modulation wave vectors have fine structures with double lines, which are never reported. Obviously, this quasiparticle interference phenomenon is different from that in the cuprate superconductors, where the charge modulation wave vectors shift with the bias voltage, and their change trends along 0° (antinodal) and 45° (nodal) directions are just opposite with increasing energy [38–40].
Figure 3. The LDOS images near the As (Te, Se) vacancy in the Fe sublattice B under different $U$ and $\omega$ at optimal electron doping (15\%) for $s_{++}$ pairing symmetry $\Delta_{\text{pair}} = \frac{1}{2}(\cos k_x + \cos k_y)$ with $\Delta_0 = 5.8$ meV.

Figure 4. The FCLDOS along $(\pi, 0)$ direction in (a)–(d) and $(\pi, \pi)$ direction in (e)–(h) under different $U$ and $\omega$ at optimal electron doping (15\%) for the $s_{++}$ pairing symmetry $\Delta_{\text{pair}} = \frac{1}{2}(\cos k_x + \cos k_y)$ with $\Delta_0 = 5.8$ meV.
Now we determine the modulation wave vectors in the LDOS images. Figure 5 depicts two hole Fermi surfaces \( \alpha \) band with \( u = v = 1 \) and \( \beta \) band with \( u = 1 \) and \( v = 0 \) around \( \Gamma \) point and two electron Fermi surfaces \( \gamma \) band with \( u = 0 \) and \( v = 1 \) and \( \delta \) band with \( u = v = 0 \) around \( M \) point of iron-based superconductors at optimal electron doping \([12]\). According to the analytic expression of the Green’s function or the LDOS, we found that the interband transition is only allowed for those bands with the same index \( \nu \). In figure 5, \( \mathbf{q}_0 \) (or \( \mathbf{q}_1 \)) \((\tau = 1 \) and 2\) represent the allowed nesting vectors connecting to two outer (inner) Fermi surfaces around \( \Gamma \) and \( M \) points, and \(|\mathbf{q}_{01}\| > |\mathbf{q}_{11}| > |\mathbf{q}_{02}| > |\mathbf{q}_{12}|\). We analyze in detail the numerical values of the modulation wave vectors in figure 4 and the nesting vectors in figure 5, and conclude firmly that the nesting vectors \( \mathbf{q}_\nu \), and their vector differences \( \mathbf{q}_{\nu 1} - \mathbf{q}_{\nu 2} \) are nothing but the modulation wave vectors in the LDOS images.

In summary, we have explored the impact of a single As \((\text{Te, Se})\) vacancy on the electronic states in iron-based superconductors. The ligand vacancy can induce two robust resonance peaks in the superconducting energy gap at the fixed symmetric positions about zero energy, which are consistent with the STM experiments. The resonance peaks are independent of the phase of the superconducting order parameter in the bulk, similar to zero energy bound state produced by the interstitial Fe ions. Because a magnetic field that is not too strong changes predominately the phase of the superconducting order parameter, we predict that these two bound states keep unchanged with increasing magnetic field strength, which could be detected by STM experiments. The energy-dependent LDOS images possess 0° and 45° stripes with multiple periods. The modulation wave vectors come from the nesting vectors of the Fermi surfaces, which are independent of the local hoping correction and the bias voltage. The quasiparticle interference patterns induced by As \((\text{Te, Se})\) vacancies are undoubtedly originated in the nesting effect in iron-based superconductors.

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References

[1] Bednorz J G and Muller K A 1986 Z. Phys. B 64 189
[2] Kamihara Y et al 2008 J. Am. Chem. Soc. 130 3296
[3] Ren Z A et al 2008 Chin. Phys. Lett. 25 2215
[4] Chen X H et al 2008 Nature 453 761
[5] de la Cruz C et al 2008 Nature 453 899

Figure 5. The Fermi surfaces of iron-based superconductors at optimal electron doping (13%) and the allowed nesting vectors.
[6] Chen G F et al 2008 Phys. Rev. Lett. 100 247002  
[7] Wen H-H et al 2008 Europhys. Lett. 82 17009  
[8] Li A et al 2016 arXiv:1602.04937  
[9] Yin J-X et al in preparation  
[10] Liu C et al 2018 Phys. Rev. B 97 024502  
[11] Song C-L et al 2011 Science 332 1410  
[12] Zhang D 2009 Phys. Rev. Lett. 103 186402  
Zhang D 2010 Phys. Rev. Lett. 104 089702  
[13] Ding H et al 2008 Europhys. Lett. 83 47001  
[14] Lu D et al 2008 Nature 455 81  
[15] Liu C et al 2008Phys. Rev. Lett. 101 177005  
[16] Kondo T et al 2008 Phys. Rev. Lett. 101 147003  
[17] Evtushinsky D V et al 2009 Phys. Rev. B 79 054517  
[18] Nakayama K et al 2009 Europhys. Lett. 85 67002  
[19] Zabolotnyy V et al 2009 Nature 457 569  
[20] Terasihina K et al 2009 Proc. Natl Acad. Sci. 106 7330  
[21] Sekiha Y et al 2009 New J. Phys. 11 023020  
[22] Miao S et al 2012 Phys. Rev. B 85 094506  
[23] Grothe S et al 2012 Phys. Rev. B 86 174503  
[24] Shan L et al 2011 Nat. Phys. 7 325  
[25] Gao Y et al 2011 Phys. Rev. Lett. 106 027004  
[26] Chuang T-M et al 2010 Science 327 181  
[27] Li G et al 2012 Phys. Rev. B 86 060512(R)  
[28] Huang H et al 2011 Phys. Rev. B 83 134517  
[29] Li B et al 2013 New J. Phys. 15 103018  
[30] Yin J-X et al 2015 Nat. Phys. 11 543  
[31] Zhang D 2015 Physica C 519 43  
[32] Huang H et al 2016 Phys. Rev. B 93 064519  
[33] Laplace Y et al 2009 Phys. Rev. B 80 140501  
[34] Julien M-H et al 2009 Europhys. Lett. 87 37001  
[35] Zhou T, Zhang D and Ting C S 2010 Phys. Rev. B 81 052506  
[36] Balatsky A V, Vekhter I and Zhu J-X 2006 Rev. Mod. Phys. 78 373  
[37] Yin Y et al 2009 Phys. Rev. Lett. 102 097002  
[38] Hoffman J E et al 2002 Science 295 466  
[39] Wang Q-H and Lee D-H 2003 Phys. Rev. B 67 020511  
[40] Zhang D and Ting C S 2003 Phys. Rev. B 67 100506  
Zhang D and Ting C S 2004 Phys. Rev. B 69 012501