Journal of Physics and Chemistry of Solids 112 (2018) 246–251

Contents lists available at ScienceDirect

Journal of Physics and Chemistry of Solids

journal homepage: www.elsevier.com/locate/jpcs

Quasiparticle interferences in the coexistence phase of iron pnictides based on a five-orbital model

Dheeraj Kumar Singh [a,b]

[a] Harish-Chandra Research Institute, Chhatnag Road, Jhunsi, Allahabad, 211019, India
[b] Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai, 400085, India

ARTICLE INFO

Keywords:
Iron pnictides
Coexistence phase
Quasiparticle interference

ABSTRACT

We investigate quasiparticle interference in the coexistence phase of spin-density wave state and *s*-wave superconductivity using a five-orbital tight-binding model. We examine underdoped and overdoped cases, one with magnetic-exchange gap significantly larger than the superconducting gap, and other with both gaps being comparable. In the former case, QPI peaks are very weak or absent near $(0, \pm\pi)$ for either of the states with s^{+-}- or s^{++}-wave symmetry while they are present near $(\pm\pi, 0)$ in each case, thus making any differentiation between them difficult. In the latter case, a clear distinction between the two types of states is obtained as the peaks are intense near $(0, \pm\pi)$ and $(\pm\pi, 0)$ for the s^{+-}- and s^{++}-wave symmetry, respectively.

1. Introduction

Phase diagram characteristics such as magnetic order exhibited by the parent compounds and appearance of the superconductivity on doping either holes or electrons in the iron pnictides is similar to those of the cuprates, though nature of the magnetic order or superconducting state (SC) is entirely different [1–3]. Unlike cuprates, parent compound is a metallic spin-density wave (SDW) state with ferromagnetic arrangement of spins along one direction and antiferromagnetic arrangement along the perpendicular direction. The SDW state is electronically highly anisotropic as observed in the experiments such as transport measurements [4,5], scanning-tunneling microscopy (STM) [6] etc. On the other hand, the SC state exhibits a sign-reversing *s*-wave (s^{+-}-wave) symmetry. An important difference from the cuprates is also the coexistence phase (SDW + SC) [7–9] which is found to be sandwiched between the SDW and SC phases in the temperature vs doping phase diagram, implying that it represents a state with competition rather than cooperation between the two ordering tendencies. Such a complex state may show unusually extreme sensitivity to an external perturbation such as disorder, magnetic field etc.

Nature of the SC order parameter in the coexistence phase is expected to be of the s^{+-}-wave symmetry because of the proximity to the pure SC state that has the same symmetry. Several theoretical works [10,11] also indicate that the SC state with s^{+-}-wave symmetry is more favorable to coexist with the SDW state than the sign-preserving s^{++}-wave symmetry.

Experimentally, quasiparticle interference (QPI) obtained by using spectroscopic imaging scanning tunneling microscopy (SI-STM) is a powerful technique to unravel the symmetry of the SC order parameter [12–14]. The method has also been used to probe the electronic structure of other type of ordered states [6] as well as topological insulators [15,16]. It involves the detection of interference of quasiparticles through the modulation of local density of state (LDOS) caused by the randomly distributed impurity atoms [17], which can be realized by measuring the differential conductance. Fourier transform of the real space data then gives the wave vectors at which the dominant scatterings occur.

In iron pnictides, apart from detecting the existence of quasi-one dimensional electronic nanostructures in the SDW state [6,18–20], QPI patterns suggest that the SC state has s^{+-} symmetry [21–23]. In the SDW state, Fourier transform of highly anisotropic real-space LDOS modulation consists of a quasi-one dimensional peak and two additional parallel running peaks at $(\pm\pi/4, 0)$, several features of which have been captured by studies based on the band and orbital models [24–28]. Whereas in the SC state, s^{+-} and s^{++}-wave symmetry can be distinguished by the relative intensity of QPI corresponding to the intrapocket and interpocket scatterings [29–36]. However, QPI in the SDW + SC state has not attracted a similar attention as in a pure SDW or SC state.

It is expected that the QPIs in the overdoped region of the coexistence phase will be more close in appearance to that in a pure SC state because of the presence of a very small magnetic-exchange gap. However, it is not clear whether the anisotropy will be similar or different for the s^{++} or s^{+-} symmetry. Furthermore, if the magnetic exchange gap is increased to correspond to that in the underdoped region, it is desirable to know the

E-mail address: dheerajsingh@hri.res.in.

https://doi.org/10.1016/j.jpcs.2017.09.028
Received 3 July 2017; Received in revised form 4 September 2017; Accepted 18 September 2017
Available online 21 September 2017

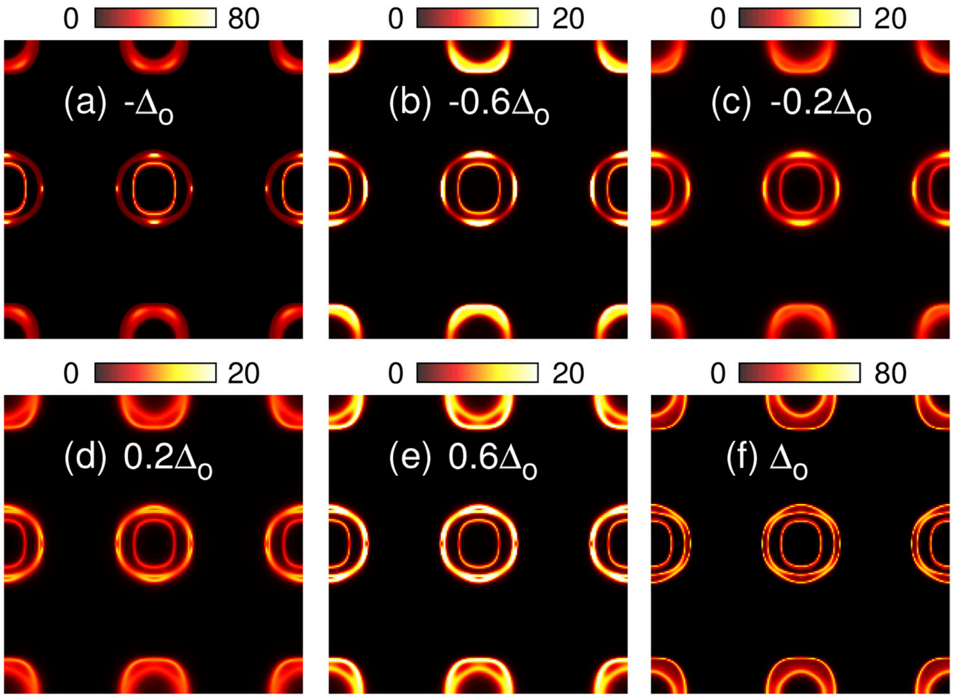

Fig. 1. Constant energy maps of the spectral functions $\mathscr{A}(\mathbf{k},\omega)$ in the coexistence phase SDW + SC for the bandfilling $n = 6.03$. Various quasiparticle energies are considered in terms of the SC gap $\Delta_o = 25$ meV. The range of k_x and k_y is [-π, π].

fate of QPI peaks near ($\pm\pi$, 0) and (0, $\pm\pi$), which has been often been used to differentiate between the two type of SC order parameters in the pure SC state. In this work, we address these two issues by focusing in the electron-doped region and using a five-orbital tight-binding model.

2. Theory

We consider following mean-field Hamiltonian in the coexistence phase with (π,0) SDW order and s-wave superconductivity

$$\mathscr{H} = \sum_{\mathbf{k}} \Psi^{\dagger}(\mathbf{k})\hat{H}(\mathbf{k})\Psi(\mathbf{k}) = \sum_{\mathbf{k}} \Psi^{\dagger}(\mathbf{k}) \begin{pmatrix} \hat{\varepsilon}(\mathbf{k}) & \hat{\Delta}^{m} & \hat{\Delta}^{s}(\mathbf{k}) & \hat{O} \\ \hat{\Delta}^{m} & \hat{\varepsilon}(\mathbf{k}+\mathbf{Q}) & \hat{O} & \hat{\Delta}^{s}(\mathbf{k}+\mathbf{Q}) \\ \hat{\Delta}^{s}(\mathbf{k}) & \hat{O} & -\hat{\varepsilon}(\mathbf{k}) & \hat{\Delta}^{m} \\ \hat{O} & \hat{\Delta}^{s}(\mathbf{k}+\mathbf{Q}) & \hat{\Delta}^{m} & -\hat{\varepsilon}(\mathbf{k}+\mathbf{Q}) \end{pmatrix} \Psi(\mathbf{k}). \tag{1}$$

Here, the operator $\Psi^{\dagger}(\mathbf{k}) = (d^{\dagger}_{\mathbf{k}1\uparrow}, d^{\dagger}_{\mathbf{k}2\uparrow}, \ldots, d^{\dagger}_{\mathbf{k}+\mathbf{Q}1\uparrow}, d^{\dagger}_{\mathbf{k}+\mathbf{Q}2\uparrow}, \ldots d_{-\mathbf{k}1\downarrow}, d_{-\mathbf{k}2\downarrow}, \ldots d_{-\mathbf{k}-\mathbf{Q}1\downarrow}, d_{-\mathbf{k}-\mathbf{Q}2\downarrow})$ in the Nambu formalism. Subscript indices 1, 2, 3, 4, and 5 corresponds to the orbitals $d_{3z^2-r^2}$, d_{xz}, d_{yz}, $d_{x^2-y^2}$, and d_{xy}, respectively. $\hat{\varepsilon}(\mathbf{k}) = \hat{\varepsilon}'(\mathbf{k}) + \hat{N}$ is a 5×5 matrix, where hopping matrix $\hat{\varepsilon}'(\mathbf{k})$ [37]. $\hat{O}$ is a 5×5 null matrix. $\hat{\Delta}^{s}(\mathbf{k})$ and $\hat{\Delta}^{m}$ are 5×5 diagonal matrices. For simplicity, same SC gap $\Delta^{s}_{ll'} = \Delta_o\delta_{ll'} \cos k_x \cos k_y$ is considered for all the orbitals. Elements of diagonal matrix $\hat{N}$ are $N_{ll'} = \frac{5J-U}{2} n_l$ and those of off-diagonal matrix $\hat{\Delta}^{m}$ are $2\Delta^{m}_{ll'} = Um_l + J\sum_{l\neq l'} m_{l'}$. For further simplification, orbital-resolved magnetization and charge densities are obtained self-consistently by setting SC order parameters to zero. Diagonal matrix and off-diagonal matrix elements corresponding to $\hat{N}$ and $\hat{\Delta}^{m}$, respectively, are obtained within the mean-field approximation of standard on site Coulomb interaction given by

$$\begin{aligned} \mathscr{H}_{int} &= U\sum_{\mathbf{i},\mu} n_{\mathbf{i}\mu\uparrow}n_{\mathbf{i}\mu\downarrow} + \left(U' - \frac{J}{2}\right)\sum_{\mathbf{i},\mu<\nu} n_{\mathbf{i}\mu}n_{\mathbf{i}\nu} \\ &\quad -2J\sum_{\mathbf{i},\mu<\nu} \mathbf{S}_{\mathbf{i}\mu}\cdot\mathbf{S}_{\mathbf{i}\nu} + J\sum_{\mathbf{i},\mu<\nu,\sigma} d^{\dagger}_{\mathbf{i}\mu\sigma}d^{\dagger}_{\mathbf{i}\mu\bar{\sigma}}d_{\mathbf{i}\nu\bar{\sigma}}d_{\mathbf{i}\nu\sigma}. \end{aligned} \tag{2}$$

U and U' are the intraorbital and the interorbital Coulomb interaction, respectively. J is the Hund's coupling. U and U' are related by the condition $U' = U$ - 2J.

We consider a single non-magnetic impurity with δ-potential to examine the QPI in the SDW + SC state. Then, the modification introduced in the Green's function of the coexistence phase is given by

$$\delta\hat{G}(\mathbf{k},\mathbf{k}',\omega) = \hat{G}^{0}(\mathbf{k},\omega)\hat{T}(\omega)\hat{G}^{0}(\mathbf{k}',\omega) \tag{3}$$

$\hat{G}^{0}(\mathbf{k},\omega) = ((\omega + i\eta)\hat{\mathbf{I}} - \hat{H}(\mathbf{k}))^{-1}$ is the mean-field Green's function, $\hat{\mathbf{I}}$ is a 20×20 identity matrix and

$$\hat{T}(\omega) = \left(\hat{1} - \hat{V}\hat{\mathscr{G}}(\omega)\right)^{-1}\hat{V}. \tag{4}$$

here,

$$\hat{\mathscr{G}}(\omega) = \frac{1}{N}\sum_{\mathbf{k}} \hat{G}^{0}(\mathbf{k},\omega) \tag{5}$$

and

$$\hat{V} = V_o \begin{pmatrix} \hat{1} & \hat{1} & \hat{0} & \hat{0} \\ \hat{1} & \hat{1} & \hat{0} & \hat{0} \\ \hat{0} & \hat{0} & -\hat{1} & -\hat{1} \\ \hat{0} & \hat{0} & -\hat{1} & -\hat{1} \end{pmatrix} \tag{6}$$

V_o is the impurity potential and $\hat{1}$ is a 5×5 identity matrix. Therefore, corresponding change in the DOS $\delta\rho(\mathbf{q},\omega)$ is given by

$$\delta\rho(\mathbf{q},\omega) = -\frac{1}{\pi}\sum_{\mathbf{k},i\leq 10} Im\delta G^{ii}(\mathbf{k},\mathbf{k}',\omega) \tag{7}$$