Magnetic excitations in the normal and nematic phases of iron pnictides

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Abstract
In this paper, we theoretically study the behaviors of the magnetic excitations (MEs) in the normal and nematic phases of iron pnictides. The normal state MEs exhibit commensurability to diamond and square-like structure transition with the increase of energy. This structure transition persists in the spin and orbital scenarios of nematic phases, although the MEs show anisotropic behaviors due to the $C_4$ symmetry breaking induced by the nematic orders. The MEs exhibit distinct energy evolution behaviors between the spin and orbital scenarios of nematicity. For the spin-nematic scenario, the anisotropy of the MEs persists up to the high energy region. In contrast, for the orbital-nematic scenario, it reduces dramatically in the low energy region and is negligible in the high energy region. These distinct behaviors of the MEs are attributed to the different origins between the spin and orbital scenarios of nematic orders.

Keywords: magnetic excitations, spin-nematic order, orbital order

(Some figures may appear in colour only in the online journal)

1. The introduction

The unconventional superconductivity found in iron pnictides has been of great interest in recent years. The superconductivity arises when the carriers are doped into the parent compounds, which exhibit the collinear spin density wave (SDW) order below $T_N$. Due to the proximity of the SDW and superconductivity phases, the magnetic fluctuations are proposed to be responsible for the emergence of the unconventional superconductivity [1–4]. Experimentally, it was found that the SDW transition is generally accompanied by a lattice distortion with the onset temperature $T_d$ above or coincident with $T_N$ [5–7]. It has been confirmed that the lattice structure transition is attributed to the electronic nematicity which is characterized by the $C_4$ rotational symmetry breaking [8]. So far, it was proposed that the nematicity originates from the magnetic or orbital fluctuations [8–12]. Due to the tight relation between the SDW and the nematic phases, it is believed that there exists an intrinsic interplay between the nematicity and the magnetic fluctuations [9–11, 13, 14]. Thus, the study of the normal state behaviors of the magnetic excitations (MEs) and their relation to nematicity is highly desired as it may shed light on the mechanism of unconventional superconductivity.

So far, extensive inelastic neutron scattering (INS) experiments have been performed to investigate the behaviors of the MEs in various iron-based compounds. It was found in the $122$ [15, 16], $111$ [17, 18] and $11$ [19] materials that the MEs exhibit rich structure in the energy-momentum space. The low energy MEs are dominated by the commensurate peaks centered at $(\pi, 0)$ and $(0, \pi)$. With the increase of energy, the MEs turn to be a diamond-like structure centered at $(\pi, \pi)$. A diamond to square structure transition occurs for the MEs with the further increase of energy. In addition, it was found that the MEs develop the anisotropic behaviors below a temperature $T^*$ which is basically coincident with the onset of the nematic fluctuations [20–22]. The low energy MEs are dominated by the peaks around $(\pi, 0)$ and $(0, \pi)$. However, they exhibit distinct intensity and temperature evolution between these two regions below $T^*$.

Theoretically, the behaviors of the MEs have been studied by some previous works. Especially, the effects of nematicity on the MEs are discussed within the orbital-nematic scenario. It was found [23] that the low energy MEs are dominated by peaks around $(\pi, 0)$ and $(0, \pi)$. However, the peaks are different in intensity in the presence of the orbital order. This ME behavior is qualitatively consistent with the INS data [21, 22].
The energy evolution behaviors of the MEs are detailed in [24] over a wide energy region. Indeed, the theoretical results show that the MEs exhibit a structure transition with the increase of energy, similar to that observed by the INS experiments [15–19]. However, the origin of this structure transition has not been addressed. Besides, these previous works focus on the feedback effects of the orbital order on the MEs. However, the influences of the spin-nematic order on the behaviors of the MEs have not been studied so far. As we know, a detailed comparison of the MEs between the spin and orbital scenarios of nematicity is essential to understand the origin of nematicity [8] by using the INS technique.

In this paper, we study the behaviors of the MEs in the normal and nematic phases of iron-pnictides. For the normal state, the low energy MEs are dominated by the peaks centered at \((\pi, 0)\) and \((0, \pi)\). With the increase of energy, the commensurate MEs give way to a diamond-like structure with peaks centered at \((\pi \pm \delta, \pi)\) and \((\pi, \pi \pm \delta)\). With the further increase of energy, the MEs turn to be dominated by a square-like structure with peaks centered at \((\pi \pm \delta, \pi \pm \delta)\) and \((\pi \mp \delta, \pi \mp \delta)\). Thus, these energy evolution behaviors of the MEs are qualitatively consistent with the INS observations [15–19]. Further analysis shows that the structure transition coincides with the energy evolution of the topology of the constant energy contours (CECs). The main features of the MEs are dominated by the intraorbital particle-hole excitations. Furthermore, it was found that the MEs exhibit a resonance-like peak at \((\pi, \pi)\) with the characteristic energy as high as 0.34, which is comparable to the energy scale of the collective mode suggested by the ARPES observations [26]. The structure transitions of the MEs remain in the spin and orbital scenarios of nematic phases, although anisotropy of the MEs develops due to the \(C_4\) symmetry breaking induced by the nematic orders. In the spin-nematic scenario, the anisotropy of the MEs persists up to the high energy region. While, for the orbital-nematic scenario, it decreases dramatically with the increase of energy and is negligible in the high energy region.

2. The model and formulas

The Hamiltonian we use to carry out the calculations can be divided into three parts: the tight binding part, the Coulomb interacting part, and the part that models the spin or orbital driven nematic phase.

We adopt the five orbital tight binding Hamiltonian of [27] which reproduces the LDA energy bands. Following the previous studies [24, 25], a band renormalization factor \(z = 3\) is introduced. This magnitude of \(z\) is compatible with the experimental observations and the numerical simulations [28–33]. In this way, the tight binding Hamiltonian reads

\[
H_0 = \sum_{k,a,b} \sum_{\sigma, \sigma'} z^{-1} \epsilon_{ab}(k) C_{\sigma a}^\dagger C_{\sigma b},
\]

where \(a, b\) and \(\sigma\) are the orbital and spin indices, respectively. The parameters for \(\epsilon_{ab}(k)\) are given in [27] and the energy unit eV will be used throughout the paper.

As usual, the Coulomb interaction Hamiltonian \(H_{\text{int}}\) is given by,

\[
H_{\text{int}} = U \sum_{i,a} n_{ia} n_{ia} + U' \sum_{i,a} n_{ia} n_{ib} + J \sum_{i,a,b} C_{\sigma a}^\dagger C_{\sigma b} C_{-\sigma b} C_{-\sigma a} + J' \sum_{i,a,b} C_{\sigma a}^\dagger C_{\sigma b} C_{\sigma b} C_{\sigma a},
\]

where \(n_{ia} = n_{ia} + 1\) is the electron number of orbital \(a\) at site \(i\) with \(n_{ia} = C_{\sigma a}^\dagger C_{\sigma a}\), \(U, U', J, J'\) are the coefficients of the intraorbital interaction, interorbital interaction, Hund coupling and pair hopping terms, respectively. \(U = U' + J + J'\) and \(J = J'\) are assumed as required by the spatial rotational symmetry.

In iron-pnictides, the nematic order breaks the \(C_4\) symmetry but restores the spin rotational symmetry. As proposed theoretically, the simple interacting term

\[
H_n = U_0 \sum_{i,a} (\vec{S}_{ia} \cdot \vec{S}_{ia+\delta} - \vec{S}_{ia} \cdot \vec{S}_{ia+\delta})
\]

is adopted to model the spin driven nematicity [9–11]. Where \(V_n\) is the spin-nematic order, \(\vec{S}_{ia}\) is the spin operator of orbital \(a\) at site \(i\). \(\delta_x\) and \(\delta_y\) are unit vectors along the \(x\) and \(y\) axes, respectively. Generally, there are other possible spin-nematic terms allowed by symmetry. For simplicity, we focus on the present form of the spin-nematic order. We believe that the main physics of the spin driven nematicity have been captured by the model shown above. While in the orbital-nematic scenario, the orbital orders are used to model the orbital driven nematicity [12, 34–36]. The explicit form of the orbital orders is established in [36] based on the symmetry analysis. For simplicity, we focus on the orbital order of the form

\[
H_n = \sum_{\mathbf{k},\mathbf{q}} \lambda_0 \delta(\cos k_x \cos k_y, \cos \lambda_0) + \lambda_0 \cos k_x - \cos k_y, C_{\mathbf{k}+\mathbf{q},\mathbf{r}} \rightleftharpoons C_{\mathbf{k},\mathbf{r}} + \lambda_1 \cos k_x, C_{\mathbf{k},\mathbf{r}} \rightleftharpoons C_{\mathbf{k},\mathbf{r}} + \lambda_1 \cos k_y, C_{\mathbf{k},\mathbf{r}} \rightleftharpoons C_{\mathbf{k},\mathbf{r}}
\]

which dominates the band splitting behaviors around the Fermi level [37, 38], where \(\lambda_0\) and \(\lambda_1\) are the orbital order parameters. Thus, the full Hamiltonian reads

\[
H = H_0 + H_n
\]

for the spin-nematic phase, while it reads

\[
H = H_0 + H_n + H_{\text{int}}
\]

for the orbital-nematic phase. With these Hamiltonians, the spin susceptibility is calculated within the random phase approximation (RPA) method. For the spin and orbital scenarios, the quadratic terms \(H_0\) and \(H_0 + H_n\) are used to construct the Green’s functions, while the quartic terms \(H_{\text{int}} + H_n\) and \(H_{\text{int}}\) are considered as the interaction between the particle-hole pairs, respectively.

In the present model, the Green’s function can be defined in the orbital basis as \(G_{\mathbf{k}a}(\mathbf{k}, \tau) = \langle \mathbf{C}_{\mathbf{k}a}(\tau) C_{\mathbf{k}a}(0) \rangle\). Due to the spin rotational symmetry in the present model, it is adequate to study the transverse spin susceptibility, which is defined as

\[
\chi_{\mathbf{k}a,\mathbf{k}b}(q, \tau) = \langle \mathbf{S}_{\mathbf{q}a}(\tau) \mathbf{S}_{\mathbf{q}b}(0) \rangle
\]

where \(S_{\mathbf{q}a}(q) = \frac{1}{N} \sum_{\mathbf{k}} C_{\mathbf{k}a}(\mathbf{k} + q) C_{\mathbf{k}a}(\mathbf{k})\) and \(S_{\mathbf{q}b}(q) = \frac{1}{N} \sum_{\mathbf{k}} C_{\mathbf{k}b}(\mathbf{k} + q) C_{\mathbf{k}b}(\mathbf{k})\) are the spin flip operators with \(N\) the number of the lattice sites. The bare spin susceptibility can be expressed as

\[
\chi^{0}_{\mathbf{k}a,\mathbf{k}b}(q, \tau) = \frac{1}{N^2} \sum_{\mathbf{k},\mathbf{\omega}_n} G_{\mathbf{k}a}(\mathbf{k}, -\mathbf{\omega}_n) G_{\mathbf{k}b}(\mathbf{k} + q, \mathbf{\omega}_n + \mathbf{i} \omega_n)\]

where \(\beta = 1/T\) is the inverse of temperature \(T\).

In the spin-nematic scenario, the nonzero elements of the interaction matrix read as

\[
U_{\mathbf{k}a,\mathbf{k}b}(q) = V(q) = \langle \mathbf{C}_{\mathbf{k}a}(\mathbf{k}, \tau) \mathbf{C}_{\mathbf{k}b}(\mathbf{k} + q) \rangle = \langle \mathbf{C}_{\mathbf{k}a}(\mathbf{k}, \tau) \mathbf{C}_{\mathbf{k}b}(\mathbf{k} + q) \rangle = \langle \mathbf{C}_{\mathbf{k}a}(\mathbf{k}, \tau) \mathbf{C}_{\mathbf{k}b}(\mathbf{k} + q) \rangle = \langle \mathbf{C}_{\mathbf{k}a}(\mathbf{k}, \tau) \mathbf{C}_{\mathbf{k}b}(\mathbf{k} + q) \rangle
\]

and

\[
U_{\mathbf{k}a,\mathbf{k}b}(q) = V(q) = \langle \mathbf{C}_{\mathbf{k}a}(\mathbf{k}, \tau) \mathbf{C}_{\mathbf{k}b}(\mathbf{k} + q) \rangle = \langle \mathbf{C}_{\mathbf{k}a}(\mathbf{k}, \tau) \mathbf{C}_{\mathbf{k}b}(\mathbf{k} + q) \rangle = \langle \mathbf{C}_{\mathbf{k}a}(\mathbf{k}, \tau) \mathbf{C}_{\mathbf{k}b}(\mathbf{k} + q) \rangle = \langle \mathbf{C}_{\mathbf{k}a}(\mathbf{k}, \tau) \mathbf{C}_{\mathbf{k}b}(\mathbf{k} + q) \rangle
\]
and $\hat{U}_{ab,ab+b}(q) = J$. While in the orbital scenario, they read $\hat{U}_{aa,aa}(q) = U$, $\hat{U}_{aa,bb(a+b)}(q) = J$, $\hat{U}_{ab,bb(a+b)}(q) = U'$ and $\hat{U}_{ab,ab+b}(q) = J'$. Thus, the RPA spin susceptibility can be constructed as

$$\chi(q, \omega_{\pm}) = \chi^{0}(q, \omega_{\pm})(I - \hat{U}(q)\chi^{0}(q, \omega_{\pm}))^{-1},$$

where $\chi^{0}$, $\hat{U}$ and $\chi$ are the bare spin susceptibility, the interaction matrix and the RPA renormalized spin susceptibility, respectively. It should be noticed that our definitions of the $\hat{U}$ and $\chi$ matrices are different from those in [27]. $\hat{U}_{ab,cd}$ and $\chi_{ab,cd}$ in this paper correspond to $\hat{U}_{ba,cd}$ and $\chi_{ab,de}$ in [27], respectively. After the analytic continuation, the spectra of the MEs can be obtained through the analysis of the imaginary part of the retarded spin susceptibility which reads

$$\chi^{R}(q, \omega) = \sum_{a,b} \text{Im} \chi_{aa,bb}(q, \omega).$$

Without loss of generality, $U = 0.35$ and $J = U/4$ are used throughout the paper. Due to the introduction of $z$, $U$ reduces to be about $z^{-1}$ of that in [27]. This magnitude of $U$ is adopted to keep the system near the magnetic instability. The temperature is set to be $T = 0.001$. $V_{c}$ and $\lambda_{c}$ are the order parameters for the spin and orbital scenarios of nematicity, respectively. Here, the calculations are carried out on a $128 \times 128$ lattice.

### 3. The magnetic excitations

#### 3.1. The normal state magnetic excitations

We begin with the study of the normal state MEs. In figures 1(a)–(c) and (d)–(f), we show the energy evolution of the MEs for $n = 6.03$ and $n = 5.95$, respectively. As shown in figure 1(a), the four peaks of the MEs are the larger electron pockets around $(0,0)$ and $(\pi,0)$, which are well nested. As a result, the electron pockets around $(0,0)$ and $(\pi,0)$ are well nested. As a result, the MEs are dominated by the peaks at $(\pi,0)$ and $(0,\pi)$, while the thin line parts correspond to $\omega = -0.1$. The dominating scattering process is indicated by the black arrow in figure 2(b). It should be noticed that the above scattering process is intraorbital dominated by $d_{xy}$. When the energy increases to be $0.2$, the corresponding CECs change dramatically in structure. The typical CECs are shown in figure 2(c) for $\omega = -0.1$ and 0.1. The CECs for $\omega = 0.1$ are the electron pockets centered at $(0,\pi)$ and $(\pi,0)$, while the thin line parts correspond to $\omega = -0.1$. The dominating scattering process is indicated by the black arrow in figure 2(b).
We perform which, respectively. \( U \) for and the minimum singular value \( \omega \) of the structure transition of MEs has not been addressed by related to the intraorbital particle-hole scatterings. This cause increase of energy. The main features of the MEs are directly due to the changing of the CECs with the increasing of the doping level. The MEs are composed of two parts in the whole energy region. As a result, the main features of the MEs do not change qualitatively with the changing cases in the normal state MEs. To show the momentum and energy dependence of the MEs, we plot in figure 3 the MEs along the high symmetry direction of the Brillouin zone. Figures 3(a) and (b) are the normal state MEs for \( n = 6.03 \) and \( n = 5.95 \), respectively. The intensity is in logarithmic scale in these two panels. (c) and (d) are the energy dependence of the imaginary part of the bare spin susceptibility \( \chi_0(q', \omega) \) and the minimum singular value of \( \hat{I} - \hat{\mathbf{U}}(q') \chi_0(q', \omega) \) for \( n = 6.03 \) and \( q^* = (\pi, \pi) \), respectively.

Figure 2. Schematic shown of the particle-hole scattering between the negative and positive constant energy contours (CECs) for \( n = 6.03 \). The colors show the dominating orbital components of the CECs. The thin and thick lines correspond to the CECs of the negative and positive energies, respectively. (a) is the CEC of \( \omega = -0.02 \) and 0.02. (b) and (c) are the same with (a) but for \( \omega = -0.04, 0.08 \) and \( \omega = -0.1, 0.1 \), respectively.

Figure 3. (a) and (b) are the normal state MEs for \( n = 6.03 \) and \( n = 5.95 \), respectively. The intensity is in logarithmic scale in these two panels. (c) and (d) are the energy dependence of the imaginary part of the bare spin susceptibility \( \chi_0(q', \omega) \) and the minimum singular value of \( \hat{I} - \hat{\mathbf{U}}(q') \chi_0(q', \omega) \) for \( n = 6.03 \) and \( q^* = (\pi, \pi) \), respectively.

As revealed by previous experiments [20, 21, 43–45], the nematic phase is accompanied by the anisotropic magnetic structure of the MEs. With the further increase of energy, intensity peaks develop gradually along the \( (\pi, \pi) - (0, 0) \) direction. As a result, a diamond to square structure transition occurs in this energy region. On top of that, a resonance-like mode develops around \( (\pi, \pi) \) with the characteristic energy of 0.34 eV. This is qualitatively consistent with the DMFT simulation for the doped 122 materials [16]. It is interesting to notice that the recent ARPES data indicates the existence of a collective mode with the characteristic energy of 0.5 eV [26] which is comparable to our result. As shown in figure 3(c), the imaginary part of the bare spin susceptibility exhibits no singular behavior around \( \omega = 0.34 \) for \( q^* = (\pi, \pi) \). We perform the singular value decomposition of \( \hat{I} - \hat{\mathbf{U}}(q') \chi_0(q', \omega) \) which is the denominator of the RPA spin susceptibility. The energy dependence of the minimum singular value \( S_{\min} \) is shown in figure 3(d). It can be seen that \( S_{\min} \) exhibits minima exactly at 0.34, thus the resonance-like mode arises from the pole-like effects of the RPA spin susceptibility. Unlike the bound states of the MEs, which occur below \( 2\Delta_0 \) in the superconducting state [39–42], the resonance-like mode develops at much higher energies and it is strongly damped due to its deep in the particle-hole continuum. Actually, no real pole occurs for the RPA spin susceptibility due to the finite value of the imaginary part of the bare spin susceptibility as shown in figure 3(c).

3.2. The MEs in the spin and orbital scenarios of nematicity
excitations and band splitting between $d_{xz}$ and $d_{yz}$. It was theoretically proposed that the nematicity may originate from the spin or orbital fluctuations [8–12]. Here, we study the feedback effects of the spin and orbital scenarios of nematic orders on the behaviors of the MEs. In figure 4, we show the energy evolution of the MEs in the spin and orbital driven nematic phases for $V_n = 0.01$ and $\lambda = 0.030$, respectively.

In panels (a)–(c) of figure 4, we show the energy evolution of the MEs for the spin case of $n = 6.03$. For a low energy of $\omega = 0.04$, the MEs are dominated by a commensurate peak centered at $(\pi, 0)$. In contrast, the intensity of the MEs around $(0, \pi)$ is much weaker. This is attributed to the spin-nematic orders which break the $C_4$ rotational symmetry. For positive $V_n$, the spin interaction is enhanced around $(\pi, 0)$, while it is depressed around $(0, \pi)$. Thus, the MEs show larger intensity around $(\pi, 0)$. When the energy increases to $\omega = 0.12$, the MEs turn to be dominated by the structure around $(\pi, \pi)$. Two peaks centered at $(\pi, \pi \pm \delta)$ dominate the main features of the MEs. There are two additional peaks centered at $(\pi \pm \delta, \pi)$, however they are much weaker in intensity. This is attributed to the spin-nematic order which enhances the spin interaction along the vertical direction while depresses it along the horizontal direction around the $(\pi, \pi)$ region. The four peaks exhibit the similar diamond-like structure with those shown in figure 1(b). With the further increase of energy, the pattern of the MEs changes gradually and it is dominated by four diagonal peaks which form a square-like structure when the energy is around 0.2. As shown in figures 4(a)–(c), the structure transition of the MEs in the spin-nematic scenario is quite similar to that depicted in figures 1(a)–(c). However, due to the spin-nematicity induced $C_4$ rotational symmetry breaking, the MEs is distorted in structure. As shown in figures 4(g)–(i), similar behaviors of the MEs exist for the hole doped case of $n = 5.95$. It was checked that the above established features of the MEs persist in the spin-nematic phase when $n$ is around 6.0.

It should be noticed that quite similar structure transition of the MEs occurs in the orbital-nematic scenario. In figures 4(d)–(f) and (j)–(l), the energy evolution behaviors of the MEs are shown for $n = 6.03$ and $n = 5.95$, respectively. A commensurability to diamond structure transition occurs when the energy increases from $\omega = 0.04$ to $\omega = 0.12$. At a high energy of $\omega = 0.2$, the MEs exhibit a square-like structure around $(\pi, \pi)$. It was checked that the structure transition is qualitatively unchanged when the momentum dependent orbital order $\lambda_1$ is taken into account. Thus, the established behaviors of the MEs are robust phenomenon in the orbital-nematic case. Compared to the spin-nematic case, the anisotropy of the MEs is weaker in the orbital-nematic scenario. Especially, it weakens significantly with the increase of energy. As shown in figures 4(e) and (k) for the orbital cases of $n = 6.03$ and 5.95, the MEs are dominated by four peaks with comparable intensity around $(\pi, \pi)$. In contrast, for the spin-nematic case, the vertical peaks have significantly larger intensity than the horizontal ones. This has been shown in figures 4(b) and (h). Considering that the magnitude of $V_n$ is smaller than that of $\lambda_0$, it is clearly that the spin-nematic order has more prominent influences on the behaviors of the MEs.

As shown above, both the spin and orbital nematic orders give rise to the anisotropic behaviors of the MEs. However, the energy evolution behaviors of the anisotropy are distinct between these two cases. Here, we introduce a quantity

Figure 4. Energy evolution of the magnetic excitations in the spin and orbital scenarios of nematic phases. (a)–(f) show the energy evolution of the MEs for the spin and orbital driven nematicity for $n = 6.03$, respectively. (g)–(l) show the energy evolution of the MEs for the spin and orbital driven nematicity for $n = 5.95$, respectively.

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\[ \chi_{\text{AN}}^{\omega}(\omega) = \frac{\chi_0^{\omega}(\omega) - \chi_\lambda^{\omega}(\omega)}{\chi_0^{\omega}(\omega) + \chi_\lambda^{\omega}(\omega)} \] to characterize the energy dependence of the anisotropy of the MEs, where \[ \chi_\lambda^{\omega}(\omega) = \sum_{q \in |q|} \chi_\lambda^q(q,\omega) \] and \[ \chi_0^{\omega}(\omega) = \sum_{q \in \Delta} \chi^q(q,\omega). \] In figure 5, the red and blue lines are the energy dependence of \( \chi_{\text{AN}}^{\omega}(\omega) \) for \( V_n = 0.01 \) and 0.005 for the spin-nematic scenario of \( n = 6.03 \), respectively. \( \chi_{\text{AN}}^{\omega}(\omega) \) decreases with the increase of energy, and persist to be finite around 0.2. Thus, the anisotropy of the MEs persists up to the high energy region for the spin-nematic scenario. As shown in figure 5, \( \chi_{\text{AN}}^{\omega}(\omega) \) decreases with the reduction of \( V_n \). However, it exhibits quite similar energy dependence when \( V_n \) varies. The purple and green lines are the energy dependence of \( \chi_{\text{AN}}^{\omega}(\omega) \) for \( \lambda_0 = -0.03, \lambda_0 = 0 \) and \( \lambda_0 = -0.01, \lambda_0 = -0.01 \) for the orbital-nematic scenario, respectively. These two sets of orbital orders give rise to the same splitting energy between the \( d_{xz} \) band around \((\pi,0)\) and the \( d_{yz} \) band around \((0,\pi)\). The magnitude of the splitting energy is comparable to the experimental data on FeSe [37, 38]. In this case, \( \chi_{\text{AN}}^{\omega}(\omega) \) decreases dramatically in the low energy region and it is rather small when the energy is above 0.1. Thus, the anisotropic MEs are expected to be observed in the low energy region for the orbital-nematic scenario.

The distinct energy evolution behaviors of \( \chi_{\text{AN}}^{\omega}(\omega) \) between the spin and orbital cases can be attributed to the different origins of the nematic orders. For the spin scenario, the anisotropic MEs arise from the anisotropic interaction within the RPA treatment of the spin susceptibility. In contrast, for the orbital scenario, the anisotropy of the MEs is directly related to the anisotropic band structure induced by the orbital orders. We find that the band distortions induced by the orbital orders do not occur in the full energy region. As shown in figure 6(a), the anisotropy of the energy bands is mainly reflected in the energy region ranging from the bottom of the \( d_{xz} \) band to energies slightly above the Fermi level. For illumination, we show the quasiparticle spectral functions (QSFs) in figures 6(b)–(d) for \( \omega = -0.13, -0.06 \) and 0.02, respectively. As shown in figure 6(b) for the QSFs near the bottom of the \( d_{xz} \) band, there are small anisotropy between the \((0,\pi)\) and \((\pi,0)\) regions. With the increase of energy, significant anisotropy develops in the momentum space. The typical QSFs are shown in figure 6(c) for \( \omega = -0.06 \). The anisotropy of the QSFs weakens gradually when the energy is above the Fermi level. The typical features of the QSFs are shown in figure 6(d) for \( \omega = 0.02 \). It is interesting to notice that the anisotropy of the QSFs is much stronger when the energy is around the Dirac-cone dispersions locating around \((\pi,0)\) and \((0,\pi)\). As shown in figure 6(a), the Dirac-cone dispersions dominate the energy bands in the energy region from \(-0.12\) eV to \(-0.01\) eV. This energy separation is slightly larger than 0.1 eV above which the anisotropy of the MEs is rather small in the orbital-nematic case. Thus, the anisotropic MEs are attributed to the Dirac-cone dispersions induced by the orbital orders in the orbital scenario of nematicity. Actually, the density of states is rather large when the energy is around the Dirac-cone due to the small velocity of the \( d_{xz} \) and \( d_{yz} \) bands around \((\pi,0)\) and \((0,\pi)\), respectively. This coincides with the previous study that the Dirac-cone dispersions play the major role in the features of the quasiparticle scattering interference patterns [36]. Thus, the distinct energy evolution behaviors of \( \chi_{\text{AN}}^{\omega}(\omega) \) can be traced back to the different origins between the spin and orbital scenarios of nematic orders which give rise to anisotropic interaction and distorted band structure, respectively.

4. Summary and conclusions

In conclusion, we have studied the behaviors of MEs in the normal and nematic phases of iron-pnictides. In the normal state, the MEs exhibit structure transitions with the increase of energy. In the low energy region, the MEs are dominated by the commensurate peaks centered at \((\pi,0)\) and \((0,\pi)\). In the intermediate energy, the MEs turn to be dominated by peaks at \((\pi \pm \delta,\pi)\) and \((\pi,\pi \pm \delta)\), which form the diamond-like
structure. With the further increase of energy, a square-like structure of the MEs develops in the high energy region. These behaviors of the MEs are attributed to the energy evolution of the CECs. The main features of the MEs are dominated by the intraorbital particle-hole scatterings. Meanwhile, the established energy evolution behaviors of the MEs are qualitatively consistent with the INS observations [15–19]. Besides, we find that the MEs exhibit a resonance-like peak around $(\pi, \pi)$ with the characteristic energy as high as 0.34, which is comparable to that suggested by the ARPES data [26]. This mode shares the similar origin with the magnetic resonance mode in the superconducting state [39–42], although it is strongly damped due to its deep in the particle-hole continuum. The structure transition of the MEs remains when the spin and orbital nematic orders are taken into account, although anisotropy develops due to the nematicity induced $C_4$ symmetry breaking. However, the MEs exhibit distinct energy evolution between the spin and orbital scenarios of nematicity. The anisotropy of the MEs persists to the high energy region and is negligible in the high energy region for the spin-nematic case. These are directly related to the different origins between the spin and orbital scenarios of nematic phases. Thus, these distinct behaviors of the MEs between the spin and orbital cases can be used to distinguish the origin of the nematic phase by using the INS technique.

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