Physics Letters A 380 (2016) 2008–2012

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Influence of orbital nematic order on spin responses in Fe-based superconductors

Yuehua Su [a,*], Chao Zhang [a], Tao Li [b,*]

[a] Department of Physics, Yantai University, Yantai 264005, PR China
[b] Department of Physics, Renmin University of China, Beijing 100872, PR China

ARTICLE INFO

Article history:
Received 29 December 2015
Received in revised form 10 April 2016
Accepted 11 April 2016
Available online 14 April 2016
Communicated by L. Ghivelder

Keywords:
Fe-based superconductors
Orbital nematic order
Spin fluctuations

ABSTRACT

Electronic nematicity is ubiquitous in Fe-based superconductors, but what the primary nematic order is and how the various nematic phenomena correlate with each other are still elusive. In this manuscript we study the physical consequence of the orbital nematic order on the spin correlations. We find that the orbital nematic order can drive a significant spin nematicity and can enhance the integrated intensity of the spin fluctuations. Our study shows that the orbital nematic order has strong effect on the spin correlations and it can not be taken as an unimportant secondary effect of the nematic state in Fe-based superconductors.

1. Introduction

The electronic nematic state is a novel state in nature which breaks rotational symmetry spontaneously but is translationally invariant [1]. In the newly discovered Fe-based superconductors (FeSCs), the rotational symmetry breaking is ubiquitous. It has been observed in different experimental probes, charge resistivity [2,3], angle-resolved photoemission spectroscopy (ARPES) [4–9], neutron scattering [10–13], optical conductivity [14,15], nuclear magnetic/quadrupole resonance (NMR/NQR) [16–18], magnetic torque measurement [19], scanning tunneling microscope/spectroscopy (STM/STS) [20–22], Raman scattering [23], X-ray diffraction [24], etc. (Some reviews are given in References [25,26].) The rotational symmetry breaking leads to a nematic phase transition at critical temperature T_c. This nematic phase transition shows close correlation to the structural and magnetic phase transitions [27–29]. The origin of the nematic phase transition and its correlation with superconductivity are now active topics in the field.

One complexity to study the electronic nematicity comes from the fact that the rotational symmetry breaking manifests itself in different channels simultaneously. Table 1 shows the various nematic parameters in experiments. From Landau's principle of symmetry breaking, the multiplicity of the nematic parameters can be easily understood. Consider the symmetry breaking of Fe-site symmetry group from D_{2d} to D_2 in Fe-1111 and Fe-122 families. Any function O_η which is invariant under the operations of D_2 but not that of D_{2d} can be defined as a nematic parameter. It can be defined mathematically as

$$O_\eta = \sum_\gamma C_\gamma \Psi_\gamma, P_g[O_\eta] = O_\eta, \forall g \in D_2, \tag{1}$$

where Ψ_γ are basis of one irreducible non-identity representation of D_{2d} and P_g is the corresponding operation of a group element g of D_2.

The various nematic parameters show diverse manifestations of the electronic nematicity in FeSCs. In ARPES, the nematicity shows itself as orbital-relevant band shift [4–9]. In inelastic neutron scattering (INS), it manifests anisotropic spin-wave excitations (dispersion and damping) [10] and nematic dynamical spin fluctuations [12,13], the much low-energy part of the latter is also shown in $1/T_1T$ [16]. In charge transport resistivity and conductivity, the nematicity shows as a combined effect of the anisotropic Fermi velocity and the anisotropic microscopic scattering. The latter is proven as a dominant factor for the nematicity in STM/STS [20–22,30]. It is also remarkable that the nematicity in optical conductivity shows in a very large energy range from zero frequency to high energy of about 2 eV [14].

The diverse experimental manifestations leads to hot debates on the primary driving mechanism of the nematicity in FeSCs. Among the various nematic parameters, the Ising spin (localized or itinerant) nematic order [26,31–34] and the orbital nematic order [35–37] are the most popular candidates as the primary one. Another potential nematic order is related to the Fermi-surface Pomeranchuk instability [38]. Now it is still elusive which one is

* Corresponding authors.
E-mail addresses: suyh@ytu.edu.cn (Y. Su), litao_phys@ruc.edu.cn (T. Li).

http://dx.doi.org/10.1016/j.physleta.2016.04.016
0375-9601/

Table 1
Examples of the various nematic parameters O_η in different experimental techniques. Whether the corresponding responses are static (S) or dynamical (D) and whether they are related to rotational symmetry breaking in spatial (S) or magnetic (M) spaces are also explicitly shown [39]. $\sigma_{\alpha\alpha}$ are the conductivity along α-axis, and $\chi_{\alpha\alpha}(\mathbf{q},\omega)$ (or $\chi(\mathbf{q},\omega)$) are spin magnetic susceptibility at momentum $\mathbf{q}$ and frequency ω with spin polarization along α-axis (without spin polarization). $\mathbf{Q}_1=(\pi,0)$, $\mathbf{Q}_2=(0,\pi)$ and $\mathbf{Q}=\mathbf{Q}_1$ or $\mathbf{Q}_2$ are antiferromagnetic momenta. ω_N in $1/T_1T$ is the nuclear resonance frequency which is too small as compared to the electronic energy scales, $\gamma(\mathbf{q})$ is a form factor.

Experimental technique	Nematic parameter O_η	S/D response	Symmetry breaking in S/M space
Resistivity/Conductivity	$\sigma_{xx}-\sigma_{yy}$	S/D	S
ARPES	$\Delta(\mathbf{k})\left\langle d^\dagger_{\mathbf{k},xz}d_{\mathbf{k},xz}\pm d^\dagger_{\mathbf{k},yz}d_{\mathbf{k},yz}\right\rangle$	S	S
INS			
spin flip	$\chi_{xx}(\mathbf{Q},\omega)-\chi_{yy}(\mathbf{Q},\omega)$	D	M
spin wave	$\chi(\mathbf{q},\omega)$ in $\mathbf{q}$ variation	D	S
spin fluctuations	$\chi(\mathbf{Q}_1,\omega)-\chi(\mathbf{Q}_2,\omega)$	D	S
NMR			
Knight shift	$\chi_{xx}-\chi_{yy}$	S	M
$1/T_1T$	α-dependent $\sum_{\mathbf{q}}\gamma(\mathbf{q})\chi_{\alpha\alpha}(\mathbf{q},\omega_N)$	S	M
Torque	$\chi_{xx}-\chi_{yy}$	S	M
Raman	$\langle\rho^\mu\rho^\mu\rangle$, ρ^μ Raman density	D	S
STM/STS	local density of states (LDOS)	S	S

the primary driving force and how these nematic orders correlate with each other.

In this manuscript, we will focus our study on the orbital nematic order. From symmetry analysis we proposed recently a general form of the orbital nematic order $O=\sum_{iajb}F_{ia,jb}d^\dagger_{ia}d_{jb}$, which involves a local form factor $F_{ia,jb}$ (i, j denote lattice site and a, b denote 3d orbital) [37]. The local form factor $F_{ia,jb}$ can be on-site s-wave, nearest-neighbor d-wave and nearest-neighbor extended s'-wave, etc. These orbital nematic orders can be defined in momentum space as,

$$\begin{aligned} O_s &= \sum_{\mathbf{k}}\left(d^\dagger_{\mathbf{k},xz}d_{\mathbf{k},xz}-d^\dagger_{\mathbf{k},yz}d_{\mathbf{k},yz}\right),\\ O_d &= \sum_{\mathbf{k}}\Delta_d(\mathbf{k})\left(d^\dagger_{\mathbf{k},xz}d_{\mathbf{k},xz}+d^\dagger_{\mathbf{k},yz}d_{\mathbf{k},yz}\right),\\ O_{s'} &= \sum_{\mathbf{k}}\Delta_{s'}(\mathbf{k})\left(d^\dagger_{\mathbf{k},xz}d_{\mathbf{k},xz}-d^\dagger_{\mathbf{k},yz}d_{\mathbf{k},yz}\right), \end{aligned} \tag{2}$$

where $\Delta_d(\mathbf{k})=(\cos k_x-\cos k_y)/2$ and $\Delta_{s'}(\mathbf{k})=(\cos k_x+\cos k_y)/2$.

The on-site orbital nematic order O_s has been taken extensively as a nematic order in FeSCs. However a detailed investigation on the ARPES data shows that the orbital-dependent band shift is strong momentum-dependent [4–9]. In $BaFe_2As_2$ [4,7] and FeSe [8,9] families, the band shift is much larger at momentum near $\mathbf{Q}_1=(\pi,0)$ and $\mathbf{Q}_2=(0,\pi)$ than that near Γ point $\mathbf{k}=(0,0)$. Obviously it can not be accounted for by a simple on-site orbital nematic order O_s. This unusual momentum-dependent band shift can be naturally interpreted by a *bond* d-wave orbital nematic order O_d as we have proposed [37,40,41]. The bond orbital nematic orders we have introduced for the nematic state of FeSCs are very similar to the bond charge-density-wave (CDW) order which is proposed for the CDW state of the cuprate superconductors [42]. Compared to the on-site order, the *bond* order can avoid the energy enhancement from strong local Coulomb interaction, thus makes the system in a more stable and lower energy state. A similar idea has been proposed in a recent study [41].

In our recent study, we have shown that the orbital nematic order can enhance the condensation energy of the magnetic state [37]. In this manuscript, we will follow this study to investigate the influence of the orbital nematic order on the nematic spin correlations. Recent INS experiment shows strong nematic spin fluctuations in FeSCs, where the spin fluctuations at antiferromagnetic (AFM) momentum $\mathbf{Q}_1$ are much larger than those at AFM momentum $\mathbf{Q}_2$ [12]. Moreover the integrated strength of the AFM spin fluctuations is enhanced sharply when across the nematic phase transition [13]. In this manuscript, we introduce a finite orbital nematic order for the nematic state of FeSCs. We show that a finite orbital nematic order can drive a significant spin correlation nematicity and can enhance the integrated intensity of the spin fluctuations as observed in the INS experiments [12,13]. Our results show that the orbital nematic order has strong effect on the spin nematicity, and it should not be taken as a simple secondary effect caused by the symmetry breaking from the spin nematicity.

Our manuscript is arranged as following. In Sec. 2 we specify a simplified model Hamiltonian for the nematic state of FeSCs. In Sec. 3 we study the spin correlations with a finite orbital nematic order. Sec. 4 shows our discussion and conclusion.

2. Model Hamiltonian

At present a well-defined theory for the nematic state of FeSCs is absent. This is due to the entanglement of the various nematic responses as observed in diverse experimental probes. In our study, we will simplify our focus on how the orbital nematic order makes influence on the spin fluctuations in FeSCs. We thus introduce a simplified Hamiltonian which includes a mean-field part H_0 for the ordered nematic state and an interacting part H_I to account for the interaction-renormalized spin fluctuations.

The mean-field Hamiltonian H_0 is defined as $H_0=H_t+H_{mf}$, where H_t describes the electronic band structure with the 3d orbitals involved and H_{mf} is the mean-field contribution from a finite orbital nematic order. Following Kuroki et al. [43], we define H_t as

$$H_t=\sum_{iajb\sigma}t_{ia,jb}d^\dagger_{ia\mu}d_{jb\mu}, \tag{3}$$

where $d_{ia\mu}$ and $d^\dagger_{ia\mu}$ are the annihilation and creation operators respectively for 3d electrons. The subscripts i/j, a/b and μ are indices for lattice site, orbital and spin degrees of freedom, respectively. H_{mf} describes the orbital nematic state in mean-field approximation and is defined by

$$H_{mf}=-\Delta\ O_\eta, \tag{4}$$

where O_η is given in Eq. (2). Here we make approximation that an unknown microscopic origin of the orbital nematic order from such as multi-orbital Hubbard interaction or beyond is not considered. The recent ARPES data [8,9] shows that the band shift has a mean-field-like temperature dependence, we thus propose that the orbital nematic order follows $\Delta=\Delta_0(1-T/T_c)^{1/2}$. In our study, we set 100 meV as an energy unit and set $\Delta_0=0.33$ ($\sim$ 33 meV) following ARPES data of Yi et al. [4] and $T_c=0.13$ ($\sim$ 140 K).