Driving force of the orbital-relevant electronic nematicity in Fe-based superconductors

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Abstract
The electronic nematic responses in Fe-based superconductors have been observed ubiquitously in various experimental probes. One novel nematic character is the d-wave bond orbital-relevant nematic charge order which was firstly proposed by symmetry analysis and then confirmed by angle-resolved photoemission spectroscopy. In this paper, we present a mechanism that the driving force of the orbital-relevant nematic charge order is the reduction of the large Hubbard energy in the particle-hole charge channel by virtual hopping processes. This is one scenario from strong-coupling consideration. The same virtual hopping processes can lead to a super-exchange interaction for the spin magnetic order in the particle-hole spin channel and a pairing interaction for the superconducting order in the particle-particle channel. Thus the electronic nematic order, the spin magnetic order and the pairing superconducting order are intrinsically entangled and they can all stem from the same microscopic virtual hopping processes in reduction of the Hubbard energy. The electronic nematicity, the spin magnetism and the pairing superconductivity in unconventional superconductors are proposed to be unified within this mechanism.

Keywords: electronic nematicity, driving force, Fe-based superconductors

The electronic nematic state is one universal electronic state with spontaneous rotational symmetry breaking \([1]\). It shows novel unconventional physics \([2–6]\). Recently, the electronic nematic state has been observed in Fe-based superconductors (FeSCs) with ubiquitous nematic responses in various experimental probes \([7–10]\). One special character of the electronic nematicity in FeSCs is the unusual momentum-dependent electronic band deformation with large value at \((\pi,0)/(0,\pi)\) and small value at \(\Gamma\) point as observed in ARPES \([11–15]\). This special nematic character rules out the on-site orbital order of the different occupation of the \(d_{xz}\) and \(d_{yz}\) electrons, which is confirmed consistently by the Raman scattering in \(B_{1g}\) channel \([9, 16]\) and the other ARPES data \([17, 18]\). This novel nematic character has been attributed to a d-wave bond orbital-relevant nematic charge order which was firstly proposed by our symmetry analysis \([19, 20]\). The orbital-relevant nematic charge order in FeSCs can enhance the magnetic condensation energy \([20]\). It can also lead to the static \([19]\) and the dynamical \([10]\) magnetic nematic responses which have been observed in the magnetic torque \([21]\) and the neutron scattering spectra \([22]\). Thus the orbital-relevant electronic nematicity plays important roles in the low-energy physics of FeSCs.

The driving force of the ubiquitous nematicity in FeSCs is still elusive. The driving nematic order may be an Ising spin nematic order \([23–25]\), an itinerant magnetic nematic order \([26, 27]\), an orbital-relevant nematic charge order \([19, 20]\), or a Pomeranchuk nematic order of Fermi surface instability \([28–32]\). Other possible driving mechanisms of the electronic nematicity are also proposed, such as to reduce the Huud’s coupling energy \([33]\) or to reduce the nearest-neighbour Hubbard energy \([34–36]\).

In this paper, we will study the driving force of the orbital-relevant electronic nematicity in FeSCs. Our starting point is the multi-orbital Hubbard model with relatively large Hubbard interactions to account for the relatively strong correlation of...
the 3d electrons in FeSCs. This is one scenario for FeSCs from strong-coupling consideration. The one-orbital Hubbard model with strong Hubbard interaction has been extensively studied in understanding the unconventional superconductivity and the novel normal states of cuprate superconductors in the last three decades [37]. Within this scenario, the bond orbital-relevant nematic charge order can arise from the virtual hopping processes in reduction of the large Hubbard energy in the particle-hole charge channel. The same virtual hopping processes can lead to a super-exchange interaction for the spin magnetic order in the particle-hole spin channel and an effective pairing interaction for the superconducting order in the particle-particle channel. Thus the electronic nematic order, the spin magnetic order and the pairing superconducting order are unified to stem from the same microscopic virtual hopping processes. We also propose that the electronic nematicity, the spin magnetism and the pairing superconductivity in unconventional superconductors come from the same mechanism of reduction of the Hubbard energy by virtual hopping processes.

Before a further study on the driving force of the orbital-relevant electronic nematicity in FeSCs, we firstly summarize the most possibly relevant nematic operators from the Landau’s principle of symmetry breaking [38]. With a structural phase transition from a tetragonal to an orthorhombic phase, the Fe-site symmetry group is reduced from $D_{2d}$ to $D_2$ [19, 20]. Following the Landau’s principle, the electronic nematicity can be described by introducing a symmetry breaking term $\delta H$ into the Hamiltonian $H_0$ which belongs to the identity representation of the $D_{2d}$. Now the Hamiltonian $H = H_0 + \delta H$ belongs to the identity representation of the $D_2$ but not that of the $D_{2d}$. $\delta H$ can be expanded by the irreducible representations of the $D_{2d}$ [10, 38], i.e.

$$\delta H = \sum_{j,n,\mu} h_{j,n,\mu}^{(j)} O_{n,\mu}^{(j)},$$

(1)

where $\{O_{n,\mu}^{(j)}; \mu = 1, 2, \cdots, d_j\}$ form the basis functions of the $j$th irreducible representation of the $D_{2d}$, $d_j$ is the corresponding dimension. $n$ denotes the different groups of the $j$th representation. $h$ can be regarded as the conjugate field of the nematic operator $O$. This expansion can be easily obtained by projection operations and the summation does not include the identity representation of the $D_{2d}$. It is shown that there is only one channel in the symmetry reduction from $D_{2d}$ to $D_2$, i.e. $\delta H$ belongs to the $B_1$ representation of the $D_{2d}$.

In tables 1 and 2, we present the on-site, the nearest-neighbour bond and the next-nearest-neighbour bond orbital-relevant nematic operators in the particle-hole charge channel. They are defined as

$$O(k) = \sum_{\alpha \sigma \tau} d_{\alpha \nu \sigma}^{\dagger} \Xi_{\alpha \nu \sigma}(k) d_{\alpha \nu \sigma},$$

(2)

where $a, b$ are the orbital indices and $\sigma$ are the spin indices. Three orbitals near Fermi energy, $\{d_{xz}, d_{xc}, d_{xy}\}$, are considered. The lattice versions of the orbital-relevant nematic charge operators with five 3d orbitals have been provided in the articles [19, 20]. The d-wave orbital-relevant nematic charge operator, $O(k) = \sum_{\alpha \sigma \tau} (\cos k_x - \cos k_y) d_{\alpha \nu \sigma}^{\dagger} d_{\alpha \nu \sigma}$ with $\{d_{xc}, d_{xz}\}$ orbitals involved, has been introduced to account for the unusual electronic band deformation as observed in ARPES [19, 20, 34, 35]. As a simple d-wave orbital-relevant nematic charge order cannot account for all the details of the band deformation, especially near $\Gamma$ point, here we present the most possibly orbital-relevant nematic operators for further investigation of the electronic band deformation. It should be noted that the combination of the nearest-neighbour extended s-wave and d-wave bond orbital-relevant nematic charge orders can lead to a band deformation with both $(\pi, 0)/(0, \pi)$ and $\Gamma$ points involved. Moreover, since the next-nearest-neighbour hopping integrals of the 3d electrons in FeSCs are not ignorable in magnitude, the next-nearest-neighbour bond orbital-relevant nematic charge operators may also arise, with one example defined as $O(k) = \sum_{\sigma} (\cos k_x \cos k_y) \left( d_{kx,s}^{\dagger} d_{kx,\sigma} - d_{kx,\sigma}^{\dagger} d_{kx,s} \right)$ which has also been proposed recently in study of the Huud’s coupling in FeSCs [33].

The orbital-relevant nematic operators defined in equation (2) are the on-site or the bond ones in the particle-hole charge channel. There are many available orbital-relevant nematic operators in other channels. One special example is the orbital-relevant nematic operator in the particle-hole spin channel defined by

$$S_{ij} = \sum_{\alpha \sigma \tau_1} \sum_{\alpha \sigma \tau_2} \rho_{i,j} d_{\alpha \nu \sigma_1}^{\dagger} \left( \frac{\sigma_1}{2} \right)_{\alpha \sigma_1,\tau_1} d_{\alpha \nu \sigma_2},$$

(3)

\begin{table}
\centering
\caption{Orbital-relevant nematic operators in the particle-hole charge channel with three 3d orbitals $\{d_{xz}, d_{xc}, d_{xy}\}$ near Fermi energy involved. The pure $\{d_{xc}, d_{xz}\}$-relevant ones are shown in table (1). The representation (repst.) of $D_{2d}$ in the last column are shown as $G_1 \otimes G_2 = G_1$ with $G_1$ and $G_2$ the symmetries of the components of $O(k)$. The first two rows are for nearest-neighbour bond and the third row is for next-nearest-neighbour bond.}
\begin{tabular}{|c|c|}
\hline
$\Lambda(k)$ & $O(k)$ & $\Omega$ & repst. of $D_{2d}$ \\
\hline
on-site & $c =$ const. & $\tau_3$ & $A_1 \otimes B_1 = B_1$
\hline
nn-bond & $\cos k_x + \cos k_y$ & $\tau_3$ & $A_1 \otimes B_1 = B_1$
\hline
nnn-bond & $\cos k_x - \cos k_y$ & $\tau_3$ & $B_1 \otimes A_1 = B_1$
\hline
nnn-bond & $\sin k_x \sin k_y$ & $\tau_2$ & $B_2 \otimes A_2 = B_1$
\hline
\end{tabular}
\end{table}

\begin{table}
\centering
\caption{Orbital-relevant nematic operators in the particle-hole spin channel with five 3d orbitals $\{d_{xc}, d_{xz}, d_{xy}\}$ involved.}
\begin{tabular}{|c|c|}
\hline
$O(k)$ & $\text{repst. of } D_{2d}$ \\
\hline
$(\cos k_x - \cos k_y) d_{kx,\sigma}^{\dagger} d_{kx,\sigma}$ & $B_1 \otimes A_1 = B_1$
\hline
$\left( d_{kx,\sigma}^{\dagger} d_{kx,\sigma} \right) \left( \frac{\sigma_1}{2} \right)_{\alpha \sigma_1,\tau_1} d_{kx,\sigma}$ & $A_2 \otimes B_2 = B_1$
\hline
\end{tabular}
\end{table}
where $\rho_\sigma$ is an orbital-relevant phase factor and $\sigma$ are the Pauli matrices. It should be noted that the nematic operators we have introduced in equation (2) and (3) are the extended orbital-relevant Pomeranchuk nematic operators in the respective charge and spin channels. The original Pomeranchuk nematic operators are defined in band models without explicit orbital character as

$$n_k = \sum_\sigma \phi_\sigma d^\dagger_\sigma d_\sigma, \quad S_k = \sum_{\sigma_1\sigma_2} \phi_\sigma d^\dagger_{\sigma_1} \left( \frac{\sigma}{2} \right)_{\sigma_1\sigma_2} d_{\sigma_2},$$

where $\phi_\sigma$ is a $k$-dependent form factor [39]. The recent functional and parquet renormalization group studies found a Pomeranchuk nematic order in FeSCs with d-wave Fermi surface deformation [28–32]. It should be noted that what exact form factor of the proposed Pomeranchuk nematic order can not be explicitly presented in the renormalization group formulations since these theoretical formulations are established only near Fermi pockets.

Any other operator which follows equation (1) of the Landau’s principle can be taken as nematic operator. Examples in higher-order charge or spin channels can be defined such as

$$O_a = \sum_i (n_{ia}n_{i+\delta a} - n_{ia}n_{i+\delta a}), \quad O_s = \sum_i (S_{ia} \cdot S_{i+\delta a} - S_{ia} \cdot S_{i+\delta a}).$$

$O_s$ is the Ising spin nematic operator introduced to account for the spin nematic responses [23–25]. The diverse nematic responses in different channels stem from the diverse nematic operators which manifest themselves by a finite coupling to the driving nematic order operator.

Now let us study the driving force of the orbital-relevant electronic nematicity in FeSCs. Our starting point is the Hubbard model with relatively large Hubbard interactions. This assumption is based upon the following experimental results: i) the linear-temperature dependent magnetic susceptibility shows strong local spin magnetic fluctuations [40]; ii) both the local magnetic moment and the ordered magnetic moment are large [41]; iii) the electronic band structure near Fermi energy is largely renormalized [42, 43]. These experimental results together with the theoretical studies [44, 45] show obviously the relatively strong correlation of the 3d electrons in FeSCs.

Let us firstly focus on the one-orbital Hubbard model with Hamiltonian $H = -\sum_{(ij)\sigma} t_{ij} d^\dagger_{i\sigma} d_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$, where the hopping integrals are only defined on the nearest-neighbour bonds. In the large-$U$ limit near half-filling, the Hubbard model involves the Mott physics which are proposed to be essential in cuprate superconductors [37]. This is a strong-coupling scenario for cuprate superconductors. In the large-$U$ limit near half-filling, the virtual hopping processes between the paired singly-occupied sites lead to an effective Hamiltonian in second-order perturbations, $H_{\text{eff}} = -V \sum_{(ij)\sigma} P_i d^\dagger_{i\sigma} d_{j\sigma} d^\dagger_{j\sigma} d_{i\sigma}, P$, where $P$ is a Gutzwiller projector and $V = \frac{2\pi}{\sigma^2}$. The relevant physics of this effective Hamiltonian are extensively studied for cuprate superconductors [37]. There are particle-hole charge physics involved in $H_{\text{eff}}$, which can be described by

$$H_\chi = -V \sum \chi_{ij} \chi_{ji}, \quad (4)$$

where a bond charge operator $\chi_{ij}$ is defined in the particle-hole charge channel as

$$\chi_{ij} = \sum_\sigma d^\dagger_{i\sigma} d_{j\sigma}. \quad (5)$$

The projector $P$ is not explicitly shown in equation (4). The Pomeranchuk charge operator $n_k$ is the momentum version of the bond charge operator $\chi_{ij}$ with a local form factor. The bond charge order parameters, such as a d-wave nematic charge order, an extended s-wave charge order, or a staggered flux order with special local form factor, have been proposed in the study of the $t – J$ model for cuprate superconductors [37, 46]. The virtual hopping processes also involve the physics in the spin channel described by a super-exchange interaction

$$H_s = 2V \sum_{(ij)} \left( S_i \cdot S_j + \frac{1}{4} n_i n_j \right). \quad (6)$$

Obviously, an antiferromagnetic order is favoured at low temperature. The virtual hopping processes also involve the pairing physics in the particle-particle channel. They can be described by a new expression of $H_{\text{eff}}$ as

$$H_\Delta = V \sum_{(ij)} \Delta_{ij}^{(s,1)} \Delta_{ij}^{(s,1)} + \Delta_{ij}^{(s,-1)} \Delta_{ij}^{(s,-1)} + \frac{1}{2} \Delta_{ij}^{(s,0)} \Delta_{ij}^{(s,0)} - \frac{1}{2} \Delta_{ij}^{(s,1)} \Delta_{ij}^{(s,1)}, \quad (7)$$

where the pairing operators are defined as $\Delta_{ij}^{(x,1)} = d_{ij} d_{ji}$, $\Delta_{ij}^{(s,1)} = d_{ij} d_{ji}$ and $\Delta_{ij}^{(s,0)} = (d_{ij} d_{ji} + d_{ji} d_{ij})$. The pairing Hamiltonian $H_\Delta$ shows that a stable singlet pairing state can come from the virtual hopping processes.

This simple analysis on the one-orbital Hubbard model from strong-coupling consideration shows that the same virtual hopping processes in reduction of the on-site Hubbard energy involve various physics in different channels. Therefore the bond charge order, the spin magnetic order and the pairing superconducting order are unified to stem from the same microscopic virtual hopping processes but in different channels. This is our principal idea on the driving force of the bond nematic charge order in FeSCs and its intrinsic correlation with the spin magnetism and the pairing superconductivity.

The multi-orbital Hubbard model for FeSCs is simplified as

$$H = -\sum_{(ij)\sigma\rho} t_{ij}^{\sigma\rho} d^\dagger_{i\sigma\rho} d_{j\rho\sigma} + U \sum_i n_{i\uparrow\sigma} n_{i\downarrow\sigma} + U \sum_{i<\rho} n_{i\rho\uparrow} n_{i\rho\downarrow}$$

where $(ij)$ includes both the nearest-neighbour and the next-nearest-neighbour hoppings of the 3d electrons, and the on-site chemical potential terms are not explicitly shown. In the case with large $U$, the virtual hopping processes in second-order perturbations with singly-occupied orbitals involved can be described by an effective Hamiltonian $H_{\text{eff}} = -\sum_{(ij)\sigma\rho} V_{ij}^{\sigma\rho} d^\dagger_{i\sigma\rho} d_{j\rho\sigma} d^\dagger_{j\rho\sigma} d_{i\sigma\rho}, P$, where $V_{ij}^{\sigma\rho} = 2(\pi\sigma^2) / U$ and $a, b$ are the indices of the singly-occupied orbitals. In the particle-hole charge channel, $H_{\text{eff}}$ can be rewritten as
\[ H_\chi^\prime = - \sum_{(ij)ab} V_{ij}^{ab} \chi_{ij,ab}^\dagger \chi_{ij,ab}, \]  

where the orbital-relevant bond charge operator is defined as \( \chi_{ij,ab} = \sum_{\sigma} d_{ij,ab,\sigma}^{\dagger} d_{ij,ab,\sigma} \). Of all the singly-occupied orbitals involved in \( H_\chi^\prime \), if two orbitals are degenerate and the associated hopping integrals are weakly orbital dependent \( t_{ij} \approx t_{ij} \), then the contribution of these two orbitals in \( H_\chi^\prime \) can be simplified as 

\[ H_\chi^\prime = - \sum_{(ij)} 2V_{ij} \left( \bar{S}_{ij} \cdot \bar{S}_\chi + \frac{1}{4} \bar{\chi}_{ij}^\dagger \bar{\chi}_{ij} \right), \]  

where \( V_{ij} = \frac{2t_{ij}^2}{U} \), and the pseudo-spin operator \( \bar{S}_{ij} \) and the orbital-relevant bond charge operator \( \bar{\chi}_{ij} \) are defined as 

\[ \bar{S}_{ij} = \sum_{\alpha} d_{ij,\alpha}^{\dagger} \left( \frac{\tau}{2} \right)_{\alpha} d_{ij,\alpha}, \quad \bar{\chi}_{ij} = \sum_{\alpha} d_{ij,\alpha}^{\dagger} d_{ij,\alpha}. \]  

\( \tau \) are the Pauli matrices defined in the paired degenerate singly-occupied orbital space. The orbital-relevant nematic operators we proposed for FeSCs in equation (2) [19, 20] are the bond charge operators \( \chi_{ij,ab} \) with rotational-symmetry-breaking local form factors. Similar to the one-orbital Hubbard model, the virtual hopping processes also give rise to a super-exchange interaction in the particle-hole spin channel, 

\[ H'_\chi = \sum_{(ij)ab} 2V_{ij}^{ab} \left( S_{ia} \cdot S_{ib} + \frac{1}{4} n_{ia} n_{ib} \right), \]  

where \( S_{ia} \) and \( n_{ia} \) are the on-site spin and charge operators, respectively. In the particle-particle channel, \( H'_\text{eff} \) has a pairing form as 

\[ H'_\Delta = \sum_{(ij)ab} V_{ij}^{ab} \left( \Delta_{ij,ab}^{(1)} \dagger \Delta_{ij,ab}^{(1)} + \Delta_{ij,ab}^{(s,-1)} \dagger \Delta_{ij,ab}^{(s,-1)} \right) + \frac{1}{2} \Delta_{ij,ab}^{(s,0)} \Delta_{ij,ab}^{(s,0)} - \frac{1}{2} \Delta_{ij,ab}^{(s,1)} \Delta_{ij,ab}^{(s,1)}, \]  

where the pairing order operators are defined as \( \Delta_{ij,ab}^{(1)} = d_{ja,\dagger} d_{ia,\dagger} \), \( \Delta_{ij,ab}^{(s,-1)} = d_{ja,\dagger} d_{ia,\dagger} \), and \( \Delta_{ij,ab}^{(s,0)} = (d_{ja,\dagger} d_{ia,\dagger} \pm d_{ia,\dagger} d_{ja,\dagger}) \).

Some remarks on our approximate treatment of the multi-orbital Hubbard interactions should be noted. Firstly, there are other virtual hopping processes in second-order perturbations. One special class is described by \( \tilde{H}'_\text{eff} = - \sum_{(ij),a \neq b} V_{ij}^{ab} P_{ij,ab} d_{ja,\dagger}^{\dagger} d_{ia,\dagger} d_{ja,\dagger} d_{ia,\dagger} P \). Since each term of \( \tilde{H}'_\text{eff} \) is not self-Hermitian, it describes higher-order perturbations compared to \( H'_\text{eff} \) [47]. For examples, \( \tilde{H}'_\text{eff} \) has a new form in the spin channel as 

\[ \tilde{H}'_\text{eff} = \sum_{(ij),a \neq b} 2V_{ij}^{ab} \left( S_{ia} \cdot S_{ib} + \frac{1}{4} n_{ia} n_{ib} \right), \]  

where \( S_{ia} = \sum_{\sigma} d_{ia,\sigma}^{\dagger} \left( \frac{\tau}{2} \right)_{\sigma,\sigma} d_{ia,\sigma} \), and \( n_{ia} = \sum_{\sigma} d_{ia,\sigma}^{\dagger} d_{ia,\sigma} \) which describe the inter-orbital spin and charge physics.

In the pairing channel, \( H'_\text{eff} \) can be reexpressed as 

\[ \tilde{H}'_\Delta = \sum_{(ij),a \neq b} V_{ij}^{ab} \left( \Delta_{ij,ab}^{(1)} \dagger \Delta_{ij,ab}^{(1)} + \Delta_{ij,ab}^{(s,-1)} \dagger \Delta_{ij,ab}^{(s,-1)} + \frac{1}{2} \Delta_{ij,ab}^{(s,0)} \right) - \frac{1}{2} \Delta_{ij,ab}^{(s,1)} \Delta_{ij,ab}^{(s,1)} \]  

where the pairing operators are defined as \( \Delta_{ij,ab}^{(s,1)} = d_{ja,\dagger} d_{ia,\dagger} \), \( \Delta_{ij,ab}^{(s,-1)} = d_{ja,\dagger} d_{ia,\dagger} \), and \( \Delta_{ij,ab}^{(s,0)} = (d_{ja,\dagger} d_{ia,\dagger} \pm d_{ia,\dagger} d_{ja,\dagger}) \). 

\( \tilde{H}'_\Delta \) describes the inter-orbital pairing couplings. Secondly, we have neglected the exact configurations of the local orbital occupation in the effective Hamiltonian \( \tilde{H}'_\text{eff} \), where the interaction constants \( V_{ij}^{ab} \) only include the contribution of the paired singly-occupied orbitals \( (ia, jb) \). In the multi-orbital model for FeSCs, the realistic configuration of the local orbital occupation will lead to correction to the effective interaction constants \( V_{ij}^{ab} \) from local correlations of other orbitals. Thirdly, we have not included the Huud’s coupling in the above study, which has been assumed to be much smaller than \( U \). The inclusion of the Huud’s coupling would lead to slightly spin- and orbital-dependent correction to the effective interaction constants \( V_{ij}^{ab} \) [47, 48], which is ignored at our first study. It will lead to a Kugel–Khomskii spin-orbital model for FeSCs [49], which involves too complex spin-orbital physics to be well studied within an intuitive phenomenological theory. Finally, it should be noted that the effective Hamiltonian \( \tilde{H}'_\text{eff} \) mainly focuses on the low-energy physics driven by the large on-site Hubbard interactions, where the singly-occupied orbitals are mostly involved. Since the crystal-field splitting of the five 3d orbitals and the exact local electronic configuration of the Fe ions in FeSCs are not definitely defined, the singly-occupied orbitals involved in \( \tilde{H}'_\text{eff} \) can be extensively defined. They can include the orbitals which are singly-occupied and the orbitals which have both finite probability to be singly-occupied and finite probability to be doubly-occupied\(^3\).

\[ H'_\chi^\prime, H'_\chi, H'_\Delta \] from the virtual hopping processes in the multi-orbital Hubbard model describe different physics in FeSCs in the respective particle-hole charge, particle-hole spin and particle-particle channels. Thus the bond nematic charge order, the spin magnetic order and the pairing superconducting order are intrinsically entangled and can come from the same microscopic virtual hopping processes in reduction of the Hubbard energy.

In the above study, we show that the reduction of the Hubbard energy by virtual hopping processes can be a driving force of the orbital-relevant nematic charge order. The same virtual hopping processes can also lead to a spin \( J_1 - J_2 \) model for FeSCs, which involves an Ising spin nematic order [23–25]. Thus the orbital-relevant nematic charge order we have proposed [19, 20] and the Ising spin nematic order come from the same microscopic virtual hopping processes in reduction of the Hubbard energy. However, this driving force of the orbital-relevant nematic charge order is very different to that of the itinerant magnetic nematic order [26, 27], the latter of which is assumed to stem from high-order magnetic fluctuations of the itinerant electrons. One challenge in the scenario of the itinerant magnetic nematicity is how to produce a strongly momentum-dependent electronic band deformation

\(^3\) A properly realistic phenomenological model for FeSCs can be defined by \( H = H_s + H_\chi + H'_\text{eff} \), where \( H_s \) are the multi-orbital on-site Hubbard interactions including the Huud’s coupling, and \( H'_\text{eff} \) does not involve the Gutzwiller projector \( P \). This is one extended multi-orbital model of the \( t - U - J \) model for the Gossamer superconductivity in the cuprate superconductors [50, 51].
with d-wave symmetry. The Pomeranchuk nematic orders in the functional and parquet renormalization group theories come from the instability of the itinerant electrons in particle-hole charge channels with zero momentum of center of mass [28–30, 32]. The reduction of the nearest-neighbour Hubbard interactions as a driving force [35, 36] is different to the one in our theory, as the latter of which comes from the reduction of the on-site Hubbard energy by virtual hopping processes and can unify the electronic nematicity, the spin magnetism and the pairing superconductivity.

Although the orbital-relevant nematic order we have proposed is one extended orbital-relevant Pomeranchuk nematic order, its driving force comes from a strong correlation mechanism. There are two steps in energy gain in the formation of the orbital-relevant nematic charge order we proposed. One is the reduction of the Hubbard energy in strong correlation processes, and the other is a further Fermi-surface instability. Only a pure Fermi-surface instability in weak-coupling scenario drives the Pomeranchuk nematic order [39]. The associated nematic phase transition in our theory is one from a normal Gutzwiller projected Fermi liquid to an ordered Gutzwiller projected nematic liquid. The nature of this nematic phase transition and the possible difference to the Pomeranchuk nematic phase transition [2–5] is one interesting issue for future study.

As a summary, we have firstly presented all possible electronic nematic operators for FeSCs from the Landau’s principle of symmetry breaking. We then have presented a driving mechanism that the reduction of the Hubbard energy by virtual hopping processes can drive the electrons into a charge nematic state. The same mechanism is also the driving force for the spin magnetic state and the pairing superconducting state. Following these results, we propose that the bond orbital-relevant nematic order in the particle-hole charge channel is the driving nematic order in FeSCs with the reduction of the Hubbard energy as the driving force. Moreover, since the electronic nematic order, the spin magnetic order and the pairing superconducting order are universal characters of many unconventional superconductors [1, 7], they should all stem from one universal microscopic mechanism. We propose that the reduction of the Hubbard energy by virtual hopping processes is the driving mechanism, and the electronic nematicity, the spin magnetism and the pairing superconductivity in unconventional superconductors can then be unified within this mechanism.

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