Antiferromagnetism with ferro-orbital order in Fe pnictides

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Abstract. We investigate the magnetism of a two-orbital model proposed for Fe pnictides by using the Hartree-Fock approximation. In this study, we include possibility of orbital order on an equal footing with magnetic order. Antiferromagnetic order occurs with ordering vector $\left(\pi, 0\right)$. We find that this antiferromagnetic state inevitably accompanies ferro-orbital order, since the ordering with $\left(\pi, 0\right)$ breaks the equivalence of $x$ and $y$ directions, and as a result, the occupancies of $d_{xz}$ and $d_{yz}$ orbitals become different. Through an electron-lattice interaction, the lattice should be distorted from a tetragonal to orthorhombic structure in the antiferromagnetic state. We also show that a band gap does not open at some points in the Brillouin zone even in the antiferromagnetic state due to multiorbital nature of the bands as long as the Coulomb interaction is not too large.

1. Introduction

Since the discovery of superconductivity in LaFeAsO$_{1-x}$F$_x$ with a high transition temperature $T_c = 26$ K [1], Fe pnictides have attracted much interest. In particular, the mechanism of the superconductivity is one of the most important issues. In Fe pnictides, superconductivity occurs around the magnetic phase boundaries [1, 2, 3, 4, 5] as in high-$T_c$ cuprates, and magnetism is probably playing an important role in the emergence of superconductivity. Thus, it is highly desirable to understand magnetism characteristic to Fe pnictides from a microscopic view point.

The magnetism in Fe pnictides is much different from that in cuprates. For example, ordering vector of the antiferromagnetism is $\left(\pi, \pi\right)$ in the cuprates, while it is $\left(\pi, 0\right)$ in Fe pnictides in the unfolded Brillouin zone with one Fe ion per unit cell [6, 7, 8, 9]. Another important difference is conductivity. The antiferromagnetic states are metallic [2, 3, 4, 10, 11, 12] in Fe pnictides while insulating in undoped cuprates. In Fe pnictides, a structural transition occurs at [7, 8, 9, 13, 14] or near [6] the antiferromagnetic transition.

In this study, we investigate magnetism of the two-orbital model proposed for Fe pnictides [15, 16] by applying Hartree-Fock approximation. In particular, we consider orbital order on an equal footing with antiferromagnetic order, and show that the antiferromagnetic order accompanies ferro-orbital order. While the two-orbital model has already been studied by the Hartree-Fock approximation [17], the orbital-order, which is a main topic of this study, has not been investigated.
2. Model and Method

We consider a square lattice of Fe ions with \( d_{zx} \) and \( d_{yz} \) orbitals [15, 16]. Then, the model Hamiltonian is given by

\[
H = \sum_{k,\tau,\sigma} c_{k\tau\sigma}^\dagger c_{k\tau\sigma} + U \sum_{i,\tau} n_{i\tau\uparrow} n_{i\tau\downarrow} + U' \sum_i n_{ix} n_{iy} + J \sum_{i,\tau} n_{ix} n_{iy} + J' \sum_{i,\tau} n_{ix} n_{iy}
\]

where \( c_{i\tau\sigma} \) is the annihilation operator of the electron at site \( i \) with orbital \( \tau \) and spin \( \sigma \) (\( \uparrow \) or \( \downarrow \)) and \( c_{k\tau\sigma} \) is the Fourier transform of \( c_{i\tau\sigma} \). \( \tau = x \) and \( y \) denote \( d_{zx} \) and \( d_{yz} \) orbitals, respectively. The number operators are defined as \( n_{i\tau\sigma} = c_{i\tau\sigma}^\dagger c_{i\tau\sigma} \) and \( n_{i\tau} = \sum_\sigma n_{i\tau\sigma} \). \( U, U', J, \) and \( J' \) denote the intraorbital Coulomb, interorbital Coulomb, exchange, and pair-hopping interactions, respectively. The relations \( U = U' + J + J' \) and \( J = J' \) hold for \( d_{zx} \) and \( d_{yz} \) orbitals [18] and we use them. For the kinetic energy term, we use the parameters proposed by Raghu et al. [15]:

\[
\epsilon_{kxx} = -2t_1 \cos k_x - 2t_2 \cos k_y - 4t_3 \cos k_x \cos k_y, \quad \epsilon_{kxy} = -2t_1 \cos k_x - 2t_1 \cos k_y - 4t_3 \cos k_x \cos k_y,
\]

and \( \epsilon_{kxy} = -4t_4 \sin k_x \sin k_y \), where \( t_1 = -t, t_2 = 1.3t, t_3 = 3t = -0.85t \), and we have set the lattice constant unity.

In the Hartree-Fock approximation, we assume that the expectation value of the number \( n_{i\tau\sigma} \) has the following form:

\[
\langle n_{i\tau\sigma} \rangle = \left\{ [n + m_o(\delta_{\sigma\uparrow} - \delta_{\sigma\downarrow}) + m_{so}(\delta_{\sigma\uparrow} - \delta_{\sigma\downarrow})(\delta_{\tau\uparrow} - \delta_{\tau\downarrow})] + [n_q + m_{sq}(\delta_{\sigma\uparrow} - \delta_{\sigma\downarrow}) + m_{oq}(\delta_{\tau\uparrow} - \delta_{\tau\downarrow}) + m_{soq}(\delta_{\sigma\uparrow} - \delta_{\sigma\downarrow})(\delta_{\tau\uparrow} - \delta_{\tau\downarrow})]e^{i\mathbf{q}\cdot \mathbf{r}_i}/4, \right. \tag{2}
\]

where \( \mathbf{q} = (\pi, \pi) \) or \( (\pi, 0) \equiv \mathbf{Q} \), \( \mathbf{r}_i \) denotes the position of site \( i \), and \( n \) is the number of electrons per site. The order parameters are \( m_s, m_o, m_{so}, n_q, m_{sq}, m_{oq}, \) and \( m_{soq} \). We can explicitly express them by using Eq. (2). For example, \( m_o = \frac{1}{N} \sum_{i,\tau,\sigma,\alpha} \langle c_{i\tau\sigma}^\dagger \sigma^\alpha c_{i\tau\sigma} \rangle \) and \( m_{soq} = \frac{1}{N} \sum_{i,\tau,\sigma,\alpha} e^{i\mathbf{q}\cdot \mathbf{r}_i} \langle c_{i\tau\sigma}^\dagger \sigma^\alpha c_{i\tau\sigma} \rangle \), with \( \alpha = z \), where \( \sigma^\alpha \) is the Pauli matrix. We determine the lowest energy state among the solutions of the Hartree-Fock approximation. Although here we consider \( \alpha = z \) for the orbital state, we also considered order parameters with \( \alpha = x \) and \( y \). Then, we found that the \( z \)-component ordered state with \( \mathbf{q} = \mathbf{Q} = (\pi, 0) \) always has lower energy than the other ordered states within the parameter range we investigate here.

3. Result

Figure 1(a) shows \( U \) dependence of the order parameters \( m_o \) (for ferro-orbital order), \( m_{soQ} \) (for antiferromagnetic order), and \( m_{soQ} \) (for antiferro-spin-orbital order) at \( n = 2 \) and \( J = 0.1U \). We find that the other order parameters are zero. As shown in this figure, \( m_{soQ} \) jumps to a

![Figure 1](image-url)
small but finite value at $U/t \simeq 2.97$. At the same point, $m_o$ and $m_{so}Q$ also have jumps to finite values as shown in Fig. 1(b). Thus, the transition to the antiferromagnetic state is of first order. In the antiferromagnetic state with $q = Q = (\pi, 0)$, $x$ and $y$ directions are not equivalent and the occupations of $d_{zx}$ and $d_{yz}$ become different in general. Thus, the antiferromagnetic state is inevitably accompanied by ferro-orbital order, i.e., finite $m_o$. In the coexistent state of antiferromagnetism and ferro-orbital order, $m_{so}Q$ also becomes finite as shown in Fig. 1. Through the electron-lattice interaction, the ferro-orbital order should induce lattice distortion. The obtained small value of $m_o$ indicates such lattice distortion will be small, and is consistent with the observed weak lattice anomaly [13].

Figure 2 shows the band structure in the ordered state for several values of $U$ at $n = 2$ and $J = 0.1U$. For $U/t = 6$, band gaps open at some points at the Fermi level, while not on the lines $(0, 0)$-$(\pi/2, 0)$ and $(0, \pi)$-$(\pi/2, \pi)$. At $k_y = 0$ and $\pi$, the off-diagonal element $\epsilon_{k_x}$ in the kinetic energy term is zero, and $d_{zx}$ and $d_{yz}$ orbitals do not mix. The mean field in the ordered state mixes electrons with $k$ and $k + Q$ in the same orbitals, and $d_{zx}$- and $d_{yz}$-orbital states are not mixed even in the ordered state at $k_y = 0$ and $\pi$. The two bands crossing at around the Fermi level are different orbitals on both $(0, 0)$-$(\pi/2, 0)$ and $(0, \pi)$-$(\pi/2, \pi)$ lines, and a gap cannot open there. Thus, the system remains metallic even in the antiferromagnetic state as in experimental observations.

However, by increasing $U$, the band crossing points on $(0, 0)$-$(\pi/2, 0)$ and $(0, \pi)$-$(\pi/2, \pi)$ lines move to $(\pi/2, 0)$ and $(\pi/2, \pi)$, respectively, as shown in Fig. 2(b). By increasing $U$ further, the band crossing disappears as shown in Fig. 2(c), and finally a gap opens in whole the Brillouin

![Figure 2](image_url)

**Figure 2.** Band structure around the metal-insulator transition for $n = 2$ and $J = 0.1U$. The Fermi energy is set to be zero in these figures.
zone as shown in Fig. 2(d). The metal-insulator transition takes place at $U/t \simeq 6.7$ for $n = 2$ and $J = 0.1U$. This metal-insulator transition is a continuous transition and the order parameters show no anomaly at the transition as shown in Fig. 1(a). Note that the metal-insulator transition occurs even if the orbital order is not considered [17]. However, the antiferromagnetic state of Fe pnictides is still metallic, and thus, $U$ cannot be very large.

4. Summary

To summarize, we have shown that the antiferromagnetic order with ordering vector $(\pi, 0)$ accompanies ferro-orbital order. This ferro-orbital order should induce tetragonal to orthorhombic lattice distortion through the electron-lattice interaction. We have also shown that the system remains metallic even in the antiferromagnetic state as long as the Coulomb interaction is not very large. This feature is due to the multi-orbital nature characteristic to Fe pnictides. However, by increasing the Coulomb interaction, the system can become insulating, since the band structure changes. Thus, the Coulomb interaction in Fe pnictides has to be of moderate size.

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