FAST TRACK COMMUNICATION

The role of Hund’s coupling in the stabilization of the \((0, \pi)\) ordered spin density wave state within the minimal two-band model for iron pnictides

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Abstract
Spin wave excitations and the stability of the \((0, \pi)\) ordered spin density wave (SDW) state are investigated within the minimal two-band model for iron pnictides including a Hund’s coupling term. The SDW state is shown to be stable in two distinct doping regimes—for finite hole doping in the lower SDW band for small second-neighbour hoppings, and for low electron doping in the upper SDW band for comparable first-neighbour and second-neighbour hoppings. In both cases, Hund’s coupling strongly stabilizes the SDW state due to the generation of additional ferromagnetic spin couplings involving the inter-orbital part of the particle–hole propagator. The spin wave energies for the two-band model are very similar to the one-band \(t-t'\) Hubbard model results obtained earlier, and are in agreement with the findings from inelastic neutron scattering studies of iron pnictides.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Single-crystal neutron scattering studies of iron pnictides have indicated a commensurate magnetic ordering of iron moments ordered ferromagnetically in the \(b\) direction and antiferromagnetically in the \(a\) and \(c\) directions [1]. Inelastic neutron scattering measurements for \(\text{AFE}_3\text{As}_2\) \((\text{A} = \text{Ca}, \text{Ba}, \text{Sr})\) yield well-defined spin wave excitations up to the zone boundary on an energy scale \(\sim 200\ \text{meV}\) [2–4]. The realization of a \((0, \pi, \pi)\) ordered SDW state has opened the possibility of observing phenomena in this class of compounds which are characteristically associated with both the antiferromagnetic (AF) state—such as quantum spin fluctuations, hole/electron motion in an AF background, and spin fluctuation mediated pairing—and the metallic ferromagnetic (F) state—such as carrier induced spin interactions, correlation induced spin–charge coupling, and non-quasiparticle states.

A minimal two-band model consisting of two degenerate orbitals \(d_{xz}\) and \(d_{yz}\) per Fe ion on a two-dimensional square lattice [5] has been widely studied recently [6–11], in efforts to understand the magnetic ordering and excitations in doped iron pnictides. \textit{Ab initio} calculations [12] using the local density approximation suggest that the Fermi surface is determined by bands having mostly \(d_{xz}\) and \(d_{yz}\) character, as also indicated by polarized angle-resolved photoemission spectroscopy (ARPES) [13]. The hybridization of Fe 3d orbitals with themselves as well as through the As 3p orbitals lying above and below the square plaquettes formed by the Fe atoms leads to effective hopping parameters of the two-orbital model as shown schematically in figure 1.

However, the roles of inter-orbital exchange interaction (Hund’s coupling) in the spin wave energies and the stability of the \((0, \pi)\) ordered SDW state have not been investigated within the minimal two-band model. This study would also allow for...
and three dimensions was shown to be stabilized by the AF anisotropic intra-orbital hoppings as well as the carrier induced F spin couplings as in metallic asymmetric and peaked electronic spectral distribution due to Hund’s coupling is known to stabilize metallic ferromagnetism (compared with the one-band model results obtained earlier involving the two orbitals d_{x^2-y^2} and d_{yz} orbitals of interest for iron pnictides, with the four hopping terms $t_1−t_4$ as shown in figure 1. The inter-orbital density interaction term $V_{n_{1x},n_{2y}}$ has been dropped as it does not play any role in the magnetism up to the random phase approximation (RPA) considered here.

We consider the (0, $\pi$) ordered SDW state of the above two-band model, with F and AF spin orderings along the $x$ and $y$ directions, respectively. For the single-band model, this SDW state can be conveniently represented in a two-sublattice basis [14, 15]. Extending this approach to a composite two-orbital ($\alpha\beta$), two-sublattice (A B) basis, the Hartree–Fock (HF) level Hamiltonian matrix in this composite basis ($\alpha \alpha \beta \beta$) assumes the form

$$H^\alpha_\text{HF}(\mathbf{k}) = \begin{bmatrix} -\sigma \Delta_\alpha + \epsilon^{1x}_k & 0 & \epsilon^{2y}_k + \epsilon^{3y}_k & \epsilon^{4y}_k \\ 0 & -\sigma \Delta_\beta + \epsilon^{2x}_k & \epsilon^{4x}_k & \epsilon^{4y}_k \\ \epsilon^{2y}_k + \epsilon^{3y}_k & \epsilon^{4x}_k & -\sigma \Delta_\alpha + \epsilon^{1x}_k & 0 \\ \epsilon^{3y}_k & \epsilon^{4x}_k & \epsilon^{4y}_k & -\sigma \Delta_\beta + \epsilon^{2x}_k \end{bmatrix}$$

(2)

where $\alpha$ and $\beta$ refer to the $d_{x^2−y^2}$ and $d_{yz}$ orbitals, the band energies

$$\begin{align*}
\epsilon^{1x}_k &= -2t_1 \cos k_x \\
\epsilon^{2y}_k &= -2t_2 \cos k_x \\
\epsilon^{3y}_k &= -4t_3 \cos k_x \\
\epsilon^{4y}_k &= -4t_4 \cos k_x
\end{align*}$$

(3)

correspond to different hopping terms in different directions, and the self-consistently determined exchange fields are

$$2\Delta_\alpha = U_\alpha m_\alpha + J m_\beta \\
2\Delta_\beta = U_\beta m_\beta + J m_\alpha$$

(4)
in terms of the sublattice magnetizations $m_\alpha$ and $m_\beta$ for the two orbitals. For a given Fermi energy $E_F$, the sublattice magnetization $m_\mu$ for orbital $\mu$ was obtained from the corresponding electronic densities as

$$m_\mu = n^{\mu A}_1 - n^{\mu A}_2 = n^{\mu B}_1 - n^{\mu B}_2 = n^{\mu A}_1 - n^{\mu B}_1$$

$$= \sum_{\mathbf{k}l} \left( \phi^{\mu A}_{l\mathbf{k}t} \right)^2 - \left( \phi^{\mu B}_{l\mathbf{k}t} \right)^2 \theta(E_F - E_{k\mathbf{t}})$$

(5)

and hole (electron) doping was obtained as the deviation from 1 of the band filling (1/2) $\sum_{\mathbf{k}l} \theta(E_F - E_{k\mathbf{t}})$. Here $E_{k\mathbf{t}}$ and $\phi_{k\mathbf{t}}$ are the eigenvalues and eigenvectors of the Hamiltonian matrix (2), where the index $l$ refers to the four eigenvalue branches. Quantum corrections to sublattice magnetization resulting from inter-band spectral weight transfer due to electron–magnon interaction should contribute to the substantially reduced magnetic moment observed in iron pnictides.

It is instructive to consider two limiting cases which connect to the SDW state of the one-band model. When $t_1 = t_2 = t, t_3 = t'$, and $t_4 = 0$, the two orbitals in equation (2)
get decoupled and are also exactly degenerate as \( t_1 = t_2 \), and equation (2) identically reduces to the SDW state Hamiltonian for the one-band \( t'-t'' \) Hubbard model [15]:

\[
H_{\text{HF}}^{\sigma}(\mathbf{k}) = \begin{bmatrix}
-\sigma \Delta + \epsilon_{k} & \epsilon_{k}^x \\
\epsilon_{k}^x & \sigma \Delta + \epsilon_{k}'
\end{bmatrix}
\]

(6)

where \( \epsilon_{k}^{x(y)} = -2t \cos k_{x(y)} \) and \( \epsilon_{k}' = -4t' \cos k_x \cos k_y \).

In the more relevant limiting case \( t_1 = -t_2 = -t \), \( t_3 = -t' \), and \( t_4 = 0 \), although the two orbitals in equation (2) again get decoupled, they are no longer degenerate as \( t_1 \neq t_2 \). For the \( \beta \) orbital, although the off-diagonal terms have exactly opposite sign as compared to equation (6) for the one-band model due to the \( t_1, t_3 \) sign reversal, the energies and amplitudes remain unchanged due to energy band folding in the SDW state. For the \( \alpha \) orbital, the transformation \( k_x \rightarrow k_x + \pi \) cancels the effect of the \( t_1, t_3 \) sign reversal on both diagonal and off-diagonal terms, and again renders the SDW state identical to equation (6) for the one-band model.

The above equivalence also implies identical spin wave dispersion as for the one-band model. In the following, we will investigate the effects of finite band mixing term \( t_4 \) on the spin wave energies in the \((0, \pi)\) ordered SDW state.

3. Transverse spin fluctuations in the broken-symmetry state

In the random phase approximation, the transverse spin fluctuation propagator for the two-band model includes both \( U \) and \( J \) ladders, and hence retains its usual form:

\[
\tilde{\chi}_{\text{RPA}}^{ij}(\mathbf{q}, \omega) = \frac{\chi^{ij}(\mathbf{q}, \omega)}{1 - [U] \chi^{ij}(\mathbf{q}, \omega)}
\]

(7)

where the interaction matrix \([U]\) includes the Hund’s coupling term \( J \) as off-diagonal matrix elements, as given below (1). Spin wave energies were obtained approximately from poles of equation (7) in terms of the largest eigenvalue of the real part of \([U] \chi^{ij}\). The bare particle–hole propagator:

\[
\chi^{ij}(\mathbf{q}, \omega)_{ab} = \sum_{k, \sigma} \frac{\phi_{k \downarrow}^{a} \phi_{k \downarrow}^{b} \phi_{q-k \downarrow}^{b} \phi_{q-k \downarrow}^{a}}{E_{k \downarrow} - \epsilon_{k} - \omega - i\eta}
\]

(8)

is evaluated in the orbital–sublattice basis by integrating out the fermions in the \((0, \pi)\) ordered SDW state. Here \( E_{k\sigma} \) and \( \phi_{k\sigma} \) are the eigenvalues and eigenvectors of the Hamiltonian matrix \((2)\), the orbital–sublattice basis indices \( a, b \) run through \( 1–4 \), and \( l, m \) indicate the four eigenvalue branches. The superscripts \(+ (-)\) refer to particle (hole) energies above (below) the Fermi energy \( E_F \), and both inter-band and intra-band particle–hole terms are included.

The bare propagator \( [\chi^{ij}] \) has a finite imaginary part representing (low energy) intra-band and (high energy) inter-band particle–hole excitations, resulting in finite spin wave damping and linewidth even at the RPA level, as in metallic antiferromagnets [18]. The spin–charge coupling mechanism, relevant for metallic ferromagnets such as manganites, will also contribute due to the decay of spin waves into longer wavelength modes accompanied with internal charge excitations [19]. Indeed, this has been suggested from the absence of any steep increase in damping at higher energy indicative of a Stoner continuum [3]. From the observed high energy behaviour of the spin wave damping ascribed to particle–hole excitations [4], it has been inferred that the full excitation spectrum cannot be understood in terms of the local moment picture. Weakly damped spin waves near the ordering wavevector have been obtained within multiband models from the imaginary part of the spin fluctuation propagator [20–22].

Figure 2 shows the spin wave dispersion in the \((0, \pi)\) state of the two-band model, showing the stabilization of the F–AF state for small Hund’s coupling. For \( J = 0 \), the spin wave energy becomes negative for small \( q_x \) near the \( M \) and \( \Gamma \) points, indicating instability with respect to long wavelength spin twisting modes in the ferromagnetic ordering direction. Here, the hopping terms are \( t_1 = -1.0, t_2 = 1.0 \), and \( t_3 = t_4 = -0.3 \), the exchange field \( \Delta = 3.0 \), and the hole doping concentration \( x \approx 35\% \) at Fermi energy \( E_F \approx 2.5 \), for which the self-consistency condition (4) yields \( U + J \approx 11 \). Also shown is the single-band result obtained by simply setting \( t_4 = 0 \). We have set \( |t_1| = 1 \) as the unit of the energy scale, and the spin wave energies are shown for \( |t_1| = 200 \) meV.

Evidently, the electronic spectral function modification due to the band mixing term \( t_4 \) reduces the F spin couplings and destabilizes the F–AF state. The additional spin coupling \( J^2 [\chi^{0}\phi_{k\sigma}]^{bb} \) generated by Hund’s coupling due to the inter-orbital

![Figure 2. The spin wave dispersion obtained for the two-band model with Hund’s coupling \((J = U/4)\), without Hund’s coupling \((J = 0)\), and for the single-band case \((t_4 = 0)\). Here \( t_1 = t_4 = -0.3 \), and the hopping energy scale \(|t_1| = 200 \) meV.](image)
Figure 3. (a) Hole doping dependence of the spin wave dispersion for the two-band model with Hund’s coupling included. Here $t_3 = t_4 = -0.7$ and $\Delta = 2$. (b) Without Hund’s coupling ($J = 0$), the spin wave energies become negative over a larger part of the Brillouin zone.

Figure 4. (a) Spin wave energies for the two-band model with same hopping parameters as in [5], showing strong enhancement (suppression) in the F (AF) ordering direction with increasing electron doping $y$. (b) Spin wave energies are strongly enhanced when a small Hund’s coupling term is included.

component of the particle–hole propagator restores the stability of the F–AF state.

Figure 2 also shows that for small $t_4$, the overall structure of the spin wave dispersion for the two-band model, with Hund’s coupling included, is very close to that for the one-band model obtained earlier [15], with respect to anisotropic spin wave velocities, spin wave dispersion, and energy scale. Significantly, the spin wave dispersion clearly shows a maximum at $(\pi, \pi)$ in agreement with neutron scattering experiments [2–4].

For larger second-neighbour hoppings $t_3 = t_4 = -0.7$ and somewhat smaller exchange field $\Delta = 2$, the hole doping dependence of spin wave dispersion is shown in figure 3(a). The self-consistency condition yields $U + J \approx 8$ for $x = 20\%$ (at $E_F = -0.75$). While the peak spin wave energy in the AF direction is indeed enhanced, as expected from the stronger second-neighbour AF spin couplings generated, the F–AF state is evidently not robust with respect to fluctuations in the F ordering direction. For $x = 10\%$, the spin wave energy becomes negative near X and $M'$, indicating instability with respect to zone boundary modes, whereas at higher hole doping $x = 30\%$, the spin wave energy becomes negative near $\Gamma$ and $M$, indicating instability with respect to long wavelength modes.

For the relatively stable case at $x = 20\%$, the spin wave energies with and without Hund’s coupling are compared in figure 3(b). Again, Hund’s coupling is seen to play a crucial role in stabilizing the F–AF state, as indicated by the negative spin wave energies obtained for $J = 0$ over a larger part of the Brillouin zone.

Finally, we consider the set of hopping parameters $t_1 = -1.0$, $t_2 = 1.3$, $t_3 = t_4 = -0.85$, which yields circular electron and hole pockets near the bottom of the upper band [5]. At half-filling, the spin wave dispersion (figure 4(a), $y = 0$) is very similar to that derived for the single-band $t–t'$ model [14], for which the spin wave energy vanishes at the zone boundary in the ferromagnetic direction due to absence of any ferromagnetic spin coupling in the insulating state.

For low electron doping in the upper SDW band, finite F spin couplings are generated which further stabilize the F–AF state, as seen from the spin wave dispersion in figure 4(a). Here $\Delta = 3$ and a small Hund’s coupling has been included. The Fermi energies are in the range 1.3–2.6 for the electron dopings considered. At $y = 8\%$, the spin wave energy at the
F zone boundary X exceeds that at the AF zone boundary, as observed experimentally. The F–AF state is seen to be stable for very low electron doping, and becomes rapidly destabilized with increasing electron doping due to the suppression of AF spin couplings. This behaviour is in agreement with the observed rapid suppression of magnetic order in iron pnictides with electron doping (due to F substitution of O atoms in LaO1−xFexAs or Ni substitution of Fe atoms in BaFe2−xFexAs2) [24].

Notably, the spin wave dispersion, energy scale, and doping behaviour for the electron doped SDW state are all very similar to those of figure 2 for the hole doped SDW state as well as the single-band model. Evidently, it is the generation of the ferromagnetic spin couplings in all three cases which is the common crucial factor in stabilizing the (0, π) ordered SDW state. For Δ = 2, the SDW state effective gap ~400 meV is well above the maximum spin wave energy, which prevents spin wave excitations from rapidly decaying into a particle–hole continuum, as is indeed not observed experimentally up to energies of 200 meV.

4. Conclusions

Spin wave energies were obtained in the (0, π) ordered SDW state of the minimal two-band model for iron pnictides including the term for Hund’s coupling of the degenerate dxy and dxz Fe orbitals. Negative spin wave energies were taken as signalling instability of the (0, π) SDW state with respect to transverse spin fluctuations, indicating significantly weakened F or AF spin couplings. A robust (0, π) SDW state was found in two distinct doping regimes—finite hole doping in the lower SDW band for small second-neighbour hoppings (squarish electron/hole pockets), and low electron doping in the upper band for comparable hopping terms (circular electron/hole pockets).

In both cases, the Hund’s coupling term J was found to strongly stabilize the (0, π) SDW state due to the generation of additional ferromagnetic spin couplings J′[χ0|ux⟩|uy⟩] involving the inter-orbital part of the particle–hole propagator. Furthermore, the spin wave dispersion, energy scale, and doping behaviour were in both cases found to be very similar to those for the one-band model, which was ascribed to the carrier induced ferromagnetic spin couplings as the common crucial factor in stabilizing the (0, π) ordered SDW state. The emergence of F spin couplings at finite hole/electron doping results in a characteristic peak spin wave energy at (π, π), in agreement with neutron scattering experiments on iron pnictides, and also accounts for the large planar anisotropy observed between the AF and F spin couplings in the ab plane.

Evidence of Fermi surface folding associated with the SDW state has been observed in recent ARPES studies [23]. Electronic quasiparticle dispersion and spectral function renormalization in the (0, π) ordered SDW state due to electron–magnon interaction and multiple magnon emission–absorption processes should therefore be of interest.

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