Magnetic spectrum of the $J_1 - J_2$ model for pnictides

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Abstract. We calculate the magnetic excitation spectrum of the $J_1 - J_2$ model for iron pnictides within the framework of the nonlinear sigma model. We find, in addition to the usual acoustic spin-wave branch, a second, optical spin-wave branch, not captured by previous theoretical studies. We also find that the spin-wave velocity has a planar directional anisotropy, resulting from the collinear/striped structure of the antiferromagnetic ground state. Finally, we include single ion anisotropy, which fully gaps all branches, and we discuss the relevance of the modified, multi-branched, fully gapped character of the spectrum to the understanding of neutron scattering results for SrFe$_2$As$_2$

1. Introduction
The discovery of superconductivity above 50 K in RFeAsO$_{1-x}$F$_x$ (R = La, Ce, Sm, etc.) [1] brought the new iron-based pnictide compounds, including the MFe$_2$As$_2$ (M = Ba, Sr, etc.) family [2], into the class of the so called high-temperature superconductors. Like cuprates, pnictides also exhibit a layered spin density wave (SDW) ordered structure in the parent compound, which gives room to superconductivity upon doping [3]. From the theoretical point of view, the magnetism of the parent compounds could be, in principle, described in terms of localized magnetic moments at the Fe positions, interacting antiferromagnetically both via a superexchange $J_1$ between nearest Fe neighbors, Fe–Fe, and a second superexchange $J_2$ between As bridged next-to-nearest Fe neighbors, Fe–As–Fe [4]. Although an itinerant description in terms of band electrons, Fermi surface nesting, and spin-density-wave (SDW) instability, is also a good candidate for the understanding of the magnetism in iron pnictides [5, 6], in the following we shall adopt an effective description in terms of local moments.

2. The Model
Let us start by considering the $J_1 - J_2$ spin-Hamiltonian

$$\hat{H} = J_1 \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \hat{S}_i \cdot \hat{S}_j,$$

where $J_1 > 0$ and $J_2 > 0$ are, respectively, the antiferromagnetic superexchanges between nearest-neighbors, $\langle i, j \rangle$, and next-to-nearest neighbors, $\langle\langle i, j \rangle\rangle$, spins $\hat{S}_i$ on a two dimensional
square lattice. The existence of two superexchanges $J_1$ and $J_2$ in the spin Hamiltonian (1) renders the antiferromagnetism collinear, with wave vectors at $(\pi, 0)$ and/or $(0, \pi)$ [7]. This is in agreement with recent inelastic neutron scattering experiments in (Sr,Ba)Fe$_2$As$_2$ [7, 8], which exhibit clear peaks at the antiferromagnetic zone center $Q = (1, 0, 1)$, for energies between 5−15 meV. Such wave vector degeneracy in the classical ground state of the Hamiltonian (1) gives rise to an extra Ising symmetry [9, 10, 11], which is broken at a different temperature than the AF ordering one.

Previous linear spin wave studies of the $J_1 − J_2$ model have considered, as a starting point, a classical ground state with a two sublattice structure, and have obtained that the quantized magnetic spectrum would be composed by a single gapless spin-wave branch [12], with $\hbar \omega(k) \sim |k|$ for small wave vector $k$. The existence of such gapless mode reflects the full rotational invariance of the spin Hamiltonian (1) and is in agreement with Goldstone’s theorem. We shall refer to this branch as the acoustic branch. As we shall soon see, the actual four sublattice structure of the AF/Ising broken classical ground state, with two coupled, interpenetrating Néel ordered states, gives rise to a second, optical spin-wave branch.

For $J_2 \approx 2J_1$, as the experiments suggest, the ground state is a collinear antiferromagnet, composed by two coupled, interpenetrating Néel ordered states. Thus, we can spin spins in a coherent basis for each of these Néel states, which we shall label as $A$ and $B$, and we write

\[ \hat{S}_i^A = S \Omega_i^A = S \left[ e^{iQ \cdot \mathbf{n}_A} \mathbf{n}_A \sqrt{1 - \left( \frac{L_A}{s} \right)^2} + \mathbf{L}_A \right], \hat{S}_i^B = S \Omega_i^B = S \left[ e^{iQ \cdot \mathbf{n}_B} \mathbf{n}_B \sqrt{1 - \left( \frac{L_B}{s} \right)^2} + \mathbf{L}_A \right], \]

where $Q = (\pi/a, \pi/a)$ is the ordering wave vector for each Néel state, $\mathbf{n}_{A,B}$ and $\mathbf{L}_{A,B}$ are, respectively, the staggered and uniform components of the spins belonging to the two states, and $s = S/a^d$ is the density of spin in the unit cell. We use the fixed length constraint $\mathbf{n}_{A,B}^2 = 1$.

After integrating out the uniform (fast) components $\mathbf{L}_{A}$ and $\mathbf{L}_{B}$ of the spins we arrive at the action that describes the low-energy, long-wavelength fluctuations of the staggered (slow) order parameter $\mathbf{n}_{A,B}$ (as usual we use $\beta = 1/k_B T$)

\[ S(\mathbf{n}_A, \mathbf{n}_B) = \frac{\rho_s}{2\hbar} \int_0^{\hbar\beta} d\tau \int d^2x \left\{ |\nabla \mathbf{n}_A|^2 + |\nabla \mathbf{n}_B|^2 \right\} + \frac{1}{\xi^2} \left\{ |\partial_x \mathbf{n}_A|^2 + |\partial_x \mathbf{n}_B|^2 \right\} + \gamma \left( \mathbf{n}_A \cdot \partial_x \mathbf{n}_B + \mathbf{n}_B \cdot \partial_x \mathbf{n}_A \right) + \eta \mathbf{n}_A \cdot \mathbf{n}_B - \frac{1}{\xi^2} \left\{ (\mathbf{n}_A \cdot \mathbf{\partial}_x \mathbf{n}_B)(\partial_x \mathbf{n}_A \cdot \partial_x \mathbf{n}_B) − (\mathbf{n}_A \cdot \partial_x \mathbf{n}_B)\mathbf{n}_B \cdot \partial_x \mathbf{n}_A \right\}. \]

(2)

The first line contains the action for two nonlinear sigma models corresponding to the order parameters $\mathbf{n}_A, \mathbf{n}_B$. The second line contains their coupling, through $\gamma$, within the AF/Ising broken phase, where the term $\mathbf{n}_A \cdot \mathbf{n}_B$ is allowed (this model was derived explicitly for the $(\pi, 0)$ magnetic configuration, which breaks explicitly the Ising symmetry). For the Ising symmetric part of the phase diagram, such term would have been absent, but integration over fluctuations would give rise, instead, to a term like $(\mathbf{n}_A \cdot \mathbf{n}_B)^2$, which is Ising invariant [9]. Finally, the fourth line contains interacting dynamical terms that also arise from the integration over the uniform components.

All couplings in (2) are expressed in terms of the original parameters. The spin stiffness is $\rho_s = 2J_2 S^2 a^{2-d}$, the spin-wave velocity equals $c_0 = 2\sqrt{2} S a \sqrt{4J_2^2 − J_1^2}/\hbar$, we will also have a contribution from $c_1 = c_0(J_2/J_1)$, while the couplings between $\mathbf{n}_A$ and $\mathbf{n}_B$ are

\[ \gamma = \frac{2J_1}{J_2} \left( 1 + \frac{J_f^2/4}{4J_2^2 − J_1^2} \right) \quad \text{and} \quad \eta = \frac{2}{a^2} \left( \frac{J_1}{J_2} \right) \frac{J_f^2}{4J_2^2 − J_1^2}. \]

(3)

The bare values of the parameters described above are, as expected, higher than the measured values. For example, for $a = 5.695$ Å, $J_1 = 20$ meV, and $J_2 = 40$ meV, we find $\hbar c_0 = 1.2$ eV Å.
while the typical values are actually around 0.25 eV Å. For a theory like the one described by Eq. (2), which is highly interacting, a full renormalization procedure is required to reduce the values of all couplings. For now, and for the purposes of comparison with experiments in this letter, we shall use the already established values for some of these constants.

3. The Magnetic Spectrum

To find the magnetic excitation spectrum we look at the poles of the staggered spectral function, $A(k, \omega)$. Within the Green’s function formalism, these are obtained from the imaginary part of the retarded Green’s function, $G_{\text{ret}}(k, \omega)$, for transverse staggered fluctuations, usually denoted by $A(k, \omega) = -(1/\pi) \lim_{\delta \to 0} \text{Im}[G_{\text{ret}}(k, i\omega_n \to \omega + i\delta)]$, where $\omega_n = 2\pi n/\beta$ are the Matsubara frequencies. Thus, we consider a configuration such as $n_A = (\sigma_A, \pi_A^x, \pi_A^y)$ and $n_B = (\sigma_B, \pi_B^x, \pi_B^y)$, in which case the coefficient of the quadratic part in the transverse fluctuations, $(\pi_{A,B}^x)^2 G^{-1} \pi_{A,B}^y$, is written, in reciprocal space, as

$$G^{-1} = \begin{bmatrix}
\epsilon_0(k, \omega_n) & b\sigma_B \omega_n & -\epsilon_1(k, \omega_n) & -b\sigma_B \omega_n \\
b\sigma_B \omega_n & \epsilon_0(k, \omega_n) & b\sigma_A \omega_n & -\epsilon_1(k, \omega_n) \\
-\epsilon_1(k, \omega_n) & -b\sigma_A \omega_n & \epsilon_0(k, \omega_n) & b\sigma_A \omega_n \\
b\sigma_B \omega_n & -\epsilon_1(k, \omega_n) & -b\sigma_A \omega_n & \epsilon_0(k, \omega_n)
\end{bmatrix},$$

where

$$\epsilon_0(k, \omega_n) = k^2 + \frac{1}{c_0^2} \omega_n^2 + \frac{2i\hbar \lambda_{A,B}}{\rho_s}, \quad (4)$$
$$\epsilon_1(k, \omega_n) = \gamma k_x k_y + \frac{\sigma_A \sigma_B}{2c_0^2} \omega_n^2 - \frac{n}{2}, \quad (5)$$

Here $\lambda_{A,B}$ are the Lagrange multipliers for the fixed length constraint, while $\sigma_A$ and $\sigma_B$ are the renormalized order parameters of the two Néel ordered states.

The structure of the magnetic spectrum then follows from the zeroes of the determinant of the transverse propagator matrix, det $G = 0$, or simply

$$(\epsilon_0^2 - \epsilon_1^2)^2 - b^2 (\sigma_A + \sigma_B)^2 \omega_n^2 (\epsilon_0 - \epsilon_1)^2 = 0, \quad (6)$$

with $\epsilon_0$ and $\epsilon_1$ given by Eqs. (4) and (5), after the replacement $i\omega_n \to \omega$. The condition for stationary action determines the saddle point to be at $i\lambda_A = i\lambda_B = \eta \rho_s / 4\hbar$ and $\sigma_A = -\sigma_B = \sigma$.

The first set of poles correspond to

$$\hbar \omega(k) = \hbar c_{\text{SW}} \sqrt{k_x^2 + \gamma k_x k_y}, \quad (7)$$

where $\frac{1}{c_{\text{SW}}} = \left(\frac{1}{c_0^2} - \frac{\omega_n^2}{2c_0^2}\right)$. This is the usual acoustic spin-wave branch also found in linear spin wave theory [12], which is gapless at the zone center, $\hbar \omega(0) = 0$, in agreement with Goldstone’s theorem. Notice that the observable spin-wave velocity $c_{\text{SW}}$ increases by a factor $\sqrt{1 + \gamma}$ as one moves from the $k_y = 0$ (or $k_x = 0$) line to the $k_x = k_y$ direction (along the spin stripes), showing that the spin-wave dispersion has a planar directional anisotropy, see Fig. 1, a consequence of the collinear character of the antiferromagnetic order.

The second set of poles correspond to

$$\hbar \Omega(k) = \hbar c_{\text{op}} \sqrt{k_x^2 - \gamma k_x k_y + \eta}, \quad (8)$$

where $\frac{1}{c_{\text{op}}} = \left(\frac{1}{c_0^2} + \frac{\omega_n^2}{2c_0^2}\right)$. Here, instead, we find an optical gap, $\hbar \Omega(0) = \Delta_{\text{op}} \neq 0$, at the antiferromagnetic zone center (1, 0, 1), given by

$$\Delta_{\text{op}} = \hbar c_{\text{op}} \sqrt{\eta}, \quad (9)$$
which corresponds to long lived optical excitations. Notice now that the optical spin-wave
velocity along the \( k_x = k_y \) line decreases with respect to the \( k_y = 0 \) (or \( k_x = 0 \)) directions,
see Fig. 1, exactly the opposite from the case for the acoustic branch. The optical gap hardens
as \( J_1 \) increases, see inset in Fig. 1, and eventually diverges at \( J_1 = 2J_2 \), when the classical
configuration changes and the action (2) has to be modified.

4. Comparison with Experiments

In Fig. 1 we show our results for the magnon dispersion of the acoustic and optical modes, as a
function of momentum. As we can clearly see, the dispersion is anisotropic in both cases. We
also compare our results to neutron diffraction experiments from Ref. [7] in the right panel of
Fig. 1, where clearly a second magnon gaps is observed at higher energies, which becomes softer
as the temperature is increased.

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