Neutron polarization analysis as a probe of spin-orbital coupling in iron pnictide superconductors

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Phase diagrams of copper oxide and iron arsenide superconductors.

What are the effective exchange couplings in FeAs?

Localized magnets

La$_2$CuO$_4$

What about FeAs?

Coldea et al. PRL 86 5377 (2001)

Fermi surface nesting in metals

Exchange couplings between local moments

$J = 112$ meV
The effective of electron and hole doping?

The doping dependence of the phase diagram
Are there direct evidence for itinerant electron contribution to AF order in Ba122?
Wave vector dependence of spin-waves in BaFe$_2$As$_2$
Model calculation of spin-waves in BaFe$_2$As$_2$

$SJ1a = 59$ meV $SJ1b = -9$ meV $SJ2 = 13$ meV $SJ3 = 2$ meV,

Harriger, PRB 84, 054544(2011).
Evolution of spin-excitations in Ni-doped BaFe$_2$As$_2$
Electron doping evolution of spin excitations in \( \text{BaFe}_{2-x}\text{Ni}_x\text{As}_2 \)

Is there local moments in 10% Ni-doped Ba122 compounds?

Doping dependence of dynamic susceptibility in Ni-doped Ba122 compounds
For electron overdoped Ba122, a large spin gap opens near AF wave vector.
Comparison of spin excitations in optimally hole and electron doped Ba-122

How to estimate magnetic exchange energy?

\[ \Delta E_{ex}(T) = 2J (\langle S_{i+x} \cdot S_i \rangle_N - \langle S_{i+x} \cdot S_i \rangle_S) \]
Temperature dependence of the neutron spin resonance in (Ba,K)Fe$_2$As$_2$
Temperature dependence of the neutron spin resonance energy in (Ba,K)Fe$_2$As$_2$
Can changes in spin excitations account for the superconducting condensation energy?

\[ \Delta E_{ex}(T) = 2J(\langle S_{i+x} \cdot S_i \rangle_N - \langle S_{i+x} \cdot S_i \rangle_S) \]

\[ \langle \hat{S}_i \cdot \hat{S}_j \rangle = \frac{3}{\pi g^2 \mu_B^2} \int \frac{d\mathbf{q}^2}{(2\pi)^2} \int d\omega [1 + n(\omega, T)] \chi''(\mathbf{q}, \omega) \cos[\mathbf{q} \cdot (\mathbf{i} - \mathbf{j})], \]

\[ \frac{d^2 \sigma}{d\Omega dE} \frac{k_i}{k_f} = \frac{2(\gamma r_e)^2}{\pi g^2 \mu_B^2} |F(\mathbf{Q})|^2 [1 + n(\omega, T)] \chi''(\mathbf{q}, \omega), \]

\[ \Delta E_{ex} = -0.33 \text{ meV/Fe.} \]

\[ U_c = -17.3 \text{ J/mol} \]

\[ = -17.3 \frac{1 \text{ eV}}{1.6 \times 10^{-19}} \frac{1}{6.02 \times 10^{23} \text{ f.u.}} \]

\[ = -17.3 \frac{1 \text{ eV}}{1.6 \times 10^{-19}} \frac{2 \times 6.02 \times 10^{23}}{\text{Fe}} \]

\[ = -0.09 \text{ meV/Fe} \]
Neutron polarization analysis can conclusively identify the spin excitation anisotropy and longitudinal spin excitations in solids.
Neutron polarization analysis to sort out magnetic excitation anisotropy.

\[
\begin{align*}
\sigma_{x}^{SF} &= \frac{R}{R+1}(\sin^2 \theta M_a + \cos^2 \theta M_c) + \frac{R}{R+1} M_b + B, \\
\sigma_{y}^{SF} &= \frac{1}{R+1}(\sin^2 \theta M_a + \cos^2 \theta M_c) + \frac{R}{R+1} M_b + B, \\
\sigma_{z}^{SF} &= \frac{R}{R+1}(\sin^2 \theta M_a + \cos^2 \theta M_c) + \frac{1}{R+1} M_b + B
\end{align*}
\]
Spin nematic phase in electron-doped Ba122

(a) $T^*$ vs Ni doping $x$ with $x=0.096$

(b) Lattice distortion $\delta = (a_o - b_o) / (a_o + b_o)$

(c) $T^* = 70(10)$ K for $P = 0$ and $P > P_0$

(d) $T_C = 19.8$ K and $T_N = 33(2)$ K

Tet. PM
Ort.
C-AF
SC
Neutron polarization analysis to determine magnetic anisotropy in nearly optimally Ni-doped Ba122
Isotropic to anisotropic spin excitation transition in the paramagnetic tetragonal phase.
Spin anisotropy occurs in tetragonal phase with $\text{Ma}\sim\text{Mc}>\text{Mb}$

Final Messages

High-Tc superconductivity in iron pnictides has two important ingredients:
1. Need high-energy spin excitations to maintain large effective J.
2. Need low-energy itinerant electron-spin excitation coupling to have superconductivity.
3. There are strong evidence for spin-orbit coupling in the tetragonal phase of optimal Ba122, as seen in spin excitation anisotropy.
4. Similar anisotropy is also seen in the parent compound.