Spin Dynamics and Exchange Interactions in the A-type Antiferromagnetic State of $Pr_{0.5}Sr_{0.5}MnO_3$

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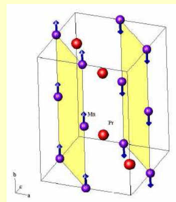
Motivation

•Layered A-type antiferromagnetic structure is realized in manganites with different type of orbital ordering and with different levels of hole doping.
Examples: undoped case - $LaMnO_3$ ($d_{3x^2-r^2}$ / $d_{3y^2-r^2}$) [ref. 1]
half-hole doped case - $PrSrMnO_3$ (CMR) ($d_{x^2-y^2}$)
(below the Nèel temperature 150 K)
•The motivation of this study is to understand the correlation between spin dynamics and orbital ordering in manganites.

Magnetic structure of $Pr_{0.5}Sr_{0.5}MnO_3$



Note that the ferromagnetic planes are rotated by 45 degree w. r. t. the crystal ab or bc planes.

Experimental setup

HB-3 thermal triple-axis spectrometer at HFIR

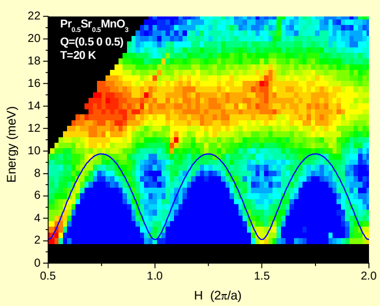
Instrument setup:
PG(002) monochromator
PG(002) analyzer
E_f = 13.7 meV
Collimation: 120'-40'-40'-120'
Energy transfer = 2 to 25 meV

• A single crystal of 2.5 gram was used in the Inelastic neutron scattering experiments.
• Most of the data were collected as the constant energy scans in the (h 0 h) or (h 0 3-h) scattering planes.

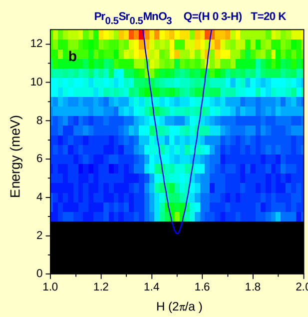
Results

a) Inelastic Neutron Scattering: Antiferromagnetic Spin Waves

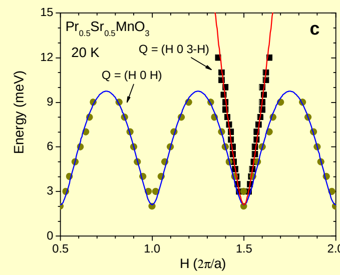
spin wave dispersion for Q perpendicular to the ferromagnetic planes



spin wave dispersion for Q parallel to the ferromagnetic planes

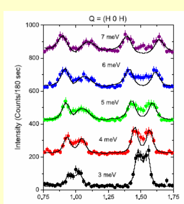


Highly anisotropic spin waves in the layered antiferromagnetic state

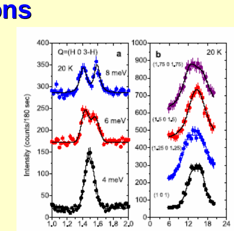


spin wave dispersion for Q parallel to the ferromagnetic planes is much steeper than the dispersion for Q perpendicular to the ferromagnetic planes. The solid lines are best fits by the spin wave dispersion of the 3D Heisenberg model with single ion isotropy. Strong crystal field excitations of Pr ions appear on top of the spin wave dispersion between 10 and 20 meV.

b) Constant energy scans show magnon excitations



Magnon excitations for Q along the antiferromagnetic direction (0.5 0 0.5)
Solid lines are best fits by the structure factor
(dominated by Mn sub-lattice)



a) Magnon excitations for Q parallel to the ferromagnetic planes (h 0 3-h). Solid lines are best fits by the structure factor (dominated by Mn sublattice)
b) Two crystal field excitations of Pr ions appear on top of the dispersion at 12.8 meV and 15.35 meV. Solid lines are the best fits by the structure factor
(dominated by the Pr sub-lattice)

c) *Spin wave analysis: dispersion of the 3D Heisenberg model with Single Ion Anisotropy*

Hamiltonian: $H = -J_f \sum_{ij \parallel planes} S_i \cdot S_j + J_a \sum_{ij \perp planes} S_i \cdot S_j - D \sum_i S_i^2$ [ref. 2 and ref. 3]

J_f is the in-plane ferromagnetic coupling, J_a is the out-of-plane antiferromagnetic coupling [ref. 3]

Spin wave dispersion: $h\omega(q) = 2S\,[\,\{2J_f(1-\gamma_{\parallel q}) + J_a + D/2\}^2 - \{J_a\,\gamma_{\perp q}\}^2\,]^{1/2}$

J_a = 3.07 meV
J_f = 5.83 meV
D = 0.15 meV is single-ion anisotropy energy
$\gamma_{\parallel q}$ and $\gamma \perp q$ are the spin wave structure factors

$$S(Q,\omega) = \Sigma_m A_m f_{Mn}^2(Q)\frac{\omega_m \Gamma_m (1+n(\omega_m,T))}{(\omega-\omega_m)^2+\Gamma_m^2} + \Sigma_p B_j f_{Pr}^2(Q)\frac{2\Gamma_p}{4\pi(\omega-\omega_p)^2+\Gamma_p^2}$$

is the dynamic structure factor [ref. 3]

Conclusions

•The ferromagnetic exchange interaction is nearly twice larger than the superexchange interaction.
•The hole doping mobilizes the e_g electrons and changes the type of orbital ordering in the half-doped manganite, and enhances the exchange interactions.
•The type of orbital ordering plays a role in the anisotropy of exchange interactions.

References: .

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3) V. V. Krishnamurthy, J. L. Robertson, R. S. Fishman, M. D. Lumsden, and J. F. Mitchell, submitted to Phys. Rev. Lett.