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To cite this version:
J. Cooke, J. Blackman. MAGNETIC EXCITATIONS IN TRANSITION METAL SYSTEMS. Journal de Physique Colloques, 1988, 49 (C8), pp.C8-81-C8-82. <10.1051/jphyscol:1988827>. <jpa-00228439>

HAL Id: jpa-00228439
https://hal.archives-ouvertes.fr/jpa-00228439
Submitted on 1 Jan 1988

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MAGNETIC EXCITATIONS IN TRANSITION METAL SYSTEMS

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Abstract. — An expression for the neutron scattering cross section based on itinerant electron theory within RPA has been derived which incorporates the most general form of the exchange matrix consistent with crystal symmetry. Numerical results indicate a wider range of spin-wave behavior than found previously.

The magnetic properties of transition metal systems are difficult to calculate because the electrons which produce the magnetism are itinerant and highly correlated. Regardless of the level of approximation of the many-body theory, there remains the difficult task of evaluating the relevant expressions which depend necessarily on electronic band structure. This complexity, however, can lead to unusual properties not found in local moment systems. For example, the existence of spin waves only over a part of the Brillouin zone, and "optic" spin wave modes which result from multi-band and multi-symmetry effects.

The prediction [1, 2] and subsequent observation [3, 4] of these as well as other effects indicates that itinerant theory provides an excellent description of the low temperature properties of transition metal ferromagnets. This is not to say that this description is exact. The prediction that the lower branch of the spin wave dispersion curve persists out to the Brillouin zone boundary along [100] in nickel [1] has not been confirmed experimentally. In addition, calculations based on local density theory [5] do not yield the "optic" spin wave branches which have been predicted by our theoretical approach and observed experimentally.

One of the most striking features of the predicted dispersion curves is that they exist to quite high energies along [100]; about 300 meV for nickel and 700 meV for iron. Experimental results obtained at these higher energies, however, may be more difficult to interpret because the spin-wave peaks are both smaller and broader and other contributions to the total magnetic scattering, such as the orbital term, could become important. It appears, therefore, that a calculation of the magnetic part of the total inelastic neutron scattering cross section on an absolute scale would not only provide a more general test of itinerant electron theory but could be useful in helping to interpret experimental data at these higher energies.

The magnetic cross section is generally segmented into a spin part, which is the sum of transverse and longitudinal terms, and an orbital part. The form of these terms is based on an expansion of the electronic wave function in terms of symmetry orbitals \( \phi_{\mu} \),

\[
\psi_{nk\sigma}(r) = \sum_{\mu} a_{n\mu\sigma}(k) \phi_{\mu}(r); \quad (1)
\]

where \( n, \sigma, \) and \( \mu \) are the band, spin, and symmetry indices, respectively. The results are given in terms of the following quantities:

\[
W_{\mu\nu\eta\xi}^\sigma(q, z) = \int \phi_{\mu}(r) \phi_{\nu}(r') V_{\sigma}(r, r') \times \phi_{\eta}(r') \phi_{\xi}(r) d^3 r d^3 r', \quad (2)
\]

\[
\Gamma_{\mu\nu\eta\xi}^\sigma(q, z) = \frac{1}{N} \sum_{nm} \frac{f_{nk\sigma} - f_{mk\nu\sigma'}}{z - E(mk + q\sigma') + E(nk\sigma)} a_{n\mu\sigma}(k)
\times a_{m\nu\sigma'}(k + q) a_{n\sigma\eta}(k) a_{m\xi\sigma'}(k + q), \quad (3)
\]

\[
F_{\mu\nu}^{(s)}(q) = \int \phi_{\mu}(r) e^{-i q \cdot r} \phi_{\nu}(r) d^3 r, \quad (4)
\]

\[
F_{\mu\nu}^{(o)}(q) = \int \tilde{\phi}_{\mu}(r) q \cdot p \phi_{\nu}(r) d^3 r, \quad (5)
\]

\[
\tilde{\Gamma}^\sigma_{\mu\nu\eta\xi}^{\sigma'}(q, z) = [I + \Gamma^\sigma_{\mu\nu\eta\xi}^{\sigma'}(q, z) W^*]^{-1} \Gamma^\sigma_{\mu\nu\eta\xi}^{\sigma'}(q, z). \quad (6)
\]

In these expressions \( V_{\sigma} \) is the screened coulomb interaction and \( p \) is the linear momentum operator. The transverse and longitudinal parts of the spin term are then given by

\[
\frac{d^2 \sigma}{d\omega dE'}|_{\text{TRANS}} = C_0 \text{Im} \left\{ \sum_{\mu\nu \eta\xi\sigma} F_{\mu\nu}^{(s)}(q) \tilde{\Gamma}_{\mu\nu\eta\xi \sigma}^{\sigma'}(q, z) F_{\eta\xi}^{(s)}(q) \right\}, \quad (7)
\]

\[
\frac{d^2 \sigma}{d\omega dE'}|_{\text{LONG}} = \frac{C_0}{2} \text{Im} \left\{ \sum_{\mu\nu \eta\xi\sigma} F_{\mu\nu}^{(s)}(q) \tilde{\Gamma}_{\mu\nu\eta\xi \sigma}^{\sigma'}(q, z) F_{\eta\xi}^{(s)}(q) \right\}.
\]

Article published online by EDP Sciences and available at http://dx.doi.org/10.1051/jphyscol:1988827
\[ m_\sigma \left[ I - \sum_g \langle \sigma, q, z \rangle V(q) \right]^{-1} \langle \sigma' \sigma' \rangle (q, z) V(q) \langle \sigma' \sigma' \rangle \langle \mu' \mu' \rangle F_{\mu' \mu'}^\sigma(q) m_\sigma \]

where \( m_\sigma = \pm 1 \) for spin up and down respectively, \( C_0 \) is a constant factor, and \( V(q) \) is the Fourier transform of the bare coulomb interaction. The expression for the orbital term is the same as the longitudinal term except for the overall factor, the replacement of the orbital for the spin form factor, and the replacement of \( m_\sigma \) by 1. The second term in the expression for the longitudinal (and orbit) contribution can be written in terms of the RPA dielectric function and therefore includes plasmon effects. Plasmon energies are, however, generally above the energy range considered here but the contributions from these terms could still be significant.

In this formalism the \( W_{\mu \nu \sigma \tau}^\sigma \) are treated as parameters. In previous work only the two parameters diagonal in the symmetry indices (\( e_g \) and \( t_2g \)) were retained [6]. It turns out that there are only ten independent d-symmetry parameters that are not related by symmetry. Two of these parameters are fixed by the spin-splitting energy which is obtained from the band calculation. Calculations of the transverse part of the cross section for arbitrary values of the eight independent parameters have revealed a wider variety of spin wave behavior than that obtained from the two parameter theory. Some of the results obtained from calculations along [100] based on bands generated from Slater-Koster parameters proposed by Callaway et al. [7] for nickel are shown in figure 1. In addition to the case where both branches persist out to the zone boundary, which was predicted previously, there are cases where one branch exists everywhere, one branch exists only over part of the zone, or only small portions of the upper branch exist over a limited region. These results are representative for a number of proposed band structures.

These results may help explain why only one spin wave branch was found in the local density calculation. Local density theory apparently generates exchange matrix elements which are consistent with the single branch case which is, of course, inconsistent with experiment. The results obtained thus far do not, however, yield a case where the lower branch dies out before reaching the zone boundary. It is possible that changes in the band structure could produce this result and this is currently being pursued. Another possibility is experimental in origin. Because of finite resolution the scattering cross section may depend significantly on what happens off the symmetry line in a region where the dispersion curve is highly anisotropic. Calculations off the symmetry line require large amounts of computer time and work is underway to develop methods for carrying out a systematic study of this possibility.

Fig. 1. – Spin wave energy for nickel along [100] for various choices of the \( W^\sigma \) parameters. These results are illustrative of the type of behavior that has been found.

Calculations of the non-interacting part \( (W^\sigma = 0) \) of the first term in the expression for the longitudinal (Eq. (8)) and orbit terms indicate that longitudinal terms is small and the orbit term is larger than the transverse term over a broad range of energy and wave vector in the higher energy range. In addition, both the spin and orbit terms exhibit considerable structure which can be correlated with the electronic energy bands. Inclusion of the spin wave and plasmon enhancement factors could, of course, alter these results.

Acknowledgments

This research was sponsored by the Division of Materials Sciences, U.S. Department of Energy under contract DE-AC05-840R21400 with Martin Marietta Energy Systems, Inc.