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The investigation of Neutron Scattering In Spin Waves Theory of Ferromagnetic Crystals

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ABSTRACT

Inelastic neutron scattering, probing the temporal spin-spin correlation at the different microscopic scale, is a powerful technique to study the magnetic behaviour of ferromagnetic crystals. In addition, high penetration power of neutron in samples has made it as a useful way for spin-spin interaction in neutron scattering. Changes in the magnetic cross section in term of different energy transfer and temperatures are calculated for nickel and iron as transition metals in Heisenberg model versus spin wave theory by considering atomic form factor. Finally, the effect of magnetic structure and behaviour of crystal in measuring cross-section shows that increasing temperature results in the Cross-section increase Also, the existence of propagating spin waves below Tc is compared in Ni and Fe in different momentum transfers. The relation of spin wave energy with temperature dependence of nickel has created different behaviour in the changes of cross section rather than iron.

| scattering cross section | Heisenberg model | spin waves | form factor | magnons |

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1. INTRODUCTION

Quantum Heisenberg magnetic models are famous for defining ferromagnetic metals. The perception of spin wave theory or magnons is so useful that most experiments is explained by spin wave or magnon theory [1]. Also, neutron scattering is a unique technique to probe the magnon spectrum of propagating spin waves. Since some other researcher tried to consider itinerant-electron model of ferromagnetism for transition elements, in this research, we consider Heisenberg model for an electronic state for nickel and iron which is localized in real space. The effects of neutron scattering from these kinds of ferromagnetism in a localized system are investigated. Moreover, Physical spin wave theories are limited below temperature and it is necessary to treat the unphysical states in higher temperature. Nevertheless, without regard to this fact, inelastic neutron scattering has been used to investigate the temperature dependence of cross section from 0 to above Curie temperature in nickel and iron. Also, we have measured the ferromagnetic scattering for scattering vector (κ) for nickel and iron and by considering appropriated interval for each of them; we investigate cross section changes versus scattering vector.

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2. EXPERIMENTAL

2.1 Materials, method and instruments

The Heisenberg Hamiltonian for a ferromagnetic system is

$$-H = \sum_{l,l'} J\left(l \quad l'\right)\hat{s}_l \cdot \hat{s}_{l'} \ , \tag{1}$$

Is the exchange parameter between spins situated at the Bravais lattice sites and is defined such that. The energy of a spin wave is quantized and the unit of energy of a spin wave is called a magnon. There will be a series of such waves and each spin wave will possess a wavelength and quantized energy and the wave vector q are given the dispersion relation. For a ferromagnetic linear chain with nearest neighbour interaction this relation is given by

$$\hbar\omega_q = 4Js\left(1-\cos qa\right) \ , \tag{2}$$

Due to the long wavelength for this system, we consider localized model for Heisenberg ferromagnetism. Total z-component of spin commute with H. Therefore, regarding scattering cross-section in (1), scattering cross-section of system contains only the longitudinal term and the transverse. Of course, at low temperature longitudinal term gives elastic scattering. Therefore, one magnon creation and annihilation are made because of transverse term, which means it gives rise to inelastic scattering. So, Heisenberg Hamiltonian become

$$H = -\sum_{l,l'} J(l-l')\left\{\hat{s}_l^z \hat{s}_{l'}^z + \hat{s}_l^+ \hat{s}_{l'}^-\right\}, \tag{3}$$

Also, for a Bravious lattice, the generalized scattering cross section can be written as

$$\left(\frac{d^2\sigma}{d\Omega dE}\right) = r_0^2 k'/k\left(\frac{1}{2}gf(\kappa)\right)^2 e^{-2w(\kappa)}\left(\delta_{\alpha\beta} - \hat{\kappa}_\alpha\hat{\kappa}_\beta\right)\times$$
$$\sum \exp\{i\kappa.(l-l')\}\frac{1}{2\pi\hbar}\int\left\langle \hat{s}_l^\alpha \hat{s}_{l'}^\beta(t)\right\rangle \exp(-i\omega t)dt,$$

The evaluation of correlation function $\langle \hat{s}_l^+ \hat{s}_l^- \rangle$ can be written:

$$<\hat{s}_l^+ \hat{s}_{l'}^-(t)> = 1/N^2 \sum_q e^{iq.(l'-l)} <\hat{s}_q^+ \hat{s}_q^-(t)> =$$
$$2S/N \sum_q e^{-iq.(l'-l)+i\omega_q t}(1+n_q), \tag{5}$$

$$<\hat{s}_l^- \hat{s}_l^+(t)> = 1/N^2 \sum_q e^{iq.(l'-l)} <\hat{s}_q^- \hat{s}_q^+> \tag{6}$$

Where

$$n_q = \frac{1}{e^{\hbar\omega_q\beta} - 1}, \tag{7}$$

n_q is the magnon occupancy for annihilation and creation magnon. Also, n_q shows occupation number of magnon in scattering process, which possesses wave vector q. From equation (4), (5) and (6) the transverse cross section inelastic neutron scattering for annihilation and creation magnon is given by master formulas:

$$\left(\frac{d^2\sigma}{d\Omega dE}\right)^+ = r_0^2 k'/k\left(\frac{1}{2}gf(\kappa)\right)^2 e^{-2w(\kappa)}\left(1+k_z^2\right)\times\frac{1}{2}s\times(2\pi)^3/v_0$$
$$\times\sum_{\tau,q}\left(n_q+1\right)\delta\left(E-\hbar\omega_q\right)\delta\left(\kappa-q-\tau\right),$$

$$\left(\frac{d^2\sigma}{d\Omega dE}\right)^- = r_0^2 k'/k\left(\frac{1}{2}gf(\kappa)\right)^2 e^{-2w(\kappa)}\left(1+k_z^2\right)\frac{1}{2}s\times(2\pi)^3/v_0$$
$$\sum_{\tau,q} n_q\delta\left(E+\hbar\omega_q\right)\delta\left(\kappa+q-\tau\right),$$

In both formulas for the cross-section contain momentum and energy conservation condition. Also, the nature of the interaction between the spin of neutron and the spin of the electrons gives rise to the orientation factor $(1+\tilde{\kappa}_z^2)$ in (8), r_0 the classical electron radius the scattering vector $\boldsymbol{\kappa}= k_i - k_f$ and energy transfer $h\omega = E_i - E_f$ and $k_{i(f)}$ incident (scattered) neutron energy and wave vector, respectively. The magnetic form factor is denoted by $f(\boldsymbol{\kappa})$ which is defined by:

$$f(\kappa) = g_S/g\left\langle J_0\right\rangle + g_l/g\left(\left\langle J_0\right\rangle + \left\langle J_2\right\rangle\right), \tag{9}$$

Where J_0 and J_2 are spherical Bessel function, and g_s, g_l and g are the Lande factor.

3. RESULTS & DISCUSSION

We consider atomic form factor (2) for Fe as a ferromagnetism which is transition element with a $3d^6$electronic configuration. Also gl=1/2, gs=1, s=2 and l=2 [2].The total cross section change is plotted versus the scattering vector (momentum transfer) in three different Temperatures for iron in fig.1. Cross section for any temperature is well-behaved inwhole scattering vector region. It shows neutron inelastic scattering patterns for Fe with increasing scattering vector, the cross section decreases. Therefore, the diminished scattered neutron number causes to decrease the probability of reaction as inelastic. Also the cross section is very important except for the scattering vector interval 1.2-1.3 fm^{-1} when the magnetic scattering is weak at high scattering vector in fig.1. generally, there will be uncorrelated spin waves in this scattering interval for iron.

General temperature dependence of the total cross section is shown in Fig.2. As can be seen, with increasing temperature, cross section increased too. With increasing temperature long-term magnetism breaks down and magnon occupancy n_q is increased[3,4]. So, the sharp spin waves found at low temperature broaden as the temperature is increased. Therefore, with increasing magnon number, neutron scattering from spin waves increase even though, the ferromagnetic spin waves is uncorrelated . large temperature dependence of cross section at high temperature is clearly shown in Fig.2.

As can be seen in Fig.3, The general behaviour is similar to that found for iron. Nevertheless, the scattering vector dependence of cross section is larger than Fe [4]. It can be related d-band structure of nickel as well as scattering vector dependence of nickel form factor is larger than iron. Also, electronic configuration of nickel as a transition element is $3d^8$ with gl=1/2, gs=1, s=1 and l=3.

Also, magnetic scattering cross section tends to zero at $2fm^{-1}$ for nickel, whereas it is $1.3fm^{-1}$ for iron. As a result, the decrease of magnetic scattering for Fe is steeper than Ni. Therefore, as can been seen in fig.4. the smaller magnetic moment and the larger stiffness constant for Ni propagation correlated spin waves are observed in larger scattering vector interval in about 0.2Tc.

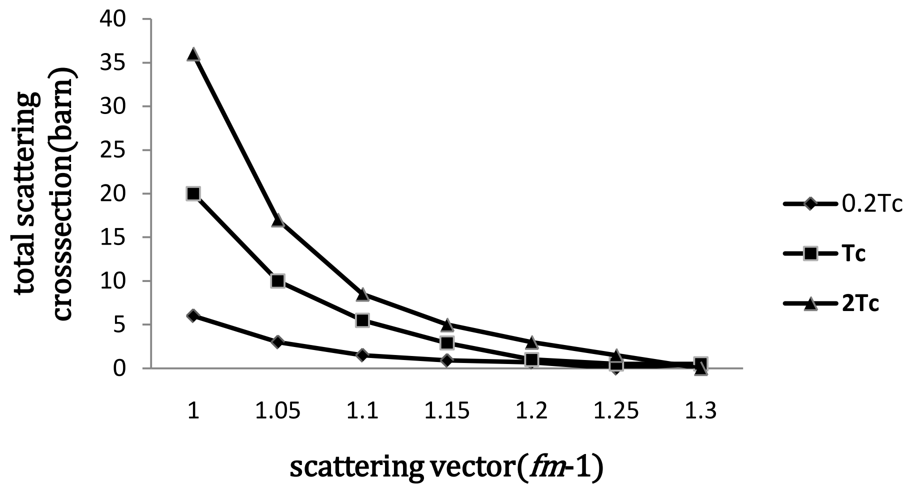

Fig. 1 The changes of total magnetic cross-section in terms of wave vector k in two different temperature in Fe

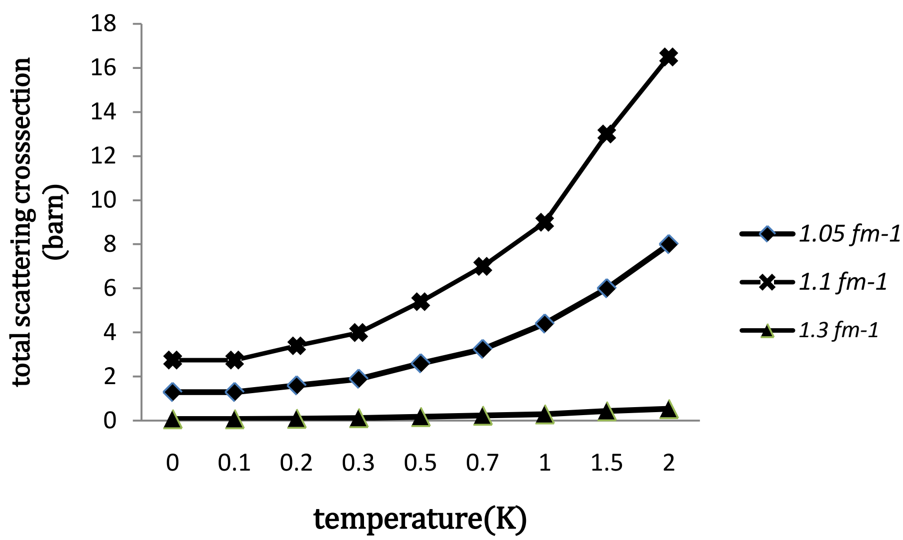

Fig. 2 the total magnetic cross section changes curves for Fe as a function of reduced temperature T/Tc in three different scattering vectors.

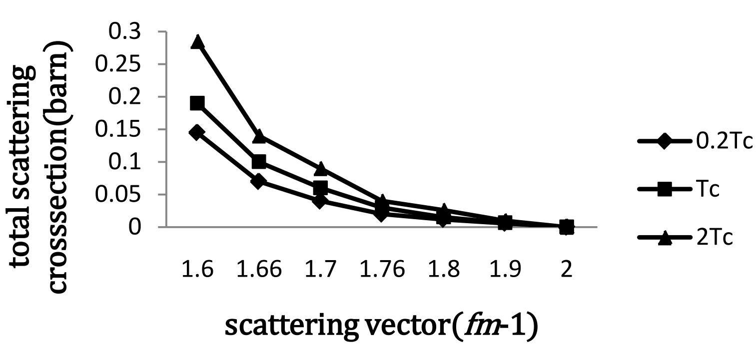

Fig. 3 Scattering vector dependence of cross section in three different temperatures for Ni

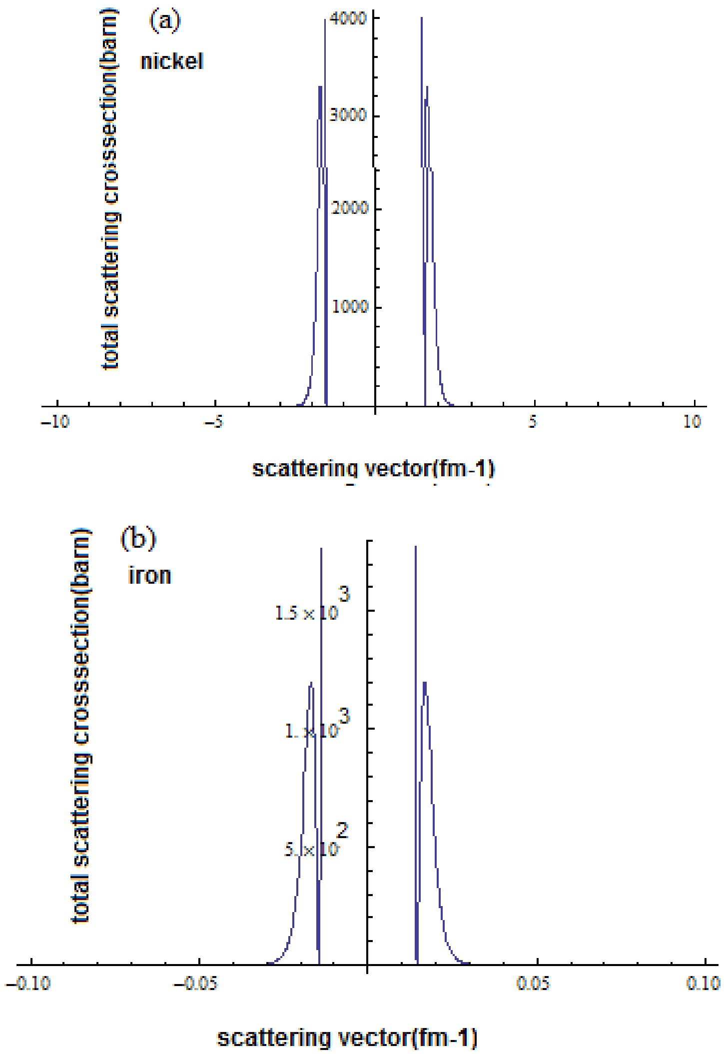

Fig.4 (a) and **(b)**, magnetic cross section as correlated spin waves in Ni and Fe at 0.2 Tc

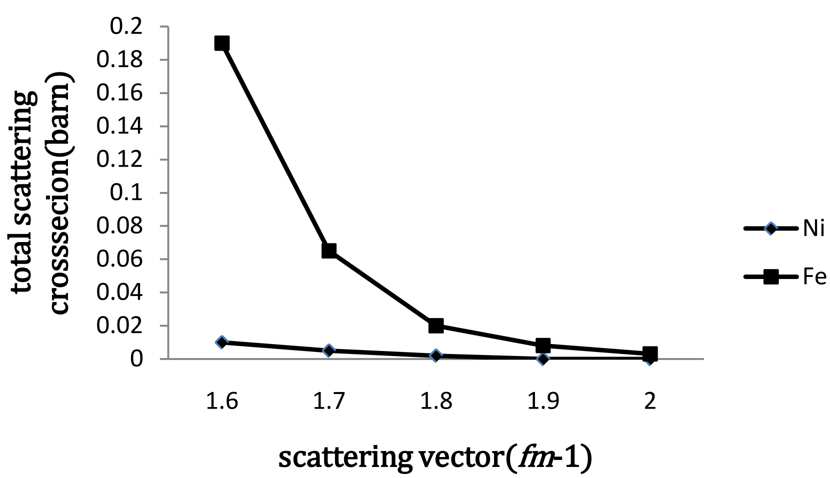

Fig.5. scattering vector dependence of magnetic cross section at T_c for iron and nickel

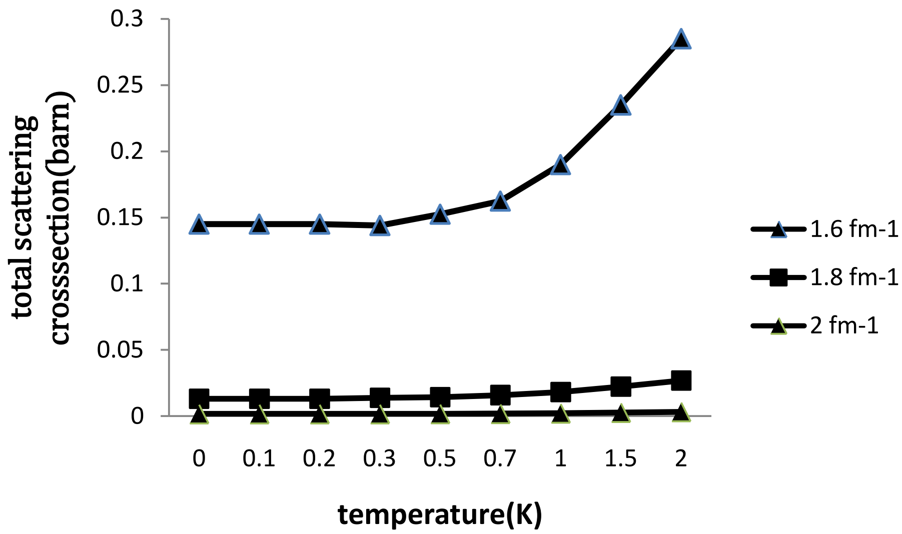

Fig.6.magnetic cross section changes in terms of temperature for Ni at three different scattering vector.

Fig.5. shows the comparison of cross section changes in terms of scattering vector for iron and nickel. iron differs from nickel by a steeper changes in a defined scattering vector interval. Moreover, the maximum obtained cross section for nickel is 0.02 barn in 1.6fm-1 whereas it is 0.2barn for iron, the results show the weak magnetic scattering from nickel spin waves.

Cross section changes are as monotonic function of temperature in whole scattering vector region which is displayed in Fig.5. as can be seen, temperature dependence of cross section at low temperature is less than iron because of high spin waves energies at low temperature for nickel [5,6,7]. So, less increase magnon number with increasing temperature for nickel causes temperature dependence of magnon occupancy to become less at low less at low temperature rather than iron.

Another important feature of fig.**6**. is the very weak response of nickel at scattering vector 1.8 fm^{-1} and 2fm^{-1}. So, it is understandable in the vicinity of the minimum value of scattering vector, the slope of curve is greater than near high scattering vector and consequently with increasing scattering vector temperature effects become less on increasing of magnetic cross section because with increasing scattering vector spin waves energies decrease.

4. CONCLUSION

Calculation of the below, at and above Curie temperature neutron scattering for ferromagnetic material like nickel and iron have revealed cross section changes versus temperature and scattering vector. These results have led to a new pictures of neutron scattering behaviour in transition metal in Heisenberg model, one in which with increasing scattering vector, cross section decreases and with increasing temperature, cross section increases. Although cross section changes in terms of scattering vector is plotted at related interval of scattering vector for iron and nickel, they have the same general behaviour in whole scattering vector region. Moreover temperature dependence of scattering cross section from nickel at low temperature is less than iron. In this research we see that neutron scattering can provide good tests of models for Heisenberg ferromagnetism. Supplementary calculation on paramagnetic crystal showed that the scattering cross section is proportional with temperature means with increasing temperature , the scattering cross section decreases then this result can be used to distinguish ferromagnetic from paramagnetic crystal. Also, The effect of temperature on scattering cross section of an unknown crystal can be used for distinguish kind of crystals .

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