SPIN FLUCTUATIONS IN PARAMAGNETIC NICKEL
P. Rusek, J. Callaway

To cite this version:
P. Rusek, J. Callaway. SPIN FLUCTUATIONS IN PARAMAGNETIC NICKEL. Journal de Physique Colloques, 1988, 49 (C8), pp.C8-53-C8-54. <10.1051/jphyscol:1988813>. <jpa-00228274>

HAL Id: jpa-00228274
https://hal.archives-ouvertes.fr/jpa-00228274
Submitted on 1 Jan 1988

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
SPIN FLUCTUATIONS IN PARAMAGNETIC NICKEL

P. Rusek (1) and J. Callaway (2)

(1) Institute of Physics, Technical University, 50-370 Wroclaw, Poland
(2) Department of Physics and Astronomy, Louisiana State University Baton Rouge, LA 70803-4001, U.S.A.

Abstract. - The temperature dependence of the cross section for inelastic magnetic scattering of neutrons in constant-q scan has been studied using results of renormalization group theory. The temperature behaviour of the peak in the cross section and its width are in good agreement with the results of computation of the cross section for paramagnetic Ni using acurate energy bands.

The spin fluctuations above Curie temperature in 3d ferromagnetic metals are still unresolved problem. Experimentally those fluctuations have been widely studied by means of inelastic neutron scattering (usually Fe and Ni are used in such experiments) [1, 2].

The cross section for scattering of neutron in the constant-energy scan has well defined peak in paramagnetic phase, which dispersion law is similar to dispersion of spin waves below $T_c$. It has been interpreted as the propagating spin excitations above $T_c$. The persistance of spin waves into paramagnetic phase in ferromagnetic metals predicts Moriya's theory [3] and they naturally appear in paramagnetic phase in the local band theories [4]. However, relatively large half-width of this peak, the absence of any peak in cross section above $T_c$ and possibility to derive it using dynamic scaling arguments [5] suggest that this peak should be ascribed to the conservation law of magnetic moment rather than to spin wave like excitations.

The experimental results in constant-q scan for large momentum transfer $q (q \geq 0.3 \text{ Å}^{-1}$ for Ni) are controversial. There are measurements which indicate existence of the peak in cross section above $T_c$ for relatively large $q$ vector ($q \geq 0.3 \text{ Å}^{-1}$ for Ni at $T = 650 \text{ K}$) [2] but in other measurements [1] no peak has been found.

In view of those controversies the computer calculation of cross section in constant-q scan has been especially desired. It gives possibilities to study system in controversial range of parameters.

In our previous papers [6] we reported results of computation of neutron scattering cross section, in constant-q scan for Ni in paramagnetic phase using accurate energy bands. The calculations were based on computation of the dynamical susceptibility $\chi(q, \omega)$ which is straightforward related to the scattering function $S_q(q, \omega)$ that is proportional to the neutron cross section.

$$S_q(q, \omega) = \frac{2}{(1 - e^{-\omega/kT})} \text{Im} \omega(q, \omega) = 2\chi(q)\omega(1 - e^{-\omega/kT})^{-1} F(q, \omega),$$

where $F(q, \omega)$ is the spectral weight function. The dynamical susceptibility $\chi(q, \omega)$ of ferromagnetic metals can be written as

$$\chi(q, \omega) = \chi_{\text{0}}(q, \omega)[1 - I_{\text{ef}}(q, \omega)\chi_{\text{0}}(q, \omega)]^{-1}.$$

Here $\chi_{\text{0}}(q, \omega)$ is susceptibility of free electrons and $I_{\text{ef}}(q, \omega)$ describes correlations between spin fluctuations. In RPA $I_{\text{ef}}(q, \omega) \rightarrow I$ where $I$ is Coulomb integral. To evaluate the temperature dependence of $I_{\text{ef}}$ the dynamical susceptibility $\chi(q, \omega)$ was calculated in the approximation in which the vertex part of $\chi(q, \omega)$, $\Gamma(q, \omega)$ was approximated by two full dressed spin-triplet scattering amplitude. That approximation is justified for temperatures not too far from $T_c$. It has been found that $I_{\text{ef}} \sim T^{4/3}$ [7] and consequently the Curie-Weiss law is satisfied by $\chi(0, 0)$. With that temperature dependence of $I_{\text{ef}}$ the scattering function $S_q(q, \omega)$ was computed for several $q$ and wide range of temperatures.

At $T = 1.03 T_c$ (for Ni $T_c = 631 \text{ K}$), for large momentum transfer $q \geq 0.31 \text{ Å}^{-1}$, there is peak in the cross section for non zero energy transfer $\omega$. With increasing $q$ this peak shifts to higher energy, it becomes better defined and over a substantial range of $q$ its width is proportional to $q^{2.5}$. Its position and width is well described by critical dynamics but its detail structure depends on the energy bands structure of Ni. As temperature increases from 1.03 $T_c$ to 1.5 $T_c$ the peak shifts to higher energy and its width increases. However, temperature dependence of the width is stronger than temperature dependence of the peak position. The same behaviour of the position of the cross section maximum and its width is observed in constant-energy scan. This peak can not be interpreted in terms of propagating spin excitations due to its relatively large width compare to its position. Moreover, that peak is not accompanied by any peak in Im $\chi(q, \omega)$.

In this note we explain the temperature dependence of the cross section for magnetic scattering of neutrons in constant-q scan applying the results of renorma-
tion group theory. According to the dynamic scaling hypothesis the spectral function $F(q, \omega)$ has the form

$$\phi \left( \frac{\omega}{\omega_c}, q \xi \right)$$

for sufficient small arguments, where characteristic frequency scales as $\omega_c(q, \xi) = Aq^{2-\delta} \Omega(q \xi)$. The correlation length $\xi = \xi_0(T / T_c - 1)^{-\nu}$ (for Ni $\xi_0 = 0.62 \, \AA$, $\nu = 0.7$) is decreasing function of temperature. In the region where the dynamic scaling works $\omega \ll kT$ the detail balance factor $\frac{\omega}{kT} \approx 1$ and consequently we may expect the same temperature dependence of the peak position and the half-width of $F(q, \omega)$. In the region where the dynamic scaling works $\omega \ll kT$ the detail balance factor $\frac{\omega}{kT} \approx 1$ and consequently we may expect the same temperature dependence of the peak position and the half-width because the peak position and the half-width scale in the same manner. Moreover, in the region of $q \xi$ which is considered the scaling function $\Omega(x)$ increases as a result of the deep minimum in $\Omega(x)$ [7]. Therefore the peak position and the width should decrease with temperature. Those discrepancies with results of out computations can be removed in the frame of renormalization group theory.

In an experiment and in our computation $\omega / kT$ varies in the range 0.2-0.9 and thus in that case the detail balance factor is important [9, 10]. We have assumed that in that range of $\omega / kT$ the spectral function fulfills scaling law $F(q, \omega) \sim \phi \left( \frac{\omega}{\omega_c}, q \xi \right)$ but we remained in scattering function (1) the exact form of detail balance factor. The shape function $\phi(s, x)$ for arbitrary $q$, $\omega$ and $T - T_c$ calculated in the first order in $\epsilon = 6 - d$ has the form [11]

$$\phi(s, x) = 2 \text{Re} \times \left( -is + f(x) \pi (x, isf(x)(1 + x^{-2})) \right)^{-1}, \quad (2)$$

with

$$\pi(x, iw) = \left[ \left( 1 + \frac{3.16}{x^2} \right)^{5/4} - 0.46 iw \right]^{3/5},$$

and

$$f(x) = [1 - 0.51 \arctan (0.46 (1 + x^{-2}) \times \left( 1 + 3.16 x^{-2} \right)^{-1})]^{-1} \left( 1 + 3.16 x^{-2} \right)^{-3/4},$$

and the scaling function $\Omega(x)$ is well approximated by

$$\left( 1 + x^{-2} \right) \left( 1 + 3.16 x^{-2} \right)^{-3/4}. \quad (3)$$

The functions (2) and (3) satisfy asymptotic scaling law and they are in good agreement with experiment [6, 12], despite the fact that they were calculated far from real dimension.

We carried out calculation of cross section (1) in constant-$q$ scan with the shape function (2) in temperatures range of $1.03 T_c - 1.5 T_c$ and in $q$ range of $0.31 - 0.57 \, \AA^{-1}$. The temperature dependence of the peak position and the half-width at $q = 0.46 \, \AA^{-1}$ is shown in figure 1.

The shape function $\phi(s, x)$ does not have peak for finite $s$ for any $(x \epsilon)$, however the cross section (1) does. It originates from competition of detail balance factor and the shape function. Asymmetry in cross section for $\omega \rightarrow -\omega$, which is introduced by detail balance factor, is less than 10% in the range of $s$ and $x$ which are considered. It is remarkable the weak temperature dependence of the peak position, relatively stronger temperature dependence of the half-width and they monotonically increase with temperature. Those effects are due to temperature dependence not only the with but the shape function also. $\phi(s, x)$ changes from non-Lorentzian in critical region i.e. $x \rightarrow \infty$ to a Lorentzian in the hydrodynamic region $x \rightarrow 0$. For the peak position the change with temperature in width is compensated by the change of shape. The similar temperature behaviour of peak position and its width is observed in experiment in constant-energy scan [9].