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Neutron Scattering Study of MnSi Proving No "Exchange Hole"

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ABSTRACT

Neutron scattering experiments have been performed in MnSi below T_C with the double-axis powder scattering technique using unpolarized neutrons, and also with the polarization analysis technique. The magnetic scattering intensity has not shown any anomaly around $q = 0.5$ $Å^{-1}$, in contrast to the previous results of Ziebeck et al. who found a large intensity peak at this momentum transfer. Thus the hypothesis of Ziebeck et al. of observing an "Exchange Hole" is excluded.

Among many different ferromagnetic materials, MnSi belongs to a class where the magnetism is governed by the itinerant 3-d electrons . Below T_c = 29.5 K, this material orders magnetically with a long helical spiral period of 175 Å in zero external field but becomes ferromagnetic in an applied external field $H_{ext} > 7$ kG,. In an earlier neutron scattering measurement below T_c at T = 5K in H_{ext} = 10 kG, Ishikawa et al. found a clear spin wave excitation followed by a broader intensity maximum in the Stoner-continuum extending along the spin wave dispersion line $E = \hbar\omega = Dq^2$, where D = 50 meV.Å^2. No magnetic scattering in any other part of the ω-q plane was found. Recently at Grenoble, Ziebeck et al.[3] developed a method to measure the energy-integrated magnetic scattering intensity of polarized neutrons, and applied it to MnSi.[3] Below T_c at T = 11 K in $H_{ext} \sim 0$, they found a clear maximum of the diffuse magnetic scattering intensity around q = 0.5 Å^{-1}, and concluded it to be a direct observation of an antiferromagnetic-like correlation of the electron spin densities due to the quantum exchange correlation among itinerant electrons, i.e., an "Exchange Hole".

Since such an "Exchange Hole" is not consistent with the earlier observation[2], we performed neutron scattering experiments at Brookhaven (BNL) in MnSi below T_c, which we report on in this article. We first employed the conventional double-axis technique with unpolarized neutrons for a powdered specimen to obtain the energy-integrated intensity of the diffuse scattering. The powder scattering intensity I(q) can be put onto an absolute scale using the integrated intensity

ΣI_B of a Bragg peak using the relation

$$\frac{I(q)}{\Sigma I_B} = \frac{d\sigma}{d\Omega} \cdot \frac{N_m \cdot V_c \cdot (\Delta 2\theta) \cdot 8\pi \cdot \sin\theta \sin 2\theta}{\lambda^3 \cdot PF_N^2} \qquad (1)$$

where θ is the scattering angle of the Bragg peak, F^2 and P respectively represent its nuclear structure factor and the multiplicity, $\Delta 2\theta$ denotes the angular step of the powder scan around the Bragg peak, λ is the wave length of the incident neutrons, and V_c is the volume of the unit cell containing N_m magnetic atoms. Using eq. 1 with $N_m = 4$, the diffuse scattering intensity $d\sigma/d\Omega$ is obtained for each Mn atom and is plotted in Fig. 1. Assuming the following relation for diffuse paramagnetic scattering

$$\frac{d\sigma}{d\Omega} = \frac{2}{3} \gamma_o^2 \quad S(S + 1) \cdot f_m^2 (q) \qquad (2)$$

where $\gamma_o = 0.291$ barns/str and f_m^2 is the magnetic form factor, we can express the intensity in terms of the number of effective Bohn magnetons ($M=2\sqrt{S(S+1)}$) of a Mn spin S, and directly compare the results of Ziebeck et al.[3] as in Fig. 1.

We performed the measurements with two different incident neutron energies, $E_i = 30.5$ and 87 meV at T = 5K, and obtained almost identical results as shown in Fig. 1. This indicates that the major contribution to the intensity is low-energy scattering and suggests that the experimental results are rather independent on a range of energy integration as long as $E_i \gtrsim 30$ meV. Since we used unpolarized neutrons, the measured intensity of the BNL data includes both magnetic and nuclear scattering, and the nearly constant intensity at $q > 0.7$ Å^{-1} should be due principally to the nuclear incoherent and phonon scattering from MnSi. Nevertheless, the BNL data represents the upper limit of the magnetic scattering. Therefore, the present experiment is totally inconsistent with the ILL-Grenoble results since we found a smooth variation of intensity over the entire observed range of q with much smaller absolute intensity around $q = 0.5$ Å^{-1} as compared to the result of Ziebeck et al.[3] Thus, no "Exchange Hole" is observed in the present experiment.

To investigate further details, we also performed polarization analysis with neutrons spin-polarized parallel and perpendicular to the scattering vector q, i.e., the technique used by Ziebeck et al.[3] Rather than use poor energy resolution intentionally, however, we used a better resolution of FWHM $\Delta E \sim 2$-5 meV with lower constant final energies $E_f = 30.5$ and 60 meV, and attempted to map the intensity contour of the magnetic scatterings in the ω-q plane. Selecting the spin-flip scatterings, the difference in the intensity for $\vec{q}$ parallel (horizontal field) and $\vec{q}$ perpendicular (vertical field) to the neutron polarization was measured with powder and single crystal specimens of MnSi at T = 5K. Although the observable range was limited as shown in Fig. 2 due to energy and momentum conservation requirements at low-angles, no anomaly was found around $q = 0.5$ Å^{-1} for any combination of specimens and E_f.

Rather, the intensity exhibited a maximum along the spin-wave dispersion line as shown in Fig. 2. An "Exchange Hole" was therefore not indicated in this measurement either.

We might point out possible explanations for the peak at $q = 0.5$ $Å^{-1}$ observed at Grenoble. In our initial experimental arrangement for polarized neutrons, a similar but spurious peak was observed around $q = 0.5$ $Å^{-1}$ for neutron energies higher than ~ 100 meV. However, this could be removed by increasing the shielding to eliminate stray neutrons. The "defocussed" configuration of the analyzer, which takes the counter away from the direct beam, was also helpful in removing such spurious peaks. In the powder measurement at room temperature, Ziebeck et al.[3] observed some nuclear Bragg peaks of Mn_5Si_3 indicating the presence of about 7% Mn_5Si_3 in their MnSi specimen. This could give another explanation to the spurious peak at $T = 11$ K, since Mn_5Si_3 produces its strongest magnetic Bragg peak at $q = 0.5$ $Å^{-1}$ below its Neel temperature of 68K [4]

In conclusion, the results of two different measurements, shown in Figs. 1 and 2, demonstrate that the "Exchange Hole" does not exist in MnSi below T_c. Details will be discussed elsewhere.

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Figure Captions

Fig. 1. Neutron scattering intensity of powdered MnSi at T = 5K observed at Brookhaven (BNL) using the energy-integrating double-axis powder scattering technique with unpolarized neutrons. The intensity is normalized for each Mn atom, and is compared to the results of Ziebeck et al.[3] observed at ILL, Grenoble for T = 11K. The intensity scale is also given in effective Bohr magnetons M of a Mn moment. The ILL data represents purely magnetic intensity while the BNL data includes both magnetic and nuclear scattering.

Fig. 2. Magnetic scattering intensity observed in powdered MnSi at T = 5K using polarization analysis of the scattered neutrons with constant final energy E_f = 60 meV. The ω-q range above the straight line is not accessible due to energy and momentum conservation restrictions. The broken line represents the spin-wave dispersion relation observed in Ref. 2.

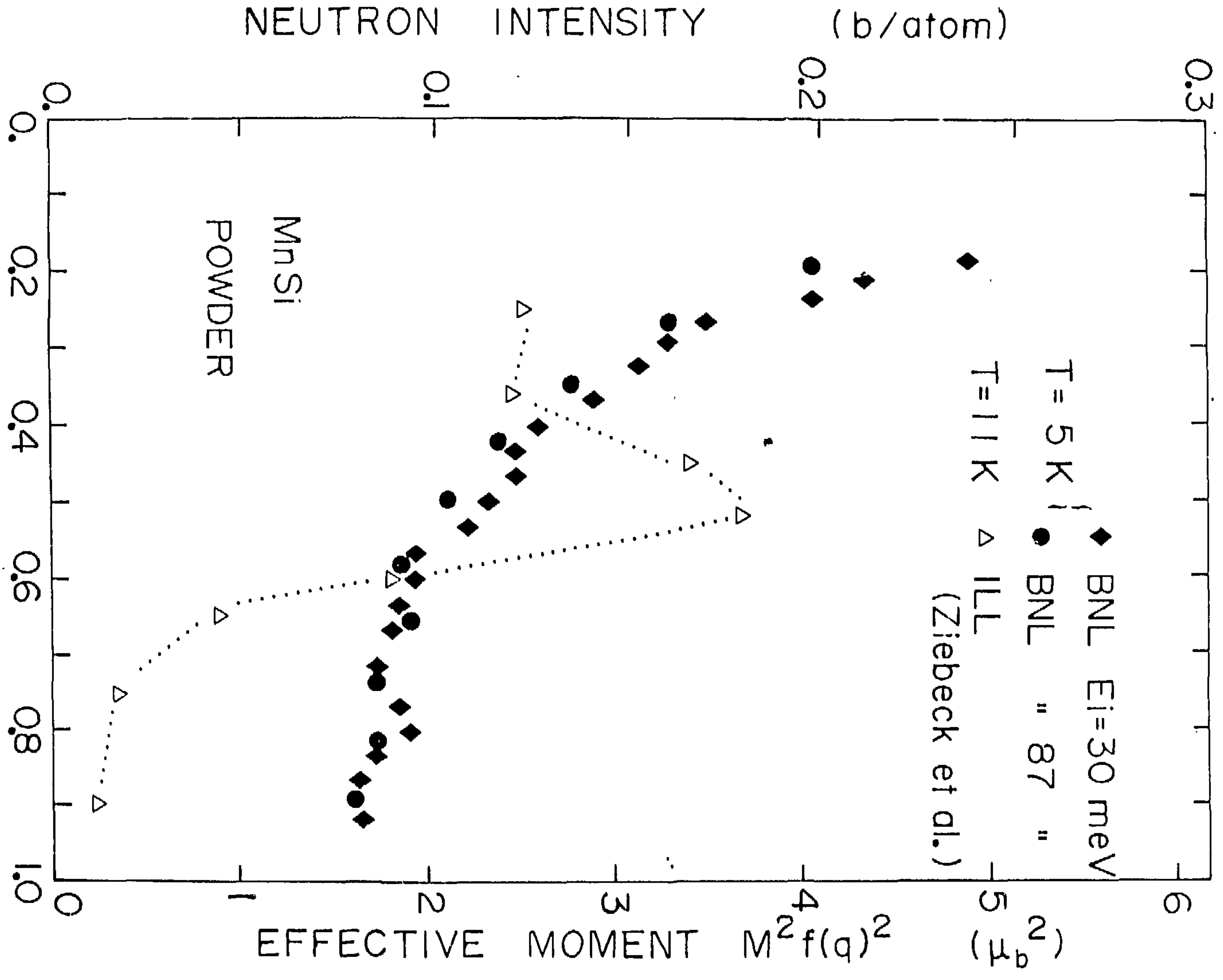
NEUTRON INTENSITY (b/atom)
0.
0.1
0.2
0.3
0.0
0.2
0.4
0.6
0.8
1.0
q (Å^{-1})
MnSi
POWDER
T = 5 K
◆ BNL Ei=30 meV
● BNL " 87 "
T=11 K
△ ILL
(Ziebeck et al.)
0
1
2
3
4
5
6
EFFECTIVE MOMENT M^{2}f(q)^2 (μ$_b$^{2})

Figure 1

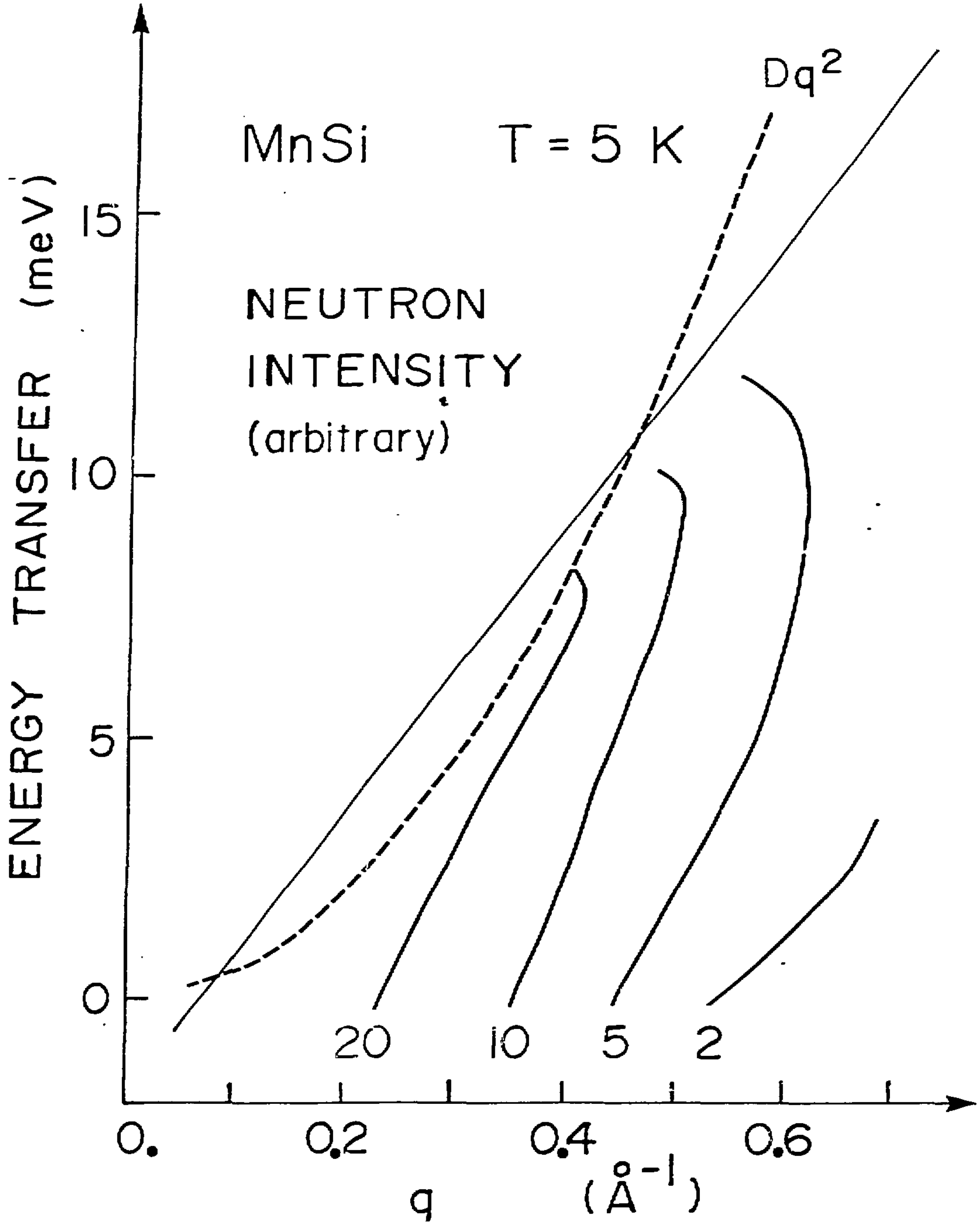
MnSi T = 5 K
NEUTRON INTENSITY (arbitrary)
Dq²
ENERGY TRANSFER (meV)
15
10
5
0
20
10
5
2
0.
0.2
0.4
0.6
q (Å⁻¹)

Figure 2