

Comparison of the critical magnetic scattering from the Heisenberg system EuO with renormalization-group theory

P. Böni, M. E. Chen, and G. Shirane
 Brookhaven National Laboratory, Upton, New York 11973
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The paramagnetic scattering from the isotropic Heisenberg ferromagnet EuO has been investigated by inelastic neutron scattering in order to test the predictions of asymptotic renormalization-group theory. The scattering cross sections are in excellent agreement with theory over a wide range of momentum and energy ($q < 0.3 \text{ \AA}^{-1}$, $\omega < 0.4 \text{ meV}$).

I. INTRODUCTION

The critical magnetic scattering of several isotropic ferromagnets has been studied in detail during the last decade by neutron scattering techniques. One of the most outstanding results is the almost perfect agreement of the q dependence of the linewidth Γ with the predictions of dynamical scaling $\Gamma = Aq^z$ with $z = 2.5$ over at least four decades in energy in EuO [Fig. 1 (Ref. 1)] and Fe (Refs. 2 and 3). During the course of these investigations, the magnetic scattering was parametrized in terms of the scattering function

$$S(q, \omega) = 2kT\chi(0) \frac{\kappa_1^2}{\kappa_1^2 + q^2} F(q, \omega) \frac{\omega/kT}{1 - e^{-\omega/kT}}, \quad (1)$$

where $\chi(0)$ is the static susceptibility, κ_1 the inverse correlation length and the other symbols have their usual meaning. The spectral weight function $F(q, \omega)$ defines the line shape as measured in constant-momentum-transfer (constant- q) scans. In almost all neutron scattering measurements to date a simple Lorentzian

$$F(q, \omega) = \frac{1}{\pi} \frac{\Gamma}{\Gamma^2 + \omega^2} \quad (1a)$$

was used to determine the linewidth of the paramagnetic scattering. The line shape itself was only of secondary importance because their influence on Γ was minor, when compared with the resolution corrections and statistical errors of the measurements.

With the advances in neutron scattering, which resulted in higher intensities and better resolution, clear deviations of the measured spectra from a Lorentzian have been observed.^{1,3} Actually these deviations were expected from theory and had led DeGennes⁴ to introduce a "cutoff Lorentzian" nearly 30 years ago. When we conducted the comprehensive neutron scattering studies in Fe and EuO the correct shape function $F(q, \omega)$ was not known. Therefore, we have modified the Lorentzian in a heuristic way and could improve the quality of the fits significantly at the expense of an additional shape parameter. The extracted line widths followed the predictions of dynamical scaling up to about 1/3 of the zone boundary.

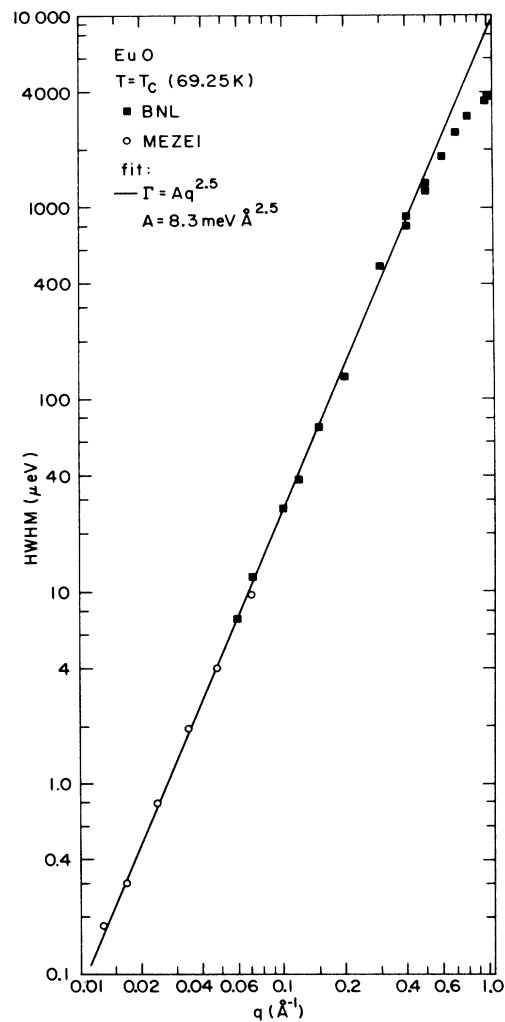


FIG. 1. Linewidth of the quasielastic scattering at T_c follows the predictions of dynamical scaling theory over 4 decades in energy [after Böni and Shirane (Ref. 1)]. HWHM represents half width at half maximum.

Although the obvious way to measure $F(q, \omega)$ is the determination of the spectrum itself (as described above), nonmagnetic background contributions often preclude an exact characterization of $F(q, \omega)$, especially in the tail sections of the cross section where the intensities are small. An elegant method to compare theoretical line shapes with measurement is the constant-energy (constant- E) scan technique. These scans show a rather sharp peak at finite q for a diffusive type scattering function. The peak position is extremely sensitive to the exact profile of $F(q, \omega)$ and it can be measured accurately and compared with theory. It turns out that Eq. (1) together with a Lorentzian shape function Eq. (1a) predicts peaks at $q_0 = (E/3A)^{0.4}$ in contrast to the measurements which are well parametrized by $q_0 = (E/1.27A)^{0.4}$ (Ref. 5). Actually these latter deviations have motivated Wicksted *et al.*³ to introduce the modified Lorentzian spectral weight function mentioned above.

In order to remove the discrepancies between the measured constant- E data and the predictions of Eqs. (1) and (1a) a breakdown of dynamical scaling at larger q has been proposed.⁶ Recently Folk and Iro^{7,8} have demonstrated, however, that asymptotic renormalization group theory yields a cross section which is in good agreement with the available constant- E data from Fe and no contradiction to dynamical scaling was found. Moreover, asymptotic renormalization group theory justifies the use of the modified Lorentzian, because the two cross sections are in almost perfect numerical agreement with each other.

The purpose of the present study is to demonstrate that peak positions as well as peak profiles of the critical magnetic scattering from the isotropic Heisenberg ferromagnet EuO are in excellent agreement with the predictions of renormalization-group theory. We have chosen this system, because the quasielastic scattering is theoretically well understood up to the zone boundary and the dynamical scaling prediction $z = 2.5$ ($z = 2.46$, if Fisher exponent is included) is valid over at least four decades in energy.¹ EuO has, however, the disadvantage that it absorbs neutrons and since the spin-wave energies are low,⁹ it is difficult to conduct constant- E scans in the most interesting region of small energies, because the scans are more or less tangential to the dispersion curve.

II. EXPERIMENTAL PROCEDURE

The measurements were performed on the same powder sample of isotopically enriched ^{153}EuO used in previous studies by Passell *et al.*⁹ and Mezei.^{10,11} The sample weighed 0.75 g, was 24 mm high, 12 mm wide, and 0.5 mm thick. EuO crystallizes in the NaCl structure. The lattice constant is $a = 5.12 \text{ \AA}$ at $T = T_c$ and the nearest inverse neighbor distance is therefore $d_{111}^* = 2.12 \text{ \AA}^{-1}$. The experiments were performed on triple axis spectrometers at the Brookhaven High Flux Beam Reactor. We have determined the Curie temperature by measuring the temperature dependence of the critical scattering and obtained $T_c = 69.25 \pm 0.05 \text{ K}$.

The data was collected in the forward direction keeping fixed either the final neutron energy E_f or incident neutron energy E_i . Pyrolytic graphite crystals set for the

(002) reflection were used as monochromator and analyzer for most of the experiments. Higher-order neutrons were removed either by a cooled Be filter for E_f or E_i smaller than 5 meV or by a pyrolytic graphite filter for $E_f = 14.7 \text{ meV}$. The collimations are defined in the figure headings. For more details see Ref. 1.

III. PARAMAGNETIC SCATTERING AT T_c

Before we present some of our new results we would like to introduce the scattering function which has been discussed recently in detail by Folk and Iro^{7,8} and is based on the renormalization-group approach performed by Dohm for an isotropic ferromagnet at T_c in $6-\epsilon$ dimensions¹² and on an interpolation formula by Bhattacharjee and Ferrell¹³

$$S(q, \omega) = 2kTC \frac{1}{Aq^{4.5}} \frac{1}{\pi} \times \text{Re} \frac{1}{is + \alpha \left[1 + i \frac{\beta}{\alpha} s \right]^{-0.6}} \frac{\omega/kT}{1 - e^{-\omega/kT}}, \quad (2)$$

where $\alpha = 0.78$, $\beta = 0.46$, $C = \lim_{T \rightarrow T_c} \chi(0) \kappa_1^2$, and $s = \omega/Aq^{2.5}$, which is equivalent to $s = \omega/\Gamma$. All parameters in this scattering function are known in contrast to the modified Lorentzian, mentioned above, where an additional shape parameter had to be introduced to parametrize the data.

In Fig. 2 we present a typical scan for $q = 0.15 \text{ \AA}^{-1}$. The elastic background at $\omega = 0$ was 50 counts/4.5 min and has already been subtracted. The broken and solid lines are fits to Eqs. (1) and (2), convoluted with the resolution function with A fixed at $8.3 \text{ meV \AA}^{2.5}$. The single fitted parameter for the solid line in Fig. 2(a) is a normalization constant for the paramagnetic scattering. The broken line is simply normalized to the data points around $\omega = 0$. The energy-independent background has been kept fixed at its value measured below T_c . The cross section based on renormalization-group theory fits the data almost perfectly, whereas the Lorentzian profile yields overly large wings which cause an overly large width for the resolution convoluted profile. The fitted parameters in Fig. 2(b) are a normalization constant for the magnetic scattering and a constant background. The fits demonstrate that both scattering functions seem to represent the data well. They deviate significantly from each other only at energy transfers exceeding 0.2 meV. The renormalization group fit yields the correct background [see Fig. 2(a)], whereas the Lorentzian fit yields 0 counts, which is unreasonably low. The latter happens because of the large tail of the Lorentzian. We conclude that renormalization-group theory represents the data significantly better than a Lorentzian.

Knowing the normalization constants for both scattering functions from the constant- q data in Fig. 2(b) we are able to calculate constant- E scan profiles and compare them with experiment. We have performed scans for energies $0.07 \text{ meV} < \omega < 3 \text{ meV}$. Some typical raw data is shown in Figs. 3 and 4. All scans exhibit a relatively sharp peak at finite q , as expected. The data points at

small q have been omitted because of contamination by the direct beam. The solid and broken lines have been calculated by convoluting either the scattering function based on renormalization-group theory or the Lorentzian scattering function, respectively, with the resolution function, using the known normalization constants. The constant background (the only free parameter in the calculation) was adjusted in such a way that χ^2 was minimized. The comparison between data and calculation shows that renormalization-group theory reproduces peak shape and intensity well up to about 0.3 meV (see Fig. 3). Above $\omega=0.5$ meV, i.e., far outside the critical region, where asymptotic renormalization-group theory is expected to break down, we observe clear deviations between experiment and theory (Fig. 4). The Lorentzian spectral weight

function, on the other hand, does not reproduce the data at all.

IV. DISCUSSION

In the preceding section we have shown that asymptotic renormalization-group theory accounts well for all our magnetic scattering measurements from EuO obtained for $q < 0.3 \text{ \AA}^{-1}$ and $\omega < 0.4$ meV. This range is much wider than what we expected to be the critical region for which the theory was made for. Mezei¹¹ conducted recently constant- q scans at very small q in EuO and found that the line shape closely resembles a Lorentzian in disagreement with the prediction of renormalization-group theory [Eq. (2)]. Further neutron scattering studies are necessary to resolve this problem.

In Fig. 5 we compare the present constant- E data from EuO with data from other isotropic ferromagnets. The peak positions follow the prediction of renormalization group theory up to $\zeta=0.15$, well into the region where Lynn reported a breakdown of dynamical scaling.⁶ Ac-

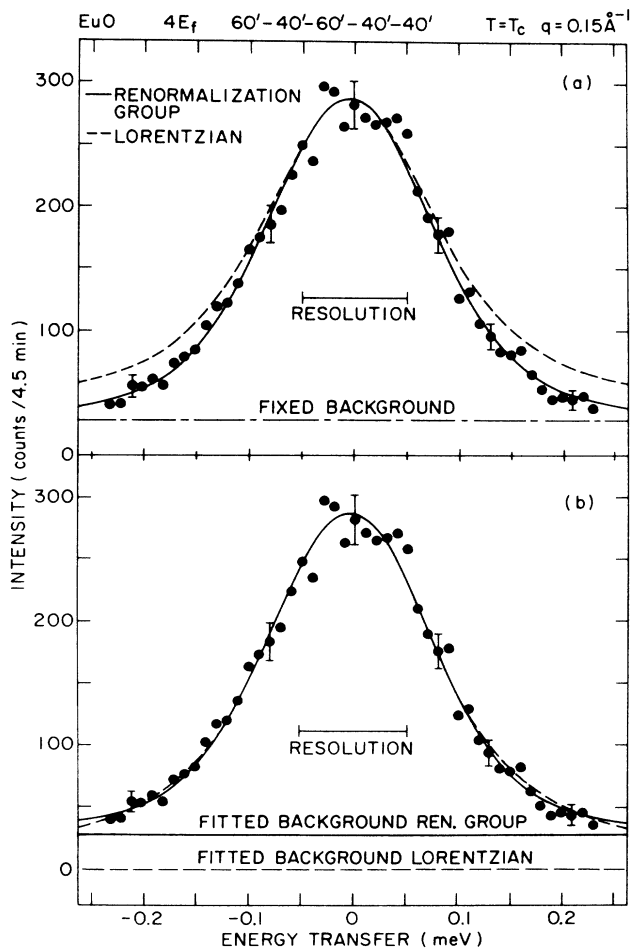


FIG. 2. Example of a constant- q scan at 0.15 \AA^{-1} measured at T_c . The elastic background around $\omega=0$ has already been subtracted. The broken and solid curves are fits to Eqs. (1) and (2), respectively, keeping fixed the linewidth (for details see text). In (a) the constant background has been kept fixed at the value determined by measurements below T_c (chain line). In (b) the background has been fitted too. The fit to the Lorentzian cross section gives 0 counts background (broken line) whereas the fit to renormalization-group theory yields the correct background (solid straight line).

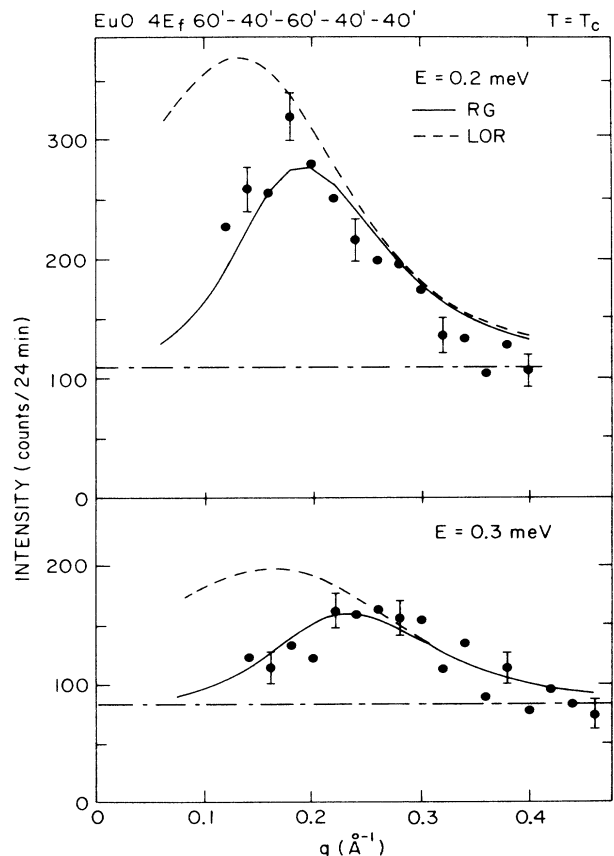


FIG. 3. Constant- E scans measured at T_c . The lines have been calculated according to Eqs. (1) and (2) with the normalization constant for the magnetic scattering fixed at the value obtained from fits to the constant- q scan in Fig. 2(b). Renormalization-group theory (RG) (solid line) accounts well for the observed peak profiles. The chain line represents the constant background.

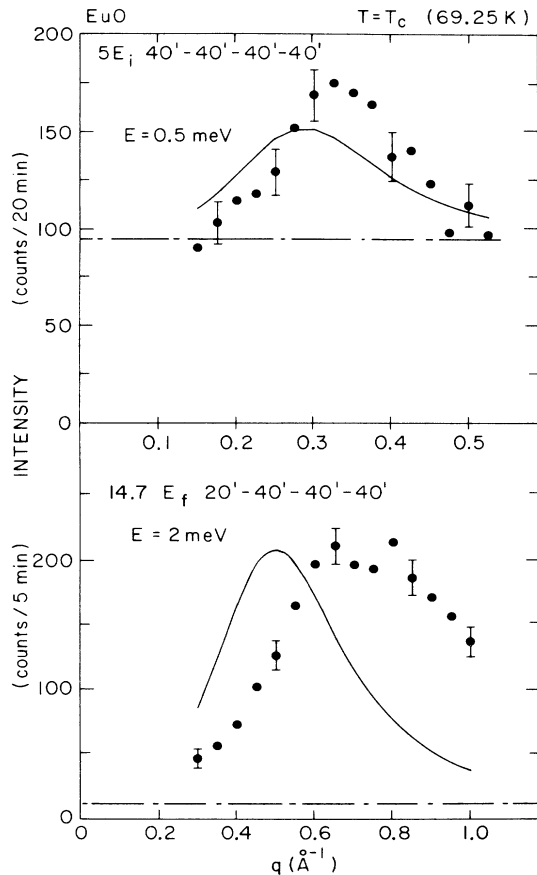


FIG. 4. For the sake of completeness we show constant- E scans measured far outside the critical region where renormalization-group theory is not valid. The normalization constants used have been determined in a similar way as for the measurements in Fig. 3. Note the different experimental conditions. The nearest zone boundary is at $q = 1.06 \text{ \AA}^{-1}$.

According to Lynn, dynamical scaling should break down around a characteristic wave vector q_c defined by $q_c = (kT_c/3A)^{0.4}$, i.e., when the thermal energy is of the same order of magnitude as the energy width of the magnetic scattering. For Ni, $\zeta_c = 0.10$ and for EuO $\zeta_c = 0.27$ ($\zeta_c = q_c/d_{111}^*$). However, according to Fig. 5, Ni follows the predictions of dynamical scaling at least as far as in EuO, in disagreement with Lynn's energy considerations.

The shape of the constant- E curve for Fe at larger q is apparently different from the curves for the localized systems EuO and Pd_2MnSn because the data for Fe follows the predictions of renormalization-group theory up to nearly half way to the zone boundary whereas the data for the localized systems starts to bend over near $\zeta = 0.15$. It is an interesting feature of Fe, that the linewidth mea-

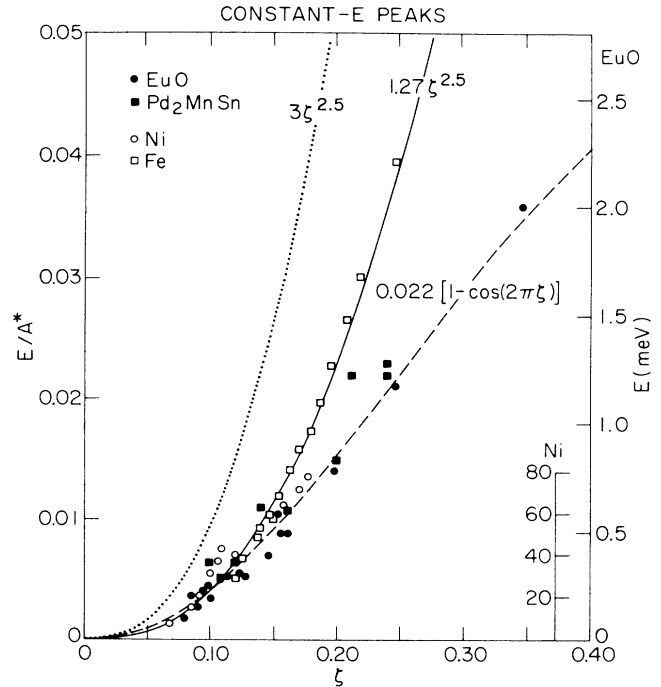


FIG. 5. Constant- E peak positions in itinerant and localized systems [after Böni and Shirane (Ref. 5)] plotted vs momentum. The energy has been scaled by $A^* = (Ad_{111}^*)^{2.5}$, where d_{111}^* is the nearest inverse plane distance and momentum is given in units of d_{111}^* . The dotted line is the prediction of the double Lorentzian scattering function [Eq. (1)] and the solid line is the parametrization of the data by $E/A^* = 1.27\zeta^{2.5}$, which is very close to the prediction of renormalization-group theory $E/A^* = 1.3\zeta^{2.5}$. The data of the localized systems EuO and Pd_2MnSn is well parametrized by $E/A^* = 0.022[1 - \cos(2\pi\zeta)]$ near the zone boundary ($\zeta = 0.5$). Note the very different energy scales for EuO and Ni.

surements too are in accord with dynamic scaling up to nearly half way to the zone boundary.¹⁴ The trend for Ni is not clear because of the lack of high-energy data.

In summary, we have demonstrated that linewidths and peak profiles of the paramagnetic scattering from the isotropic Heisenberg ferromagnet EuO are in excellent agreement with the predictions of asymptotic renormalization-group theory and the dynamical scaling predictions in the critical region at T_c .

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¹P. Böni and G. Shirane, Phys. Rev. B 33, 3012 (1986).

²F. Mezei, Phys. Rev. Lett. 49, 1096 (1982).

³J. P. Wicksted, P. Böni, and G. Shirane, Phys. Rev. B 30, 3655 (1984).

⁴P. G. De Gennes, J. Phys. Chem. Solids 4, 223 (1958).

⁵P. Böni and G. Shirane, J. Appl. Phys. 57, 3012 (1985).

⁶J. W. Lynn, Phys. Rev. Lett. 52, 775 (1984).

⁷R. Folk and H. Iro, Phys. Rev. B 32, 1880 (1985).

- ⁸R. Folk and H. Iro, *Phys. Rev. B* 34, 6571 (1986).
- ⁹L. Passell, O. W. Dietrich, and J. Als-Nielsen, *Phys. Rev. B* 14, 4897 (1976); 14, 4908 (1976); 14, 4923 (1976).
- ¹⁰F. Mezei, *J. Magn. Magn. Mater.* 45, 67 (1984).
- ¹¹F. Mezei, *Physica* 136B, 417 (1986).
- ¹²V. Dohm, *Solid State Commun.* 20, 657 (1976).
- ¹³J. K. Bhattacharjee and R. A. Ferrell, *Phys. Rev. B* 24, 6480 (1981).
- ¹⁴G. Shirane, P. Böni, and J. P. Wicksted, *Phys. Rev. B* 33, 1881 (1986).