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Paramagnetic neutron scattering and renormalization-group theory for isotropic ferromagnets at T_c

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The results of the asymptotic renormalization-group theory at T_c are compared with neutron scattering data and a satisfactory agreement is found.

Recently a breakdown of dynamic scaling for an isotropic ferromagnet outside the region of small wave vectors has been concluded from neutron scattering experiments by Lynn.[1] He found strong disagreement between the measured scattering function and what was taken as the results of dynamic-scaling theory. However, for not too large wave vectors, most of these discrepancies can be traced back to the use of a Lorentzian (the result of the van Hove theory) for the shape function for large arguments, whereas the renormalization-group (RG) theory predicts a different behavior.[2-4] Moreover, the shape function at T_c has already been calculated within RG theory.[3,4] But so far, to our knowledge, these results have not been compared quantitatively with experiments. A reason for this may be that the critical dimension $d_c=6$ is very far from the physical dimension $d=3$, and one could question the significance of an ϵ-expansion calculation for $\epsilon=3$ $(\epsilon=6-d)$. Fortunately, within the RG theory one can deduce exact statements, especially about the critical exponent z $(z=2.5)$ and the scaling behavior of the shape function for small and large arguments.[2] We show that a simple shape function,[4] which fulfills these exact requirements and which is compatible with the ϵ expansion,[3] is in satisfactory agreement with experiment.

In order to remove the discrepancies with experiments Wicksted, Böni, and Shirane[5] modified the Lorentzian shape function in a heuristic way. However, this approach did not prove or disprove the validity of dynamic scaling, since no connection of the modification with a theory involving dynamical scaling was established. One of the results of this paper is that RG theory leads to a shape function that numerically agrees with their function in the experimental range.

Following Ma and Mazenko,[6] the dynamics of the magnetization density $\mathbf{S}(\mathbf{x},t)$ for an isotropic ferromagnet is described by the equation of motion

$$\dot{\mathbf{S}}=\lambda f\mathbf{S}\times\frac{\delta H}{\delta\mathbf{S}}+\lambda\Delta\frac{\delta H}{\delta\mathbf{S}}+\boldsymbol{\zeta}\ , \tag{1}$$

where $\boldsymbol{\zeta}$ is a stochastic force connected with the damping constant λ, f is a coupling constant, and H is the usual Landau-Ginzburg-Wilson functional

$$H=\int d^dx\left[\frac{1}{2}(\nabla\mathbf{S})^2+\frac{r}{2}\mathbf{S}^2+\frac{u}{4!}\mathbf{S}^4\right]\ . \tag{2}$$

Then the dynamic magnetization correlation function

$$C(\mathbf{q},\omega)\delta^{\alpha\beta}=\int d^dx\int dt\, e^{-i(\mathbf{q}\cdot\mathbf{x}-\omega t)}\langle S^\alpha(\mathbf{x},t)S^\beta(0,0)\rangle \tag{3}$$

obeys the asymptotic scaling law[2]

$$C(q,\omega)\sim q^{-(2+z-\eta)}\phi(x)\ , \tag{4}$$

where the scaling variable $x=\omega/Aq^z$ contains the nonuniversal factor A. The shape function behaves as

$$\phi(x)\sim\text{const for } x\rightarrow 0\ , \tag{5a}$$

and

$$\phi(x)\sim x^{-(z+4)/z}\text{ for } x\rightarrow\infty\ . \tag{5b}$$

The critical exponent z is, below $d_c=6$, given exactly by

$$z=\frac{d+2-\eta}{2}\ . \tag{6}$$

Since η is small ($\eta\simeq0.05$, Ref. 7) it will be neglected in the following. Whereas (4)–(6) are general results of the RG theory, the explicit form of the shape function $\phi(x)$ can only be found by some perturbation calculation in the coupling f. To first order in ϵ this has been carried out by Dohm[3] and his result has been confirmed in Ref. 4. In a strict ϵ expansion $\phi(x)$ may be written in the form

$$\phi(x)=[1+\epsilon F(0)]\,\text{Re}\frac{1}{1+ix+\epsilon F(x)}\ , \tag{7}$$

where $F(x)$ can be found in Ref. 3. For large x the logarithmic behavior of $F(x)\sim-\frac{1}{8}\ln(ix)$ has to be exponentiated to lead to the dependence according to (5b) with the ϵ-expanded exponent $(z+4)/z\simeq2+\epsilon/8$. However, to take into acount (5b) exactly we use the interpolation function proposed in Ref. 4. This means $F(x)$ in (7) is substituted by

$$\epsilon F(x)=(1+\beta ix)^{(z-4)/z}-1\ , \tag{8}$$

where

$$\beta=\frac{z}{4}(6+6\ln2-3\pi)\ . \tag{9}$$

Thus, the correlation function (3) has been determined up to the nonuniversal scale factor A appearing in x, which has to be taken from experiment.

The neutron scattering function, taking into account detailed balance, is given by the dynamic susceptibility $\chi(q,\omega)$,[8] namely,

$$S(q,\omega)=\text{const}\frac{2}{1-e^{-\beta\hbar\omega}}\,\text{Im}\chi(q,\omega)\ . \tag{10}$$

In the frame of RG theory we calculate $\text{Im}\chi$ via the classical fluctuation-dissipation theorem

$$\mathrm{Im}\chi(q,\omega)=\frac{\omega}{2}C(q,\omega)\ , \tag{11}$$

thus leading to the approximation

$$S(q,\omega)=\mathrm{const}\frac{\omega}{1-e^{-\beta\hbar\omega}}C(q,\omega)\ . \tag{12}$$

The ω-dependent prefactor corrects for the fact that our $C(q,\omega)$ does not fulfill detailed balance-conditions.[9] For $d=3$, we get from (4), (7), and (8),

$$C(q,\omega)\sim q^{-4.5}\mathrm{Re}\frac{1}{ix+(1+0.46ix)^{-0.6}}\ . \tag{13}$$

We fix the scale factor A by the requirement that the half-width Γ of (12) at fixed q agree with the experimental value. For Fe, for instance, we have[5] $\Gamma=142q^{2.5}$ with Γ and q in units of meV and Å^{-1}, respectively, which implies $A=111$ meV Å$^{2.5}$. For other cubic ferromagnets we obtain $A=274$ (Ni), 47 (Pd_2MnSn), and 6.8 (EuO) meV Å$^{2.5}$ (see Table I in Ref. 10).

Now, *without any further adjustable parameter*, we can compare the theoretical prediction for the constant-energy scans with experiment. Here we restrict ourselves to Fe (see Refs. 5 and 11). In these scans the intensity shows peaks at nonzero q_0 values, which depend on energy. The scaling property of the asymptotic shape function implies the relation $\omega=Bq_0^{2.5}$. B is determined by the shape of $\phi(x)$ for values of x larger than the half-width (for Fe, $B=175$ meV Å$^{2.5}$). Figure 1 shows the excellent agreement of the result of the RG theory with the data for Fe. This also clearly demonstrates that for large arguments x, the Lorentzian is inadequate, and no contradiction to dynamic scaling is deducible from these data, contrary to Ref. 1.

A further test of $\phi(x)$ is shown in Fig. 2. There the width Δq of the constant-energy peaks is plotted against the peak position. Any scaling function yields a linear dependence $\Delta q=cq_0$, where c depends on the shape function. The value $c=0.75$ obtained from RG theory is a considerable improvement over the result $c=1.57$ as found by Lynn[1] from a Lorentzian.

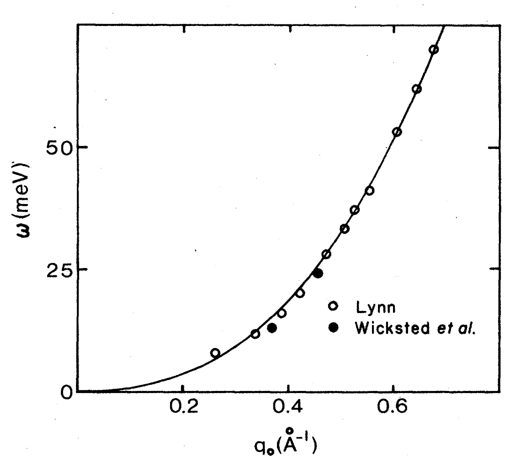

FIG. 1. Energy ω vs peak position q_0 of constant-energy scans. Solid curve: theoretical prediction of asymptotic RG theory. The data are from Refs. 5 and 11.

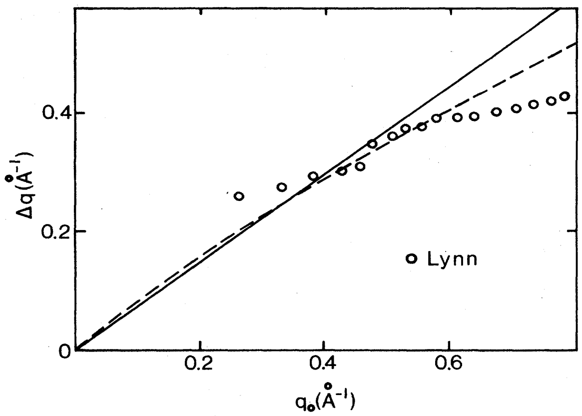

FIG. 2. Width Δq of the peak in the constant-energy scan vs peak position q_0. Solid curve: theoretical prediction of asymptotic RG theory. The dashed line results from the heuristic shape function of Refs. 5 and 12. Data from Ref. 11.

A similar agreement with experiments like that in Fig. 2 has been found in Refs. 5 and 12 using a heuristic shape function, which however, besides A, contains a further fit parameter. With the help of this parameter their function was adjusted to the data of Fig. 1. Since their shape function [a comparison with $\phi(x)$ is given in Fig. 3] does not have the scaling property they obtain a curvature, which is in slightly better agreement at larger q_0 values in Fig. 2, where a crossover to nonscaling behavior is expected. In the RG theory the nonasymptotic shape function, appropriate for the large-q and -ω region, depends in a nonuniversal way on q and ω (Ref. 13) separately. Such a nonuniversality at larger q_0 values can also be found by extending Fig. 1 to other cubic ferromagnets (see Fig. 6 of Ref. 10). One may suppose that such effects could be treated within the framework of a nonasymptotic RG theory.

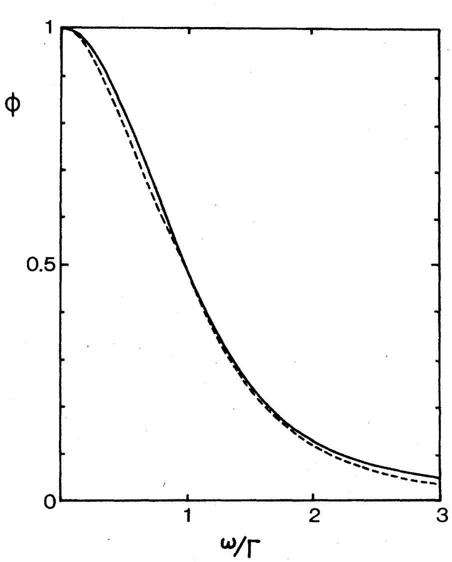

FIG. 3. Comparison of the shape function ϕ, Eq. (12) (solid line) with the heuristic shape function of Refs. 5 and 12 (dashed line) at $q=0.2$ Å^{-1}. Note that $\omega/\Gamma=1.28x$.

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[13]A further uncertainty could be the extrapolation to T_c of the experimental data measured at finite $T-T_c$. Therefore, it would be worthwhile to consider also the temperature dependence of the shape function.