NMR determination of the order-parameter exponent β in $Fe_{0.46}Zn_{0.54}F_2$

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We report NMR second-moment measurements of ^{19}F in crystalline $Fe_{0.46}Zn_{0.54}F_2$. The inhomogeneous broadening was studied below and above the critical temperature $T_c = 35.395$ K. The line profile is Gaussian for $|t| = |(T-T_c)/T_c| \gtrsim 3\times10^{-2}$ and approaches a Lorentzian for $|t| \lesssim 3\times10^{-2}$. In the random-field region, the second moment was obtained from the fitting of an effective line shape to the experimental data. We assume that the line-profile second moment scales with the sublattice magnetization in all ranges of temperature. Below T_c, we observe a crossover from a random-exchange Ising model to a random-field Ising model, with the magnetization exponent $\beta = 0.35$ and 0.125, respectively. Above T_c, the data can be treated according to a scheme proposed by Heller.

We obtained estimates for the β magnetization critical exponent from NMR measurements of the resonance of the F^- ion in crystalline[1] $Fe_{0.46}Zn_{0.54}F_2$. We worked in a range of temperature where it is relatively easy to observe the resonance associated with the F^- ions without magnetic nearest neighbors, the so-called F_0 resonance.[2] The NMR spin-echo amplitude was monitored in a phase-coherent pulsed spectrometer, at 77 MHz fixed frequency, as the magnetic field is varied by 3–5 times the observed linewidth, about the resonance value $H_0 = 19.3$ kG. The tank circuitry was tuned up at almost all the temperatures of measurement.

The linewidths $\Delta H_{1/2}$ ($\Delta H_{1/4}$) at half (quarter) intensity were obtained directly from the experimental data. The relations $(\Delta H_{1/4}/\Delta H_{1/2})^2$ vs T are shown in Fig. 1 for H parallel and perpendicular to the [001] direction (c axis), respectively. The plot of $(\Delta H_{1/4}/\Delta H_{1/2})^2_{\parallel}$ vs T shows the change from a Gaussian $[(\Delta H_{1/4}/\Delta H_{1/2})^2 = 2]$ into a Lorentzian profile $[(\Delta H_{1/4}/\Delta H_{1/2})^2 = 3]$, as T becomes closer to the critical temperature T_c. The spin-echo intensity, which has been measured in an extra run

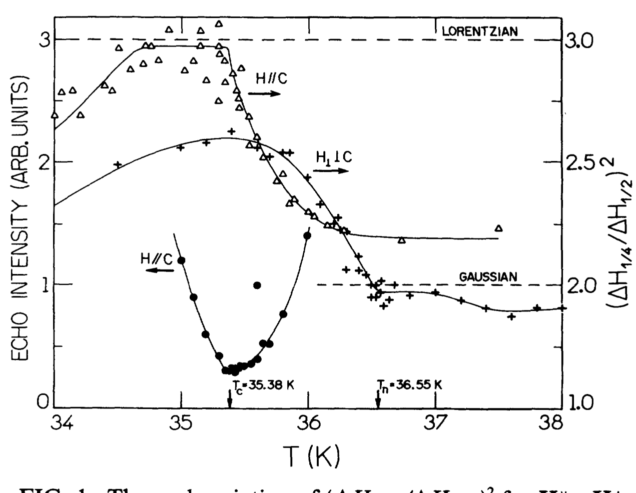

FIG. 1. Thermal variation of $(\Delta H_{1/4}/\Delta H_{1/2})^2$ for $\mathbf{H}\parallel c$, $\mathbf{H}\perp c$, and echo intensity in an independent run. The solid lines are guides for the eyes.

at fixed $\mathbf{H}_0$ (parallel to the c axis), reaches a minimum at the critical temperature $T_C \approx 35.38$ K ($\mathbf{H}_0 \parallel c$), as shown in Fig. 1. The relation $(\Delta H_{1/4}/\Delta H_{1/2})^2_{\parallel}$ reaches a value close to the Lorentzian prediction and stays constant down to 34.6 K. For magnetic fields applied perpendicularly to the c axis, the relation $(\Delta H_{1/4}/\Delta H_{1/2})^2_{\perp}$ is always less than 2.6; above the critical temperature $T_n = 36.55\pm0.05$ K ($\mathbf{H}_0 \perp c$), it becomes very close to the Gaussian prediction. The critical temperatures are consistent with the relation[3,4]

$$T_n - T_c = bH_0^2 + T_n(ch_{\mathrm{RF}}^2)^{1/\phi} , \quad (1)$$

where $H_0 = 19.3$ kG, bH_0^2 is the mean-field shift, h_{RF} is the reduced random field, ϕ ($=1.40$) is the crossover exponent, and c is a constant of order unity. For $T_n = 36.55$ K, Eq. (1) leads to $T_c = 35.39$ K. As T_c was established directly from the experimental data within 50 mK, without any conditions about the line profile, the critical-exponent parameters were then investigated trying various values of T_c between 35.35 and 35.45 K.

The determination of the second moment of the line profile by a numerical calculation directly from the data gives reasonable results only for a Gaussian line shape. For $|t| \lesssim 5\times10^{-2}$, where $t = (T-T_c)/T_c$, the direct numerical integration leads to a miscalculation due to the arbitrary cutoff of a line profile which goes toward a Lorentzian. In this case it is not possible to perform a power-law fit with a minimum of consistency. This miscalculation was overcome by fitting to the experimental data an effective line shape of the type

$$F(H) = I_0 \frac{e^{-a^2(H-H_0)^2}}{b^2 + (H-H_0)^2} , \quad (2)$$

which goes to a Lorentzian profile for $a \to 0$.

The second moment of this effective line shape is given by

$$M_2 = \langle (H-H_0)^2 \rangle = b \frac{e^{-a^2b^2}/a\sqrt{\pi} - b[1-\Phi(ab)]}{1-\Phi(ab)} , \quad (3)$$

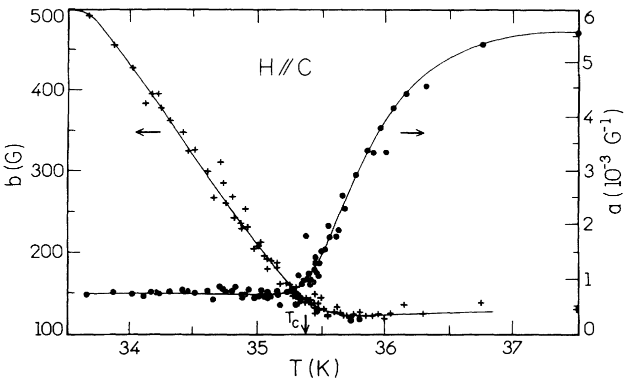

FIG. 2. Thermal variation of the fit parameters of the Gaussian-Lorentzian line profile. The dots represent the a term and crosses the b term. The solid lines are guides for the eyes.

where $\Phi(ab)$ is the error function.

We have assumed that the second moment of the line profile scales with the sublattice magnetization in all regions of temperature (random exchange, random field, and well above T_c), from 10 to 40 K, approximately.

In Fig. 2 we show the thermal variation of the fitting parameters a and b for $|t| \lesssim 5\times10^{-2}$. For $T \gtrsim 35.7$ K, since the Lorentzian parameter b is a constant, the changes in the line profile are given essentially by the Gaussian parameter a. For $T \lesssim 35.4$ K the Gaussian parameter is a constant, and so the changes in the line profile are then given by the Lorentzian parameter. It should be noted that these results are consistent with the experimental data for the relation $(\Delta H_{1/4}/\Delta H_{1/2})^2_{\parallel}$, as shown in Fig. 1.

First, consider the behavior below the critical temperature.

(i) $T<T_c$ (with $|t|>3\times10^{-2}$). For the region well below T_c, the line is Gaussian and the line-profile second moment $\sqrt{M_2}$ was obtained from a direct integration from the experimental data. In a log-log plot, $\sqrt{M_2}$ vs $|t|$ is shown in Fig. 3, for $T_c=35.395$ K. To perform the power-law fit ($\sqrt{M_2}=m_0|t|^{\beta}$), we have chosen data between two temperatures, $T_{\rm near}=34.4$ K and $T_{\rm far}=10$ K (top arrows in Fig. 3). A good fit to the experimental data is obtained with $\beta=0.351$. In order to verify the consistency of this result, we have performed several fits, changing the values of $T_{\rm near}$ and $T_{\rm far}$. In the inset we show these fits as a function of the fitting range $\tau=(T_c-T_{\rm near})/(T_c-T_{\rm far})$ for three different values of T_c. For $T_c=35.395$ and 35.45 K, the β values are not too sensitive to the choice of T_c. The average value is $\beta=0.348\pm0.010$, in good agreement with the predictions for the random-exchange Ising model (REIM) and with other experimental values listed in Table I of Ref. 3.

(ii) $T<T_c$ (with $|t|<3\times10^{-2}$). As stated before, in the random-field region, we have used the effective line shape, given by Eq. (2), to obtain the second-moment line profile.

In Fig. 4(a) we show $\sqrt{M_2}$ vs $|t|$ in a log-log scale, with $T_c=35.395$ K, for $\tau=(T_c-T_{\rm far})/(T_c-T_{\rm near})=159$. The solid line represents a reasonably good power-law fit

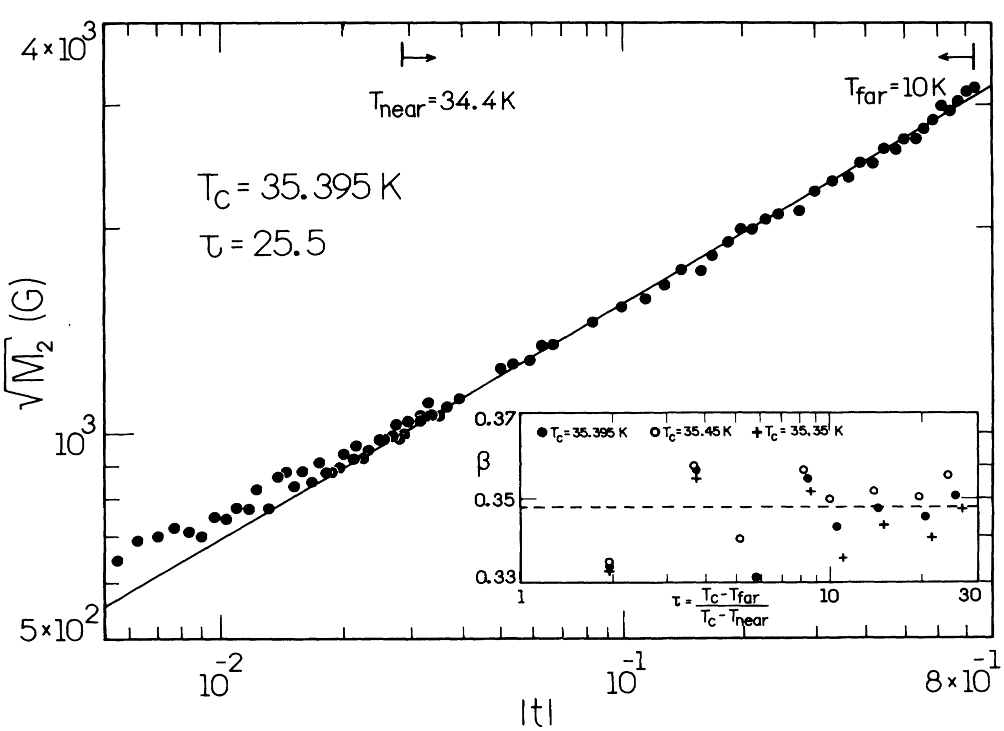

FIG. 3 $\sqrt{M_2}$ vs $|t|$ log-log plot, for $T_c=35.395$ K and $\tau=25.5$. The solid line is the curve fit of $\sqrt{M_2}=m_0|t|^{\beta}$, with $\beta=0.351$. The inset shows β vs τ, in a semilog form for three different values of T_c. The dashed line is the average β value.

to the experimental data in the region $10^{-4} \le |t| \le 10^{-2}$, with $\beta = 0.121$. The β fluctuations as function of the range fit τ are shown in Fig. 4(b). The average value from these data is $\beta = 0.125 \pm 0.015$, in agreement with predictions for the random-field Ising model (RFIM).[3]

To see the dependence on the choice of the value of T_c, similar fits were done with T_c between 35.35 and 35.45 K. There is a discontinuity in the slope of the β-vs-T_c curve, as shown in Fig. 4(c). Thus the critical temperature was chosen as $T_c = 35.395 \pm 0.005$ K.

Let us consider the behavior above the critical temperature. Well above the critical temperature, the line-profile second moment exhibits a Curie-Weiss behavior,

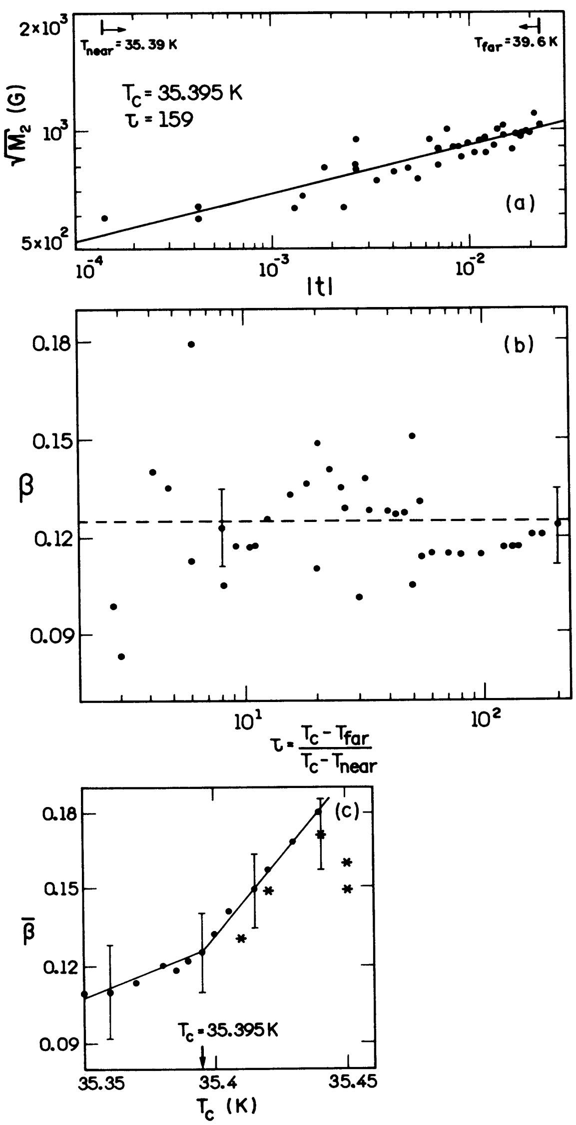

FIG. 4. (a) $\sqrt{M_2}$ vs $|t|$ log-log plot, for $T_c = 35.395$ K and $\tau = 159$. The solid line is the curve fit of $\sqrt{M_2} = m_0 |t|^{\beta}$, with $\beta = 0.121$. (b) A semilog plot of β vs τ. The dashed line is the average value. (c) Plot of β vs T_c. The solid lines are the linear fits, taking into account only the points marked by dots.

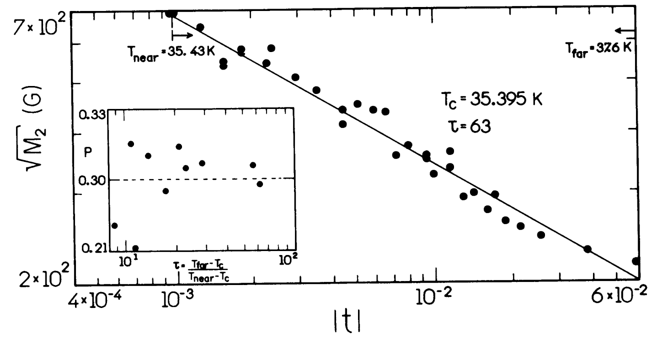

FIG. 5. $\sqrt{M_2}$ vs $|t|$ log-log plot, for $T_c = 35.395$ K and $\tau = 63$. The solid line is the curve fit of $\sqrt{M_2} = A|t|^{-p}$, with $p = 0.298$. The inset shows p vs τ in a semilog form. The dashed line is the average p value.

as already reported in Ref. 2. In the random-field region, Heller has proposed a model[5,6] for the broadening of the NMR line of the nucleus in a random magnet for $T \to T_c$ (with $|t| \lesssim 10^{-2}$ at $H_0 \approx 20$ kG). His calculations for the second moment give

$$\begin{aligned} \langle (\delta H)^2 \rangle^{1/2} &= M_2^{1/2} \\ &= c(1-x)^{1/2} |t|^{-\nu(1-2\eta)/2} H \\ &= A|t|^{-p} , \end{aligned} \tag{4}$$

where ν is the correlation-function exponent, η is the correlation-length critical exponent, and x is the concentration. To compare Heller's prediction of the scaling of the square root of the line-profile second moment, obtained with the effective line shape, the experimental data were plotted in a log-log scale, shown in Fig. 5, for $T_c = 35.395$ K. A good fit to a straight line is found in the range $10^{-3} \le |t| \le 6\times10^{-2}$, with a slope $p = 0.298$ for $\tau = (T_{\text{far}} - T_c)/(T_{\text{near}} - T_c) = 63$. The p fluctuations in the choice of the range fit τ are shown in the inset. The average value of p is 0.300 ± 0.015, which can be compared with the predictions for the $d=3$ pure Ising model[3] ($p = 0.30$), for the REIM ($p = 0.32$), and for the RFIM ($p = 0.25$). The improvement in these results, obtained with the effective line-shape function, can be checked against the results of a direct integration from the experimental lines, as shown in Fig. 3 of Ref. 2.

In conclusion, from our NMR measurements, we obtain a critical exponent β, indicating the crossover from the behavior of a random-exchange to the behavior of a random-field Ising model. Instead of the expected random-field behavior, the test of Heller's model is compatible with an exponent for the pure three-dimensional Ising model.

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