Field dependence of the susceptibility maximum temperature in ferromagnets

J. Sznajd
Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wroclaw, Poland
(Received 14 March 2001; published 25 June 2001)

It is shown within the mean-field Landau's theory that if a ferromagnet in the presence of a magnetic field can be in a phase in which the magnetization is parallel to the field, the susceptibility has a maximum at a point $t=t_h$ and under magnetic field (H) this point is shifted according to $H^{2/3}$. This 2/3 power law is independent of a spin model. The prediction of Landau's theory is examined on the one-dimensional quantum $S=1/2$ anisotropic Heisenberg model by using a linear real-space renormalization group. It has been found that for a longitudinal field only in the isotropic Heisenberg model the shift of the susceptibility maximum can be fitted satisfactory to a power law with exponent close to 2/3. In other cases the deviation from a single power law seems to be clear. On the other hand, for the field perpendicular to the easy axis the fit to a power law is excellent but a value of the exponent depends on the anisotropy constant.

DOI: 10.1103/PhysRevB.64.052401 PACS number(s): 75.10.Jm, 75.40.Cx

In a recent paper[1] Markovich, Rozenberg, Gorodetsky, Revzin, Pelleg, and Felner have shown experimentally that the electrical resistivity $\rho(T)$ of $La_{0.91}Mn_{0.95}O_3$ at ambient pressure and zero magnetic field reaches a maximum at $T_r=262$ K. Upon increasing field (H) the maximum widens and shifts towards higher temperature according to $H^{2/3}$. Assuming that the maximum of $\rho(T)$ coincides with maximum of magnetic susceptibility $\chi(T)$ the authors have attempted to explain this behavior by using a simple generalization of the Landau's theory for the anisotropic systems.[2,3] Indeed, it has been shown[2] that the susceptibility of a uniaxial ferromagnet in a transverse field reaches above the critical point a maximum which shifts according to $H^{2/3}$. However, it seems that the shift of the maximum $\chi(T)$ location according to the 2/3 *law* is more universal and to some extent does not depend on the symmetry of the system. This can support the Markovich *et al.*[1] idea to apply the relation derived, in fact, for a single crystal for the description of a polycrystalline ferromagnet.

In the first part of this paper it is shown that within Landau's theory the shift of $\chi(T)$ maximum under magnetic field according to the 2/3 law should be observed for all anisotropic ferromagnets which exhibit a phase transition to the paramagnetic phase as well as for isotropic ferromagnets in a field. In the second part the temperature dependence of the susceptibility of one-dimensional ferromagnets in a finite field will be studied by using real-space renormalization group.

Let us start with Landau's expansion for the reduced free energy of an anisotropic ferromagnet in a magnetic field,

$$f=f_o+(t-t_0)m^2+k_\alpha^{(1)}m_\alpha^2+bm^4+k_{\alpha,\beta}^{(2)}m_\alpha^2m_\beta^2-\vec{m}\vec{h}, \tag{1}$$

where t and h denote reduced temperature and field, respectively, m_α magnetization component, and $k^{(i)}$ anisotropy constants.

It is obvious that for an arbitrary symmetry of the system there are such directions of the magnetic field for which the magnetization is directed along the field at least in some temperature region. The simplest case is the field directed along an easy axis, for example, the Ising model in the longitudinal field or the Heisenberg model in any field where the magnetization is along the field at any temperature. For the anisotropic ferromagnets there are some additional directions in which directed external magnetic field does not destroy the phase transition from a phase with spontaneous long-range order to the phase with magnetization along the field[4,3,5]—the *paramagnetic phase*.

Landau's free energy of a ferromagnet with field in the paramagnetic phase can be written in the form

$$f=f_0+(t-t_k)m_h^2+bm_h^4-m_hh, \tag{2}$$

where t_k depends on the symmetry of the system and m_h denotes the magnetization component along the field. The necessary condition for the existence of the free energy (2) minimum is

$$2m_h[(t-t_k)+2bm_h^2]=h. \tag{3}$$

The magnetic susceptibility is given by

$$\chi(t)=\frac{1}{2(t-t_k)+6bm_h^2}, \tag{4}$$

and it reaches the maximum at

$$t=t_k+6bm_h^2. \tag{5}$$

Upon inserting Eq. (5) into Eq. (3) one obtains for the magnetization at the temperature $t=t_h$ at which the susceptibility reaches the maximum

$$m_h=\left(\frac{h}{16b}\right)^{1/3}, \tag{6}$$

and finally

$$t_h=A+Bh^{2/3}, \tag{7}$$

where

$$A=t_k,\quad B=\frac{3}{2}\left(\frac{b}{4}\right)^{1/3}. \tag{8}$$

In the particular case of the uniaxial ferromagnet in a transverse field[1,2] the paramagnetic phase is realized above the critical temperature $t > t_c(h)$,

$$t_c(h) = t_0 + k - 2b\left(\frac{h}{2k}\right)^2, \tag{9}$$

and the location of the $\chi(t)$ maximum is given by the formula (7) where $A = t_0$ and B is the same as in Eq. (8).

For the cubic ferromagnets in the external field along $\{100\}$ direction, described by the free energy

$$f = f_o + am^2 + bm^4 + k_4(m_x^4 + m_y^4 + m_z^4) - m_x h, \tag{10}$$

the critical temperature is given by the relation[3]

$$t_c(h) = t_0 - 2b\left(\frac{h}{4k_4}\right)^{2/3}, \tag{11}$$

and the shift of the location of the susceptibility maximum under magnetic field has again the form (7) with

$$A = t_0, \quad B = \frac{3}{2}\frac{3b + k_4}{(5b + 2k_4)^{2/3}}. \tag{12}$$

Though the shift of the critical temperature depends on the symmetry; uniaxial or cubic, and it is defined by the exponents 2 or 2/3, respectively, the shift of the location of the $\chi(t)$ maximum is in some sense universal (2/3 law for both cases).

In summary of this part *within the mean-field Landau's theory* if a ferromagnet in the presence of the external magnetic field can be in the paramagnetic phase, then the susceptibility has a maximum at the point $t = t_h$ and under magnetic field (h) this point is shifted according to $h^{2/3}$. This 2/3 power law is universal with respect to a model (Ising, XY, Heisenberg, cubic) and, of course, with respect to the lattice dimensionality.

In the remainder of this paper the Landau's theory prediction will be analyzed by using the real-space renormalization group (RSRG). The RSRG is, first of all, a powerful tool to study universal properties near a critical point, however, it can be also used to calculate thermodynamic quantities such as specific heat or susceptibility over the entire temperature range. The linear RSRG methods have been applied to study a temperature dependence of the free energy and specific heat of one- and two-dimensional quantum spin systems at zero magnetic field in Refs. 6 and 7. Below we consider one-dimensional $S = 1/2$ anisotropic Heisenberg model defined by the Hamiltonian

$$H = \sum_{\alpha = x,y,z} K_\alpha \sum_i S_i^\alpha S_{i+1}^\alpha + h\sum_i S_i^x, \tag{13}$$

where S_i^α denotes αth spin operator component at ith site of a chain, and the factor $-1/k_B T$ has already been absorbed in the Hamiltonian. Hereafter the reduced temperature is defined by $t = k_B T/K_{max}$, where K_{max} is the largest interaction K_α. Of course for the one-dimensional system there is no long-range order for any finite temperature and the magnetization is directed along the field for arbitrary small field strength. Thus for $T > 0$ a spin chain with arbitrary anisotropy is in the paramagnetic state. As mentioned above, within the Landau's theory the susceptibility of such a system should have a maximum which shifts according to $h^{2/3}$.

Dividing the Hamiltonian (13) into four-spin clusters and considering only one cluster we can find the renormalized interaction by using the following linear RSRG transformation (decimation):[6,7]

$$e^{H'(\vec{\sigma}_1,\vec{\sigma}_2)} = \frac{1}{4}\mathrm{Tr}_{\vec{S}}(1 + \vec{\sigma}_1\vec{S}_1)(1 + \vec{\sigma}_2\vec{S}_4)e^{H_0(\vec{S})}. \tag{14}$$

The renormalized Hamiltonian H' has the same form as original Hamiltonian H for new spin operators $\vec{\sigma}$ with new parameters K'_α and h':

$$K'_x = \frac{1}{4}(\lambda_4 + \lambda_3 - \lambda_2 - \lambda_1),$$

$$K'_y = \frac{1}{4}\left[\lambda_1 - \lambda_2 + \frac{1}{r}(f_y - f_z)(\lambda_3 - \lambda_4)\right],$$

$$K'_z = \frac{1}{4}\left[\lambda_1 - \lambda_2 - \frac{1}{r}(f_y - f_z)(\lambda_3 - \lambda_4)\right], \tag{15}$$

$$h' = \frac{1}{r}f_h(\lambda_3 - \lambda_4),$$

where

$$\lambda_{1,2} = \ln(a_0 - f_x \pm f_y \pm f_z),$$

$$\lambda_{3,4} = \ln(a_0 + f_x \pm r), \tag{16}$$

and

$$a_0 = \frac{1}{4}\mathrm{Tr}_{\vec{S}} e^{H_0(\vec{S})}, \quad f_\alpha = \frac{1}{4}\mathrm{Tr}_{\vec{S}} S_1^\alpha S_4^\alpha e^{H_0(\vec{S})},$$

$$f_h = \frac{1}{4}\mathrm{Tr}_{\vec{S}} S_1^x e^{H_0(\vec{S})}, \quad r = \sqrt{(f_y - f_z)^2 + 4h^2}. \tag{17}$$

As usual, in each step of the transformation a constant term independent of σ^α appears,

$$G(K_i, h) = \frac{1}{4}(\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4), \tag{18}$$

and the free energy per site can be calculated by using the formula[8]

$$f = \sum_{n=1}^{\infty}\frac{G(K_i^{(n)}, h^{(n)})}{3^n}. \tag{19}$$

For the Ising spin chain in a longitudinal field, i.e., for $K_y = 0$ and $K_z = 0$ the decimation procedure (14) can be carried out exactly and, consequently, the transformation (15)–(17) leads to the exact result for the free energy. For a quan-

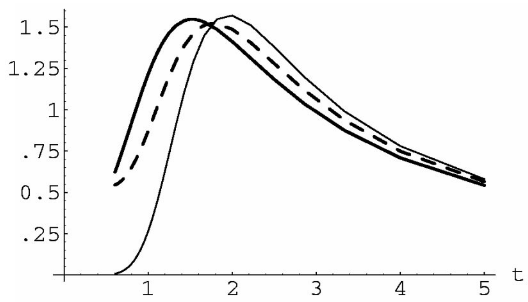

FIG. 1. The susceptibility of the Ising (thin line), Heisenberg (solid line), and XY (dashed line) models in the presence of the magnetic field $h=0.5$.

tum system, because of the noncumutativity of several terms of the Hamiltonian (13) the decimation cannot be, of course, carried out exactly and the transformation (15)–(17) is only an approximation. However, the result of this approximation leads to reasonable values of the free energy of the one-dimensional quantum anisotropic Heisenberg model in the free-field case, especially in the high-temperature region.[6,7]

Using the formulas (15)–(18) one can easily find numerically the free energy and other thermodynamic quantities of the models described by the Hamiltonian (13). We will calculate the magnetic susceptibility $\chi=\delta^2 f/\delta h^2$ for special cases of (i) $K_x=K_y=K_z$ isotropic Heisenberg model; (ii) $K_x=K_y$, $K_z=0$ XY model with field in the plane; (iii) $K_x>K_y=K_z$ uniaxial ferromagnet with field parallel to the easy axis; (iv) $K_x=K_y<K_z$ uniaxial ferromagnet with field perpendicular to the easy axis. In Fig. 1 the susceptibility of the Heisenberg (i) and XY (ii) quantum models in the presence of the external magnetic field is presented and compared with the known exact result for the Ising model in the longitudinal field.

Figure 2 shows the susceptibility of the $S=1/2$ Heisenberg model for several values of the magnetic field. According to the exact result,[9] for $h=0$ the susceptibility starts from infinity and decreases monotonically as the temperature increases. For $h\neq 0$ the susceptibility starts from zero and has a maximum which decreases, widens, and shifts to higher temperatures with increasing field. This is a characteristic behavior of the susceptibility of ferromagnets in the field parallel to the easy axis (longitudinal susceptibility). The dependence of the susceptibility maximum location t_h on the

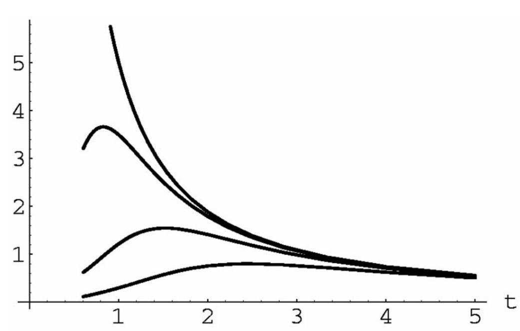

FIG. 2. The susceptibility of the Heisenberg model. The curves from bottom to the top are for $h=1$, 0.5, 0.2, and 0, respectively.

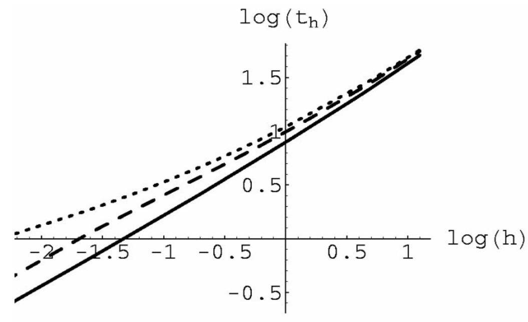

FIG. 3. Log-log plot of the field dependence of the susceptibility maximum location for: Ising (dotted line), XY (dashed line), and Heisenberg (solid line) models.

longitudinal external field for Ising, XY, and Heisenberg models is presented in log-log plot of Fig. 3. From Fig. 3, we see that only in the case of the isotropic Heisenberg model the results can be fitted satisfactory to a power law $t_h \propto h^{\upsilon}$ with $\upsilon\approx 0.696$ for $0.1<h<5$. In the other cases, Ising and XY models, the deviation from the single power law is rather clear. The same behavior is observed for the uniaxial ferromagnet with the field along the easy axis (see Fig. 6).

In case (iv), perpendicular susceptibility of the uniaxial ferromagnet in zero field, starts from finite value $\chi_o=(1-\Delta)^{-1}$ (in the limiting case of $\Delta\rightarrow 0$, the Ising model, χ_o tends to 1[9]) and has a maximum at t_o (see Fig. 4). For the finite field this maximum initially increases and shifts to lower temperatures but then, similarly as for the longitudinal susceptibility, decreases, widens, and shifts to higher temperatures with increasing field (Fig. 5). The field dependence of the susceptibility maximum location t_h-t_o of the uniaxial ferromagnet with longitudinal and transverse fields is presented in the log-log plot of Fig. 6. For the longitudinal susceptibility, the location of the maximum in zero field $t_o=0$ whereas for the transverse susceptibility t_o depends on the anisotropy constant Δ and, for example, for $\Delta=0.95$ and 0.9, $t_o=0.13$ and 0.217, respectively. It is clear from Fig. 6 that, contrary to the longitudinal susceptibility, the shift of the transverse susceptibility maximum can be described by the power law $t_h-t_o\propto h^{\upsilon}$. However, the exponent υ depends on Δ, and for $\Delta=0.95$ and 0.9, $\upsilon=0.776$ and 0.834, respectively.

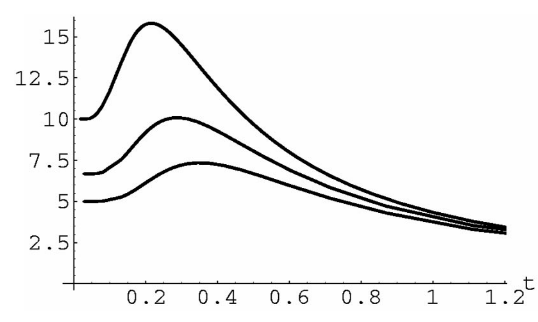

FIG. 4. The temperature dependence of the zero-field perpendicular susceptibility of the one-dimensional uniaxial ferromagnet. The curves from bottom to the top are for $\Delta=K_x/K_z=0.8$, 0.85, and 0.9, respectively.

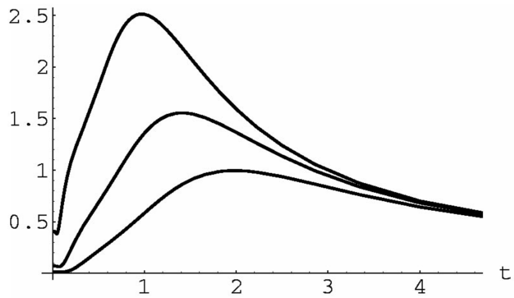

FIG. 5. The temperature dependence of the susceptibility of the one-dimensional uniaxial ferromagnet ($\Delta=0.9$) with perpendicular field. The curves from bottom to the top are for $h=0.8$, 0.5, and 0.3, respectively.

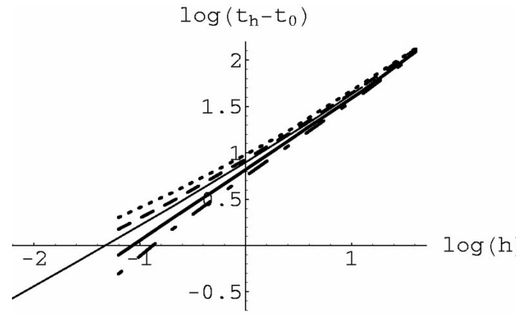

FIG. 6. Log-log plot of the field dependence of the susceptibility maximum location for: uniaxial Heisenberg with longitudinal field: $K_y=K_z=0.9K_x$ (dashed line); $K_y=K_z=0.7K_x$ (dotted line); uniaxial Heisenberg with transverse field; $K_x=K_y=0.95K_z$ (solid line); $K_x=K_y=0.9K_z$ (dashed-dotted line); and isotropic Heisenberg (thin line) models.

In conclusion, the existence of the susceptibility maximum in the paramagnetic phase of ferromagnets in the field is not, of course, connected with the critical fluctuations, so one should not expect a universal behavior—interaction-independence of the exponent υ. From the same reason the influence of the lattice dimensionality should not be so crucial as in the case of the critical behavior. Thus we can conclude that the shift of the transverse susceptibility of the uniaxial ferromagnet under magnetic field follows the power law with the exponent υ close to 2/3 for $\Delta\to 0$, and υ slowly increases with increasing anisotropy.

This paper has been motivated by the paper of Markovich *et al.*[1] who have shown experimentally that the shift of χ maximum in $La_{0.91}Mn_{0.95}O_3$ at applied field follows the 2/3 power law in accordance with Landau's theory. However, the authors have pointed out that the anisotropy in manganites is rather small and magnetic fields used in the experiment were relatively high, and under these circumstances the results of the RSRG for one-dimensional system are consistent with the Landau's theory predictions.

[1] V. Markovich, E. Rozenberg, G. Gorodetsky, B. Revsin, J. Pelleg, and I. Felner, Phys. Rev. B **62**, 14 186 (2000).
[2] J. Sznajd, Acta Phys. Pol. A **40**, 687 (1971).
[3] J. Sznajd, Acta Phys. Pol. A **47**, 61 (1975).
[4] H. Thomas, Phys. Rev. **187**, 630 (1969).
[5] G. Ritter and J. Sznajd, Acta Phys. Pol. A **58**, 283 (1979).
[6] H. Takano and M. Suzuki, J. Stat. Phys. **69A**, 426 (1979).
[7] J. Sznajd and M. Dudziński, J. Phys. Stud. **3**, 370 (1999); J. Sznajd, Phys. Rev. B **63**, 184404 (2001).
[8] M. Nauenberg and B. Nienhuis, Phys. Rev. Lett. **33**, 1598 (1974).
[9] S. Katsura, Phys. Rev. **127**, 1508 (1962).