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PHASE TRANSITION IN A COMPRESSIBLE ISING FERROMAGNET

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Within the droplet model for the Ising spin system it is shown that the magnetic specific heat C_p and the susceptibility χ_p for constant vanishing pressure and magnetic field remain finite in a compressible lattice as the critical point T_c is approached from below. This regularization of C_p and χ_p is caused by the long-range indirect spin-spin interaction, which is a consequence of the dependence of the exchange integral on the lattice spacing.

It was pointed out by Fisher[1] that constrained "hidden" variables (e.g., impurity density, elastic degrees of freedom) renormalize the critical exponents of a system undergoing a second-order phase transition. In this note we examine the effect of elasticity on the nature of the Curie point in an Ising ferromagnet with a compressible harmonic lattice. The hidden variables in this case are the deviations $u_\mu{}^m$ ($m = 1, \cdots, N$; $\mu = x, y, z$) of the mth atom from its rest position $\vec{R}^m$. The $\vec{R}^m$ are determined from the minimum of the lattice potential energy. A spin variable $\sigma^m = \pm 1$ is attached to the mth atom. External mechanical forces $\vec{K}^m$ enter the Hamiltonian via a term $-\vec{u}^m \cdot \vec{K}^m$ (summation over repeated indices is implied). If the thermal averages $\langle \vec{u}^m \rangle$ are constrained by prescribing a strain tensor $\epsilon_{\mu\nu} = \epsilon\delta_{\mu\nu}$, where $\langle u_\mu{}^m \rangle = \epsilon_{\mu\nu} R_\nu{}^m$, then, according to Fisher's theory, one expects that the specific heat C_v for constant ϵ (i.e., for constant volume V) remains finite at the Curie point, displaying a cusp-shaped maximum at T_c. The magnetic susceptibility χ_v at constant V should still diverge, but also has a renormalized exponent. The basic hypothesis made in the theory is that for constant forces $\vec{K}^m$, C_K and χ_K behave "ideally", as in a rigid lattice.[2] For example, it is assumed that $C_K \propto (T_c - T)^{-\alpha'}$ for $T \to T_c - 0 \equiv T_c{}^-$, with $\alpha' \approx \frac{1}{16}$, as is obtained from exact series expansion methods.[3]

In contrast to this hypothesis we find that C_K and χ_K remain finite in the compressible Ising ferromagnet as $T \to T_c{}^-$. Specifically, we start from an Ising model for spins on a simple cubic lattice, with an exchange integral acting only between nearest-neighbor (nn) spins and depending on the distance between them. For simplicity we consider only the case[4] $\vec{K}^m = 0$. In the Hamiltonian $H = H_L + H_S + H_{SL}$, H_L describes harmonic phonons, H_S the Ising spin system, and H_{SL} is the spin-lattice interaction, which is obtained by expanding the exchange integral in powers of $\vec{u}^m$ and keeping only the linear terms:

$$H_{SL} = -u_\mu{}^m (\nabla_\mu{}^m J^{mn}) \sigma^m \sigma^n \equiv -u_\mu{}^m F_\mu{}^m, \tag{1}$$

with $J^{mn} = J(|\vec{R}^m - \vec{R}^n|) = J(a) > 0$. The coupling term (1) can be transformed into an indirect spin-spin interaction with the help of the unitary transformation $A\vec{u}^m A^\dagger = \vec{u}^m + \vec{v}^m$, where $v_\mu{}^m = -D_{\mu\nu}{}^{mn} F_\nu{}^n$. The $D_{\mu\nu}{}^{mn}$ is the static one-phonon Green function of the lattice, described by H_L, and may be expressed in terms of the frequencies $\omega_j(\vec{q})$ and polarization vectors $\vec{e}^j(q)$ of the normal modes with wave vector $\vec{q}$, polarization index $j = 1, 2, 3$:

$$D_{\mu\nu}{}^{mn} = -\sum_j \int \frac{d\vec{q}}{(2\pi)^3} \frac{e_\mu{}^j(\vec{q}) e_\nu{}^j(\vec{q})}{\rho \omega_j{}^2(\vec{q})} e^{i\vec{q}(\vec{R}^m - \vec{R}^n)}, \tag{2}$$

where ρ denotes the mass density. The unitary transformation changes the form of the Hamiltonian into $H_A = H_L + H_S + H_S'$, where

$$H_S' = \tfrac{1}{2} F_\mu{}^m D_{\mu\nu}{}^{mn} F_\nu{}^n. \tag{3}$$

In H_A the spin system is formally decoupled from the lattice. $H_S + H_S' = H_S{}^{\text{eff}}$ can be considered as an effective Hamiltonian for spins on a rigid lattice in the (temperature-independent) configura-

tion $\{\vec{R}^m\}$. H_S' is an elastic energy due to the strains which are caused by the spin-lattice forces $\vec{F}^m$. This interaction between spin bonds was already obtained by Vaks and Larkin.[5] Its effect on the magnetic critical point was discussed by Pokrovskii,[6] using a cumulant expansion of the free energy and scaling-law arguments but neglecting its long-range part, which is, however, of decisive importance near T_c as we shall see.

The problem is now to calculate the spin free energy with the Hamiltonian H_S^{eff}. One might think of including H_S' in the numerical calculations of critical exponents using series expansions. We shall use a less ambitious approach which employs the droplet model approximation[3,7] for the free energy. First, two rigorous statements about H_S' can easily be verified: (i) $H_S' \times\{\sigma^m\} \leq 0$ for any spin configuration and (ii) $H_S'\{\uparrow\} = 0$ in the ferromagnetic ground state with all spins "up" ($\sigma^m = +1$). From this we conclude that H_S' opposes spin ordering and thus yields a reduction of the critical temperature. Consider now a spin configuration in which two localized clusters of down spins (one cluster centered at the origin, the other at $\vec{R}$) are embedded in a uniform sea of up spins. Each of these "droplets" is assumed to contain a large number $l^{(i)}$ ($i = 1, 2$) of down spins, such that their surface may be taken to be smooth on a macroscopic scale. The forces $\vec{F}^m$ due to nn spin bonds with $\sigma^m\sigma^n = -1$ are nonvanishing only near the surface of a droplet and are normal to it, with $\sum_m \vec{F}^m = 0$. The absolute value of the force on the mth atom with spin up (down) depends on the number and position of the nn down (up) spins. In a simple cubic lattice, $|\vec{F}^m(\partial J/\partial a)^{-1}|$ takes the values $0, 2, 2\sqrt{2}, 2\sqrt{3}$. We replace these microscopic forces by suitable averages, $\vec{F}(\vec{r}^{(1)}) \equiv \boldsymbol{F}^{(1)}$ and $\vec{F}(\vec{r}^{(2)} + \vec{R}) \equiv \vec{F}^{(1)}$ with $\sum_{r^{(i)}} \vec{F}^{(i)} = 0$, where $\vec{r}^{(i)}$ runs over the spin bonds which are cut by the surface of the ith droplet, and where $|\vec{F}^{(i)}| \equiv f|\partial J/\partial a|$, $f \gtrsim 2$. The energy of this spin configuration is $H_S^{\text{eff}} = E^{(1)} + E^{(2)} + E^{(1,2)}$, where $E^{(i)}$ are the "self-energies" of the droplets and $E^{(1,2)}$ is their interaction energy. If these droplets are far apart, $a \ll \max(|\vec{r}^{(i)}|) \ll |\vec{R}|$, then we have

$$E^{(1,2)} = -\tfrac{1}{2} F_{\kappa\mu}^{(1)} [\nabla_\kappa \nabla_\lambda D_{\mu\nu}(\vec{R})] F_{\lambda\nu}^{(2)}, \tag{4}$$

where $F_{\kappa\mu}^{(i)} = \sum_{\vec{r}(i)} r_\kappa^{(i)} F_\mu^{(i)}$. In order to obtain a simple asymptotic expression for $D_{\mu\nu}(\vec{R})$ for large $|\vec{R}|$, we approximate ω_j^2 in (2) by $\sum_j \omega_j^2/3$. This average tends to $(q\bar{v})^2$ for $qa \ll 1$, where $\bar{v}$ is an average phonon velocity. We then get, for $|\vec{R}| \gg a$,

$$D_{\mu\nu}(\vec{R}) \to -\delta_{\mu\nu}(4\pi\rho\bar{v}^2|\vec{R}|)^{-1}. \tag{5}$$

For closed surfaces the "force dipoles" $F_{\kappa\mu}^{(i)}$ are proportional to $\delta_{\kappa\mu}$. From this, together with (5) and (4), one finds that the long-range part of $E^{(1,2)}$ vanishes. The self-energy of a spherical cluster with radius $r \gg a$, containing $l \approx (4\pi/3)(r/a)^3$ down spins, is found to be

$$E_l = [(36\pi)^{1/3} 2J - b']l^{2/3} + bl^{1/3}, \tag{6}$$

with

$$b = (36\pi)^{2/3}(\gamma_M f J)^2 n\kappa^0, \tag{7}$$

where $\gamma_M = (V/J)\partial J/\partial V$. We also put $M\bar{v}^2 = (n\kappa^0)^{-1}$, where M denotes the atomic mass, n the particle density, and κ^0 the compressibility of the harmonic lattice (without spin-lattice coupling). In (6), the first term in brackets is the surface energy of the droplet as is obtained from H_S. The term $-b'l^{2/3} + bl^{1/3}$, with $b, b' \geq 0$, arises from H_S'. The term $bl^{1/3}$ is entirely due to the long-range part of $D_{\mu\nu}$. No simple expression is found for b', which includes the short-range part of $D_{\mu\nu}$, but one can give arguments indicating that b' is of the order of b. For the following discussion, the crucial term in (6) will be $bl^{1/3}$.

In the droplet model, the spin free energy is approximated by the free energy of a "gas" of noninteracting globular droplets (of down spins). The difference, $\Delta G(T, B) = G(T, B) - G(0, B)$, of the total free energies per spin, including a magnetic field B (in "up" direction), is given by

$$\Delta G = -k_B T \sum_l \exp(-\varphi_l/k_B T) y^l), \tag{8}$$

with $y = \exp(-g\mu_B B/2k_B T)$. $\varphi_l = E_l - TS_l$ is the free energy of an l droplet. For E_l we insert Eq. (6), which differs essentially by the term $\propto l^{1/3}$ from the droplet energy in a rigid lattice. The entropy S_l is obtained from the statistical geometry of compact spin clusters. The counting arguments involved should be independent of whether the lattice is rigid or compressible. In our model the elasticity of the host lattice only causes a change in the energy ($H_S \to H_S^{\text{eff}}$) of the spin system. The spins are otherwise considered to be attached to a rigid lattice. The detailed form of the Hamiltonian does not enter into the usual expression[7] for the entropy, $S_l = k_B(sl^{2/3} - t \ln l + \ln q_0)$, which we therefore adopt also for the compressible lattice. In the case of a rigid lattice ($b, b' = 0$) the term $l^{2/3}$ in E_l and S_l is usually replaced by l^σ, $1 > \sigma > 0$. Extending the

arguments given[7,8] for this generalization, we also replace $l^{1/3}$ in Eq. (6) by l^{λ}, assuming only that $\sigma > \lambda > 0$. Taken together, we arrive at

$$\Delta G = -k_B T q_0 \sum_l l^{-\tau} w^{l^{\lambda}} x^{l^{\sigma}} y^l, \quad (9)$$

with $w = \exp(-b/k_B T)$, $x = \exp[s(T-T_c)/T]$, and $2(36\pi)^{1/3} J - b' = s k_B T_c$.

The droplet model is supposed to provide a reasonable picture of the spin system at low temperatures. Its validity near T_c is less obvious but will be postulated. In the case $\gamma_M = 0$ ($w = 1$, rigid lattice) one then obtains, as is well known,[3,7] the ideal critical exponents expressed in terms of σ and τ, e.g., $\alpha' = 2-(\tau-1)/\sigma$. In the present case, $\gamma_M \neq 0$ ($w < 1$, compressible lattice), one easily verifies that the analytic properties of ΔG, Eq. (9), are identical to those obtained for a rigid lattice, except at the critical point, $B = 0$, $T = T_c^-$, where all derivatives of ΔG with respect to T and B remain finite. This is so because the sums over l occurring in these derivatives at $B = 0$ are convergent for $T \to T_c^-$, since $w < 1$. At the critical point, ΔG still has an essential singularity, the sum over l in (9) being divergent for $T > T_c$, even with $w < 1$.

Let us look in more detail at the specific heat. We emphasize that the derivatives of ΔG with respect to T and B are evaluated for constant external forces $\vec{K}^m = 0$. Thus, $-T^{-1}\partial^2 \Delta G/\partial T^2 = C_K$ is the specific heat per spin for constant vanishing[2,4] pressure. The singular part of C_K (strictly singular only if $\gamma_M = 0$) is given by

$$C_K^{\,\mathrm{sing}} \propto t^{-\alpha'} \int_{+0}^{\infty} dx\, x^{2\alpha'-1} \exp(-x^2 - \zeta x^{2\lambda/\sigma}), \quad (10)$$

where $t = (T_c - T)/T_c$ and $\zeta^{-1} = (st)^{\lambda/\sigma} k_B T_c/b$. In (10) we have approximated the sum over l by an integral. Its extension to the lower limit, +0, is convenient and does not change the leading temperature dependence of C_K as $t \to 0$. For convenience we now put $\sigma = 2\lambda$. Then the integral in (10) may be expressed in terms of parabolic cylinder functions. We shall give only the asymptotic expansions for large and small values of the parameter ζ:

$$\underline{\zeta \ll 1}: \quad C_K^{\,\mathrm{sing}} \propto t^{-\alpha'}\left[1 - \frac{\Gamma(\frac{1}{2}+\alpha')}{\Gamma(\alpha')} \frac{b}{k_B T_c} (st)^{-1/2} + O(t^{-1})\right]; \quad (11a)$$

$$\underline{\zeta \gg 1}: \quad C_K^{\,\mathrm{sing}} \propto 1 - 2\alpha'(1+2\alpha')(k_B T_c/b)^2 st + O(t^2). \quad (11b)$$

In (11a), Γ denotes the Gamma function.

From (11a, b) we get the following results: (i) For $t \gg t_c \equiv (b/k_B T_c)^2/s$, the specific heat behaves like in a rigid lattice, $C_K^{\,\mathrm{sing}} \propto t^{-\alpha'}$, with $\alpha' = 2-(\tau-1)/\sigma$ and b given by Eq. (7). s is a number $O(1)$; see below. (ii) For $t \ll t_c$, $C_K^{\,\mathrm{sing}}$ approaches a finite value, linearly in t, as $t \to 0$.

In order to get an idea about the size of t_c we use[3] $J = 0.4 k_B T_c$ (our J is equal to $J_{\parallel}$ of Ref. 3), neglecting the shift b' of the critical temperature. From $s k_B T_c \approx 10J$ we then find $s \approx 4$. Taking $f = 2.5$, we have $t_0^{1/2} \approx 12 \gamma_M^2 k_B T_c n \kappa^0$. The choice $\gamma_M = 1$, $T_c = 100°\mathrm{K}$, $n = 10^{22}\ \mathrm{cm}^{-3}$, and $\kappa^0 = 10^{-12}$ cm/dyn yields $t_0 \approx 3 \times 10^{-6}$. This value is only illustrative,[9] the important point being the strong dependence of t_0 on γ_M.

A similar behavior is found for the susceptibility: $\chi_K \propto t^{-\gamma'}$, for $t \gg t_0$ with $\gamma' = (3-\tau)/\sigma$, and $\chi_K \approx$ const for $t \ll t_0$.

Unfortunately, the droplet model in its present form does not allow us to draw any quantitative conclusion for $T > T_c$. But the underlying picture of the effect of H_S' on critical behavior is more generally valid. $H_S^{\,\mathrm{eff}}$ can be written as an Ising Hamiltonian with an nn exchange coupling J^{eff} depending on the spin configuration $\{\sigma^m\}$. This might be interpreted as follows: Spin-lattice forces, due to fluctuations in the spin bonds, cause inhomogeneous strains in the lattice which modulate J^{eff}, i.e., $T_c^{\,\mathrm{eff}}$. A spatial distribution of values of $T_c^{\,\mathrm{eff}}$ leads to a smearing out of critical singularities. Clearly, these considerations also apply to the paramagnetic critical region.

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[1] M. E. Fisher, Phys. Rev. 176, 257 (1968).

[2] C_K is identical to C_p for constant pressure only if $\vec{K}^m = 0$, i.e., $p = 0$, because of thermal expansion. Thus, for $p \neq 0$, C_p should be renormalized like C_v; see G. A. Baker and J. W. Essam, Phys. Rev. Lett. 24, 447 (1970); J. Swift and H. Wagner, to be published. Note that ("anomalous") thermal expansion exists even in a harmonic lattice with spin-lattice coupling, being proportional to the internal spin energy.

[3] For a review see M. E. Fisher, Rep. Progr. Phys. 30, 615 (1967).

[4] The generalization of this model to $\vec{K}^m \neq 0$ is discussed in Swift and Wagner, Ref. 2, in which elastic constants near T_c are studied. The conslusions in the present note remain valid if $\vec{K} \neq 0$.

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[6] V. L. Pokrovskii, Fiz. Tverd. Tela 10, 3694 (1968) [Soviet Phys. Solid State 10, 2852 (1969)].

[7] M. E. Fisher, Physics 3, 255 (1967), and references therein.

[8] It is conceivable that the parameters λ, σ, τ, s, and q_0 depend on γ_M, and that λ and σ differ slightly from

the naive values $\frac{1}{3}$ and $\frac{2}{3}$ due to the residual interaction between droplets (excluded-volume effects, short-range part of $E^{(1,2)}$).

[9]Numerical computation of the integral in Eq. (10) shows that $\ln C_K^{\text{sing}}$ begins to deviate from the straight line $-\alpha' \ln t$ at $t \approx 10 t_0$ and is nearly independent of $\ln t$ for $t \lesssim 10^{-1} t_0$. The author is indebted to Dr. H. Horner for help in these calculations.

PROTON-PROTON SCATTERING AT 9.690, 9.918, AND 13.600 MeV†

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Adjustments to proton-proton elastic scattering data at 9.690 and 9.918 MeV have apparently resolved a discrepancy between the data and current energy-dependent phase-shift analyses. New data at 13.600 MeV are also presented and are compatible with the phenomenological analysis. These results indicate that the energy-dependent fitting of $p+p$ data in the region of 10 MeV is now satisfactory.

A strong discrepancy in the phenomenological analysis of proton-proton scattering near 10 MeV has been pointed out by Holdeman, Signell, and Sher[1] (HSS). They indicate that the consensus of experimental information[2-4] on scattering cross sections near 10 MeV results in a $^1S_0$ phase that is markedly below reasonable phenomenological predictions,[1,5] that in order to fit the data, serious readjustment of fits to a number of well-accepted data at other energies would be necessary (see Figs. 2 and 3 of Ref. 1).

To help resolve this discrepancy we undertook two courses of action. First, since the $^1S_0$ phase is strongly affected by the absolute values of the data, we planned a thorough examination and recalibration of all experimental parameters that affect the absolute normalization in our previous measurements[2] at 9.690 and 9.918 MeV. We also restudied the assumptions and approximations made in the reduction of the data, especially at small angles. Secondly, we measured an accurate angular distribution at a nearby energy (13.6 MeV) to help tie down the absolute value and search for possible energy-dependent systematic errors.

With one exception, the recalibrations and remeasurements produced no significant results outside expected errors. We did find a gross systematic error in the device used to measure the width of the slits in the detector; and the value of the G factor and the cross sections are directly affected. The correction increases the absolute values about 2%; the final corrected values are given in Table I. As can be seen in Fig. 3 of Ref. 1, this correction brings our absolute values close to the predicted values of the multi-energy analysis of Sher, Signell, and Heller.[6] The error of the absolute scale is slightly smaller because of an improved method of slit measurement. The relative relation of the values and the relative errors have not changed.

The experimental method used for the 13.600-MeV data given in Table II is the same as presented in Ref. 2 except that the geometry-factor accuracy has been improved to ±0.20%.

Table I. Differential cross sections for $p+p$ elastic scattering.

9.918 MeV

θ_{lab} deg.	$\sigma(\theta)_{\text{lab}}$ mb/sr	$\theta_{\text{c.m.}}$ deg.	$\sigma(\theta)_{\text{c.m.}}$ mb/sr	Relative Error %	Absolute Error %
10.00	296.22	20.05	74.83	0.80	0.90
12.50	212.58	25.06	54.18	0.41	0.56
15.00	194.83	30.08	50.20	0.39	0.54
17.50	191.72	35.09	50.04	0.37	0.52
20.00	189.03	40.10	50.09	0.37	0.52
25.00	185.92	50.12	51.11	0.41	0.55
30.00	180.31	60.13	51.91	0.34	0.50
35.00	172.44	70.14	52.53	0.34	0.50
40.00	161.56	80.15	52.69	0.34	0.50
45.00	148.37	90.15	52.46	0.36	0.52
50.00	135.58	100.15	52.78	0.36	0.51

9.690 MeV

θ_{lab} deg.	$\sigma(\theta)_{\text{lab}}$ mb/sr	$\theta_{\text{c.m.}}$ deg.	$\sigma(\theta)_{\text{c.m.}}$ mb/sr	Relative Error %	Absolute Error %
13.00	215.29	26.06	54.98	0.41	0.55
15.00	201.79	30.07	51.99	0.39	0.53
20.00	196.07	40.09	51.96	0.36	0.52
25.00	192.56	50.11	52.94	0.40	0.54
30.00	186.90	60.13	53.82	0.41	0.55