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Exactly Soluble Magnetoelastic Lattice with a Magnetic Phase Transition

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We examine the soluble magnetoelastic Ising model developed by Baker and Essam and give a detailed discussion of its thermodynamic properties. Particular attention is devoted to the properties of the magnetic phase transition at zero field, which is found to be either first order or second order, depending on whether the experiment is performed at negative or positive pressure.

KEY WORDS: Magnetoelastic system; phase transition; renormalization of critical exponents; Ising model; statistical mechanics; soluble models; thermodynamics.

1. INTRODUCTION

When trying to understand the behavior of complicated physical systems one often tries to understand first the properties of a simplified model. Thus, magnetic systems have long been studied by investigating the properties of the Ising model, which is a rigid lattice model. This is clearly inadequate for describing the effects of the finite compressibility and the elastic degrees of freedom on magnetic properties.

In order to investigate these effects, various people[(1–7)] considered models

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where Ising spins are situated at the points of a compressible lattice. In order to calculate the partition function and consequently derive the thermodynamic properties of these models, these works resorted to various approximations. However, since one of the aims was to investigate the properties of the magnetic phase transition in compressible lattices, the fact that approximations which could not properly be justified had to be used was a serious drawback.

Baker and Essam[8] then developed the first soluble example of a compressible magnetic system: They considered a cubic lattice of Ising spins with elastic forces acting between nearest-neighbor spins in addition to the usual magnetic interaction. They assumed that no shear forces were present, and that both the elastic and the magnetic interactions of a nearest-neighbor pair depend only on the longitudinal component of the separation vector,

$$\xi_{ij} \equiv (\mathbf{r}_{ij} \cdot \mathbf{R}_{ij})/|\mathbf{R}_{ij}|$$

where $\mathbf{r}_{ij}$ is the actual instantaneous separation vector connecting the atoms at the pair of sites (ij), and $\mathbf{R}_{ij}$ is the equilibrium or rigid-lattice separation vector. They then found that they could reduce the classical statistical mechanics of this model to that of a rigid Ising lattice with an effective nearest-neighbor magnetic interaction coefficient J_{eff}. The original version of the Baker and Essam (henceforth to be abbreviated as BE) model assumed that the elastic interaction $\phi(\xi_{ij})$ was a quadratic function and that the magnetic interaction $J(\xi_{ij})$ was a linear function. Subsequently this was generalized by Coplan and Dresden[9] to include quadratic $J(\xi_{ij})$. The generalization to arbitrary $\phi(\xi)$ and $J(\xi)$ was recently made independently by Baker and Essam[10][4] and by Gunther.[11]

In Section 2 of this paper we present the statistical mechanics of this generalized Baker–Essam model in an ensemble (called the λ-ensemble) in which all calculations can be exactly reduced to the statistical mechanics of the rigid Ising model. Since the model is rather unphysical in that there are no shear forces at all to prevent large fluctuations in the shape, we proceed in Section 3 to discuss the question of the validity of the thermodynamic results obtained therefrom. We show that although the length of each row has abnormally large fluctuations in our ensemble, the volume in fact does not. We conclude therefore that the volume and the pressure can properly be used as thermodynamic variables to describe the state of the system. In Section 4 we calculate some of the interesting thermodynamic functions of the system, and show that Pippard's relations are satisfied. In Section 5 we discuss the changes in the nature of the magnetic phase transition of our model that arise due to the presence of elastic degrees of freedom. We find that, depending upon the externally imposed experimental conditions, the

[4] We received a preprint of this work while our work was being written.

transition either remains an "ideal" rigid Ising transition in the sense of Fisher[12] or becomes renormalized in the sense of Fisher,[12] or else gets changed into a first-order transition.[5]

More specifically, we find that if the experiment is performed at constant pressure P, then for $P > 0$ the transition is second-order renormalized, for $P < 0$ (which in our model system corresponds to perfectly stable states) the transition is first order, and for $P = 0$ the transition is second-order ideal. In Section 6 we calculate the discontinuities which characterize the first-order transition for $P < 0$ and determine their behavior (i.e., how they tend to zero) when P approaches zero.

The fact that, depending on the external conditions of the experiment, a compressible Ising lattice can have either a first- or a second-order transition has never been convincingly shown before. All previous approximate treatments of such systems which seemed to give rise to a first-order phase transition[1–5] are misleading because the approximations used always break down in the vicinity of the Ising singularity. Consequently, when applied to the Baker–Essam model they give wrong predictions regarding its first-order transition.

There is now convincing experimental evidence that the existence of first- and second-order variants of an Ising-like transition do in fact exist, namely the beautiful experiments on the order–disorder transition in solid NH_4Cl by Garland and Weiner.[14] The dividing point between the two regimes is, however, at a positive P. We expect that our finding that the dividing point is at $P = 0$ is a result of the unphysical nature of our model, namely the total absence of shear forces. Indeed, Baker and Essam[10] report that when infinitely strong shear forces are included in their model, a first-order transition occurs for all P, while when finite shear forces are included an approximate calculation leads to a division point at a finite, positive P. We have recently found that an anisotropic version of the Baker–Essam model can have the first-order transition at $P > 0$.

2. STATISTICAL MECHANICS OF THE GENERALIZED BAKER–ESSAM MODEL

Following Baker and Essam,[8] we assume a compressible Ising Hamiltonian of the form

$$H = \sum_i (P_i^2/2m) + \sum_{ij} [\phi(\xi_{ij}) + J(\xi_{ij})\, \sigma_i \sigma_j] + h \sum_i \sigma_i \tag{1}$$

In this equation the indices i, j refer to the points of a simple cubic d-dimensional lattice. The symbol $\sum_i$ stands for a sum over all the N points of the

[5] We have already reported this result briefly for a special case.[13]

lattice, while the symbol $\sum_{(ij)}$ stands for a sum over all nearest-neighbor pairs. With each lattice point is associated an Ising spin variable σ_i and a mass m, and nearest-neighbor points interact by means of both an elastic interaction ϕ and an Ising exchange interaction J. Both of these interactions depend only on the projection of the instantaneous vector separation $\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j$ of a nearest-neighbor pair onto the equilibrium vector separation $\mathbf{R}_{ij} \equiv \mathbf{R}_i - \mathbf{R}_j$. This variable is denoted by ξ_{ij}:

$$\xi_{ij} \equiv (\mathbf{r}_{ij} \cdot \mathbf{R}_{ij})/|\,\mathbf{R}_{ij}\,| \tag{2}$$

It is this property of the interactions which allows the statistical mechanics of the magnetoelastic system to be reduced to that of a similar rigid magnetic system. The physical meaning of this property is that there are no shear forces in the lattice, and that if there were no magnetic interactions, every row and column would be a one-dimensional chain whose statistical mechanics is independent of all the other rows and columns. Baker and Essam[8] originally introduced this model with a quadratic form for $\phi(\xi)$ and a linear form for $J(\xi)$. This was later generalized to a quadratic form for $J(\xi)$ by Coplan and Dresden,[9] who also used a different ensemble to get the thermodynamic properties of their model, and to general forms for both $\phi(\xi)$ and $J(\xi)$ by Baker and Essam[10] and independently by Gunther.[11] We will use the same ensemble employed by Coplan and Dresden, since it makes many results more transparent and easier to obtain than the one used by Baker and Essam.[8,10] For this reason, as well as for the sake of deriving some relations which we need, we now briefly describe the statistical mechanics of this model.

The absence of shear forces causes the system to show no resistance to sideways (i.e., shear type) deformations of its shape. In order to somewhat rectify this behavior, we nail down the first particle of each row and column so that its position is fixed. The average length of each row $\langle \sum_{(ij)\in r} \xi_{ij} \rangle$, where r denotes some row, is then determined by introducing an appropriate Lagrange multiplier λ_r into the statistical operator ρ:

$$\rho \sim \exp\left[-\beta\left(H + \sum_r \lambda_r \sum_{(ij)\in r} \xi_{ij}\right)\right] \tag{3}$$

The physical significance of λ_r is that it is equal to the force that one must exert upon the rth row in order to determine its average length. From the form of ρ it is clear that all the average separations $\langle \xi_{ij} \rangle$ that lie in a single row r of the lattice are equal—simply because ρ is symmetric in all of the ξ_{ij} that belong to a single row. To make our discussion even simpler, we will assume that the entire system is cubic (i.e., all the rows have the same number of particles $N^{1/d}$), and that all the rows in all directions have the same average length. Because we assumed identical elastic and magnetic interactions for all nearest-neighbor pairs, this means that all the λ_r are then equal. We thus obtain the "λ-ensemble," whose statistical operator is

$$\rho_\lambda \sim \exp\left[-\beta\left(H + \lambda \sum_{(ij)} \xi_{ij}\right)\right] \tag{4}$$

We now calculate the partition function Z for this statistical operator assuming, after Baker and Essam,[8] that the elastic degrees of freedom can be treated classically. The partition function can be written in the form

$$Z(\beta, \lambda, h) = (2\pi m/\beta)^{dN/2} \sum_{\{\sigma_i\}} \exp\left(-\beta h \sum_i \sigma_i\right) \prod_{(ij)} q_{ij} \tag{5}$$

where

$$q_{ij} \equiv \int_{-\infty}^{\infty} d\xi \exp\{-\beta[\phi(\xi) + \lambda\xi + J(\xi)\, \sigma_i\sigma_j]\} \tag{6}$$

and where $\prod_{(ij)}$ means a product over all nearest-neighbor pairs, while $\sum_{\{\sigma_j\}}$ stands for a sum over all the possible assignments of ± 1 to all of the σ_i. Since the product $\sigma_i\sigma_j$ can have only two values $+1$ and -1, we denote by $q_\pm$ the corresponding values of q_{ij}:

$$q_\pm(\beta, \lambda) \equiv \int_{-\infty}^{\infty} d\xi\, e^{-\beta(\phi+\lambda\xi\pm J)} \tag{7}$$

We can now write q_{ij} as follows:

$$q_{ij} = Ae^{-\beta J_{\text{eff}}\sigma_i\sigma_j} \tag{8}$$

where

$$A(\beta, \lambda) \equiv (q_+q_-)^{1/2} \tag{9}$$

$$J_{\text{eff}}(\beta, \lambda) \equiv -(1/2\beta) \log(q_+/q_-) \tag{10}$$

Note that J_{eff} is a perfectly regular function of λ and β. Therefore one can write Z in the form

$$Z = (2\pi m/\beta)^{dN/2} A^{dN} \sum_{\{\sigma_i\}} \exp\left(-\beta h \sum_i \sigma_i - \beta J_{\text{eff}} \sum_{(ij)} \sigma_i\sigma_j\right) \tag{11}$$

where the sum $\sum_{\{\sigma_i\}}$ is equal to $Z_I(\beta J_{\text{eff}}, h)$, the rigid Ising partition function with the magnetic interaction J_{eff}. One can rewrite this as

$$\log Z(\beta, \lambda, h) = \tfrac{1}{2}dN \log[(2\pi m/\beta)\, q_+q_-] + \log Z_I(\beta J_{\text{eff}}, h) \tag{12}$$

The average value of any dynamical variable of the form $\langle R(\xi_{ij})\rangle$ is calculated as follows:

$$\langle R(\xi_{ij})\rangle = (1/Q) \sum_{\{\sigma_l\}} \exp\left(\beta h \sum_l \sigma_l\right) \prod_{(mn)} q_{mn} \cdot \langle R\rangle_{ij} \tag{13}$$

where

$$Q \equiv \sum_{\{\sigma_l\}} \exp\left(\beta h \sum_l \sigma_l\right) \prod_{(mn)} q_{mn} \tag{14}$$

$$\langle R\rangle_{ij} \equiv (1/q_{ij}) \int d\xi\, R(\xi) \exp\{-\beta[\phi(\xi) + \lambda\xi + J(\xi)\, \sigma_i\sigma_j]\} \tag{15}$$

Similarly to q_{ij}, $\langle R\rangle_{ij}$ can also have only two values, $\langle R(\xi)\rangle_\pm$, where

$$\langle R(\xi)\rangle_\pm \equiv (1/q_\pm) \int d\xi\, R(\xi)\, e^{-\beta(\phi+\lambda\xi\pm J)} \tag{16}$$

$\langle R\rangle_\pm$ is clearly the average of $R(\xi_{ij})$, assuming that $\sigma_i\sigma_j = \pm 1$, respectively.

With the help of the two projection operators onto the two possible values of the product $\sigma_i\sigma_j$, namely

$$(1 \pm \sigma_i\sigma_j)/2 \tag{17}$$

we can write $\langle R\rangle_{ij}$ in the form

$$\langle R\rangle_{ij} = \langle R(\xi)\rangle_+[(1 + \sigma_i\sigma_j)/2] + \langle R(\xi)\rangle_-[(1 - \sigma_i\sigma_j)/2] \tag{18}$$

Consequently, the average $\langle R(\xi_{ij})\rangle$ will depend on $\langle\sigma_i\sigma_j\rangle$, which is equivalent to the simple rigid Ising average $\langle\sigma_i\sigma_j\rangle_\mathrm{I}$ but with the effective magnetic interaction coefficient J_eff. Hence we obtain

$$\langle R(\xi_{ij})\rangle = \langle R(\xi)\rangle_+[(1 + \langle\sigma_i\sigma_j\rangle_\mathrm{I})/2] + \langle R(\xi)\rangle_-[(1 - \langle\sigma_i\sigma_j\rangle_\mathrm{I})/2] \tag{19}$$

The two terms $\frac{1}{2}(1 \pm \langle\sigma_i\sigma_j\rangle_\mathrm{I})$ are obviously the average probabilities for finding $\sigma_i\sigma_j = \pm 1$. Thus, this formula has a very simple intuitive meaning—it is just an application of the usual theorems on conditional probability.

Similar considerations can be used to calculate $\langle S(\xi_{ij})\, \sigma_i\sigma_j\rangle$:

$$\begin{aligned}\langle S(\xi_{ij})\, \sigma_i\sigma_j\rangle &= \langle S(\xi)\rangle_+\langle\tfrac{1}{2}(1 + \sigma_i\sigma_j)\, \sigma_i\sigma_j\rangle_\mathrm{I} + \langle S(\xi)\rangle_-\langle\tfrac{1}{2}(1 - \sigma_i\sigma_j)\, \sigma_i\sigma_j\rangle_\mathrm{I} \\ &= \langle S(\xi)\rangle_+[(1 + \langle\sigma_i\sigma_j\rangle_\mathrm{I}/2] - \langle S(\xi)\rangle_-[(1 - \langle\sigma_i\sigma_j\rangle_\mathrm{I})/2]\end{aligned} \tag{20}$$

and this, too, is nothing more than a simple application of conditional probability.

3. RELIABILITY OF THE λ-ENSEMBLE

The main reason why we perform all the statistical mechanical calculations using the λ-ensemble is that only in this type of ensemble is the model we discuss rigorously reducible to the corresponding rigid model.[6] By

[6] Instead of the term $\lambda \sum_{(ij)} \xi_{ij}$, we could have added a more general type of term $\lambda \sum_{(ij)} f(\xi_{ij})$ to the exponent of the statistical operator without spoiling its solubility properties. Anything else will not do.

contrast, Baker and Essam have chosen to use a different ensemble in their calculations,[8,10] i.e., one where every row of atoms in the lattice is constrained to have a fixed length, rather than merely having its average length determined as in the λ-ensemble. Their partition function, however, is obtained by performing a saddlepoint integration over the λ-ensemble partition function. It is therefore perhaps no great wonder that similar results are obtained in both calculations. But since it is not superfluous to justify the use of saddlepoint integration in solving the model, we prefer to adhere to the simpler basic formalism of the λ-ensemble, and to show that the thermodynamic results obtained from it are expected to be reliable, i.e., that they will not change if a different but still reasonable ensemble is used.

The reliability of our thermodynamic results is open to doubt mainly due to the possibility of large fluctuations in the volume or shape.[7] We will therefore focus our attention on these aspects. Since there are no shear forces to resist shearing strains in the lattice, one might have expected to find enormous fluctuations in the shape of the system. These are largely prevented by nailing down the first atom of each row. In order to determine what still remains of these fluctuations, we first calculate some correlation functions:

$$\begin{aligned}\langle \Delta\xi_{ij}\Delta\xi_{kl}\rangle &\equiv \langle(\xi_{ij} - \langle\xi_{ij}\rangle)(\xi_{kl} - \langle\xi_{kl}\rangle)\rangle \\ &= (1/Q) \sum_{(\sigma_i)} \exp\left(-\beta h \sum_i \sigma_i\right) \prod_{(mn)} q_{mn}(\langle\xi\rangle_{ij} - \langle\xi_{ij}\rangle)(\langle\xi\rangle_{kl} - \langle\xi_{kl}\rangle) \\ &\qquad \text{for} \quad (ij) \neq (kl)\end{aligned} \tag{21}$$

Here we have introduced the notation $\Delta R \equiv R - \langle R\rangle$. Noting that, according to (18) and (19)

$$\langle\xi\rangle_{ij} - \langle\xi_{ij}\rangle = \tfrac{1}{2}(\langle\xi\rangle_+ - \langle\xi\rangle_-)\, \Delta(\sigma_i\sigma_j) \tag{22}$$

we easily find that

$$\langle \Delta\xi_{ij}\, \Delta\xi_{kl}\rangle = [\tfrac{1}{2}(\langle\xi\rangle_+ - \langle\xi\rangle_-)]^2 \langle \Delta(\sigma_i\sigma_j)\, \Delta(\sigma_k\sigma_l)\rangle_{\mathrm{I}} \quad \text{for } (ij) \neq (kl) \tag{23}$$

Using (19) to get $\langle\xi_{ij}^2\rangle$ and $\langle\xi_{ij}\rangle$, we can also find

$$\begin{aligned}\langle \Delta\xi_{ij}^2\rangle = {}& \langle\Delta\xi_+{}^2\rangle_+ [(1 + \langle\sigma_i\sigma_j\rangle_{\mathrm{I}})/2] + \langle\Delta\xi_-{}^2\rangle_- [(1 - \langle\sigma_i\sigma_j\rangle_{\mathrm{I}})/2] \\ &+ [\tfrac{1}{2}(\langle\xi\rangle_+ - \langle\xi\rangle_-)]^2 \langle\Delta(\sigma_i\sigma_j)^2\rangle_{\mathrm{I}}\end{aligned} \tag{24}$$

where

$$\Delta R(\xi)_\pm \equiv R(\xi) - \langle R(\xi)\rangle_\pm \tag{25}$$

[7] We are indebted to Michael E. Fisher for drawing our attention to this problem.

We can now calculate the mean square fluctuation in the length L of a single row:

$$\langle \Delta L^2 \rangle = \left\langle \Big(\sum_{(ij)\in r} \Delta\xi_{ij} \Big)^2 \right\rangle = [\tfrac{1}{2}(\langle\xi\rangle_+ - \langle\xi\rangle_-)]^2 \left\langle \Big(\sum_{(ij)\in r} \Delta(\sigma_i\sigma_j) \Big)^2 \right\rangle_{\mathrm{I}} + \sum_{(ij)\in r} \{\langle \Delta\xi_+^2 \rangle_+ [(1 + \langle\sigma_i\sigma_j\rangle_{\mathrm{I}})/2] + \langle \Delta\xi_-^2 \rangle_- [(1 - \langle\sigma_i\sigma_j\rangle)_{\mathrm{I}}/2]\} \tag{26}$$

On the rhs the second term is clearly of order $O(N^{1/d})$. This is also the size of the first term, notwithstanding the fact that it includes a double sum, because the correlation function

$$\langle \Delta(\sigma_i\sigma_j)\, \Delta(\sigma_k\sigma_l) \rangle_{\mathrm{I}} \tag{27}$$

where (ij), (kl) are nearest-neighbor pairs, is known to have a finite range for the two-dimensional Ising model, and is expected to have similar behavior for the Ising model in any number of dimensions. Thus, the mean square fluctuation of the length L of a row satisfies

$$\langle \Delta L^2 \rangle = O(L) \tag{28}$$

rather than

$$\langle \Delta L^2 \rangle = O(1) \tag{29}$$

which is what we would expect for a realistic system of dimensionality greater than one.

An important consequence of the previous considerations is that the correlations between different ξ_{ij} are short-ranged. This holds not only for the simple correlation given in (23), but for higher-order correlations as well.

We now define the volume of the lattice by

$$V \equiv \prod_{\alpha=1}^{d} \Big(N^{-(d-1)/d} \sum_i x_{\alpha i} \Big) = N^{-(d-1)} \prod_{\alpha=1}^{d} \sum_i x_{\alpha i} \tag{30}$$

where $x_{\alpha i}$ is a new notation for ξ_{ij} : It denotes ξ_{ij} for the case where the equilibrium separation vector $\mathbf{R}_{ij}$ lies along the positive α axis. From what we said previously, we can now estimate the difference between the average volume as defined in (30) and the much simpler expression $N\langle x \rangle^d$:

$$(1/N^{d-1}) \left\langle \prod_{\alpha=1}^{d} \sum_i x_{\alpha i} \right\rangle - (1/N^{d-1}) \prod_{\alpha=1}^{d} \left\langle \sum_i x_{\alpha i} \right\rangle \leqslant O(1) \tag{31}$$

Furthermore, we can estimate the mean square fluctuation of V:

$$(1/N^{2d-2}) \left\langle \Delta \Big(\prod_{\alpha=1}^{d} \sum_i x_{\alpha i} \Big)^2 \right\rangle = (1/N^{2d-2})\, O(N^{2d-1}) = O(N) \tag{32}$$

The last result is the usual one for $\langle \Delta V^2 \rangle$ and it means that the relative fluctuations in volume in the λ-ensemble are small and that the average volume has a well-defined value and is a perfectly respectable thermodynamic variable. Equation (31) tells us, in addition, that instead of the cumbersome expression (30), we can use $V = N\langle \xi \rangle^d$ for the average volume.

It is perhaps surprising that despite the abnormally large fluctuations in L [see Eq. (28)], the fluctuations in the total volume turn out to be perfectly normal. To see the reason for this, let us look more closely at the three-dimensional case. For a normal, realistic system the fluctuation in the length of a row is given by (29). But different rows are not independent in their fluctuations, due to the presence of shear forces in the system. In fact, from the Debye approximation for the long-wavelength part of the phonon spectrum one can show that the correlation function of the positions of two atoms in the system includes a long-range part:

$$\langle \Delta \mathbf{r}_i \, \Delta \mathbf{r}_j \rangle = O(1/|\, \mathbf{r}_{ij} \,|) \qquad \text{for large} \quad |\, \mathbf{r}_{ij} \,| \tag{33}$$

The volume of such a system can be written as

$$V \equiv a^2 \sum_r L_r \tag{34}$$

where a is the average lattice parameter and $\sum_r L_r$ stands for the sum of the lengths of all the rows lying in a certain direction. The fluctuation in V is now given by

$$\langle \Delta V^2 \rangle = a^4 \sum_r \sum_{r'} \langle \Delta L_r \, \Delta L_{r'} \rangle = a^4 \sum_r \sum_{r'} O[1/(r - r')] = O(V) \tag{35}$$

where $r - r'$ stands for the distance between the rows r, r'. The same result is obtained for the BE model in an entirely different way: Since $\langle \Delta L_r \, \Delta L_{r'} \rangle$ has a strictly finite range, we can write

$$\langle \Delta V^2 \rangle = a^4 \sum_r O(L) = O(V) \tag{36}$$

So it looks as if nature has conspired to keep the important thermodynamic variables normal in this otherwise not very physical model!

4. THERMODYNAMICS OF THE COMPRESSIBLE ISING MODEL[8]

The thermodynamic potential that is the natural function of T, λ, h—the parameters which characterize our statistical operator—is $-kT \log Z$. The

[8] Some of the results in this section have also been derived independently in Ref. 10, using a different ensemble. Our derivation is somewhat simpler, and we include it both for the sake of completeness and also because we need the thermodynamic functions in order to discuss the magnetic phase transition in Sections 5 and 6.

thermodynamic variable that is conjugate to λ is easily found by differentiating this potential with respect to λ

$$(\partial/\partial\lambda)[-kT\log Z(\beta,\lambda,h)] = dN\langle\xi\rangle \tag{37}$$

Using (19), the average interparticle distance a is given by

$$a \equiv \langle\xi\rangle = \langle\xi\rangle_+[(1+\langle\sigma_1\sigma_2\rangle_{\mathrm{I}})/2] + \langle\xi\rangle_-[(1-\langle\sigma_1\sigma_2\rangle_{\mathrm{I}})/2] \tag{38}$$

In order to calculate $(\partial a/\partial\lambda)_{T,h}$, we first need to note that

$$-(1/\beta)\,\partial\langle\xi\rangle_\pm/\partial\lambda = \langle\Delta\xi_\pm{}^2\rangle_\pm \tag{39}$$

and that

$$\frac{1}{\beta}\frac{\partial\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{\partial\lambda} = \frac{1}{\beta}\frac{\partial\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{\partial J_{\mathrm{eff}}}\frac{\partial J_{\mathrm{eff}}}{\partial\lambda} = \frac{1}{\beta}\frac{\partial\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{\partial J_{\mathrm{eff}}}\frac{1}{2}(\langle\xi\rangle_+ - \langle\xi\rangle_-) \tag{40}$$

We can now easily obtain the following result:

$$\begin{aligned} -\frac{1}{\beta}\left(\frac{\partial a}{\partial\lambda}\right)_{T,h} &= \left\langle\Delta\xi_{12}\sum_{(ij)}\Delta\xi_{ij}\right\rangle \\ &= \langle\Delta\xi_+{}^2\rangle_+\frac{1+\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{2} + \langle\Delta\xi_-{}^2\rangle_-\frac{1-\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{2} \\ &\quad -\frac{1}{4}(\langle\xi\rangle_+ - \langle\xi\rangle_-)^2\frac{1}{\beta}\frac{\partial\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{\partial J_{\mathrm{eff}}} \end{aligned} \tag{41}$$

When $h = 0$ there is a simple connection between $\partial\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}/\partial J_{\mathrm{eff}}$ and the specific heat of the rigid Ising model at $h = 0$:

$$c_{\mathrm{I}} \equiv \left.\frac{\partial(E/N)}{\partial T}\right|_{h=0} = -\left.\frac{dJ_{\mathrm{eff}}^2}{T}\frac{\partial\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{\partial J_{\mathrm{eff}}}\right|_{h=0} \tag{42}$$

As a result of this, the derivative $\partial\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}/\partial J_{\mathrm{eff}}$ which appears in (41) is negative for sufficiently small h. Therefore all the terms on the rhs of (41) are positive, and consequently

$$-(1/\beta)(\partial a/\partial\lambda)_{T,h} > 0 \tag{43}$$

for sufficiently small h. The system thus always satisfies the stability requirement for small h. For $h = 0$ we can use (42) to write (41) in the form

$$\begin{aligned} -\frac{1}{\beta}\left(\frac{\partial a}{\partial\lambda}\right)_{T,h=0} &= \langle\Delta\xi_+{}^2\rangle_+\frac{1+\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{2} + \langle\Delta\xi_-{}^2\rangle_-\frac{1-\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{2} \\ &\quad + \left(\frac{\langle\xi\rangle_+ - \langle\xi\rangle_-}{2}\right)^2\frac{c_{\mathrm{I}}}{dk\beta^2J_{\mathrm{eff}}^2} \end{aligned} \tag{44}$$

The internal energy per particle of the system is given by

$$\frac{E}{N} = \frac{1}{N}\langle H\rangle = d\frac{kT}{2} + d\left[\langle\phi(\xi) + J(\xi)\rangle_+ \frac{1+\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{2} + \langle\phi(\xi) - J(\xi)\rangle_- \frac{1-\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{2}\right] + h\langle\sigma\rangle_{\mathrm{I}} \tag{45}$$

where we have used (1), (19), and (20).

In order to calculate the specific heat at constant λ, c_λ, note that the entropy S is given by

$$S = (\partial/\partial T)[kT\log Z(\beta,\lambda,h)] = -k\beta^2(\partial/\partial\beta)[1/\beta)\log Z] \tag{46}$$

and that consequently

$$\frac{c_\lambda}{k} = \frac{T}{Nk}\left(\frac{\partial S}{\partial T}\right)_{\lambda,h} = -\frac{\beta}{Nk}\left(\frac{\partial S}{\partial\beta}\right)_{\lambda,h} = \frac{1}{N}\beta\frac{\partial}{\partial\beta}\left[\beta^2\frac{\partial}{\partial\beta}\left(\frac{1}{\beta}\log Z\right)\right]$$
$$= \frac{1}{N}\beta^2\frac{\partial^2\log Z}{\partial\beta^2} \tag{47}$$

We will calculate c_λ only for $h = 0$. In doing this, we will encounter the derivative of $\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}$ with respect to β. Besides the regular dependence of $\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}$ on β that is found in a rigid Ising lattice, we now have also J_{eff} depending on β. Therefore we write for this derivative

$$\frac{d\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{d\beta} = \frac{\partial\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{\partial\beta} + \frac{\partial\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{\partial J_{\mathrm{eff}}}\frac{\partial J_{\mathrm{eff}}(\beta,\lambda)}{\partial\beta} \tag{48}$$

Using the fact that the thermodynamic functions of the rigid Ising model depend only on the product βJ_{eff}, as well as Eq. (10) and the relations

$$-\partial(\log q_\pm)/\partial\beta = \langle\phi(\xi) + \lambda\xi \pm J(\xi)\rangle_\pm \tag{49}$$

we can now write

$$\frac{d\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{d\beta} = \frac{\partial\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{\partial\beta}\left(1 + \frac{\beta}{J_{\mathrm{eff}}}\frac{\partial J_{\mathrm{eff}}}{\partial\beta}\right)$$
$$= \frac{\partial\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{\partial\beta}\frac{1}{2J_{\mathrm{eff}}}(\langle\phi + \lambda\xi + J\rangle_+ - \langle\phi + \lambda\xi - J\rangle_-) \tag{50}$$

We now note that the rigid Ising specific heat at $h = 0$, $c_{\mathrm{I}}(\beta J_{\mathrm{eff}})$, can be written as follows:

$$c_{\mathrm{I}} = -dk\beta^2 J_{\mathrm{eff}}\,\partial\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}/\partial\beta \tag{51}$$

By using (47) together with (50) and (51), we now get, when $h = 0$,

$$\frac{c_\lambda(\beta, \lambda, h = 0)}{k} = \frac{d}{2} + d\beta^2 \Big[\langle \Delta(\phi + \lambda\xi + J)_+{}^2\rangle_+ \frac{1 + \langle\sigma_1\sigma_2\rangle_{\rm I}}{2} + \langle \Delta(\phi + \lambda\xi - J)_-{}^2\rangle_- \frac{1 - \langle\sigma_1\sigma_2\rangle_{\rm I}}{2}\Big] + \frac{c_{\rm I}(\beta J_{\rm eff})}{k}\left(\frac{\langle\phi + \lambda\xi + J\rangle_+ - \langle\phi + \lambda\xi - J\rangle_-}{2J_{\rm eff}}\right)^2 \tag{52}$$

Again, this is a sum of positive terms. By continuity, c_λ is positive for sufficiently small h.

Equations (44) and (52) show not only that $-(\partial a/\partial\lambda)_{T,h}$ and c_λ are positive, but also that if the $\langle\ \rangle_\pm$ averages exist (i.e., if the integrals are finite), then, except for the Ising phase transition point, these quantities are intensive, i.e., of order one, as they should be. This again shows that the λ-ensemble is a perfectly well behaved one away from the Ising transition: All the relative mean-square fluctuations of thermodynamic quantities are of order $1/N$.

By differentiating Eq. (38) with respect to β, using (50), (51), and the fact that

$$-\partial\langle\xi\rangle_\pm/\partial\beta = \langle\Delta\xi_\pm\,\Delta(\phi + \lambda\xi \pm J)_\pm\rangle_\pm \tag{53}$$

we get for the thermal expansion coefficient at constant λ and $h = 0$

$$-\left(\frac{\partial a}{\partial\beta}\right)_{\lambda,h=0} = \langle\Delta\xi_+\,\Delta(\phi + \lambda\xi + J)_+\rangle_+ \frac{1 + \langle\sigma_1\sigma_2\rangle_{\rm I}}{2} + \langle\Delta\xi_-\,\Delta(\phi + \lambda\xi - J)_-\rangle_- \frac{1 - \langle\sigma_1\sigma_2\rangle_{\rm I}}{2} + (\langle\xi\rangle_+ - \langle\xi\rangle_-)(\langle\phi + \lambda\xi + J\rangle_+ - \langle\phi + \lambda\xi - J\rangle_-) \times \frac{c_{\rm I}(\beta J_{\rm eff})}{4dk\beta^2 J_{\rm eff}^2} \tag{54}$$

The second-order Ising phase transition occurs at a definite value of λ for every β, $\lambda_c(\beta)$, which is determined by the equation

$$\beta J_{\rm eff}(\beta, \lambda_c(\beta)) = (\beta J)_c \qquad (= 0.4407 \text{ for } d = 2) \tag{55}$$

The slope of the line of singular points $\lambda_c(\beta)$ is determined by differentiating this equation with respect to β, giving

$$J_{\rm eff} + \beta\frac{\partial J_{\rm eff}}{\partial\beta} + \beta\frac{\partial J_{\rm eff}}{\partial\lambda}\frac{d\lambda_c}{d\beta} = 0 \tag{56}$$

With the help of (10), (49) [see also (50)], and

$$-(1/\beta)\,\partial(\log q_\pm)/\partial\lambda = \langle\xi\rangle_\pm \tag{57}$$

we get that

$$-\beta\, d\lambda_c(\beta)/d\beta = (\langle\phi + \lambda\xi + J\rangle_+ - \langle\phi + \lambda\xi - J\rangle_-)(\langle\xi\rangle_+ - \langle\xi\rangle_-) \tag{58}$$

We can compare these results with the Pippard relations, which are expected to hold at $h = 0$ along $\lambda_c(\beta)$ from general thermodynamic considerations. There are two of them:

$$\frac{c_\lambda}{k} \cong d\beta^3 \frac{d\lambda_c}{d\beta}\left(\frac{\partial a}{\partial\beta}\right)_\lambda \tag{59}$$

$$-\left(\frac{\partial a}{\partial\beta}\right)_\lambda \cong \frac{d\lambda_c}{d\beta}\left(\frac{\partial a}{\partial\lambda}\right)_\beta \tag{60}$$

where the sign $\cong$ stands for asymptotic equality of the divergent parts of each side near $\lambda_c(\beta)$. By substituting the singular parts from (44), (52), and (54), and using (42), these Pippard relations are easily seen to hold. With their help one can also obtain the general result that the specific heat at constant $a \equiv \langle\xi\rangle$, c_a, which is the same as the specific heat at constant volume c_v, has its main divergence canceled at $\lambda_c(\beta)$: Starting from the thermodynamic expression

$$\frac{c_a}{k} = \frac{c_\lambda}{k} + d\beta^3\left[\left(\frac{\partial a}{\partial\beta}\right)_\lambda^2 \Big/ \left(\frac{\partial a}{\partial\lambda}\right)_\beta\right] \tag{61}$$

and using (60), we get that

$$\frac{c_a}{k} \cong \frac{c_\lambda}{k} - d\beta^3 \frac{d\lambda_c}{d\beta}\left(\frac{\partial a}{\partial\beta}\right)_\lambda \cong 0 \tag{62}$$

where (59) was used to get the final equality. By a more detailed calculation, one can show that c_a in fact remains finite but has a cusp at $\lambda_c(\beta)$, as predicted by Fisher's renormalization theory[12] and as also found by Baker and Essam.[8,10]

5. MAGNETIC PHASE TRANSITIONS

From the previous section it is clear that the BE compressible Ising model undergoes a phase transition that is usually of the same form qualitatively as the rigid Ising phase transition when $h = 0$ and when λ is the additional externally determined thermodynamic variable; i.e., it is a second-order transition, and the critical exponents are the same as in the rigid Ising model.

An entirely different picture emerges if instead of controlling λ we control the pressure P. The pressure is calculated as follows: First we make a Legendre transformation from λ to its thermodynamically conjugate variable dNa. The appropriate thermodynamic potential is

$$\tilde{F}(T, a, h) = -kT \log Z - dNa\lambda \tag{63}$$

and this is numerically equal to the Helmholtz free energy $F(T, V, h)$. The pressure is given by

$$P \equiv -\frac{\partial F}{\partial V} = -\frac{\partial \tilde{F}}{\partial a}\frac{\partial a}{\partial V} = \frac{dN\lambda}{dNa^{d-1}} = \frac{\lambda}{a^{d-1}} \tag{64}$$

If P is given, this constitutes an equation for λ in terms of P and T, which we rewrite as

$$a = (\lambda/P)^{1/(d-1)} \tag{65}$$

A schematic drawing of both sides of this equation as functions of λ for a fixed β, $h = 0$, and several values of P is shown in Fig. 1. Although the total

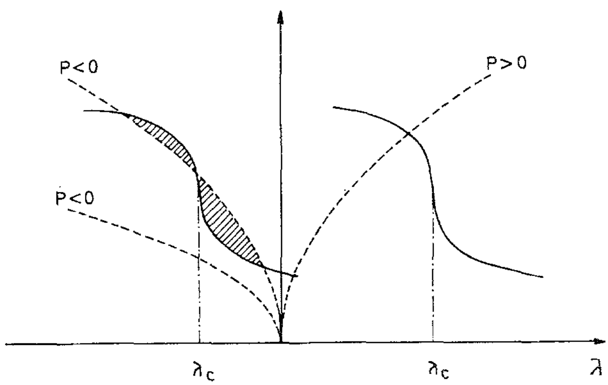

Fig. 1. Schematic drawing of the two sides of Eq. (65) as functions of λ. The two full wiggly lines represent particular cases of the function $a(\lambda)$. In the graphs we show a section of the function $a(\lambda)$ that includes a point of infinite slope λ_c, as required by Eq. (44). The three dashed lines represent $(\lambda/P)^{1/(d-1)}$ for various fixed values of P. The infinite slope of $a(\lambda)$ will clearly bring about a triple intersection in the vicinity of λ_c for $P < 0$. The hatched regions denote the area enclosed between two intersecting lines. These areas determine which of the intersection points corresponds to the stable equilibrium state.

number of solutions of this equation for any given P will depend upon details of the model such as the exact forms of $\phi(\xi)$ and $J(\xi)$, one can ensure that there will be only one solution for most values of P by making $\phi(\xi)$ increase sufficiently rapidly for large ξ. But no matter what we do, there will always be three solutions when for negative P the two curves intersect sufficiently close to λ_c, where $a(\lambda)$ has an infinite slope as required by (44).

In that case we have to examine the Gibbs free energy to determine which solution minimizes it—only that solution will correspond to a stable equilibrium state. The Gibbs free energy at $h = 0$ will be given by

$$\begin{aligned} G(T, P) &= F(T, V) + PV = -kT \log Z - dNa\lambda + (\lambda/a^{d-1})\, Na^d \\ &= -kT \log Z - (d-1)\, Na\lambda \\ &= -kT \log Z - [(d-1)\, N\lambda^{d/(d-1)}/P^{1/(d-1)}] \end{aligned} \tag{66}$$

after we have substituted λ as a function of P, T everywhere. Instead of doing that, we continue for a while to keep λ as an independent variable in the last line and define a new auxiliary function:

$$\Gamma(T, P, \lambda) \equiv -kT \log Z(\beta, \lambda) - [(d-1)\, N\lambda^{d/(d-1)}/P^{1/(d-1)}] \tag{67}$$

The derivative of this function is given by

$$\partial\Gamma/\partial\lambda = dN[a - (\lambda/P)^{1/(d-1)}] \tag{68}$$

i.e., it is equal to the difference between the ordinates of the two intersecting graphs in Fig. 1. By integrating it between two points of intersection λ_1, λ_2, one immediately finds for the difference in the Gibbs free energy

$$\Delta G = \Gamma(T, P, \lambda_2) - \Gamma(T, P, \lambda_1) = dN \int_{\lambda_1}^{\lambda_2} [a - (\lambda/P)^{1/(d-1)}]\, d\lambda \tag{69}$$

i.e., the area bounded between the two curves. One immediately sees that the middle intersection point is at best a saddle point of G, while only the two extreme points are local minima. Of these, the one next to the larger enclosed area also has the lower value of G, and thus describes the stable equilibrium state.

Consequently, if we vary P while holding T fixed, or vary T while holding P fixed, the system will usually undergo a phase transition at some point. For positive P this will be a second-order phase transition with infinite magnetic susceptibility, but with renormalized critical exponents, in agreement with Fisher's renormalization theory.[12] This was also found for this model by Baker and Essam.[8,10] But for negative P there will occur a first-order phase transition, with a finite jump in λ, a, V, and E before the second-order singularity is reached.

These properties may also be obtained in a more usual but less transparent way by first calculating the isothermal compressibility K_T:

$$\frac{1}{K_T} \equiv -V\left(\frac{\partial P}{\partial V}\right)_T = -Na^d \frac{da}{dV}\left[\frac{\partial(\lambda/a^{d-1})}{\partial a}\right]_\beta = \frac{d-1}{d} P - \frac{1}{da^{d-2}}\left(\frac{\partial \lambda}{\partial a}\right)_\beta \tag{70}$$

where we have used $V \equiv Na^d$ and $P = \lambda/a^{d-1}$. Substituting from (44) and (42), we get

$$\frac{1}{K_T} = \frac{d-1}{d} P + \frac{1}{\beta d a^{d-2}}\left[\langle \Delta\xi_+{}^2\rangle_+ \frac{1+\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{2} + \langle\Delta\xi_-{}^2\rangle_- \frac{1-\langle\sigma_1\sigma_2\rangle_{\mathrm{I}}}{2} + \frac{c_1}{4kd\beta^2 J_{\mathrm{eff}}^2}(\langle\xi\rangle_+ - \langle\xi\rangle_-)^2\right]^{-1} \tag{71}$$

The second term on the rhs is always positive and usually much larger than the first term (since $K_T \ll 1/P$ for reasonable pressures in any real solid or liquid), except at the Ising transition point, where it vanishes. Therefore, while for $P > 0$, K_T is also always positive, for $P < 0$ it will become negative in a small interval around the Ising transition point.[9] If the usual Maxwell construction is now applied, one again obtains the first-order phase transition for $P < 0$. We stress, however, that in our rigorous derivation the Maxwell construction is obtained automatically, as it should be.

When the experimental conditions are such that the volume V or the average lattice parameter a is under control, we find that the transition is always second order with renormalized coefficients. This was also found by Baker and Essam,[8,10] and is again in agreement with Fisher's renormalization theory.[12]

We would like to point out that the conditions where we find a first-order transition intervening before the second-order transition can occur are completely different from those one would expect from the various approximate methods of treatment.[2–5] Since we have treated an exactly soluble model, this means that these approximations must break down. We will analyze some of these approximations and the reasons for their failure in a future article.

Our result is also different from what one would expect from Fisher's renormalization theory,[12] but this is due entirely to an implicit assumption made by Fisher. When that assumption is removed, it is found that results of the type we have found are to be expected.[13] We will discuss this question, too, in detail in a future publication.

[9] This fact was first pointed out in Ref. 9. But they do not mention explicitly the possibility of a first-order phase transition.

6. PROPERTIES OF THE FIRST-ORDER PHASE TRANSITION

We have shown that in the region $P < 0$ if the system is cooled from a high temperature, it undergoes a first-order phase transition from a paramagnetic to a ferromagnetic or antiferromagnetic state. In order to calculate the magnitude of the various discontinuities that occur in its thermodynamic state, we must first solve the simultaneous equations

$$a(\lambda_1, T) = (\lambda_1/P)^{1/(d-1)} \tag{72}$$

$$a(\lambda_2, T) = (\lambda_2/P)^{1/(d-1)} \tag{73}$$

$$\int_{\lambda_1}^{\lambda_2} [a(\lambda, T) - (\lambda/P)^{1/(d-1)}]\, d\lambda = 0 \tag{74}$$

to determine T, λ_1, and λ_2 that characterize the transition. Here λ_1 and λ_2 are the two extreme intersection points in Fig. 1. We proceed to do this for the vicinity of the boundary between the first-order and the second-order regimes, i.e., for P close to zero.

In that case, both λ_1 and λ_2, as well as the intermediate intersection point λ_0, are very near to $\lambda_c(T)$, which is the singular point of $a(\lambda, T)$, i.e., the point of the Ising transition. From Eq. (44) and the fact that $\beta J_{\text{eff}}(\beta, \lambda)$ is a regular function of λ, it is clear that for λ close to λ_c one may write

$$a(\lambda, T) = a_c \pm b_{\mp} \mid \lambda - \lambda_c \mid^{1-\alpha_{\mp}} \qquad \text{for} \quad \lambda \lessgtr \lambda_c(T) \tag{75}$$

where $a_c \equiv a(\lambda_c(T), T)$. The coefficients b_+ and b_- and the indices α_+ and α_- characterize the critical behavior on the two sides of λ_c. To make the discussion more definite, we assume that $\lambda < \lambda_c$ corresponds to the ordered (say, ferromagnetic) state—in that case, b_- and α_- correspond to the ordered state, while b_+ and α_+ correspond to the disordered (i.e., paramagnetic) state.[10] Equation (75), where the linear term in $\lambda - \lambda_c$ is neglected, is only correct when α_+ and α_- are nonnegative, i.e., when c_{I} is infinite at λ_c, as indeed seems to be the case for the Ising model. The case where $\alpha = 0$, corresponding to a logarithmic infinity (e.g., the two-dimensional Ising model), is included in our discussion.

In order to solve Eqs. (72)–(74) we first assume that $\alpha_+ = \alpha_- \equiv \alpha$ and $b_+ = b_- \equiv b$. While this is only true for the two-dimensional Ising model, we shall see that when $b_+ \neq b_-$ (which is probably true) or even when $\alpha_+ \neq \alpha_-$ (which is probably untrue) we get qualitatively similar results.

If we use Eq. (75) to substitute in Eqs. (72) and (73) and expand the rhs in a Taylor series around λ_c, we now find

$$a_c \pm b \mid \lambda - \lambda_c \mid^{1-\alpha} = \left(\frac{\lambda_c}{P}\right)^{1/(d-1)} \pm \frac{1}{d-1} \left(\frac{\lambda_c}{P}\right)^{-(d-2)/(d-1)} \left|\frac{\lambda - \lambda_c}{P}\right| \tag{76}$$

[10] The traditional notation is α', α instead of α_-, α_+. We use the latter notation because it is more convenient and less susceptible to typographical errors.

where the upper sign refers to λ_1 and the lower sign refers to λ_2, if we assume $\lambda_1 < \lambda_c < \lambda_2$.

Using the same expansions, Eq. (74) becomes

$$(\lambda_2 - \lambda_1)\left[a_c - \left(\frac{\lambda_c}{P}\right)^{1/(d-1)}\right] + \frac{b}{2-\alpha}\left(|\lambda_1 - \lambda_c|^{2-\alpha} - |\lambda_2 - \lambda_c|^{2-\alpha}\right) - \frac{1}{2(d-1)}\left(\frac{\lambda_c}{P}\right)^{-(d-2)/(d-1)} \frac{(\lambda_1 - \lambda_c)^2 - (\lambda_2 - \lambda_c)^2}{|P|} = 0 \tag{77}$$

In order to find a solution to Eqs. (76) and (77), we note that since we have approximated $a(\lambda, T)$ by a function which is odd in $\lambda - \lambda_c$, and $(\lambda/P)^{1/(d-1)}$ by a linear function of $\lambda - \lambda_c$, we can expect λ_0, the middle intersection point in Fig. 1, to coincide with λ_c when the hatched areas are equal. Following this intuition we try to construct a solution by first choosing T to make λ_c a solution of (76). This requires that T be chosen to satisfy

$$a_c = (\lambda_c/P)^{1/(d-1)} \tag{78}$$

It immediately follows from (76) that the two extreme intersection points λ_1 and λ_2 satisfy

$$|\lambda_1 - \lambda_c| = |\lambda_2 - \lambda_c| \tag{79}$$

and consequently that (77) is automatically satisfied. What we have shown here is that the two extreme intersections in Fig. 1 are symmetric (approximately) about the middle (singular) intersection point.

From (76) and (78) we furthermore see now that

$$|\lambda_1 - \lambda_c| = \tfrac{1}{2}|\lambda_1 - \lambda_2| = |(d-1)\, b a_c^{d-2} P|^{1/\alpha} \sim |P|^{1/\alpha} \tag{80}$$

The jump in the lattice constant is given by

$$\Delta a \equiv |a(\lambda_1, T) - a(\lambda_2, T)| = 2b\,|\lambda_1 - \lambda_c|^{1-\alpha} \sim |P|^{(1-\alpha)/\alpha} \tag{81}$$

while the jump in volume V is given to lowest order in P by

$$\Delta V = dNa_c^{d-1}\,\Delta a = 2dNba_c^{d-1}\,|\lambda_1 - \lambda_c|^{1-\alpha} \sim |P|^{(1-\alpha)/\alpha} \tag{82}$$

In order to calculate the jump in the spontaneous magnetization $\langle\sigma\rangle$, we note that on one side of the transition at $\lambda = \lambda_2$, $\langle\sigma\rangle = 0$, while on the other side[11]

$$\langle\sigma\rangle \sim \left|\frac{J_{\text{eff}}(T, \lambda_1)}{k_B T} - \frac{J_{\text{eff}}(T, \lambda_c)}{k_B T}\right|^\beta \sim |\lambda_1 - \lambda_c|^\beta \sim |P|^{\beta/\alpha} \tag{83}$$

[11] See Eq. (2.40) of Ref. 12 and discussion thereof.

Here β is the critical index which characterizes the rigid Ising spontaneous magnetization. Finally, to calculate the jump in entropy S, we first note that from (46), (12), (10), and (37) it follows that the singular parts of $a(\lambda, T)$ and $S(\lambda, T)$ (i.e., the parts that have an infinite derivative) denoted by Sing(a) and Sing(S), respectively, are connected as follows:

$$\begin{aligned} -\text{Sing}(S) &= \text{Sing}\left(\frac{\partial(-kT\log Z_{\text{I}})}{\partial\beta J_{\text{eff}}}\frac{\partial\beta J_{\text{eff}}}{\partial T}\right) \\ &= \text{Sing}\left(\frac{\partial(-kT\log Z_{\text{I}})}{\partial\lambda}\frac{\partial\beta J_{\text{eff}}}{\partial T}\Big/\frac{\partial\beta J_{\text{eff}}}{\partial\lambda}\right) \\ &= -\text{Sing}(a)\cdot dN\cdot\left(\frac{\partial\lambda}{\partial T}\right)_{\beta J_{\text{eff}}=\text{const}} \end{aligned} \tag{84}$$

Since βJ_{eff} is a regular function of T and λ [see Eq. (10)], to lowest order in P we can take $\beta J_{\text{eff}} = (\beta J)_c$ [see Eq. (55)], and using (75), we can thus write

$$\text{Sing}(S) = (d\lambda_c/dT)\, dN\, \text{Sing}(a) \tag{85}$$

The jump in S thus becomes

$$\Delta S = (d\lambda_c/dT)\, dN\, \Delta a \sim |\, P\,|^{(1-\alpha)/\alpha} \tag{86}$$

From this, (82), and the Clausius–Clapeyron equation we now find

$$\frac{dP_c}{dT} = \frac{\Delta S}{\Delta V} = \frac{d\lambda_c}{dT}\frac{1}{a_c^{d-1}} \tag{87}$$

This result, valid for small $P < 0$, may be compared with the analogous result for $P > 0$ when there is no first-order transition: Differentiating the equation $\lambda = Pa^{d-1}$, we get

$$\frac{d\lambda_c}{dT} = a^{d-1}\frac{dP_c}{dT} + Pa^{d-2}(d-1)\left[\left(\frac{\partial a}{\partial T}\right)_\lambda + \left(\frac{\partial a}{\partial\lambda}\right)_T\frac{d\lambda_c}{dT}\right] \tag{88}$$

By Eq. (60), the expression in square brackets has its main divergence canceled. It may further be checked, using Eqs. (44), (54), and (58), that it is in fact finite. Consequently, in the limit when $P \to 0$ through positive values we regain Eq. (87). Thus we have shown that the line of transition points $P_c(T)$ has a continuous derivative at the boundary T_B between the second-order and the first-order regimes. Note that this result, which stems from Eq. (85), is independent of the simplifying assumptions that we made previously, i.e., $\alpha_+ = \alpha_-$, $b_+ = b_-$.

The boundary point can be shown to be a tricritical point in the sense of Griffiths.[15] The tricritical point of this model will be discussed in a forthcoming article.

Equation (87), taken together with (58), also shows that we can easily transform the critical behavior obtained in Eqs. (80)–(83) and (86) as a function of P to a critical behavior as a function of T. In these equations P and T always refer to a point on the line of first-order phase transitions. On that line, close to $P = 0$ and $T = T_B$, we can write

$$P \cong \frac{dP_c}{dT}(T - T_B) = \frac{d\lambda_c}{dT}\frac{1}{a^{d-1}}(T - T_B) \tag{89}$$

Because the coefficient of $(T - T_B)$ is neither zero nor infinity at T_B, the exponents that describe the critical behavior of the first-order discontinuities as functions of $T - T_B$ are the same as those obtained for the critical behavior in terms of P, i.e.,

$$\begin{gathered}\Delta\lambda \equiv |\lambda_1 - \lambda_2| \sim |T - T_B|^{1/\alpha}, \qquad \Delta a \sim |T - T_B|^{(1-\alpha)/\alpha} \\ \Delta V \sim |T - T_B|^{(1-\alpha)/\alpha}, \quad \langle\sigma\rangle \sim |T - T_B|^{\beta/\alpha}, \quad \langle\Delta S\rangle \sim |T - T_B|^{(1-\alpha)/\alpha}\end{gathered} \tag{90}$$

If we want to relax the assumptions that we made before and allow for $b_+ \neq b_-$ and $\alpha_+ \neq \alpha_-$, the solution of Eqs. (72)–(74) becomes more difficult, and is treated in detail in the appendix. Qualitatively though, there is very little change in the results: If we still assume $\alpha_+ = \alpha_- \equiv \alpha$, but $b_+ \neq b_-$, we still find

$$|\lambda_1 - \lambda_c| = A_1 |P|^{1/\alpha} \tag{91}$$

$$|\lambda_2 - \lambda_c| = A_2 |P|^{1/\alpha} \tag{92}$$

but $A_1 \neq A_2$, and they are no longer so easy to calculate. Instead, we find that A_1, A_2, and T are solutions of the following set of equations, obtained from (A.12)–(A.14) by setting $\alpha_+ = \alpha_- \equiv \alpha$:

$$\begin{aligned}b_-A_1^{2-\alpha} - b_+A_2^{2-\alpha} &= \frac{2-\alpha}{\alpha}A_1A_2(b_-A_1^{-\alpha} - b_+A_2^{-\alpha}) \\ b_-A_1^{1-\alpha} + b_+A_2^{1-\alpha} &= \frac{1}{(d-1)\,a_c^{d-2}}(A_1 + A_2) \\ b_+A_2^{1-\alpha} - b_-A_1^{1-\alpha} &- \frac{1}{(d-1)\,a_c^{d-2}}(A_2 - A_1) \\ &= 2\left[a_c - \left(\frac{\lambda_c}{P}\right)^{1/(d-1)}\right]|P|^{-(1-\alpha)/\alpha}\end{aligned} \tag{93}$$

From these equations one may easily see that if $\alpha \ll 1$, a good approximation to the solution is obtained by writing

$$|\lambda_1 - \lambda_c| = |(d-1)\, b_- a_c^{d-2} P\,|^{1/\alpha} \tag{94}$$

$$|\lambda_2 - \lambda_c| = |(d-1)\, b_+ a_c^{d-2} P\,|^{1/\alpha} \tag{95}$$

$$a_c - (\lambda_c/P)^{1/(d-1)} = 0 \tag{96}$$

where the last equation serves to determine T. In this approximation we again get $\lambda_0 = \lambda_c$.

If we assume $\alpha_+ \neq \alpha_-$, as well as arbitrary b_+ and b_-, we get the following results:

$$|\lambda_1 - \lambda_c| = A_1\,|\,P\,|^{1/\alpha_>}, \qquad |\lambda_2 - \lambda_c| = A_2\,|\,P\,|^{1/\alpha_>} \tag{97}$$

where $\alpha_>$ is the larger of the two exponents α_+ and α_-. If we assume, to be specific, that $\alpha_+ > \alpha_-$, then we find [see Eqs. (A.15)–(A.17)]

$$|\lambda_2 - \lambda_c| = |\,\tfrac{1}{2}(2-\alpha_+)(d-1)\, b_+ a_c^{d-2} P\,|^{1/\alpha_+} \tag{98}$$

$$|\lambda_1 - \lambda_c| = [\alpha_+/(2-\alpha_+)]|\,\lambda_2 - \lambda_c\,| \tag{99}$$

$$\alpha_+\,|(2-\alpha_+)(d-1)\, b_+ a_c^{d-2} P\,|^{(1-\alpha_+)/\alpha_+} = a_c - \left(\frac{\lambda_c}{P}\right)^{1/(d-1)} \tag{100}$$

where the last equation again serves to determine T.

From Eqs. (94), (95), (98), and (99) all the results follow in the same way as they do from (79) and (80).

APPENDIX

In order to solve Eqs. (72)–(74) for small, negative P when $b_+ \neq b_-$ and/or $\alpha_+ \neq \alpha_-$, we first assume, to make matters quite definite, that we either have $\alpha_+ = \alpha_-$ but $b_+ > b_-$, or else we have $\alpha_+ > \alpha_-$. In both of these cases we can convince ourselves that the three intersection points λ_0, λ_1, λ_2 satisfy the following inequalities (see Fig. 2)

$$\lambda_1 < \lambda_c < \lambda_0 < \lambda_2 \tag{A.1}$$

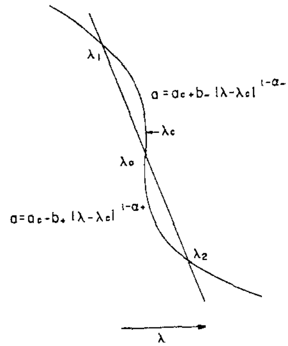

Fig. 2. Schematic drawing of $a(\lambda, T)$ (the wiggly line) and $(\lambda/P)^{1/(d-1)}$ (the straight line) as functions of λ for fixed T and P, using Eq. (75) as an approximation for a and the linear approximation for $(\lambda/P)^{1/(d-1)}$, for the case where the enclosed areas between the two curves are equal. The two approximations used for a are indicated on the graph in the appropriate regions $\lambda \lessgtr \lambda_c$. We have assumed that either $\alpha_+ > \alpha_-$, or $\alpha_+ = \alpha_-$ and $b_+ > b_-$ in order to get the intersections in the sequence indicated, i.e., $\lambda_1 < \lambda_c < \lambda_0 < \lambda_2$.

for sufficiently small P. Using (75) and a Taylor expansion for $(\lambda/P)^{1/(d-1)}$, we can write the following equations for the three intersection points:

$$a_c - \left(\frac{\lambda_c}{P}\right)^{1/(d-1)} = b_+ \mid \lambda_0 - \lambda_c \mid^{1-\alpha_+} - \frac{1}{d-1}\left(\frac{\lambda_c}{P}\right)^{-(d-2)/(d-1)} \left|\frac{\lambda_0 - \lambda_c}{P}\right| \tag{A.2}$$

$$a_c - \left(\frac{\lambda_c}{P}\right)^{1/(d-1)} = b_+ \mid \lambda_2 - \lambda_c \mid^{1-\alpha_+} - \frac{1}{d-1}\left(\frac{\lambda_c}{P}\right)^{-(d-2)/(d-1)} \left|\frac{\lambda_2 - \lambda_c}{P}\right| \tag{A.3}$$

$$a_c - \left(\frac{\lambda_c}{P}\right)^{1/(d-1)} = -b_- \mid \lambda_1 - \lambda_c \mid^{1-\alpha_-} + \frac{1}{d-1}\left(\frac{\lambda_c}{P}\right)^{-(d-2)/(d-1)} \left|\frac{\lambda_1 - \lambda_c}{P}\right| \tag{A.4}$$

To these we must add the "equal area" equation, obtained from (74) by using the same expansions:

$$(\lambda_2 - \lambda_1)\left[a_c - \left(\frac{\lambda_c}{P}\right)^{1/(d-1)}\right] + \frac{b_-}{2-\alpha_-} \mid \lambda_1 - \lambda_c \mid^{2-\alpha_-} - \frac{b_+}{2-\alpha_+} \mid \lambda_2 - \lambda_c \mid^{2-\alpha_+}$$
$$- \frac{1}{2(d-1)}\left(\frac{\lambda_c}{P}\right)^{-(d-2)/(d-1)} \frac{1}{\mid P \mid}\left[(\lambda_1 - \lambda_c)^2 - (\lambda_2 - \lambda_c)^2\right] = 0 \tag{A.5}$$

Equations (A.2)–(A.5) determine λ_0, λ_1, λ_2, and T. If we substitute in them the following ansatz,

$$\mid \lambda_0 - \lambda_c \mid = A_0 \mid P \mid^{1/\alpha_+}, \quad \mid \lambda_1 - \lambda_c \mid = A_1 \mid P \mid^{1/\alpha_+}, \quad \mid \lambda_2 - \lambda_c \mid = A_2 \mid P \mid^{1/\alpha_+} \tag{A.6}$$

where A_0, A_1, A_2 are positive coefficients which do not depend on P, we find the following equations for A_0, A_1, A_2, T:

$$\left[a_c - \left(\frac{\lambda_c}{P}\right)^{1/(d-1)}\right] | P |^{-(1-\alpha_+)/\alpha_+}$$

$$= b_+ A_0^{1-\alpha_+} - \frac{1}{d-1}\left(\frac{\lambda_c}{P}\right)^{-(d-2)/(d-1)} A_0 \tag{A.7}$$

$$= b_+ A_2^{1-\alpha_+} - \frac{1}{d-1}\left(\frac{\lambda_c}{P}\right)^{-(d-2)/(d-1)} A_2 \tag{A.8}$$

$$= -b_- A_1^{1-\alpha_-} | P |^{(\alpha_+ - \alpha_-)/\alpha_+} + \frac{1}{d-1}\left(\frac{\lambda_c}{P}\right)^{-(d-2)/(d-1)} A_1 \tag{A.9}$$

$$\left[a_c - \left(\frac{\lambda_c}{P}\right)^{1/(d-1)}\right] | P |^{-(1-\alpha_+)/\alpha_+} (A_1 + A_2)$$

$$= -\frac{b_-}{2-\alpha_-} A_1^{2-\alpha_-} | P |^{(\alpha_+ - \alpha_-)/\alpha_+}$$

$$+ \frac{b_+}{2-\alpha_+} A_2^{2-\alpha_+} + \frac{1}{2(d-1)}\left(\frac{\lambda_c}{P}\right)^{-(d-2)/(d-1)} (A_1^2 - A_2^2) \tag{A.10}$$

Since we only want to solve to lowest order in $| P |$, and since it is evident from these equations that

$$a_c - (\lambda_c/P)^{1/(d-1)} = O(| P |^{(1-\alpha_+)/\alpha_+}) \tag{A.11}$$

we will replace $(\lambda_c/P)^{-(d-2)/(d-1)}$ on the rhs of these equations by $a_c^{-(d-2)}$. By substituting the sum of Eqs. (A.8) and (A.9) into (A.10) and subtracting and adding together (A.8) and (A.9), we can write the following three equations instead of (A.8)–(A.10):

$$\frac{\alpha_-}{2-\alpha_-} b_- A_1^{2-\alpha_-} | P |^{(\alpha_+ - \alpha_-)/\alpha_+} - \frac{\alpha_+}{2-\alpha_+} b_+ A_2^{2-\alpha_+}$$

$$= A_1 A_2 (b_- A_1^{-\alpha_-} | P |^{(\alpha_+ - \alpha_-)/\alpha_+} - b_+ A_2^{-\alpha_+}) \tag{A.12}$$

$$b_- A_1^{1-\alpha_-} | P |^{(\alpha_+ - \alpha_-)/\alpha_+} + b_+ A_2^{1-\alpha_+} = \frac{A_1 + A_2}{(d-1)\, a_c^{d-2}} \tag{A.13}$$

$$b_+ A_2^{1-\alpha_+} - b_- A_1^{1-\alpha_-} | P |^{(\alpha_+ - \alpha_-)/\alpha_+} - \frac{A_2 - A_1}{(d-1)\, a_c^{d-2}}$$

$$= 2\left[a_c - \left(\frac{\lambda_c}{P}\right)^{1/(d-1)}\right] | P |^{(1-\alpha_+)/\alpha_+} \tag{A.14}$$

For the case where $\alpha_+ > \alpha_-$ we may discard in these equations the terms containing $| P |^{(\alpha_+ - \alpha_-)/\alpha_+}$, which is then a small quantity.

The equations can then be solved quite easily to yield

$$A_2 = | \tfrac{1}{2}(2 - \alpha_+)(d - 1)\, b_+ a_c^{d-2} |^{1/\alpha_+} \tag{A.15}$$

$$A_1 = [\alpha_+/(2 - \alpha_+)]\, A_2 \tag{A.16}$$

plus the following equation for T:

$$\alpha_+ |(2 - \alpha_+)(d - 1)\, b_+ a_c^{d-2} P |^{(1-\alpha_+)/\alpha_+} = a_c - (\lambda_c/P)^{1/(d-1)} \tag{A.17}$$

For the case where $\alpha_+ = \alpha_-$ we may not discard those terms, since they now include $| P |^0$. A_0 is determined, in both cases, by Eq. (A.7) and it is, in general, not equal to zero, except when both $\alpha_+ = \alpha_-$ and $b_+ = b_-$, or when $\alpha_+ = \alpha_- = \alpha$ tends to zero. Finally, we would like to point out that, as may easily be checked, any other ansatz for the solution besides (A.6) leads to an inconsistency in the equations; hence this is the only possible form for the solution.

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