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Résumé. — On réduit l'étude d'un modèle du système Ising avec spin sur un réseau compressible à un modèle d'un système Ising avec spin sur un réseau rigide. On démontre que l'équivalence des deux modèles est exacte dans l'hypothèse que les forces d'anti-déformation soient nulles ou infinies. Dans le cas de forces d'anti-déformation nulles, on renormalise les exposants critiques, en supposant que la pression extérieure n'est pas égale à zéro. Sous l'hypothèse que les forces d'anti-déformation sont infinies, on démontre l'existence d'une transition du premier ordre dans un des cas suivants : faute d'impureté, faute de magnitude finie, faute de tout arrondissement de la chaleur spécifique. Dans plusieurs intervalles expérimentaux, le système déploie les propriétés d'un des systèmes suivants : (a) transition de type d'un modèle Ising rigide, (b) transition d'un système Ising renormalisé, (c) transition du premier ordre.

Abstract. — A model of an Ising spin system on a compressible lattice is reduced exactly to that of an Ising spin system on a rigid lattice for the cases of zero and infinite anti-shearing forces. When there are no antishearing forces the critical exponents (except in zero external pressure) are renormalized. When there are infinite anti-shearing forces, a first order transition occurs (in the absence of impurity or finite size or other rounding of the specific heat). In various experimental ranges the behavior of the system will appear to be either a rigid Ising model type of transition, a renormalized Ising model type of transition, or a first order transition.

In the physical world, magnets exist not on rigid lattices but on lattices which are at least somewhat compressible. In this talk we wish to examine what modifications are necessary in the nature of the order disorder phase transition due to compressibility. As long ago as 1954, Rice [1] realized that there was a problem as to what really happens when the lattice is compressible, as all real ones are, instead of rigid. He showed that the conclusion that there is an infinite specific heat in an incompressible lattice leads to thermodynamic instability in a compressible lattice, and hence to a first-order phase transition. Wheeler and Griffiths [2] later sharpened up this result and showed that a locus of points with infinite C_V are incompatible with thermodynamic stability.

On the experimental side there are both first order transitions with a latent specific heat, and lambda-point transitions.

Domb [3] introduced a model in 1956 to investigate this problem. In his model an Ising model sits on a lattice and every nearest-neighbour bond is the same length and no fluctuations in this length are allowed. His model can be thought of as arising from a particular choice of the interatomic forces. Namely, suppose for simplicity we have a simple cubic lattice and that the interatomic force against shear deformations is infinite and the interatomic forces against compression are chosen at pleasure. Then the only allowed vibrations are for whole planes of atoms to move together, but they are so populous that we can neglect these fluctuations. He derives the relation,

$$\left(\frac{\partial p}{\partial V}\right) = \left(\frac{\partial p}{\partial V}\right)_{\text{solid}} - \frac{E_{\text{order}}\, J''}{J} + C_V T \left(\frac{J'}{J}\right)^2 \qquad (1)$$

$$\leqslant 0 \text{ for stability .}$$

Now, if $C_V \to +\infty$, then this condition is violated and a first-order transition results because of the appearance of a van der Waals loop in the isotherm. The same general type of results have been obtained by Bean and Rodbell [4], and Mattis and Schultz [5]. Calculations based on this model have been made by Garland and Renard [6] and applied to (NH_4Cl) Ammonium chloride.

Recently Domb [7] has suggested that the finite size effect limits the maximum value obtained by C_V and thus may allow, or disallow, a first order transition.

Syozi [8] and Fisher [9] have conjectured that an infinite specific heat is prevented by the presence of impurities or some other « hidden variable » through a process of « exponent renormalization ».

Swift and Wagner [10] have examined the harmonic approximation for the solid and concluded, by the neglect of several terms, that an unrenormalized second order transition occurs at constant pressure always. However, the terms neglected carry the influence of the pressure and shearing forces on the transition.

We [11] have investigated a model in which there are no forces opposing shearing deformations at all. This model and Domb's model should bracket the true case. The exact solution of this model can be given in terms of the Ising model functions. The compressibility is never negative and the Maxwell rule need not be used. Except for zero external pressure the critical indices are renormalized. That is

$$\alpha' \to -\alpha'/(1-\alpha'), \quad \beta \to \beta/(1-\alpha'), \quad \gamma' \to \gamma'/(1-\alpha') \qquad (2)$$

and also for the unprimed indices.

We [12] have studied in detail a model which preserves the good features of both Domb's model and the one we investigated previously. We obtained it by adding a type of anti-shearing force of strength Λ to the model which we had solved exactly. In the limit $\Lambda \to \infty$ the results agree with Domb's model, and in the limit $\Lambda \to 0$ we recover our previous results. An approximate derivation of the partition function is presented which interpolates between the two, exactly-known limiting cases.

We find that, except in the limit of zero antishearing

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forces, the model exhibits a first order transition. Depending on the parameters, the model can nevertheless appear to be undergoing a second order transition which will only change to first order when the specific heat is quite large. The apparent exponents can fall on either side of the asymptotic values for the rigid lattice.

Specifically, the model we consider is of the structure,

$$H = \text{K. E.} + \frac{1}{2}\sum_{\mathbf{R},\delta}\{\varphi(\delta\cdot(\mathbf{X}_{\mathbf{R}+\delta} - \mathbf{X}_{\mathbf{R}})) + \\ + \Lambda\psi(\delta \times (\mathbf{X}_{\mathbf{R}+\delta} - \mathbf{X}_{\mathbf{R}})) - \\ - J(\delta\cdot(\mathbf{X}_{\mathbf{R}+\delta} - \mathbf{X}_{\mathbf{R}}))\,\sigma_{\mathbf{R}}\,\sigma_{\mathbf{R}+\delta}\}\,. \quad (3)$$

where φ, ψ, and J are functions, $\mathbf{R}$ ranges over the lattice, δ ranges over the nearest neighbor sites, $\mathbf{X}_{\mathbf{R}}$ is the position of the particle corresponding to the $\mathbf{R}^{\text{th}}$ lattice site, and $\sigma_{\mathbf{R}}$ is its spin ($= \pm 1$). We compute the partition function as

$$Z(\beta,\lambda) = \int_{-\infty}^{+\infty} d\mathbf{X}\,\delta(\mathbf{X} - \lambda)\,Z(\beta,\mathbf{X}) \\ = \int_{-\infty}^{+\infty} d\mathbf{X}\left(\frac{N\beta}{2\pi i}\right)^3 \int_{k-i\infty}^{k+i\infty} ds\, e^{N\beta(\lambda-\mathbf{X})\cdot\mathbf{s}}\, Z(\beta,\mathbf{X}) \quad (4)$$

where $Z(\beta, \mathbf{X})$ is the partition function obtained where the first and last particles in every row are fixed in the corresponding lattice surface planes characterized by the average unit cell dimensions $\mathbf{X}$. The rest of the particle positions are free to vary over all space. We introduce the Dirac delta function, represented by a Laplace transform, to free the surface variables as well. We now use the saddle point approximation to do $\mathbf{s}$ integration.

When done in this way, we can show by an elementary calculation that the compressibility is simply related to the pressure and certain fluctuations in the system size. As both of these are non-negative, so too is the compressibility. Therefore, the system so defined is necessarily thermodynamically stable.

We have studied this model for Harmonic forces and a linear exchange force (and also more generally). In this case all the integrals over coordinate positions can be evaluated analytically, and the result is an effective spin-Hamiltonian which has two-, and four-spin terms in it.

There are two limits in which the effective spin-Hamiltonian reduces to an Ising model. One is where the shear resistance vanishes ($\Lambda = 0$, for the simple cubic lattice). In that case our results differ from those of Baker and Essam [11] by a fluctuation-type term in the exponent with its sign such as to damp fluctuations about the mean. This difference arises from employing a slightly different ensemble and does not affect the macroscopic results. The other limit is where no shear is allowed at all ($\Lambda = \infty$). In this case, the model reduces to Domb's [3] model, with one change. There is, in addition, a fluctuation type term in the exponent of the summand of the partition function. Here however its sign is such as to enhance fluctuations about the mean. Put simply the results agree with Domb's model in the one phase region, and the extra terms simply supply the Maxwell construction in the two phase region.

We have introduced the following approximation to reduce intermediate values of Λ to the Ising model. It interpolates between the limiting cases $\Lambda = 0, \infty$ and it maintains thermodynamic stability. The fourth order terms on the simple cubic lattice are proportional to

$$\sum_{\alpha,l,m,n}{}' \Upsilon^{\alpha}_{l,m,n}\,|\,Q^{\alpha}_{l,m,n}\,|^2 \quad (5)$$

where $Q^{X}_{l,m,n}$ is the Fourier transform of nearest-neighbor in the X-direction spin-spin interactions, the prime means $l = m = n = 0$ is omitted, and $\Upsilon^{X}_{l,m,n}$ is a wave number dependent coefficient

Our approximation is to replace the Υ's by a single $\bar{\Upsilon}(\Lambda/\varphi_2)$. This approximation is certainly valid for $\Lambda = 0$ or ∞. For intermediate values of Λ, there is of course, considerable variation in Υ about $\bar{\Upsilon}$. The conclusions of this model are that there is always a first order transition except when $\Lambda = 0$. However, depending on the parameters in the potential, it can easily happen that the first order transition becomes apparent only at temperatures so close to the critical temperature as to be obscured by other effects.

We have applied these calculations to β-brass. Domb's model was used because of high effective rigidity of the b. c. c. structure. The results are quite good for the order-parameter (analogue of the magnetization) as can be seen in Norvell and Als-Nielsen [13]. Our fit to the experimental ratio [13] of the amplitudes of the divergence of the analogue of the susceptibility is also good.

$$\begin{aligned} &\text{exp.} \quad t_+/t_- = 3.89 \pm 0.04 \\ &\text{Theory } t_+/t_- = 3.65 \pm 0.02 \; V \text{ constant} \\ &\text{Theory } t_+/t_- = 3.88 \pm 0.09 \; P \text{ constant.} \end{aligned} \quad (6)$$

The $t\pm$ are the temperatures above and below T_c at which equal values of the susceptibility are observed.

The fit to the specific heat data of Ashman and Handler [14] is not good at all, particularly for $T < T_c$.

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