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LATTICE MODEL FOR THE λ TRANSITION IN A BOSE FLUID*

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The critical properties of a lattice of planar classical "spins," which can be considered as a model for the λ transition in a Bose fluid, are studied using high-temperature series expansions. It is conjectured that in three dimensions the critical exponents ($T > T_c$) for the specific heat and susceptibility of the model are $\alpha = 0$ (corresponding to a logarithmic singularity) and $\gamma = 1\frac{5}{16}$, respectively.

In this Letter we report some results obtained from a relatively simple model of the λ transition in a Bose fluid proposed recently by Vaks and Larkin.[1] These authors have shown that close to the λ point (where the long-wave correlations dominate), the grand partition function of a system of interacting bosons is essentially equivalent to the partition function of a lattice of planar classical "spins" in zero external magnetic field. We can write the Hamiltonian for such a lattice of N sites, in a magnetic field $\vec{\mathrm{H}}$, as

$$\mathcal{H} = -2J\sum_{\langle ij\rangle} \vec{\mathrm{s}}_i \cdot \vec{\mathrm{s}}_j - m\vec{\mathrm{H}} \cdot \sum_{i=1}^{N} \vec{\mathrm{s}}_i, \qquad (1)$$

where $\vec{\mathrm{s}}_i$ is a two-dimensional unit vector, m is the magnetic moment per spin, and the first summation is taken over all nearest-neighbor pairs in the lattice. The direction of the magnetic field $\vec{\mathrm{H}}$ is taken parallel to the planes containing the spins. It is interesting to note that in one and two dimensions the planar-spin model has no spontaneous magnetization.[2] The spontaneous magnetization is analogous to the order parameter $|\Psi|$ in a superfluid. This suggests $|\Psi| = 0$ in one and two dimensions.[3] (In two dimensions a phase transition of the type suggested by Stanley and Kaplan[4] would not be excluded.)

The partition function and correlation functions of the planar-spin model can be evaluated exactly in one dimension[1,5] provided $\vec{\mathrm{H}} = 0$. To study the properties of the model in higher dimensions we have derived the leading coefficients in the high-temperature series expansions of the zero-field specific heat and susceptibility. The techniques which were used by the present authors to derive the high-temperature series of the classical Heisenberg model[5-7] have been applied to the planar-spin model.

The first eight coefficients of both the susceptibility (χ_0) series and the specific-heat (C_0) series have been obtained for a general lattice in zero field. For the three cubic lattices the values of the coefficients a_r and b_r, defined by

$$\chi_0 = (Nm^2/2kT) \sum_{r \geq 0} a_r K^r \qquad (2)$$

and

$$C_0 = Nk \sum_{r \geq 2} b_r K^r, \qquad (3)$$

with $K = J/kT$, are presented in Tables I and II, respectively. The susceptibility series

Table I. High-temperature susceptibility coefficients.

n	a_n (fcc)	a_n (bcc)	a_n (simple cubic)
0	1	1	1
1	12	8	6
2	132	56	30
3	1398	388	147
4	14 496	2592	696
5	148 294	17 230.667	3275
6	1503 063	112 843.333	15 171.5
7	15 132 379.25	736 900.167	70 009.125
8	151 568 185.167	4773 834.333	320 513.25

Table II. High-temperature specific-heat coefficients.

n	b_n (fcc)	b_n (bcc)	b_n (simple cubic)
2	12	8	6
3	96	0	0
4	774	276	63
5	6240	0	0
6	50 600	7453.333	970
7	418 992	0	0
8	3543 499.75	218 919.167	13 395.375
9	30 446 813.333	0	0

Table III. Successive estimates for the high-temperature specific-heat critical exponent α (fcc lattice).

n	α_n Ising spin-$\frac{1}{2}$	α_n Planar spin
3	0.4505	0.4881
4	0.3184	0.3434
5	0.1889	0.1789
6	0.0894	0.0439
7	0.0862	0.0091
8	0.1123	0.0141
9	0.1254	0.0169

have been analyzed for a singularity of the form $A(K_c-K)^{-\gamma}$ using the ratio[8] and Padé-approximant[9] methods. The final estimates obtained were

$$K_c = 0.103\,67 \pm 0.000\,06 \text{ (fcc lattice)},$$

$$K_c = 0.160\,03 \pm 0.000\,07 \text{ (bcc lattice)},$$

$$K_c = 0.2265 \quad \pm 0.0008 \text{ (simple cubic lattice)},$$

and

$$\gamma = 1.312 \pm 0.006_5$$

where the uncertainties given are not rigorous bounds but an indication of the apparent accuracy of the extrapolation procedures. The value obtained for γ is lattice independent and suggests that the exact result may be $\gamma = 1\frac{5}{16}$. In analyzing the specific heat series of the fcc lattice for a singularity of the form $B(K_c-K)^{-\alpha}$, the estimate for K_c obtained from the susceptibility series has been used to form the sequence

$$\alpha_n = nK_c(b_n/b_{n-1}) - n + 1 \quad (\alpha_n \to \alpha \text{ as } n \to \infty).$$

This sequence and the equivalent one for the spin-$\frac{1}{2}$ Ising model are presented in Table III. It is evident that the critical exponent α of the planar-spin model is considerably smaller than that of the Ising model which is now established as $\frac{1}{8}$ with only a small uncertainty.[10] From Table III and other such sequences it may be concluded that

$$0 \leq \alpha \leq \tfrac{1}{32}.$$

The expected lattice independence of α has not been verified because the series for the loose-packed lattices (which have $b_{2n+1} = 0$) are too short for accurate extrapolation.

Buckingham, Fairbank, and Kellers[11] have demonstrated that the specific heat of liquid He^4 has a logarithmic singularity ($\alpha = \alpha' = 0$) at the λ point.[12] The above estimate for the critical exponent α of the planar-spin model is therefore in good agreement with experiment. It appears plausible that the exact result for the planar-spin model is $\alpha = 0$. However, further terms in the series expansion of the specific heat are needed to exclude the possibility that α is a small positive number. The conjecture $\gamma = 1\frac{5}{16}$ cannot be tested by experiment with liquid He^4 since the analog of the magnetic susceptibility for the Bose fluid is nonphysical. It would be interesting if a magnetic system could be found which has a Hamiltonian similar to that of the planar-spin model.

If we assume the values $\alpha = 0$ and $\gamma = 1\frac{5}{16}$ then, using the scaling laws,[13] we should expect to find all the other critical exponents. Unfortunately, for the isotropic planar-spin model this procedure is not without difficulties since the zero-field susceptibility may well be infinite for $T < T_c$.

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MORIN TRANSITION IN α-Fe_2O_3 MICROCYRSTALS*

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Surface effects depress the Morin transition in microcrystals of α-Fe_2O_3 by increasing the lattice spacing homogeneously throughout the whole microcrystal volume.

We have investigated the Morin transition in microcrystals of α-Fe_2O_3 (hematite). Due to surface effects the lattice spacing in these microcrystals is larger than in bulk crystals. The Morin transition temperature is found to be depressed under this negative "equivalent pressure" at a rate comparable with the increase observed in bulk under hydrostatic pressures. The sharpness of the transition indicates that the change in the lattice spacing is homogeneous throughout the whole volume of the microcrystals.

Changes in the lattice spacing as a function of particle size have been observed before, for example, in gold microcrystals,[1] where they have been related[2] to observed increases[3] in the Debye-Waller factor. We have investigated this relationship quantitatively for α-Fe_2O_3 microcrystals. The microcrystals were produced either by the technique described by Kündig et al.[4] using silica gel, or by heating nitrate solutions at controlled temperatures for short periods. To measure at the same time both the particle size and the lattice parameter, the various-sized crystallites were used as targets in a Co x-ray spectrometer. The Bragg peaks broaden with decreasing particle size, and are displayed as the lattice spacing changes from the bulk value. The change of lattice spacing with microcrystalline size is shown in Fig. 1. These results were obtained by evaluating several Bragg lines for each sample following the analysis of King and Alexander.[5] The lattice spacing increases with decreasing particle size, and this increase is inversely proportional to the particle diameter. This inverse proportionality is similar (but opposite) to that occurring in a liquid drop under surface tension; it can be expressed as a negative free surface energy and is related to the modification of covalent bonds.[6,7] Drickamer has studied the pressure dependence of the lattice spacing in hematite.[8] At +180 kbar the volume change is $dV/V = -6.4\%$, which is equivalent in magnitude to the lattice spacing change $da/a = +2.1\%$ which we observe in 50-Å-diam particles. So we might say that 50-Å particles are under a pressure equivalent to minus 180 kbar.

Bulk α-Fe_2O_3 undergoes a spin flip near 260°K,

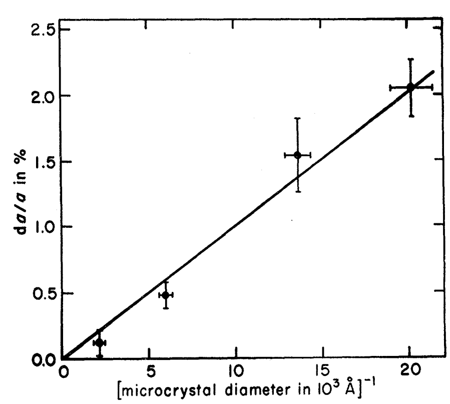

FIG. 1. Particle size versus fractional lattice-spacing change da/a for various-sized samples of hematite microcrystals.