Effects of Lattice Compressibility on Critical Behavior

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The effects predicted by Baker and Essam are estimated to be very small for real crystals. On the other hand, the theory clarifies some long-standing conceptual difficulties.

In an illuminating paper, Baker and Essam[1] have treated a model which, though in some ways artificial, is realistic enough to show the essential features of a phase transition when the interatomic distances can vary. It should be stated at once that I have no criticisms of the model or the analysis. I want only to point out that estimates can be made of the size of the effects stressed by the authors, namely, exponent renormalization and rounding of the heat capacity, which show that these effects would be very difficult to observe. The considerable value of this investigation lies instead in the clarification it brings to a long-standing problem, and it is the dispelling of misconceptions which should be emphasized.

The final results of Baker and Essam, [1] Eqs. (15) and (16), can be rearranged as

$$C_V/3R = 1 + 1/(3R/C_I + \sigma), \tag{15a}$$

$$\frac{C_p}{3R} = 1 + \left(1 + \frac{2pa_T}{\varphi_2}\right) \Big/ \left[\frac{3R}{C_I} + \frac{2pa_T}{\varphi_2}\left(\frac{3R}{C_I} + \sigma\right)\right], \tag{15b}$$

where C_I is the ideal Ising heat capacity, and $\sigma = J_1^2/\beta\varphi_2 J^2$. The deviations from "ideal" behavior are determined by σ, which we want to estimate.

To get φ_2, we note that the "normal" compressibility (i.e., well away from the critical temperature) at zero pressure is just

$$\kappa_n = 3a_T/\varphi_2.$$

To get J_1, we might assume that the exchange integral varies as some inverse power m of the interatomic distance, whence

$$J_1 = \frac{\partial J}{\partial x} = \frac{J}{a_T}\frac{\partial \ln J}{\partial \ln x} = -m\frac{J}{a_T}.$$

Another possibility is to use the observed slope of the transition line in the p-T plane, which can be shown to be

$$\frac{d\ln T_c}{dp} = -\frac{J_1 a_T^2}{J(\varphi_2 + 2pa_T)}.$$

Of the Curie-point slopes measured by Patrick, [2] that of Gd is the largest among the pure metals – 1.2 °C/kbar. Taking for κ_n the typical value 10^{-6} bar^{-1}, this gives $m = 12$, which is not unreasonable. With $a_T = 3$ Å, we find $\sigma \cong 0.2$.

Consider first the effect on C_p. Unless measurements are made at extremely high pressures, $pa_T/\varphi_2 \ll 1$, Eq. (16a) reduces to

$$\frac{C_p}{3R} = 1 + \frac{1}{3R/C_I + 2pa_T\sigma/\varphi_2},$$

and the heat capacity would be just the sum of the classical vibrational value and that of the ideal Ising model until the temperature is such that

$$\frac{C_I}{3R} \simeq \frac{\varphi_2}{2pa_T\sigma} = O(10^6) \quad \text{at } p = 1 \text{ bar}.$$

Therefore, the rounding of C_p would not (if $\alpha = \frac{1}{8}$) start to show up until $(T_c - T)/T_c$ was $O(10^{-50})$. It is clear that even if σ has been grossly underestimated, the Baker-Essam theory predicts that the anomalous part of C_p is always very close to the value for the rigid Ising model.

Consider now the effect on C_V. The rounding of C_V is determined by σ itself, and would seem to be more easily observable than the rounding of C_p. This is somewhat deceptive, however, because it is just the difference between C_p and C_V that exhibits the rounding; this difference depends on the expansion coefficient and compressibility, and the anomalies in these quantities *directly* measure the interaction between the spin ordering and interatomic distance, without the necessity of evaluating C_V. For the simple cubic lattice, using the heat-capacity equations of Gaunt and Domb, [3] and $\sigma = 0.2$, the compressibility would be only about 20% more than the normal value at $\Delta t = 10^{-3}$ below T_c. Above T_c, where the heat capacity is less than it is below T_c for the same Δt, the same fractional effect would only appear at $\Delta t \simeq 3\times 10^{-5}$, which is uncomfortably small.

It should also be mentioned that there is essentially no temperature region in which the renormalized negative α could be measured with any accuracy.

Because the Baker-Essam model is not altogether realistic (as, for example, in the absence of forces resisting shear), and because the parameters in it may vary considerably from system to system, it would not be safe to draw general conclusions

that depended strongly on these details. However, in the light of the foregoing, it does seem that for a wide range of parameters, the character of the transition as reflected in C_p would be negligibly different from that in a rigid lattice. From Baker and Essam's exact solution it is now clear that the thermodynamic constraint to a finite C_V still admits the possibility that a model that has infinite C_V may be a good description of a real system in all but a very small temperature region. It is also clear now (although in retrospect it should have been recognized earlier) that it is fallacious to compare the rigid-lattice heat capacity to the experimental C_V, as has often been attempted, because the constant-volume condition is not sufficient to prevent fluctuations of the interatomic distances.

I have had the benefit of numerous discussions with H. A. Kierstead on the subject of this comment.

[1]G. A. Baker, Jr., and J. W. Essam, Phys. Rev. Letters 24, 447 (1970).

[2]L. Patrick Phys. Rev. 93, 384 (1954).

[3]D. S. Gaunt and C. Domb, J. Phys. C 1, 1038 (1968).

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Bulk (H_{c2}) and Surface (H_{c3}) Nucleation Fields of Strong Coupling Superconducting Alloys, Gert Eilenberger and Vinay Ambegaokar [Phys. Rev. 158, 332 (1967)]. We wish to report an error in the final evaluation of our formulas, which renders spurious the former good agreement between experimental and theoretical results. Formula (4.7) was transcribed incorrectly from the Bardeen-Stephen paper, it reads correctly

$$I_1 + I_1' = (2\pi)^{-1} \left(\frac{\partial H_c(T_c)}{\partial T} \right)^2 . \tag{4.7}$$

Consequently,

$$\left(\frac{H_{c2,\mathrm{obs}}}{H_{c2,\mathrm{BCS}}} \right)_{T \to T_c} = \left(\frac{H_{c,\mathrm{obs}}^2}{H_{c,\mathrm{BCS}}^2} \right)_{T \to T_c} . \tag{4.13}$$

The predicted strong coupling correction for lead turns out to be only

$$\frac{H_{c,\mathrm{obs}}^2 \, \Delta_{\mathrm{obs}}^2}{H_{c,\mathrm{BCS}}^2 \, \Delta_{\mathrm{obs}}^2} = 1.2, \tag{5.10}$$

$$-\left(\frac{\partial H_{c3}}{\partial T} \right)_{T_c} = 115 \, \chi^{-1}(\rho) \ \mathrm{Oe/^\circ K} \tag{5.11}$$

in serious disagreement with the experimental value 206 Oe/°K. Since we have reduced our formulas to a consistency check between quantities that are measurable with good accuracy [with the possible exception of the factor $(S/S_0)^2 = 0.5$ contained in the right-hand side of (5.11)] this discrepancy remains to be explained. A similar discrepancy seems to exist for the ratio $\kappa_2(T=0)/\kappa_2(T=T_c)$ of dirty lead alloys [K. Usadel (private communication)]. We wish to thank K. Usadel for pointing out to us the error in our Eq. (4.7).

Microwave, Flux Flow, and Fluctuation Resistance of Dirty Type-II Superconductors, Richard S. Thompson [Phys. Rev. B 1, 327 (1970)]. The right-hand side of Eq. (27) should be divided by $[1 + (2\tilde{\omega})^2]$.

Five lines above Eq. (27) the expression replacing q^{-2} should read

$$\frac{\xi^4 q^2}{(\pi\omega/8T_c)^2 + (\xi q)^4} .$$

The right-hand sides of Eq. (25)–(27) should be multiplied by σ.

Above Eq. (15) the last factor in the expression for the momentum element should be $d\theta/2\pi$.

The expression $\mathrm{Re}\, Q' \cdots$ appearing at the beginning of Eq. (12) should be moved up to appear at the beginning of Eq. (11).