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Phase Transitions, Diffraction Studies and Marginal Dimensionality

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Continuous phase transitions and the associated critical phenomena have been one of the most active areas of research in condensed matter physics for several decades. This short review can only be one cut through this huge subject and we have chosen to emphasize diffraction studies as a basic experimental method and illustrate how diffraction experiments have revealed the role of dimensionality in the general classification of phase transitions.

An Elementary Example: β-Brass

Beta-brass is an alloy of Cu and Zn in almost equal amounts. The crystalline structure is body centred cubic and at room temperature, Cu atoms (open circles in Fig. 1B) occupy the cube corners, whereas Zn atoms (hatched) occupy cube centres. In the elementary argument for scattering of X-rays from a crystalline structure one considers the interference between a ray scattered from the top layer of atoms with that scattered from the next layer, and so on. In Fig. 1B we first consider neighbour layers of unit cells, that is the scattering from layers Nos. 0 and 2. With incident angle θ and unit cell size d, these two rays interfere constructively whenever $2d\sin\theta$ is an integer number n times the wavelength λ. But for $n=1$ the ray scattered from layer No. 1 will be exactly out of phase with that from No. 0, the ray scattered from layer No. 3 will be exactly out of phase with that from No. 2, and so on. If the scattering power of an odd-numbered plane equals that of an even numbered-plane the resulting intensity is zero; in crystallographic terminology one says that the (1,0,0) reflection is forbidden for the b.c.c. structure. However, for β-brass at room temperature the scattering power of odd-numbered planes is due to Zn atoms and that of even-numbered planes is due to Cu atoms, so although the rays scattered from consecutive planes of atoms are exactly out of phase when $\lambda = 2d\sin\theta$ there is nevertheless a finite Bragg intensity proportional to the square of the difference in scattering lengths, $(f_{Zn}-f_{Cu})^2$. For $n=2$ the interference is constructive and the intensity is proportional to $(f_{Zn}+f_{Cu})^2$ as illustrated in the top part of Fig. 1A.

An alternative formulation of Bragg's law to be used in the following, is also il-

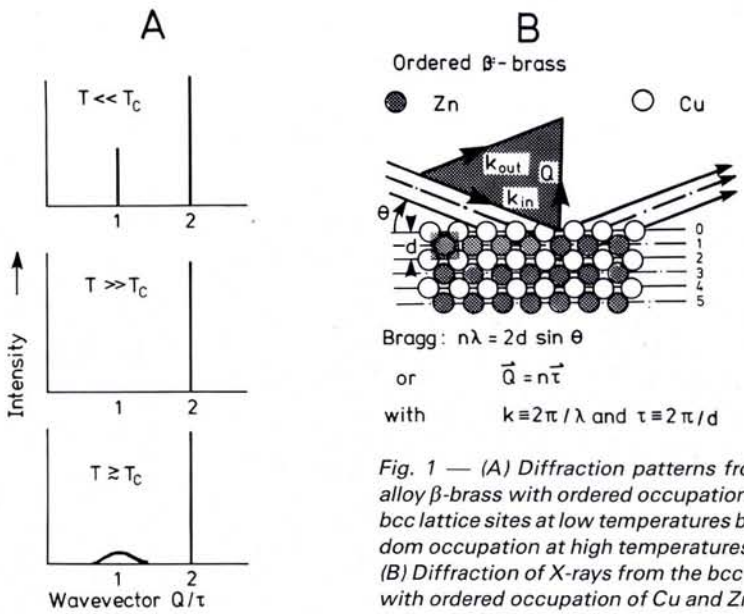

Fig. 1 — (A) Diffraction patterns from the alloy β-brass with ordered occupation of the bcc lattice sites at low temperatures but random occupation at high temperatures. (B) Diffraction of X-rays from the bcc lattice with ordered occupation of Cu and Zn.

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lustrated in Fig. 1B. The incident and scattered rays are given by the wavevectors $\mathbf{k}_{in}$ and $\mathbf{k}_{out}$, respectively, both with modulus $(2\pi/\lambda)$. The wavevector transfer $\mathbf{Q} = \mathbf{k}_{out} - \mathbf{k}_{in}$ has then modulus $2|k|\sin\theta$. For the crystal one defines the reciprocal lattice vector τ with direction normal to the considered reflecting planes and with modulus $2\pi/d$. In terms of $\mathbf{Q}$ and τ, Bragg's law is simply $\mathbf{Q} = n\tau$.

When β-brass is heated above room temperature the occupation of the b.c.c. lattice sites with Cu or Zn atoms becomes gradually more random as readily observed by a corresponding decrease of the (1,0,0) Bragg intensity. At very high temperatures, the peak around the (1,0,0) reflection has vanished corresponding to a completely random occupation of lattice sites, *cf* the middle part of Fig. 1A. The transition from the ordered phase to the disordered phase is continuous and at the transition temperature T_c the (1,0,0) *Bragg* intensity vanishes. This does not mean that all intensity has vanished for $T \geq T_c$ as illustrated in the bottom part of Fig. 1A, and we shall now discuss how this is interpreted in terms of occupation of lattice sites. The Bragg scattering in Fig. 1A is shown as delta-functions because it corresponds to the coherence from the average occupation of a very large number of lattice sites. Above T_c there is, on average, equal occupation by Cu and Zn atoms of say cube corners, but that does not exclude that in a certain region of the lattice, Cu atoms are predominantly on corners, Zn atoms in centres because in another region the situation may be reversed. The scattering from such a region of spatial extent ξ is of course less coherent than the Bragg scattering involving the entire lattice and the peak has therefore a finite width equal to ξ^{-1}.

The continuous phase transition takes place in the following way. At very high temperatures, the occupation of lattice sites is random. As the temperature is lowered correlated regions are formed, in some with predominantly Cu atoms on corners and Zn atoms in centres, in others with predominantly Zn atoms on corners and Cu atom in centres, so that on average over the entire lattice there are just as many Cu atoms as there are Zn atoms on either corner or centre sites. The dimension ξ of these ordered regions grows continuously as the temperature is lowered and actually diverges at a critical temperature T_c. At this temperature the symmetry is broken, the choice between predominantly Cu or Zn on corner sites is made. For $T < T_c$ the occupation of the two type of sites is no longer symmetric between Cu and Zn when averaged over the entire crystal and the excess occupation by one of the species increases towards saturation as the temperature is lowered to values much less than T_c.

This description turns out to be much more general than for just the order-disorder transition in an alloy [1]). All that is needed is to talk about a general order parameter rather than the specific occupation of lattice sites by the elements of an alloy. The magnetic analogue of the order-disorder transition in β-brass is obviously the uniaxial antiferromagnet where the magnetic moments below T_c are predominantly up on one sublattice and down on the other sublattice. Conceptually the uniaxial ferromagnet is even simpler and we shall use that example in establishing the general nomenclature.

Let S_r denote the atomic spin on lattice site $\mathbf{r}$ and for simplicity let us assume that S_r can only take the values $+1$ or -1. The local order parameter is then the local magnetization $M_r = g\mu_B \langle S_r \rangle$ where the brackets indicate the thermal average. Also for simplicity we set $g\mu_B = 1$ in the following. The pair correlation function $\langle S_o S_r \rangle$ is decomposed as

$$\langle S_o S_r \rangle = \langle S \rangle^2 + g(\mathbf{r}) \qquad (1)$$

with $\langle S \rangle$ being denoted long range order and $g(\mathbf{r})$ the short range order correlation function. A scattering probe which couples to the order parameter $\langle S_r \rangle$ measures the Fourier transform of $\langle S_o S_r \rangle$ and the decomposition corresponds to Bragg scattering of intensity proportional to $\langle S \rangle^2$ and so-called critical scattering proportional to the Fourier transform of the short range order correlation function. The long range order, $\langle S \rangle$, for a ferromagnet is a measure of the spontaneous bulk magnetization and it is natural to speculate whether $g(\mathbf{r})$ is also related to a magnetic bulk property. The answer lies in the bulk susceptibility χ which diverges at the critical temperature. So does the range of $g(\mathbf{r})$ and therefore $\Sigma g(\mathbf{r})$ as well. Let χ^o denote the susceptibility for non-interacting spins. The wanted relation is then $\Sigma g(\mathbf{r}) = \chi/\chi^o$. It is very useful to generalize this relation by, on the one hand considering the Fourier transform of $g(\mathbf{r})$, which is directly observed in a scattering experiment, and on the other, the wavevector-dependent susceptibility χ_q. For discussing the latter consider in general the field H conjugate to the order parameter M, but assume now that this field can vary in space $H = H_r$. In particular the field variation may be sinusoidal, $H_r = H_q \exp(i\mathbf{q}\cdot\mathbf{r})$. The response M_r will then also vary sinusoidally with the same wavevector, $M_r = M_q \exp(i\mathbf{q}\cdot\mathbf{r})$, and the generalized susceptibility χ_q is accordingly given by $M_q = M_q(H_q = 0) + \chi_q H_q$.

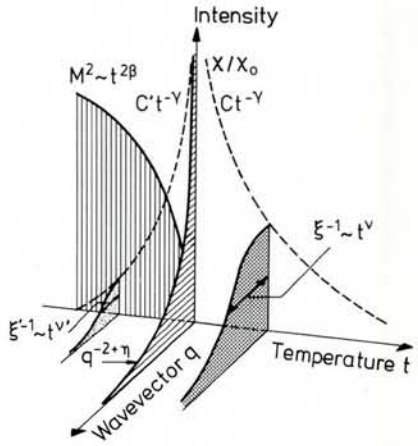


Fig. 2 — Intensity versus temperature and wavevector in a diffraction study of a continuous phase transition. In magnetic nomenclature the q=0 plane yields the bulk susceptibility, which diverges at T_c, and the spontaneous magnetization, which vanishes above T_c. The wavevector dependence gives the correlation range of short range order clusters.

For more complicated magnetic structures than a ferromagnet, $\mathbf{q}$ is defined as the difference between the applied-field wavevector and the wavevector describing the ordered structure. The largest response always occurs when the applied field wavevector coincides with that of spontaneous order, so χ_q will exhibit a maximum at $\mathbf{q} = 0$. The general fluctuation-susceptibility theorem states the relation between χ_q and the Fourier transform of $\langle S_o S_r \rangle$ measured in a diffraction experiment:

$$\Sigma_r \langle S_o S_r \rangle \exp(i\mathbf{q}\cdot\mathbf{r}) = \chi_q/\chi^o + \langle S \rangle^2 \delta(\mathbf{q}) \qquad (2)$$

In Fig. 2 we recapitulate the wavevector and temperature dependence of the quantities measured in a diffraction experiment and give the conventional nomenclature for critical exponents.

Mean-Field Approximation, Scaling and Marginal Dimensionality

The simplest discussion of χ_q which nevertheless elucidates the basic physical features is the mean-field approximation or MFA. We first consider temperatures above T_c. We seek the response to a sinusoidally varying applied field $H_n^{app} = H_q \exp(i\mathbf{q}\cdot\mathbf{r}_n)$, the lattice site $\mathbf{r}_n$ now being specified by index n. If the spins did not interact the response would be $\chi^o H_n^{app}$. The idea is now to approximate the real interaction between the spin S_n and its neighbours S_m, $f(\mathbf{r}_{nm})S_n S_m$, by its average value $f(\mathbf{r}_{nm})S_n \langle S_m \rangle$ which from all neighbours m is equivalent to a mean field $H_n^{MF} = \Sigma_m f(\mathbf{r}_{nm}) \langle S_m \rangle$. The

total field on S_n is the sum of H_n^{app} and H_n^{MF} and the response therefore $\chi^o(H_n^{app} + H_n^{MF})$. One readily finds

$$\chi_q = \chi^o/(1-\alpha_q\chi^o) \qquad (3a)$$

with

$$\alpha_q \equiv \Sigma f(\mathbf{r})\exp(i\mathbf{q}\cdot\mathbf{r}) \qquad (3b)$$

In all its simplicity, eqs. (3) contain most of the salient features of the phase transition as depicted in Fig. 2. Let us first discuss $\mathbf{q} = 0$. Recalling that $\mathbf{q}$ is the *deviation* between the wavevector of the applied field and that describing the ordered structure, α_q clearly has a maximum for $\mathbf{q} = 0$. The denominator in eq. (3a) becomes zero when $\alpha_o\chi^o = 1$. Since χ^o varies as T^{-1} one has $\alpha_o\chi^o = T_c/T$ with $T_c = \Sigma f(\mathbf{r})$ in suitable dimensionless units. The exponent γ in Fig. 2 is therefore unity in MFA.

Next, consider an expansion of α_q for small wavevectors. The simplest case is the isotropic case

$$\alpha_q = \alpha_o(1-\xi_o^2q^2) \qquad (4a)$$

revealing an isotropic critical scattering in wavevector space as found experimentally in for example β-brass. With eq. (4a) inserted into (3a) the critical scattering cross section or equivalently the wavevector dependent susceptibility near T_c becomes:

$$\chi_q/\chi^o = (\xi/\xi_o)^2\,[1+(\xi q)^2]^{-1} \qquad (4b)$$

with $\xi^2 = \xi_o^2 t$, t being the reduced temperature $(T/T_c - 1)$. The critical exponent ν, *cf* Fig. 2, is thus 1/2 in MFA, and the line shape of critical scattering is Lorentzian. A similar approach below T_c leads to $\gamma' = \gamma$, $\nu' = \nu$, $\beta = 1/2$, $\eta = 0$ and the susceptibility amplitude ratio of $C/C' = 2$.

As indicated in eq. (4b) the temperature dependence of χ_q/χ^o can just as well be expressed as a dependence on ξ using $\xi = \xi_o t^{1/2}$. In terms of q and ξ, χ_q/χ^o in eq. (4b) has the remarkable simple property of scaling: If the unit of length is chosen as ξ rather than for example Ångstrøm, then χ_q/χ^o has the same shape at all temperatures and that applies of course also to its Fourier transform, the pair correlation function. Explicitly this means that a correlated region of a predominantly up-spin cluster in a ferromagnet at say a reduced temperature of 10^{-3} looks exactly as the cluster at say $t = 10^{-4}$ provided that we enhance the length scale by the ratio of the two corresponding correlation ranges.

Although the small wavevector expansion of eq. (4a) seems fairly general there is an outstanding counter example which can be, and has been, investigated thoroughly experimentally, and that is the uniaxial, dipolar-coupled ferromagnet. As we shall see, this system has different scaling properties from those discussed above leading to a profoundly different accuracy of the mean field approximation. The dipolar interaction between two spins pointing in the z direction and situated at the origin and at $\mathbf{r} = (x,y,z)$ is $f(\mathbf{r}) = (3z^2-r^2)/r^5$. In the long-wavelength limit the Fourier transform of $f(\mathbf{r})$ is of the form

$$\alpha_o[1-\xi_o^2q^2 - g\xi_o^2\,(q_z/q)^2 + h\xi_o^2q_z^2]. \qquad (5a)$$

The coefficients ξ_o^2, g and h are readily calculated when the lattice and the size of the magnetic moments are specified. This form of α_q is very peculiar since the limiting value of α_q when $\mathbf{q} \to 0$ depends on the direction of $\mathbf{q}$: if $\mathbf{q} \to 0$ along the x axis $\alpha_q \to \alpha_o$, but if $\mathbf{q} \to 0$ along the z axis the limiting value is $\alpha_o(1-g\xi_o^2)$. Any limiting value between these two extremes may be obtained by choosing the appropriate direction of $\mathbf{q}$.

Proceeding as before in inserting eq. (5a) into eq. (3a), and using the reduced temperature $t = 1-\alpha_o\chi^o$ and defining the temperature dependent correlation range $\xi = \xi_o t^{-1/2}$ one finds readily:

$$\chi_q/\chi^o = (\xi/\xi_o)^2\,[1+(\xi q)^2 + g\,(\xi^2q_z/\xi q)^2 - (h/\xi^2)\,(\xi^2q_z)^2]^{-1} \qquad (5b)$$

to be compared with eq. (4b).

Up to this point the role of dimensionality has not appeared in the MFA. On the other hand it is known that exact solutions of the phase transition problem can easily be obtained in one dimension with the result that $T_c = 0$ K to be contrasted with $T_c^{MF} = \Sigma f(\mathbf{r})$, and with a mathematical tour-de-force following Onsager [2*]) in two dimensions gives $T_c^{MF}/T_c^{2d} = 1.76$ and critical exponents quite different from those of MFA, notably $\eta = 1/4$. The reason why the MFA fails so badly at $d = 1$ and also at $d = 2$ is of course that MFA underestimates the role of fluctuations and these become more and more important with decreasing dimensionality.

Following Ginzburg [1*]) we shall now see explicitly that the MFA is self-consistent only if d exceeds a certain value d^*, the marginal dimensionality. Consider a region Ω below T_c in which we compare the mean-squared fluctuation of the order parameter, δM_Ω^2, with the squared, average order parameter M_Ω^2. Let the number of spins in the region be N_Ω. We have then explicitly

$$\delta M_\Omega^2 = N_\Omega\,\Sigma'_i[<S_oS_i> - <S>^2] \qquad (6a)$$

$$M_\Omega^2 = (N_\Omega<S>)^2 \qquad (6b)$$

so the ratio $\delta M_\Omega^2/M_\omega^2 \sim N_\Omega^{-1}$ can always be made small by choosing Ω big enough. The appropriate region for assessing the validity of the MFA is a region of correlated spins. Therefore, in the case of isotropic scaling as in (4b) we have $N_\Omega = (\xi/\xi_o)^d$, but in the case of the dipolar coupled uniaxial ferromagnet with χ_q given by eq. (5b), N_Ω becomes $(\xi/\xi_o)^{d+1}$. The Ginzburg criterion is

$$\delta M_{\Omega(\xi)}^2 << M_{\Omega(\xi)}^2 \qquad (7)$$

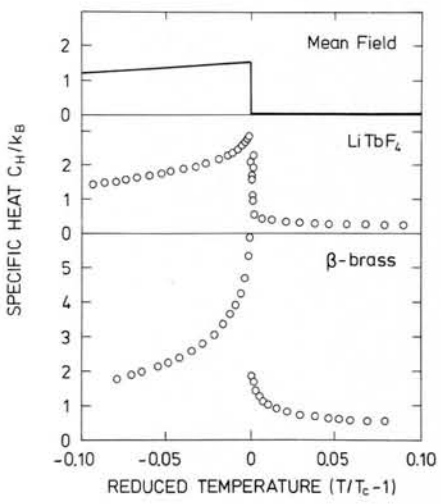
Inserting (6a) and (6b) into (7) noting that the primed sum in (6a) is only over spins within $\Omega(\xi)$ and therefore is a constant fraction of the susceptibility χ, as given by eq. (2) for $\mathbf{q} = 0$, we find

$$N_{\Omega(\xi)}\,\chi << N_{\Omega(\xi)}^2 <S>^2 \qquad (8)$$

With $N_\Omega = (\xi/\xi_o)^d \cong t^{\nu\cdot d}$, $\chi \sim t^{-\gamma}$ and $<S> \cong t^\beta$ the condition (8) requires $t^{(\nu d-\gamma-2\beta)} << 1$ for $t \to 0$, i.e. $d > d^* = (\gamma+2\beta)/\nu = (1+2\cdot 1/2)/(1/2) = 4$ but in the case of the dipolar coupled ferromagnet with $N_\Omega = (\xi/\xi_o)^{d+1}$, the marginal dimensionality is not 4 but 3, the value realized in the experiment on a three-dimensional crystal.

In summarizing, one derives the marginal dimensionality d^* from the scaling properties of χ_q as evaluated in MFA. If the actual dimensionality d exceeds d^* MFA is self-consistent and critical exponents, amplitude ratios etc. are as given already. If $d = d^*$ the famous theory of phase transitions developed by K. Wilson in the early seventies [1*]), known as the renormalization group theory which does use the MFA expression for χ_q as a basis, is exact. The critical behaviour is almost like the MFA but the power laws have logarithmic corrections, for example $\chi \sim t^{-1}\,|\ell nt|^{1/3}$. If $d < d^*$ one can use the MFA results as a basis for an expansion in the deviation from marginal dimensionality, $\varepsilon = d^*-d$. This ε-expansion, devised by Wilson and Fisher [1*]), has been carried out to second, and sometimes higher, order in ε for many model systems and it provides accurate results even for $\varepsilon = 1$. The reader might wonder how one can con-

Fig. 3 — The specific heat anomaly in mean field theory, in the uniaxial, dipolar-coupled ferromagnet $LiTbF_4$ exhibiting marginal dimensionality, and in the 3-dimensional Ising system beta brass.



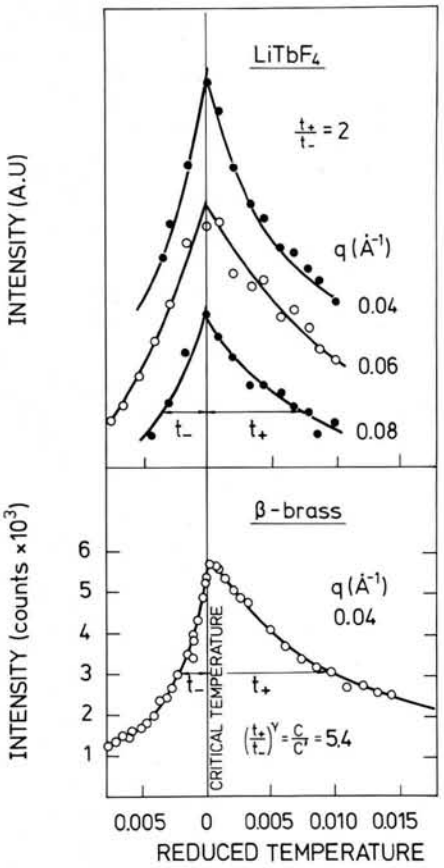


Fig. 4 — The susceptibility asymmetry around T_c is mean-field-like for $LiTbF_4$ but much more pronounced for the 3-d Ising system β-brass.

sider "many" model systems as the expression (4b) already seems fairly general. The point here is that in addition to the dimensionality d of interaction space one also has to consider the dimensionality, usually called n, of order-parameter space. In the cases we have discussed so far $n=1$ (the so-called Ising model) — spins were supposed to be uniaxial and for the alloy the occupation variable is obviously also one-dimensional in the sense of being +1 or −1, "on" or "off" etc. But the spin space may not be uniaxial and in that case $n > 1$, or the order parameter might be a density wave with an amplitude as well as a phase etc. We shall not go further into this discussion here.

The last point to be mentioned in this brief and largely phenomenological description of continuous phase transitions is the case where the fluctuations are so strong that they prevent the onset of true long range order. For the Ising case, $n=1$, we have already mentioned that $d=2$ has long range order but $d=1$ has not. In the more general case of $n > 1$ one must consider a lower marginal dimensionality d^+ at which true long range order is prevented by the fluctuations.

EXPERIMENTS

Ising systems β-brass and $LiTbF_4$

The principles of diffraction studies of the order-disorder transition in the alloy β-brass were presented in the introduction. Here we shall only add that experiments [2*]) were carried out using neutron scattering rather than conventional X-ray scattering to take advantage of the rather large difference in scattering power of Cu and Zn for neutrons, a difference that can be further enhanced using isotopically enriched Cu.

$LiTbF_4$ is a model system for the dipolar-coupled Ising ferromagnet. The magnetism is due to the unfilled 4f-electron shell of Tb giving a large magnetic moment of 9 Bohr-magnetons of the free ion Tb^{3+}. The crystalline electric field forces the 4f electron cloud to a uniaxial orientation and splits the $J=6$ multiplet into an almost ideal doublet-ground state with a magnetic moment of 8.9 Bohr magnetons and excited states several hundred degrees above, to be compared with the critical temperature of 2.87 K. The most detailed confirmation [3]) that the dipolar forces dominate the magnetic interaction has been obtained from paramagnetic neutron scattering at around 20 K. The peculiar wavevector dependence of χ_q discussed in connection with eq. (5a) is strikingly exhibited.

In Fig. 3 is shown the specific heat of β-brass, $LiTbF_4$ and MFA theory; clearly the divergence in β-brass is much stronger than in $LiTbF_4$. The reason is that $LiTbF_4$ is a system *at* marginal dimensionality, and the deviation from MFA is only a logarithmic correction which has been beautifully demonstrated experimentally by Ahlers *et al.* [1*]). Another striking difference in critical behaviour is the asymmetry around T_c of the susceptibility. This is shown in Fig. 4. At marginal dimensionality the amplitude ratio C/C', equals the MFA value of 2, whereas high temperature expansion results derived in the late sixties by Fisher and Burford [1*]) yield $C/C' = 5.1$ for the short-range coupled, three-dimensional Ising model. The data in Fig. 4 are in excellent agreement with these predictions.

When it comes to the temperature dependence of the correlation range the difference is less striking as shown in Fig. 5. The reason is that MFA already gives a rather strong singularity, $\xi^2_{MFA} \sim t^{-1}$, which is enhanced slightly *at* marginal dimensionality and should be compared with the high temperature expansion or ε-expansion prediction of $\xi^2 \sim t^{-1.29}$. Nevertheless, the data [4]) for $LiTbF_4$ in Fig. 4 are of fundamental importance because they provide a very direct experimental confirmation of the exact renormalization group equations. These lead, as pointed out by Aharony and Halperin [1*]) to the following relation between the correlation range ξ, the uniaxial correlation range $\xi_\parallel = g^{1/2}\xi^2$ (*cf* eq. 5b) and the specific heat C:

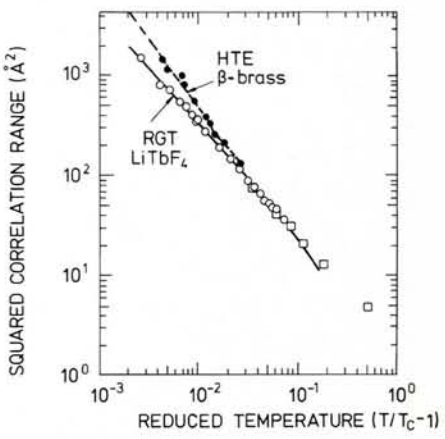
$$\xi^2 \cdot \xi_\parallel \cdot C = (3/32\pi)t^{-2}\ell n(t/t_o) \quad (9)$$

With the neutron data for ξ and g, the specific heat data for C (and t_o) this relation has been accurately confirmed as indicated in Fig. 4 by the full line.

Smectic A Phase of Liquid Crystals

Liquid crystals consist of rod-like molecules with a rich variety of phases corresponding to different combinations of their position and orientation. Here we shall consider the smectic A phase depicted in Fig. 6a. The molecules have a common orientation and are positioned in layers perpendicular to this orientation with a well-defined repetition distance between layers. Within a layer there is however no order and the structure is therefore loosely speaking that of a crystalline solid in one direction and a simple liquid in the two perpendicular directions. In Fig. 6b we consider now sinusoidal fluctuations around this average structure. When the wavevector is along the molecular axis q_z one has regions of compression and others of dilatation. There is a restoring force as in crystals and a free energy contribution of the form $1/2\, Bq_z^2u_q^2$ where B is a stiffness constant and u_q the amplitude of the fluctuation. However, when the wavevector is perpendicular to the molecular axis, $q_\perp$, the density is homogeneous as shown in Fig. 6c and the only contribution to the free energy derives from the non-parallelism of the mole-

Fig. 5 — Squared correlation range in β-brass (filled circles) in comparison with the high temperature expansion of Fisher and Burford (dashed curve) and in $LiTbF_4$ (open circles) to be compared with an exact result from renormalization group theory (full line) relating the specific heat and the correlation ranges.



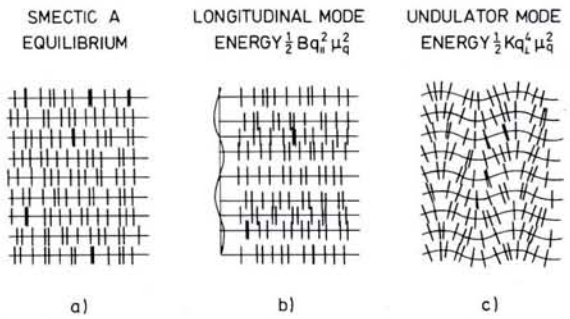


Fig. 6 — (a) The smectic A-phase is like a crystal in one direction with a well defined repetition distance between layers, but is like a liquid within each layer. (b) Longitudinal sinusoidal fluctuation around the average structure. (c) Transverse sinusoidal fluctuation, the so-called undulator mode.

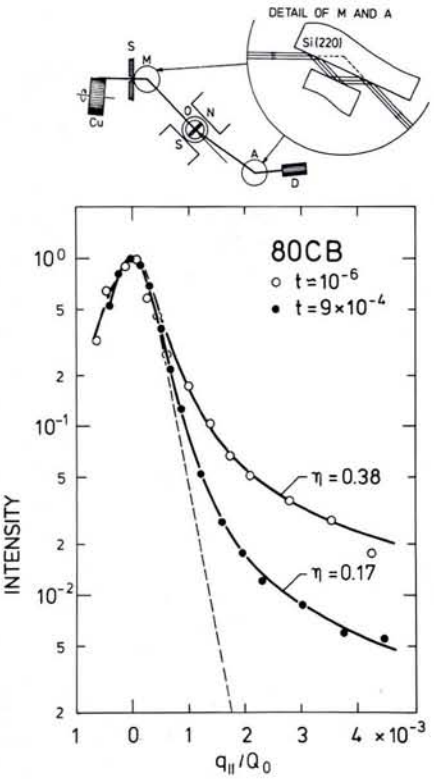
cules is this mode. One can easily see that the free energy of this mode is of the form $1/2\ q_\perp^4 u_q^2$ where K is a stiffness constant for the parallelism of the molecules. As noted already in the thirties by Landau and Peierls [5]) this leads to the paradox that the mean squared fluctuations $<u^2>$, which of course is derived by proper summation of all wavevector modes, diverges logarithmically with sample size. In other words, the undulator mode fluctuations of Fig. 6c prevent true long range order. It is possible, in the harmonic approximation, to derive the X-ray scattering profile of this structure. The result for wavevector transfer Q_z along the z-axis, $Q_z = (2\pi/d) + q_z$, is a divergence of the form

$$I(q_z) = Aq_z^{-2+\eta} \qquad (10)$$

with the parameter η being related to the stiffness constants B and K by

$$\eta = (\pi/2)\ kTd^{-2}\ (KB)^{-1/2} \qquad (11)$$

Fig. 7 — (Top) Experimental set-up for high resolution X-ray diffraction studies. S: input slit; M: monochromator; O: sample oven; A: analyzer crystal as M; D: detector. (Bottom) Line profiles of the $Q_0 = (0,0,1)$ reflection.



The difference between the divergence of eq. (10) and a true delta function response as in normal Bragg scattering is in practice small and in order to be observable the experimental resolution in **q**-space must be narrow and sharp.

Both requirements can be fulfilled by using perfect crystals as collimators for the incident and scattered X-rays. The narrow resolution is then determined by the so-called Darwin width of perfect crystals, which is a few seconds of arc only, and the sharpness is obtained by several consecutive Bragg scattering processes in each crystal, see top part of Fig. 7. The line profile from smectic layers obtained with this set-up is shown in the bottom part of Fig. 7 [6]). For true long range order the line profile would have been as the dashed line. The data are consistent with the prediction of eq. (10) when properly folded with the experimental resolution; in particular the temperature dependence of the line profile should be emphasized. The harmonic approximation expression, eq. (11), for η indicates that η increases as the transition from the smectic A phase to the nematic phase is approached because the layer stiffness constant B vanishes at the transition. The best fit values of η in Fig. 7 are in good agreement with the prediction of eq. (11) where there are no adjustable parameters.

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