is a concept that all of us understand but find difficult to quantify. The only rational approach through which we can assess this and maintain a communication line with other engineers, scientists and public is with the help of probability and statistics. In this sense aseismic design at present is more a passive insurance, at non-zero risk levels, which will be effective if and when an earthquake occurs. The risk of failure due to earthquakes can be lessened to small levels. But such an exercise will invariably be very expensive. This is not just an engineer's problem. It is for the planners to calmly decide how much the country can spend in relation to how much risk the public can tolerate in the postulated scenario of a seismic failure of the Tehri dam in the culturally important Himalayas. The planners and the public should actively participate in the decision making process.

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Disorder parameter description of phase transitions

Subodh R. Shenoy

The Yoga posture, Sirshasana, or standing on ones' head, is supposed to stimulate the brain cells. It is similarly stimulating to see how far one can go in inverting conventional viewpoints. Can the picture of a phase transition as an order parameter formation on cooling, be complemented by a picture of a disorder parameter blow-out on warming?

In this article, we consider: 1. Phase transitions and their conventional 'order-parameter' description; 2. Breakdown of these conventional ideas and the introduction of a 'disorder-parameter' description for certain special two-dimensional systems; 3. Extension of the disorder-parameter description to a particular three-dimensional system with a conventional transition; 4. Suggestion of other models that might also be examined within the disorder-parameter description. As reviews exist[1,2] the subject slice is 'vertical' (following a particular model) rather than 'horizontal'.

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Order-parameter description of phase transitions

Phase transitions are all around us—in the boiling of milk, the formation of rain drops, and the onset of spontaneous magnetization when a hot iron slab is cooled. There is a drastic change of matter from one internal arrangement to another, when a control

variable like the temperature T is moved smoothly through some critical value T_c. This 'phase' or microscopic arrangement of matter could, for example, be atoms in a liquid, randomly clumping and wandering, like off-duty soldiers strolling and chatting in loose groups, on a parade ground. On cooling smoothly through T_c, the atoms form themselves into a lattice, like a soldiers' group suddenly forming a square array, in response to a whistle from an invisible drill-sergeant. The square grows, and gaps are filled by stragglers, to complete the emerging and expanding pattern. Clearly it is natural to describe a phase transition in terms of this tendency to order—a temperature-dependent average 'order parameter' $\bar{M}$ (say), that is zero for temperature T above T_c, and non-zero below it. This ordering can either occur with $\bar{M}(T)$ jumping up from zero, and with a nonzero latent heat ('first-order transition'); or $\bar{M}(T)$ smoothly rising from zero, with a zero latent heat ('second-order transition'). The idea that a common average M appears in a correlated fashion all across the system can be expressed as a 'correlation function'. This is an average of $M(r)$, the order parameter at a position r, multiplied by $M(r')$, taken at some far-off point r', so $|r-r'|$ is very large. For $T>T_c$, with no overall order, $\{\langle M\rangle=\bar{M}=0\}$ the average of this product is the product of the independent averages. $\langle M(r)M(r')\rangle \rightarrow \langle M(r)\rangle \langle M(r')\rangle = 0$. Only for $T \leq T_c$ do we have $\langle M(r)\, M(r')\rangle \rightarrow \bar{M}^2 \neq 0$ at large separations—a key idea called 'long range order' (LRO), that helps define the average order parameter, $\langle M\rangle = \bar{M}$. This is depicted schematically in Figure 1.

This general conceptual framework seemed to work for all phase transitions, and a program was successively applied to a whole host of phase transitions: (i) Identifying the order parameter (M) in each case; (ii) finding out how the appropriate energy F depended on it, and on temperature, $F=F(M,T)$; further showing that the minimum F energy corresponded to an average $\bar{M}=0$ for $T>T_c$ and $\bar{M}\neq 0$ for $T<T_c$; (iii) including fluctuations about this average, especially in the second order case.

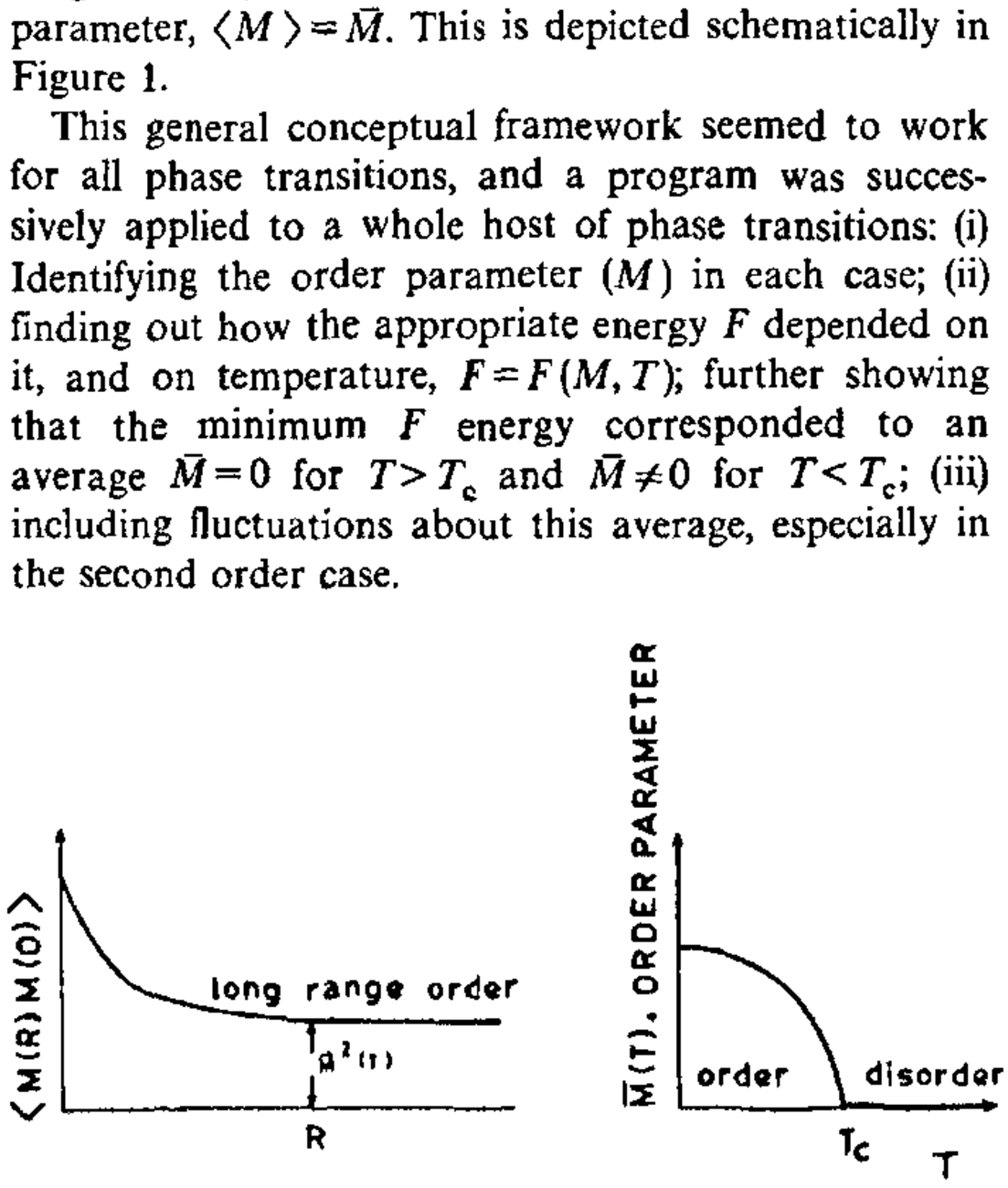

Figure 1. Long range order in correlation function, and behaviour of order parameter (for second-order transition).

Thermal fluctuations of the order parameter exist above T_c for a second order phase transition, even though the average order parameter is zero. Blobs of ordered $M(r)\neq 0$, of (temperature-dependent) size $\xi(T)$, form and disappear. Similar fluctuations of the order parameter occur below T_c. They induce remarkably simple temperature dependences around T_c, that are just the temperature difference raised to (noninteger) powers or *exponents*: $M(T)\sim(T_c-T)^{\beta}$, susceptibility $\chi\sim|T_c-T|^{-\gamma}$, specific heat $C\sim|T_c-T|^{-\alpha}$, blob size $\xi(T)\sim|T_c-T|^{-\nu}$. What is even more remarkable is that these exponents β, α, γ, ν are the same for all materials in the same 'universality class', even though lattice constants and shapes, strength of interactions and so on, could be very different. The numbers depend only on certain pure numbers common to all members of the universality class, such as space dimensionality, number of components of the order parameter, etc.

The job was to calculate these exponent values by systematically including bit by bit, these order parameter fluctuations by a rescaling procedure, called 'renormalization group', that was developed by Kadanoff of Chicago, and Wilson and Fisher of Cornell in the early seventies. One by one, the membership of the club of Understood Phase Transitions (PT) grew, with the membership card being LRO, and an order parameter. This confirmed the correctness of the conceptual picture.

But there was trouble brewing....

Thermal fluctuations of the order parameter are larger in lower dimensional systems or models, as the same disordering thermal energy, proportional to temperature T, gets squeezed into a smaller-sized arena. In fact for dimensions d at and below a (lower) critical dimension[1] d_c, $(d \leq d_c)$, fluctuations are so violent that they destroy LRO, and the average of the order parameter.

A simple model that should[3] show this absence of ordering on cooling through all nonzero temperatures, is the 'planar ferromagnet' or XY model, on a two-dimensional (2D) lattice, for which $d=d_c=2$. The model can be visualized as arrows or 'spins', at angles θ_i each on the surface of a dinner plate in the $X-Y$ plane, whose centre i is on the nodes of a square 2D grid, as in Figure 2*a*. There is clearly a relative angle $\theta_i-\theta_j$ between the arrows on neighbouring sites i and j. The energy H_{ij} between each nearest-neighbour pair of spins depends on the cosine of the angular difference,

$$\beta H_{ij} \equiv (H_{ij}/k_B T) = -K_0 \cos(\theta_i-\theta_j). \qquad (1)$$

Here K_0 is a dimensionless coupling strength and k_B is a constant. The same (2D) model effectively describes thin films of helium-4 superfluids, and superconductors

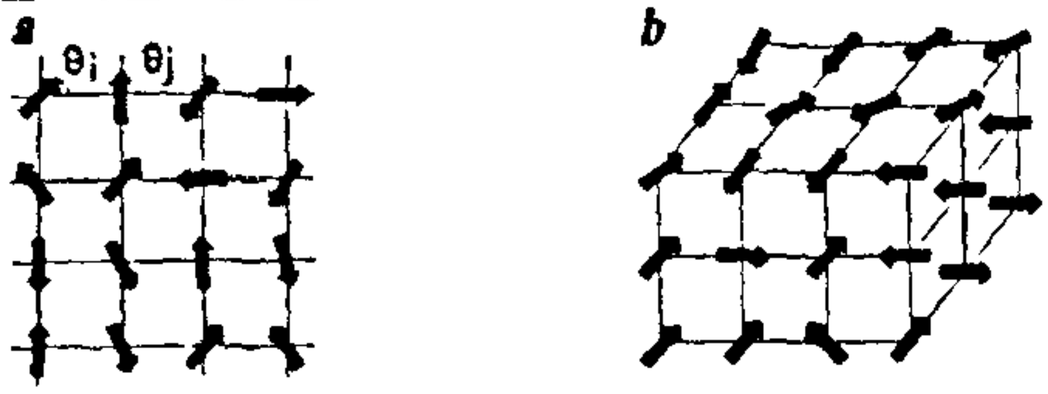

Figure 2. XY model spins, for lattice in (*a*) two dimensions, (*b*) three dimensions.

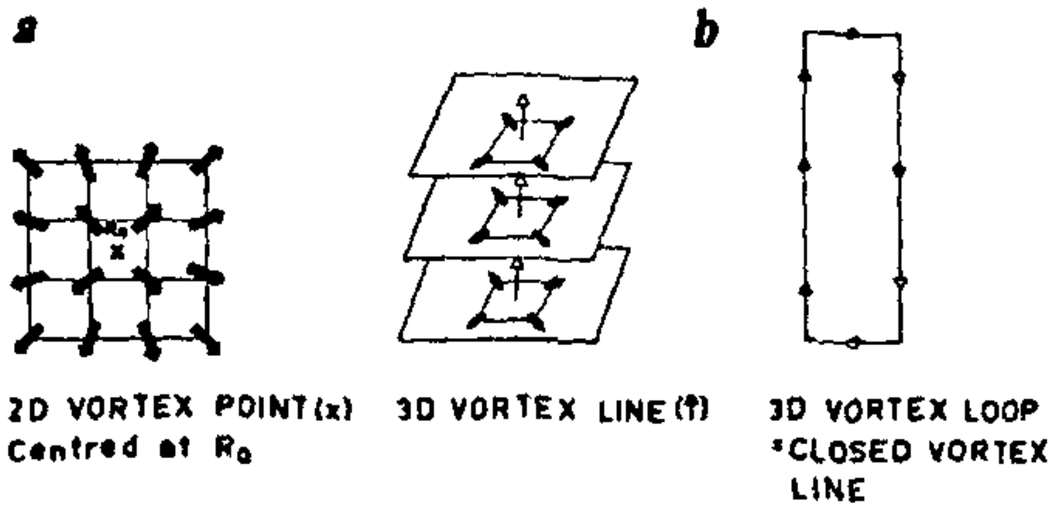

Figure 3. Vortex excitations in (*a*) 2D XY model as a point, (*b*) 3D XY model as a loop.

like aluminium, that are in the same 'universality class' of phase transitions. All such systems/models, at $d=d_c=2$ are forbidden to order, for $T\neq 0$ in the conventional order parameter picture: the angular fluctuations are too violent to permit long range order. There should be no phase transition, at any $T_c\neq 0$.

Unfortunately they happily order, on cooling, quite unaware that this is theoretically verboten! Superfluid/superconductor films have zero effective viscosity/electrical resistance, below a nonzero transition temperature $T=T_c$.

The PT club has a scruffy-looking outsider, looking in, who must be somehow admitted, perhaps by modifying the dress code. One might protest that he should be blackballed: there is no LRO. But it is hard to argue with an infinite conductivity!

Disorder parameter description in 2D

Kosterlitz and Thouless (KT)[3], in 1973, provided a way out: a new kind of phase transition, driven by the unbinding of new kinds of excitations, that sidestepped the issue of LRO.

One kind of excitation in the 2D XY model is well known. On warming from zero temperature, the spins, frozen at $T=0$ into a common angular direction $\theta_i=\theta$, can wiggle due to thermal energy, like a field of grass in a gust of wind—a 'spin wave'.

There is also another kind of excitation[3]. The four spins or arrows on the corners of an elementary lattice-square centred at R_0 can be thermally kicked to successively turn 90° with respect to the previous spin, on a clockwise (say) path. This 360° turn is also distributed over the spins of the larger square enclosing this elementary square, and so on, outwards, as in Figure 3*a*. All spins in the system are tilted by amounts that add up to 360° along any path that encloses the centre R_0. This extended object, that has a centre but no periphery, is called a 'vortex', and has vorticity (sign of successive angular tilt) that is $m(R_0)=+1$. In fact, the vortices are created in $m=\pm 1$ *pairs* from the zero vorticity ground state on warming, with a pair-creation energy E_0, and a creation probability or pair 'fugacity' y_0 given by the Boltzmann factor, $y_0\sim\exp(-E_0/k_BT)$. If the ± 1 charges happen to jump onto the same site in their travels, they annihilate in a blaze of spin waves. However, they cannot just disappear by themselves, while moving around, and are 'topologically stable'.

The word 'vortex' is nothing more than a collective noun for the swirl of spins that couple to each other by equation (1), with coupling constant K_0. The energy of a pair of vortices $m(r)$, $m(r')$ at positions r and r' varies logarithmically with the separation $|r,-r'|$, as

$$\beta H(r,r')=-2\pi K_0\, m(r)m(r')\,\ln\frac{|r-r'|}{a_0}+\beta E_0 \quad (2)$$

with $\beta E_0=\pi^2K_0$, the pair creation energy and, a_0 the minimum scale, i.e. minimum vortex separation or lattice constant in the problem. The total energy is a sum over all such pair separations.

Thus in the KT picture, the 2D XY model can be transformed into an overall neutral Coulomb gas of $m=\pm 1$ 'charges', of pair probability y_0, coupling K_0, and interpair potential $\ln R$. Whatever phase transition at some temperature T_c occurs in the Coulomb gas, is also the phase transition and critical temperature of the 2D XY model, and superfluid/superconductor thin films.

At low T there are a few vortex pairs bound in 'dipoles' ± 1 together; these increase in size and number on warming, and smaller pairs can then nest and screen the larger ones, allowing them to grow bigger still; and finally the largest (infinite) size pair unbinds, at a transition temperature T_c. This is depicted in Figure 4*a*. The vortex unbinding destroys effective superconductivity in films, by causing energy losses or dissipation from the free motion of vortices. The films thus develop voltages on application of an electric current drive, i.e. go to normal metals at $T=T_c$. In the 2D XY planar ferromagnet model, the independent

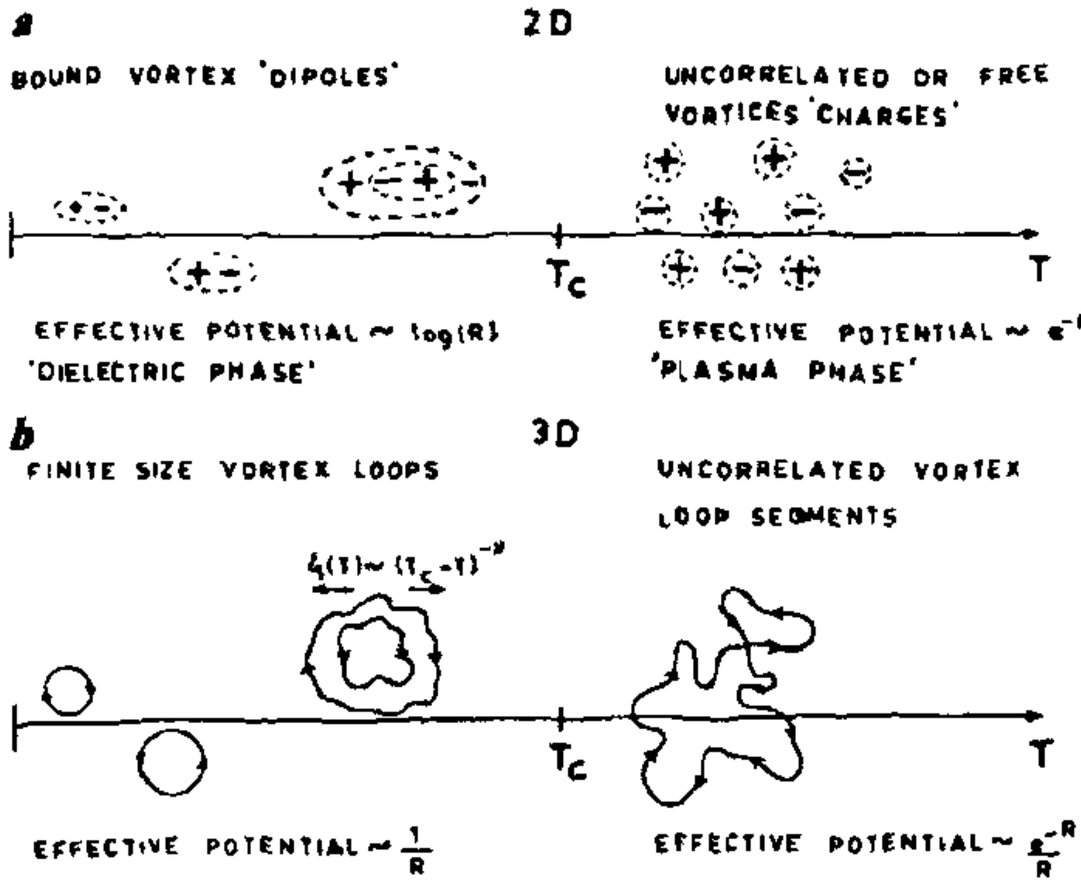

Figure 4. Disorder parameter description or vortex unbinding picture (*a*) in 2D XY case, (*b*) 3D XY case.

motion of unbound vortices stirs up all the spins randomly, for $T > T_c$. (A bound ± 1 dipole has, by contrast, compensating 'stirs' and 'anti-stirs' for $T < T_c$.) The model may be simulated on the computer[4a], with ± 1 vortices seen on the screen, and the KT picture is confirmed.

How does one extract the thermal properties? One needs to do a 'sum over states' or integration over all vortex arrangements. At first sight, this seems easy. Perhaps the $+1$, -1, vortex dipole is tightly bound as a 'molecule', and small-dipoles can then be simply added. But as mentioned, Nature is not so kind. The dipoles are nested, one inside the other, and are of *all* separations or scales, from the lattice constant a_0, through a general separation $a \equiv a_0 e^{\ell}$, to infinity. The trick is to proceed iteratively[5,6] capturing vortex pairs in separation slices da, and ultimately covering the whole scale range $a_0 < a < \infty$.

Because of nested dipole screening, the coupling constant for two test charges becomes scale-dependent, $K_0 \rightarrow K_\ell$ and is cut down compared to the bare value, K_0, as in a dielectric. This incremental dipolar screening reduction dK_ℓ, due to a small $+1$, -1 pair of size between a, and $a+da$, will depend on the fugacity or probability y_ℓ of finding such a pair, at *that* scale. (The fugacity, from equation (2) depends on the coupling, and must also becomes scale-dependent, $y_0 \rightarrow y_\ell$.) If $d_\ell = da/a$ is the fractional scale change, one finds the rate of change (A_0' is a constant) of the coupling constant with fractional scale change is

$$\frac{dK_\ell}{d\ell} = -A_0' K_\ell^2 \; y_\ell, \tag{3a}$$

where the negative sign indicates a screening or reduction of the force as one moves out.

Once we have included the screening of pairs smaller than $a+da$, this may as well be taken to be the new minimum scale for the next step of the iteration. We must track down and change any explicit dependences on the old minimum scale, a, such as in the logarithms of equation (2), or in minimum scale volume factors $(a^{-2})^2$ for the pair coordinates in the sum over states. These are to be replaced by $a+da$, and the fractional bits and pieces $\sim da/a = d\ell$ so generated can be absorbed in a new increment dy_ℓ. Thus the rate of change of fugacity on scaling up is

$$\frac{dy_\ell}{d\ell} = (4 - 2\pi K_\ell)\, y_\ell \; . \tag{3b}$$

Equations (3a) and (3b) are the famous Kosterlitz–Thouless scaling equations in 2D. The input to these 2D vortex coupling and fugacity equations is the bare or initial, smallest scale values ($K_0, y_0 = \exp(-\pi^2 K_0)$) that are temperature dependent, since $K_0 \sim T^{-1}$. Thus the behaviour of the solution K_ℓ, y_ℓ will depend on temperature. A drastic change in behaviour on a smooth change of temperature would signal a phase transition. Since equation (3b) at initial scale changes sign at $\pi K_0 \approx 2$, this could determine the transition temperature, $T = T_c$.

Figure 5*a* shows K_ℓ, y_ℓ behaviour for various temperatures. For $T < T_c$, the ± 1 pairs are pulled towards each other, and with more pairs of small separation than large, and a pair fugacity fall to zero off

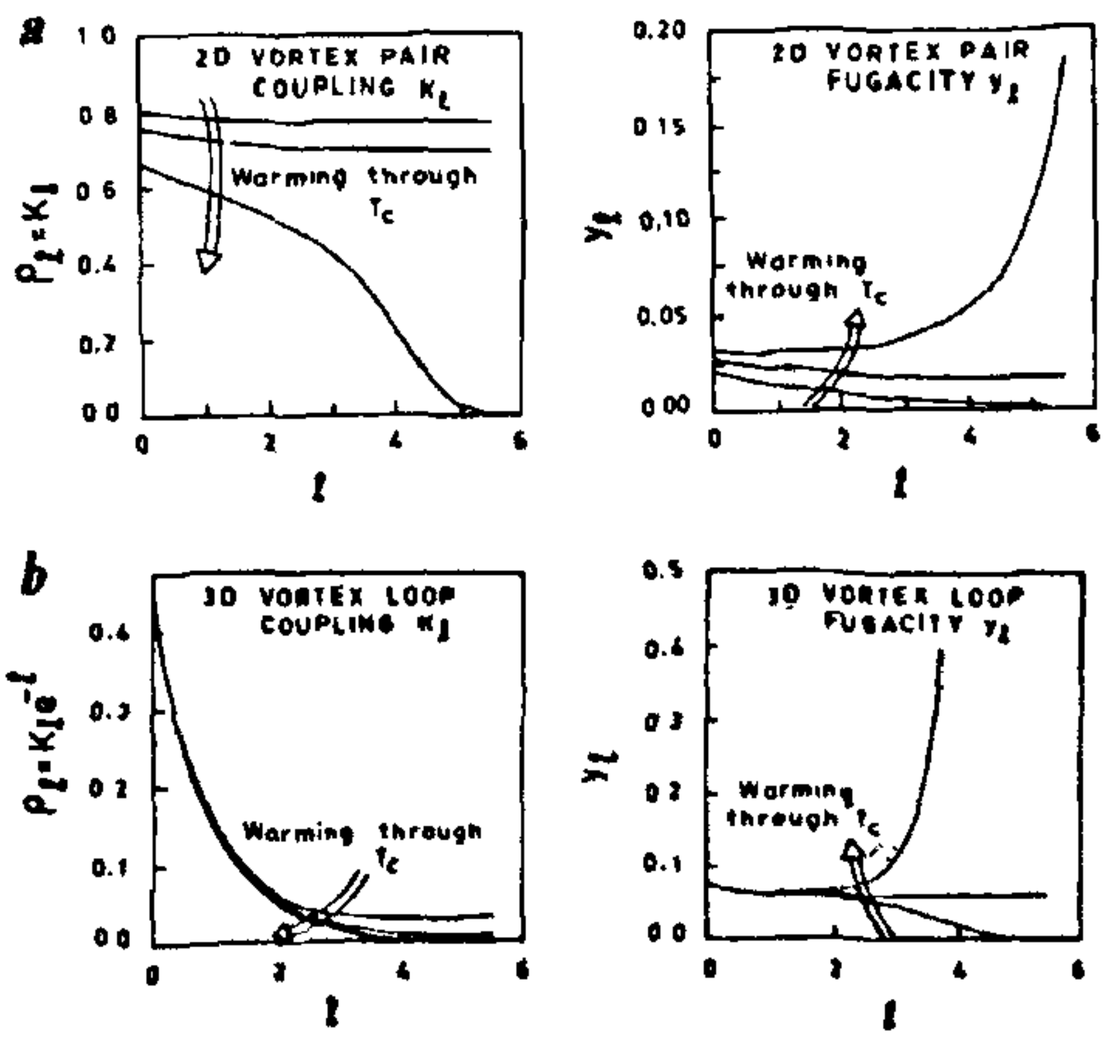

Figure 5. Coupling constant K_ℓ and vortex pair (2D) or loop (3D) fugacity y_ℓ versus ℓ, the logarithm of the pair/loop size showing drastic change of behaviour as temperature is raised through transition. For superfluid helium, the superfluid density ρ_ℓ at a given scale is related to the coupling, with $\rho_{\ell=\infty}$ The macroscopically measured value. (*a*) 2D case with $\rho_\ell = K_\ell$; (*b*) 3D case with $\rho_\ell = K_\ell e^{-\ell}$.

with distance, $y_r \to 0$: vortices are bound in (overlapping) pairs. The coupling constant of the $\ln R$ potential merely changes from one constant (K_0) to another (K_∞) i.e. there is 'dielectric' behaviour, for $T < T_c$, $K_\infty = K_0 (1/\varepsilon)$, where ε is like a vortex-charge dielectric constant. For $T > T_c$, $y_r \to \infty$ so there are more large than small ± 1 separations in the system, i.e. vortex dipole unbinding has taken place. The coupling constant is zero at large scales, $K_r \to 0$ so the potential is short-ranged, and $1/\varepsilon$ is zero, i.e. we are in a vortex 'plasma phase', for $T > T_c$.

Since unbound vortices cause a net dissipation, this means that at $T = T_c$ there is a breakdown of superfluidity or superconductivity, in thin films, and an onset of normal metal dissipation.

Thus as promised by KT, the mystery of the 2D XY model (and related systems) is resolved. It *does* have a phase transition, and must be admitted to the PT 'club as a special case, even though it does not have the LRO membership card, and only has a disorder parameter description, unlike all other phase transitions....

The Club atmosphere would be considerably more convivial, if the admitted, but ostracised, Newest Member was found to be not so 'exotic', after all. Could at least some conventional phase transitions also be treated through a disorder parameter description?

Disorder parameter description in 3D

The simplest model to consider is, naturally, the planar ferromagnet energy of equation (1), but now with the planar spins $-\pi < \theta < \pi$ on a *three dimensional* cubic lattice. This is the 3D XY model. It has a conventional phase transition, with LRO, and exponents[7] $\nu = 0.67$, $\alpha = 0.02$, $\gamma = 1.34$. It is in the same universality class as the bulk helium-4 superfluid transition.

Does it have topological excitations, like the 2D XY point vortices? Yes[8], they are *vortex loops*. Think of many vortex points, each on a 2D plane of the 3D model, and stacked one directly above the other. This induces a 'vortex line', threading the vortex centres. Each plane's spins tilt in a 360° circle around the vortex line, forming a cylinder of spin-tilts around it. Now merge the top and bottom of the vortex line, like a snake eating its own tail. What you have is a vortex loop, that is a toroidal region of tilted spins as depicted in Figure 3*b*. Just as the 2D vortex points $m = 0, \pm 1$ had a sign depending on the sense of spin-tilt, so the vortex loop is a directed *topological* current, J, with components J_x, J_y, J_z capable of taking on integer values, 0, ± 1.

It costs thermal energy to create a 3D vortex loop, just like a ± 1 2D vortex pair, so there are no loops at $T = 0$. The tumbling of a loop is a complex stirring up of the spins, especially on the scale of the loop diameter ξ of the largest loop present. The transition scenario[9,10] is analogous to the 2D case (in fact, slice a directed 2D loop and you have a ± 1 vortex pair). At low T there are a few small vortex loops; these increase in size and number on warming; smaller loops can nest and screen them, allowing them to grow bigger still; and finally the largest size loop $\xi(T) \sim |T_c - T|^{-\nu}$ blows out in size at a transition temperature T_c. This is depicted in Figure 4*b*.

The picture of a vortex-loop blow out was first proposed[2] by Onsager and by Feynman, as an explanation for the 3D superfluid transition. Computer simulations of the 3D XY transition have shown[4b] that thermally generated vortex loops are not just a figment of a theorist's imagination. At $T \neq 0$ one can keep track of the lattice squares around which spins have been twisted by 360°. The centres of these squares are found to be threaded on closed vortex loops, and the loops, indeed[4b] increase in number and complexity on warming.

In fact, Shrock and coworkers[11] found that if an externally controlled energetic cost was imposed on such vorticity-bearing squares, then the vortex loop population was suppressed, (not surprising), and the transition temperature for order-parameter formation was increased (quite interesting![10b]). Thus vortex loops not only exist, but are involved in the transition. So surely[2a], there could be a description of the phase transition[9,10], based on them?

The potential energy between two vortex-loop topological current segments $J(r)$ and $J(r')$, at r and r' turns out to depend both on their separation $|r - r'|$, and on their relative angle. In fact, it is[2] the familiar Biot–Savart 'magnetic' force law between two 'electric' currents.

$$\beta H(r, r') \simeq \pi K_0 \frac{J(r) \cdot J(r')}{|r - r'|} \tag{4}$$

but with flipped sign. Same signs repel, opposite signs attract. The self-energy E_0 of a loop of average diameter a is just the sum of such energies for segments on the same loop. The interloop interaction energy is the sum of energies for segments on different loops. The segment separations can vary from a_0 to infinity.

Figure 6 shows a possible configuration[10c] of loop segments, distributed in a doughnut or 'vada' shape about a mean circle of diameter a, with a_c being a core or fluctuation region. How can a complex structure like that be reduced to just two lengths, a, a_c? The directional form of equation (4) plays a central role.

Suppose you take a current-carrying wire and double it back along its length in a U-shape, or hairpin. The faroff magnetic field due to the hairpin is drastically less than the original straight wire, due to cancellation between oppositely directed sides. Similarly, from

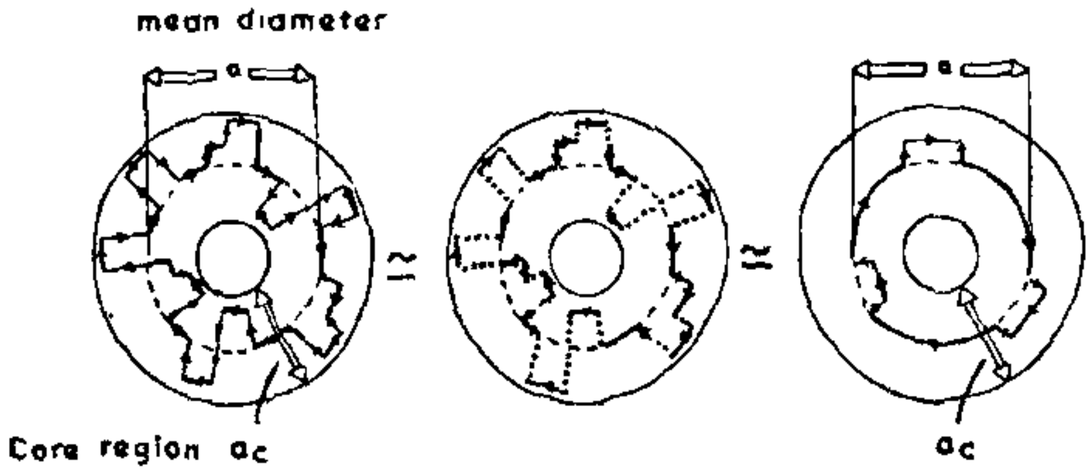

Figure 6. Directed vortex loop with mean circle diameter a, and *hairpin-like excursions from the mean circle, in a 'core' region* a_c. Fields cancel between opposite sides of harpins, and asymptotically the loop is effectively a simpler configuration of 'uncancelled' azimuthal segments.

equation (4), most segments of a hairpin excursion out from the mean diameter contribute little to the potential seen by some far-off loop. Only an uncancelled (azimuthal) segment in each hairpin may contribute. Far-off regions see only these survivors, that add up to a circle of diameter a in a core region a_c as in Figure 6. So, in the end, apparent complexity reduces to effective simplicity, because of the 'magnetic' nature of the interaction, that depends on the direction of the topological currents.

As before, we have a bare coupling K_0, and loop fugacity y_0 and a KT-type nested scaling procedure, within the physical picture above. (In fact the coupling K_0 has absorbed a minimum scale a_0, in equation (4)). The 3D scaling equations, obtained by Williams[9] and the present author[10] by different methods, are

$$\frac{dK_\ell}{d\ell} = K_\ell - A_0 K_\ell^2 y_\ell \tag{5a}$$

$$\frac{dy_\ell}{d\ell} = (6 - \pi^2 K_\ell L_\ell) y_\ell. \tag{5b}$$

Some technical comments. On comparing with equation (3), The '6' in equation (5b) comes from rescaling the minimum scale volume factor $\sim (a^{-3})^2$. The second term in equation (5a) comes from small-loops of probability y_ℓ screening the big loops, just as in equation (3a), the 2D case. The first term in equation (5a) is new and important, and comes from requiring that the minimum separation between two loops, is a if the smallest loop-diameter is a. (For 2D vortex points there is no comparable distinction, so such a term does not occur in equation (3b).) The core size a_c, enters the problem, in $L_\ell = \ln[a/a_c(\ell)] + 1$ of equation (5b).

The core region contains random hairpin excursions, and K_ℓ scales as a length, from equation (5a). A Brownian walk of length L has an rms extent $\sim L^{0.5}$, that swells, slightly with self-avoiding walk restrictions, $\sim L^{0.6}$. We assume $a_c(\ell)/a \approx K_\ell^{0.6}$, as an ansatz[10c] or model for the core. Equations (5) now form a closed system of equations, whose behaviour can be investigated, as the temperature T, and hence the inputs $K_0 \sim T^{-1}$, and $y_0 \sim \exp(-\text{constant} \times K_0)$ are varied. It turns out *there is a sharp change in behaviour, as* T *varies* through T_c: a phase transition does occur.

The fugacity y_ℓ and coupling K_ℓ show very different behaviour above and below T_c, as seen in Figure (5b), just like the 2D case. The critical exponents, obtained from this disorder parameter approach, are $\nu = 0.67$, $\alpha = -0.015$, $\gamma = 1.343$, close to values[7] from the order-parameter approach.

Thus the disorder-parameter approach can be used for a 3D system, previously described by the order-parameter approach. The two viewpoints are complementary.

Speculations on further applications

Possible applications include:

Layered 3D models

Anisotropically coupled layers of planar spins are of interest, since high T_c superconductors involve weakly coupled, phase-coherent layers[12]. Computer simulation data exist[4b]. Figure 7 shows an agreement between vortex loop theory[10c] and simulation data[4b]. The very weakly coupled layer region has some new physics, and is being investigated[13]. It would be interesting to calculate *nonlinear current-voltage characteristics* and compare with experiment[12].

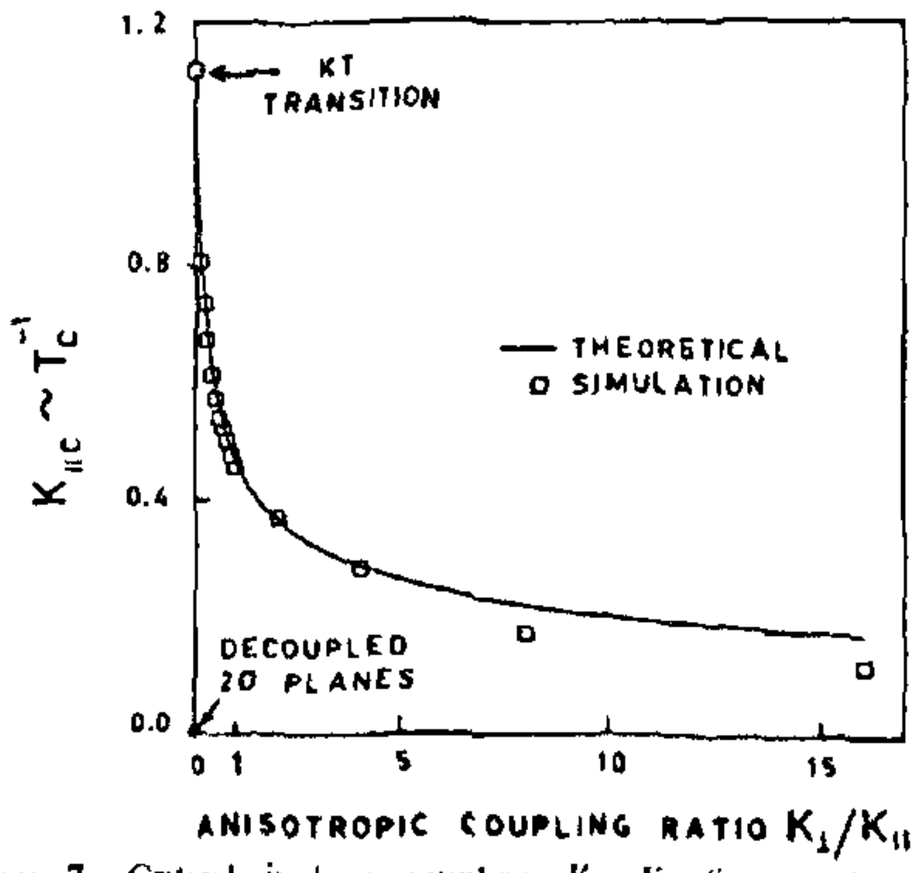

Figure 7. Critical inplane coupling $K_\parallel \simeq K_c$ (inverse transition temperature) versus anisotropy ratio $(K_\perp/K_\parallel)$ between plane/in-plane couplings. Here $K_\perp = K_\parallel$ is isotropic 3D XY case $K_\perp = 0$ is decoupled-plane 2D XY case.

Quantum fluctuations

A quantum system in d dimension can be mapped onto a classical system in $(d+1)$ dimensions, by introducing an extra label to keep track of quantum effects[14]. Thus a 2D Josephson junction array, or granular film consisting of superconducting grains separated by oxide layers, is effectively $(2+1)$ D at $T=0$, and can be described by vortex loops, now created by quantum, rather than thermal fluctuations[13]. Interesting experimental results[14] on superconductor to insulator transitions of granular films await theoretical understanding.

Other models, other topological excitations

Lattice gauge theories, of interest to particle physics, and other models, show a change in the transition temperature on suppression of relevant topological excitations[15], showing that these are somehow involved in the phase transition. Can an appropriately generalized disorder parameter scaling be developed? Hubbard models, relevant for high T_c superconductors, have their own topological excitations[16]. Vortices exist in models of the fractional quantum Hall effect[17]. Dislocation loop pictures of melting have been suggested[2].

Glassy transitions

On rapid cooling of a silica melt, the disorder of the molten liquid somehow gets trapped, in a kinetic transition to a quasi-solid without LRO, that flows like a liquid over a time-scale of centuries. If the melt can be regarded as a soup of dislocation loops[2], then a disorder parameter kinetics approach might help in making the mysterious glass transition more transparent.

Turbulence

Liquid flowing through a pipe has a parabolic velocity profile, with maximum velocity $v=v_0$ at the centre, and zero tangential velocity $v=0$ at the pipe walls, because of viscosity. As a dimensionless parameter called the Reynolds number $\mathscr{R}\propto v_0$ is increased, hydrodynamic vortices form, and beyond a critical value $\mathscr{R}>\mathscr{R}_c$, turbulence sets in[18]. Can this be regarded[19] as a nonequilibrium phase transition, driven by these nested eddies of all scales, with $\mathscr{R}_c$ analogous to the critical temperature for a disorder parameter blowout?

In conclusion, the disorder parameter approach, first regarded as applicable only to 'exotic' two-dimensional systems, is perhaps also applicable to at least one conventional three-dimensional transition. This raises the possibility that order-parameter formation on cooling, and disorder parameter blowout on warming, may be complementary approaches to yet other phase transitions, opening an interesting line of further investigation.

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Predicting the high pressure phase transformations using density functional approach

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During the last decade, there has been an intense feedback between high pressure experiments and theoretical techniques based on the density functional formalism for the analysis of phase transformations. This has resulted in increased accuracy in theoretical computations and they have now acquired predictive capabilities. Some successful examples are discussed. The existing problems and their possible solutions are indicated.

PREDICTIONS of pressure-induced phase transformations in materials from *ab initio* methods are rare. This is because it has been difficult to calculate accurately the small Gibbs free energy differences between different phases (a few mRy/atom or smaller). However, recently, electron band structure techniques based on density functional formalism have acquired such capabilities due to improvements in their formalisms as well as increases in the computational speed. Using these methods, it is now possible to correctly compute the equation of state, the most stable crystal structure of materials, phonon frequencies and other ground state properties[1,2]. The recent calculations on the element thorium, done at Trombay, describe the state of the art. High pressure experiments, done by Vohra and Akella[3], have shown that Th undergoes a fcc to bct phase change at 80 GPa and $V/V_0 = 0.6$. Figure 1 displays the variation of the computed total energy with axial ratio in the bct structure at various compressions[4]. It correctly shows the stability of the fcc ($c/a = 1.414$ in the bct axis) phase up to volume fraction of 0.6, at which the bct structure becomes more stable. The pressure of transition from the fcc to bct phase at 80 GPa agrees very well with the experimental value. In addition, the calculations accurately reproduce the experimental variation of the axial ratio (c/a) with compression in the bct phase (Figure 2) and the equation of state (Figure 3). Also they clearly bring out the important role played by the occupation of the 5f band in this structural transition in thorium.

The experimental techniques, also, have been dramatically improved during the same period. In static high pressure investigations, advances in the diamond anvil cell (DAC) technology coupled with the energy dispersive X-ray diffraction technique (EDXRD) at synchrotron radiation sources have facilitated detection of new phase transformations in solids under megabar pressures[5,6] and this has opened up new vistas for testing theoretical electronic structure calculations[7,8]. In dynamic pressure studies also, a new technique has been developed to detect phase transformations that are accompanied by small volume changes[9]. In this, a phase transformation is inferred from the observation of a discontinuity in the measured sound velocity as a function of peak pressure in the shocked state. The detection, however, like that in other shock wave techniques, is macroscopic in nature and the transition needs to be characterized either by comparison with the

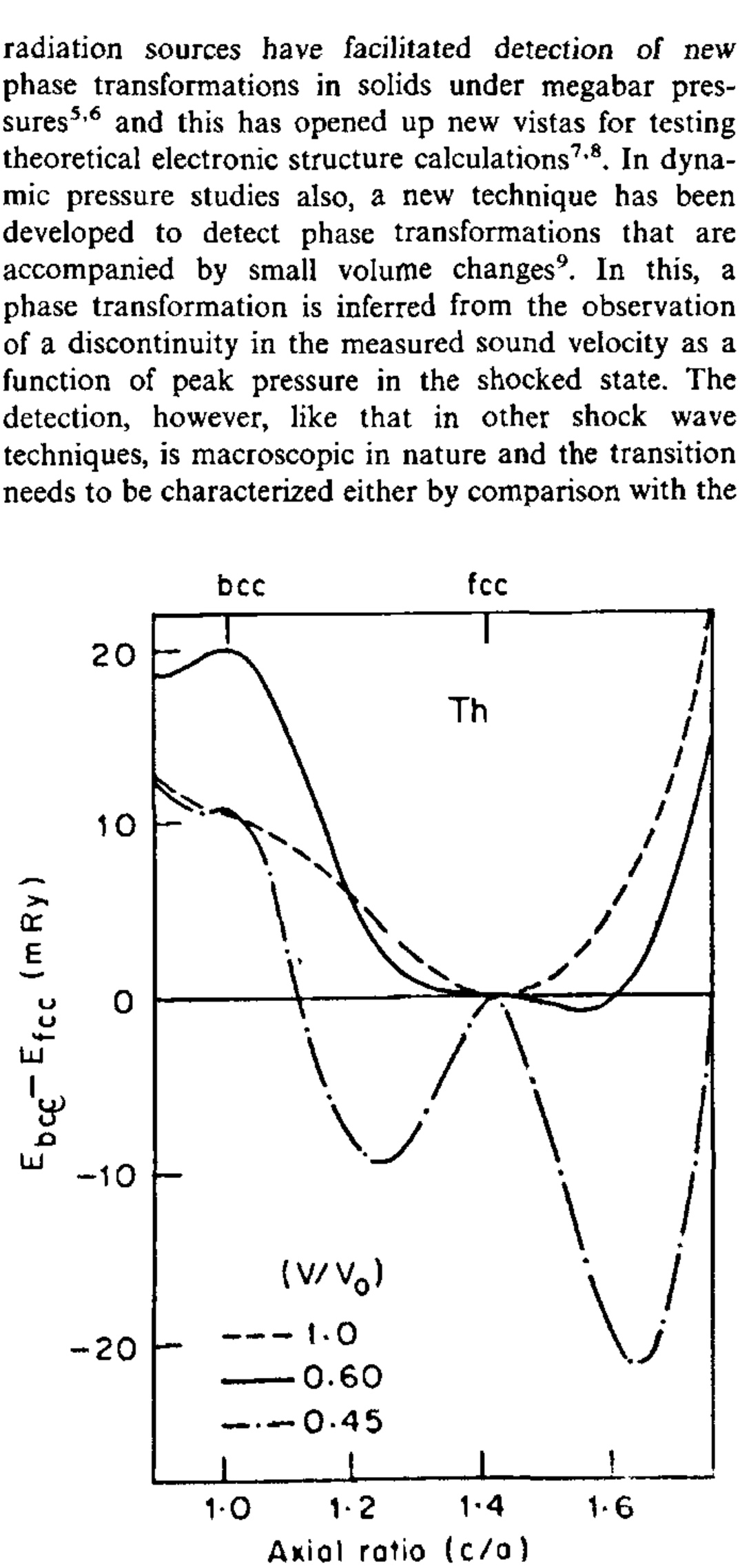

Figure 1. Total energy E_{bct} of thorium in the bct structure (relative to that in fcc phase), calculated as a function of axial ratio c/a. The curves at various compressions are as indicated in the legend (ref 4)