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The Landau model with several order parameters

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Abstract. Following Griffiths we present some further methods in the Landau model, for higher order critical points. Techniques due to Arnol'd allow us to exhibit the codimension and incidence scheme of critical points in the theory for two and three order parameters. Unlike the procedures of Griffiths who analyses the global behaviour of the free energy, the results here are obtained by pasting local solutions together. That the combination of such strata is a complete description is an assumption valid in some cases.

1. Introduction

Griffiths has previously presented a classification scheme for phase diagrams, based on topological reasoning (Griffiths 1975). As a particular case, he analyses the global behaviour of the free energy in a Landau model completely for the case of one order parameter and partially in the case of two. Such global analyses are of course hard in general: for example, Griffiths' results on the Landau model in two variables

$$\Psi(x, y)=\sum_{j,k} a_{jk}x^jy^k \tag{1}$$

in the case $a_{jk}=0$, $j+k\geqslant 3$ depend on a factorisation property of some homogeneous functions of the fourth degree in two variables, and such lucky accidents are hard to come by. If we choose on the other hand, to look at the local behaviour of a function with a critical point at the origin, say, we can proceed to fairly high order in determining the codimension and bifurcation scheme of the singularities. Of course, the global view is now lost but we can hope to recover it by pasting together local solutions and viewing the codimension of a function as a sum of the contributions from its critical point and its critical value. (Two co-existing singularities of lower codimension form an entity of higher codimension.) The meaning of and assumptions inherent in such analyses will, we hope, become clear in the following. First we recapitulate some definitions from the theory of singularities (Arnol'd 1972).

2. Definitions for local singularities

The word singularity is used interchangeably with critical point, i.e. the function we are considering has a zero and vanishing first (partial) derivatives at the critical point, supposed to be the origin as long as we look only at the local behaviour.

Moreover we are interested in second and higher order phase transitions, i.e. in degenerate singularities where one or several coefficients of the second order terms in a Landau expansion vanish at the critical point. The number of order parameters needed in a Landau expansion is the number of zero eigenvalues that the second derivatives (Hessian) matrix of the free energy with respect to the densities develops. This is termed the co-rank of the singularity since it is also the number by which the Jacobian (susceptibility) matrix drops rank. We shall assume that the co-rank is given. Krinsky and Mukamel (1975) have analysed a spin-$\frac{3}{2}$ Ising model illustrating this and other features of Landau-type theories.

We are interested in the topological type of singularities, i.e. singularities which can be made equal after a continuous change of coordinates, are to be considered equivalent (Griffiths 1975). In the usual techniques of the mathematical theory of singularities (Arnol'd 1972) a classification is made of the diffeomorphic type, i.e. up to a smooth (infinitely differentiable) change of coordinates. To help determine the topological type we make the assumption that the critical point of the lowest order terms in an order parameter expansion is isolated (i.e. $\nabla f(x)=0 \Rightarrow x=0$). We preclude therefore a line, plane, etc of singularities. This is not a restrictive assumption since most polynomials have only isolated singularities.

We now have to define the codimension and the stratification of singularities in order to be able to provide the characteristic graph. The codimension of a singularity is the dimension of the space of functions with a critical point at the origin minus the dimension of the space of functions with the given singularity. Both spaces are infinite dimensional of course and to make the codimension a precise and calculable quantity mathematicians working in the C^∞ (i.e. diffeomorphic) classification scheme gave the definition

$$\mathrm{codim}(f)=\dim M/\Delta(f). \tag{2}$$

M is the space (ideal) generated by the monomials $x, y \ldots$ (and so the space of functions vanishing at the origin) and $\Delta(f)$ is the ideal generated by the Jacobian of f, which tells us to what order f vanishes at the origin.

Thus if $f=x^2$, M_1† is generated by $(x, x.x, x.x.x, \ldots)$ and $\Delta(f)$ is generated by $(2x, 2x.x, \ldots)$ which is the same thing. The codimension of non-degenerate singularities is zero as it is designed to be.

Let us take (still with one variable) $f(x)=x^{k+1}$. Then $\Delta(f)=M_1^k$ in obvious notation and

$$\dim\left(\frac{M_1}{M_1^k}\right)=\sum_{i=1}^{k-1}\dim\frac{M_1^i}{M_1^{i+1}}=\binom{1+k-1}{k-1}-1=k-1$$

which is, of course, the obvious result. We should perhaps note that the dimension of the space of homogeneous real valued polynomials of degree k in n variables is $\binom{n+k-1}{k}$. This is because the monomials $x_1^{r_1}\ldots x_n^{r_n}$, $\sum r_i=k$ form a basis and the cardinality of this set is the number of ways one can distribute k balls among n boxes.

All this is of course well known and leads to the first conflict of the C^∞ classification scheme with what one would want in a Landau-type theory. This concerns the first genuine fourth order singularity in two variables:

$$f(x, y)=x^4+(1+\alpha)x^2y^2+\alpha y^4 \tag{3}$$

(with $\alpha \neq 0, \pm 1$ to keep the critical point isolated). The above definition (2) gives $\mathrm{codim}(f)=8$ and not 7 as we would obtain from the expansion in equation (1) with

† The subscript 1 is designed to remind us that we are dealing with one variable.

$a_{jk}=0$, $j+k \geqslant 3$ (Griffiths 1975). That is, there are ten conditions, three of which relate to the function having vanishing constant term and first partial derivatives. The proof that the codimension is 8 by formula (2) is relegated to appendix 1 which is the type of simple calculation of vector space dimensions one does in the classification of singularities.

The difference between the two numbers relates to the unsuitability of a smooth equivalence classification for one requiring only continuous equivalence. The former is easier to do however, and, as is frequently done in other contexts, we shall first look at the diffeomorphic theory and then discard what is superfluous for the homeomorphic scheme. Since requiring a coordinate change to be smooth is more restrictive than requiring it to be continuous, one obtains many singularities inequivalent under a diffeomorphism that become equivalent if only continuity is required. The form (3) is an example. If we say $f \approx g$ (f is equivalent to g) if $f(x, y)=g(\xi(x, y), \eta(x, y))$ where

$$f(x, y)=(x^2+y^2)(x^2+\alpha y^2) \tag{3}$$

and ξ, η are required to be C^∞ then α is invariant, i.e. $f_\alpha \approx f_\beta$ only if $\alpha=\beta$ (Arnol'd 1974). In a topological classification, of course, α should not matter. In this particular case the above statements are easily understood geometrically. α has the interpretation of a cross ratio of four lines and it is well known from projective geometry that: (*a*) the cross ratio is a projective invariant; and (*b*) if we allow continuous deformations, four lines with a given cross ratio can be mapped onto four lines with any different cross ratio†.

So we define a codimension for the topological type of a singularity (assuming of course that we can determine the type). We subtract from (2) the number of parameters appearing in a diffeomorphic classification. As a justification for this we use the facts that the dimension of the space of points corresponding to singularities of given $\mu \equiv \dim(M/\Delta(f))+1$ is equal to the number p of parameters needed (Gabrielov 1974) and further that at least for polynomial functions with isolated singularities the number μ‡ fixes the topological type completely. So we use the following formula for the codimension C

$$\mu=C+p+1. \tag{4}$$

The fastest way of computing μ, due to Kushnirenko (1975), is quoted without proof in appendix 2.

In order to display a characteristic graph (Griffiths 1975) we need to know how singularities bifurcate. The natural assumption that the coalescing of singularities is the only way their topological type can change§ is true for complex analytic functions (Lê Dũng Tráng and Ramanujan, to be published), can be shown to be true for functions of up to three variables (and with isolated critical points for fixed values of any parameters). So we are justified in assuming so for two and three order parameters.

† To make the appearance of parameters less mysterious, we may remark that the theory is concerned with generic singularities, i.e. singularities whose type does not change under a small deformation. This makes the introduction of parameters natural for degenerate singularities (Arnol'd 1972, 1974). In general these parameters may not have a simple geometric significance. We get them because we allow only analytic instead of merely continuous scale changes, as explained above.

‡ And not the codimension C. Care will have to be taken for spaces with the same μ and different C: their characteristic balls may not in general split.

§ In the different context of the renormalisation group theory of critical phenomena the tricritical, tetracritical, etc fixed points obtained have all been as bifurcations away from the trivial or Gaussian fixed points.

Our last comment in this section concerns the stability requirement imposed by thermodynamics, i.e. that the free energy be an absolute minimum. The typical form for the free energy at criticality will then contain only even powers of the order parameters. The global form for the free energy which will contain lower order terms and critical points of lower order computed with this free energy are not guaranteed to be absolute minima and their stability should be checked (Krinsky and Mukamel 1975). For this purpose it might be useful to have a catalogue of both the stable and unstable points that arise in a characteristic graph of a stable critical point. We do not pursue the point here, since our aim is primarily to discuss the methods available.

3. Fourth order singularities

We quote some results obtained by techniques like those outlined in appendix 1. These techniques (Arnol'd 1972) will also give results for codimension for polynomials with cubic and other terms which are ignored in a thermodynamic theory.

The singularity with non-vanishing fourth derivatives of lowest codimension is $x^4+ax^2y^2+y^4$, $a\neq\pm2$. In general topologically distinct fourth order critical points of the form

$$f(x, y)=x^{4+p}+ax^2y^2+y^{4+q} \tag{5}$$

have codimension $7+p+q$. The only critical points of lower codimension have co-rank 1, i.e. are of the form x^{2k} (or y^{2k}), $k=1, 2, 3, 4$. (This is not true if we include unstable critical points, e.g. x^3+xy^3 has codimension 6.) Still within the local picture, the incidence scheme is determined by calculating the critical points into which the given singularity breaks up under small deformations. This is done by bifurcation theory so we build up a stratification of critical points (in this case the obvious one):

$$D_2^{p,q}\to D_2\to D\to C\to B\to A$$

where we use Griffiths' notation for A, B, C, D, D_2 (Griffiths 1975) and then $D_2^{p,q}$ is of course equation (5). From the techniques available for constructing an exhaustive list of critical points there are many singularities that look like cubics etc in the above incidence scheme if one wishes to include them. For example, between D_2 and D one would get also

$$D_2\to X\to Y\to D$$

where $X=x^3+xy^3$ and $Y=x^2y+y^3$, both of codimension 6.

In this classification scheme, the fourth order expansion in three variables with codimension 16 requires ten parameters to describe its normal form! Similarly the codimension 18 object consisting of the sixth order terms requires seven parameters. We can carry this out using algorithms checking for non-degeneracy (i.e. isolated critical points), order and codimension (appendixes 1 and 2) but we might be storing up against a famine that never arrives. There are no objects between codimension $7+p+q$ and 16 if only even powers of x, y, z, ... are allowed.

4. Phase co-existence

We have defined the codimension of an isolated critical point of polynomials. To allow for phase co-existence we have to know global features of the phase diagram and not just the form of the free energy function at the critical point. There is no difficulty defining a codimension for phase co-existence

$$\bar{C} = \text{number of critical points of } f^{-1}(\psi) - 1 \tag{6}$$

where $f(x)|_{x=x^0} = \psi$. Here x_0 is a critical point and ψ the corresponding critical value. The definition then says $\bar{C} = 0$ if the critical values are all distinct. So we define the total:

$$\text{codim}(f) = C + \bar{C}. \tag{7}$$

This is effectively part of the method Griffiths uses in constructing his characteristic graph. In the mathematical literature it is proved that the hypotheses Griffiths introduces in his equation (3.3) and following it (Griffiths 1975) are consistent definitions for a space admitting a natural stratification. Formally a stratification of a topological space X is a collection of subsets $X^0, X^1, \ldots, X^i, \ldots$ which form a partition of X and $X^0 \cup X^1 \ldots \cup X^i$ is open. If X is of dimension n a natural stratification would have $X^{i+1} \subset \bar{X}^i$ with X^i a submanifold of codimension i in X. For n dimensional Euclidean space a stratification can be defined by

$$x_j = x_{j'}, \qquad 1 \leqslant j < j' \leqslant N \tag{8}$$

for all non-negative integers N. Thus the ith stratum obeys i independent algebraic equations.

For our case of the space of isolated singularities of homogeneous polynomials (plus higher order terms) we can associate with it a natural stratification: it seems clear that for points with the same codimension k the different partitions $k = C + \bar{C}$ correspond to algebraically independent spaces from the definitions of C and $\bar{C}$. Let us consider a function with N non-degenerate singularities $s_1 \ldots s_N$. Let us choose a specific order for them by $\phi(i) = s_i$, $i = 1, 2, \ldots, N$.

Then we can map a stratification of R^N onto our space V of non-degenerate singularities (all of the same codimension) by choosing mutually disjoint neighbourhoods U_i of the s_i and choosing $\phi' \in V$ such that ϕ' has a non-degenerate singularity at s'_k in U_i (and no others). The required stratification is then the image of the one in R^N by ϕ', i.e. it is $(\phi'(s'_i), \ldots, \phi'(s'_N))$.

So we can stratify our space of isolated singularities whether degenerate or not and determine the incidence scheme in this way.

We should note that μ in equation (4) has the meaning of being the number of non-degenerate critical points that the given singularity can bifurcate into. 'Nearby' functions require μ parameters—including the constant term—to describe them (Arnol'd 1972).

To get the entities corresponding to a given codimension k we are justified in partitioning k in various ways again rejecting contributions from singularities with odd powers of $x, y, \ldots$.

To get the global phase diagram however, we would need to know how many singularities of each type there were. The only global theory available is Morse theory, invalid in general for degenerate critical points (Milnor 1963). However in a thermodynamic theory with singularities being absolute minima we can use the Morse inequalities. We should emphasise that with degenerate singularities allowable in a global phase diagram the numbers N_r that enter the inequalities are no longer the number of critical points with index r. Rather N_r is greater than or equal to the number of such critical points. With this caveat, the analysis proceeds as is usual in Morse theory and as has been described in connection with phase transitions recently by Mistura (1976).

Carrying out the procedure described above we would get the graph in figure 1 perhaps incomplete in its global aspects but complete in its local.

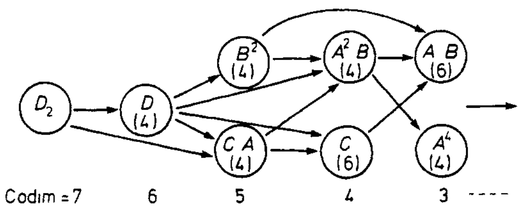

Figure 1. Incidence scheme for singularity D_2 which breaks up into $\mu = 9$ non-degenerate critical points on deformation. Knowing μ, C and the generators of a singularity determines the types available by bifurcation from it. The numbers of topologically equivalent but disconnected types are estimates obtained from μ and the co-rank and denoted in parentheses beside the singularity.

5. Conclusions

In the case where a Landau expansion of the free energy in terms of order parameters displays a critical point in the lowest order non-vanishing homogeneous part, we can determine the codimension and the form of the singularity up to topological equivalence (for up to three order parameters at least). We should note that this cannot be generalised to any analytic function since the C^∞ or C^k classification scheme requires many conditions quite irrelevant from the topological point of view†. On the other hand a purely topological attack, as far as we know, is so far from mustering any force that the renormalisation group is quite unchallenged even as a qualitative theory of real world critical points.

The second point we wish to make in this paper is that the rules that Griffiths has proposed for constructing characteristic balls are natural for such singularities as we have considered: the space has a natural stratification that is combinatorial. Again we have no comments on the purely topological problem.

Finally we may expect to give rules for determining the types arising from symmetry breaking. Basically what we need is the statement that for a finite group G there is a finite set of generators $\phi_1, \ldots, \phi_l$ for invariant polynomials, i.e. any invariant polynomial can be expressed as a polynomial function of these. (This is also true for smooth functions.) Then one can show that the local behaviour of any (polynomial or smooth) singularity can be expressed as a function of the above generators. We are not done however since the stability of such singularities has to be checked, i.e. entities that are unstable under the addition of higher order terms may become stable if required to be invariant under some group. Again in general this is a hard problem for higher singularities but with the requirement of thermodynamic stability, considerable simplifications arise. We hope to pursue this at a later date.

† As we have remarked, for isolated critical points of homogeneous polynomials, the topological type is determined by the analytic type.

Appendix 1

We look at the fourth order singularity

$$f(x, y) = (x^2 + y^2)(x^2 + \alpha y^2) \qquad \alpha \neq 0, 1, -1. \tag{3}$$

We want to show this is a genuine fourth order singularity (obvious in this case but used as an illustration) and to compute its codimension.

What we mean by 'genuine' fourth order is that terms of fifth order can be transformed away and that $f(x, y)$ itself cannot be absorbed into a lower order singularity by a change of coordinates. Mathematicians refer to this by saying that f is 4-determined but not 3-determined. For a homogeneous polynomial of course no calculation is necessary but we supply the tests for generality.

If

$$M^{k+1} \subseteq \Delta(f)M^2 \tag{A.1}$$

then f is k-determined.

We recall that M^r just means the space generated by homogeneous polynomials of degree r (in two variables in our case) denoted H_2^r. We then say $M^r = ((H_2^r))$.

We note

$$a_1 \equiv \frac{\partial f}{\partial x} = 4x^3 + 2(\alpha + 1)xy^2 \tag{A.2}$$

$$a_2 \equiv \frac{\partial f}{\partial y} = 2(\alpha + 1)x^2y + 4\alpha y^3 \tag{A.3}$$

so that $\Delta(f)M^2$ has six generators (obtained by multiplying (A.2) and (A.3) by x^2, xy, y^2). We check first that each polynomial in the list of generators is a homogeneous polynomial of degree 5. From the definition of M^5 we will be done if the six generators are a basis for the homogeneous polynomials of degree 5 (over the real numbers†). This can be easily checked by the non-vanishing of the coordinate matrix with respect to any ordered basis of H_2^5 (for $\alpha \neq 0, 1, -1$). This will show that f is 4-determined.

To show in general that a function f is not r-determined one would have to show that

$$M^r \not\subseteq \Delta(f)M. \tag{A.4}$$

To show that $\dim M/\Delta(f) = 8$ as claimed in the text we note $\Delta(f) \subseteq M^3$ and

$$\dim (M/\Delta(f)) = \dim (M/M^2) + \dim (M^2/M^3) + \dim (M^3\Delta(f))$$
$$= 5 + \dim (M^3/\Delta(f)).$$

Now we show that $((xy^2, x^2y, x^2y^2))$ span $M/\Delta(f)$ in which case they will be a basis for $M^3/\Delta(f)$‡. By writing $(f) = ((a_1, a_2))$ we see that

$$x^3 = \frac{1}{4}a_1 - \frac{1+\alpha}{4}xy^2 \qquad y^3 = \frac{1}{4}a_2 - \frac{1+(1/\alpha)}{4}x^2y$$

† It may be pertinent to note for example that the 'coordinates' used in generating M^r from H_2^r are polynomials.

‡ That $\dim M^3/\Delta(f) \geq 3$ can be checked by using that if $I \subseteq M^r \subseteq M^{\Delta(f)}$, $\dim (M^r/I) \geq \dim (M^r/M^{r+1}) - k$, if I is generated by k elements. For $r = 4$, we can show codim $(f) \geq 8$.

so

$$x^3 \equiv \frac{-(\alpha+1)}{2} xy^2 \bmod \Delta(f) \qquad y^3 \equiv -(1+1/\alpha)x^2 y \bmod \Delta(f).$$

With a little more we can show

$$x^3 y \equiv 0 \bmod \Delta(f) \qquad xy^3 \equiv 0 \bmod \Delta(f).$$

Since f is fourth order, $M^5 \subseteq \Delta(f)M \subseteq \Delta(f)$.

From the preceding five statements, we see that $((x^2y, xy^2, x^2y^2))$ span $M^3/\Delta(f)$. Our list of generators are then these and the lower order monomials: $x, y, x^2, xy, y^2, x^2y, xy^2, x^2y^2$.

Appendix 2

Kushnirenko (1975) has proved a theorem by which the codimension or rather the number μ can be easily estimated for any polynomial. Here we indicate some of the simplest computational details. In essence the method is an adaptation of Isaac Newton's for finding power series expansions for solutions of implicit equations.

The Newton polygon (for more than two variables, polyhedron) is a convex polygon constructed from the exponents of the monomials in the function and in particular one has

$$\mu(f) = n!\ V - (n-1)!\ V_1^i + (n-2)!\ V_2^{ij} \ldots \pm 1 \tag{A.5}$$

for most functions f†. The notation is as follows: V is the volume of positive orthant under the polygon, V_1^i the $(n-1)$ dimensional volume on the ith hyperplane and so forth. In the case $f(x, y) = x^4 + (1+\alpha)x^2y^2 + \alpha y^4$, V is the area under the triangle with vertices $(0, 0)$, $(0, 4)$ and $(4, 0)$ and V_1^i are the lengths of the axes to $(0, 4)$ and $(4, 0)$. This gives $\mu = 9$ or codim $(f) = 9 - 1 - 1 = 7$ by the definition (4) in the text.

We should note that algorithms can be provided for finding the generators of the singularity as well by this method but we refer to the mathematical literature for details (Arnol'd 1974).

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† In special cases $\mu >$ right-hand side.