

## Local characterization of phase diagrams

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A classification of the local topological type of phase diagrams for fluid mixtures is obtained. The classification derives from ideas of Thom and results of Arnol'd in the theory of singularities of smooth real-valued functions, together with the assumption that the state of the system corresponds to a minimum of a smooth function on a space of internal variables which can have arbitrarily high dimension. Griffiths's notions of elementary and compound entities emerge in a natural manner. The methods used are phenomenological. Some attention is given to the question of why these seem to work so well and how they might be rigorously established.

### INTRODUCTION

Our goal, in this paper, is to obtain a complete local classification of possible phase diagrams. We present a phenomenological theory dealing with phase diagrams in thermodynamic field space. Our theory subsumes the Landau model of phase transitions. But, it is deeper in the sense that it gives an insight into why the Landau theory works. We suggest how thermodynamics might be derived from the underlying statistics of the microstate of the system.

We have been very much influenced by the work of Griffiths.<sup>1</sup> We will employ his terminology and, in particular, we adopt his suggestion regarding the use of thermodynamic *field* variables (cf. Sec. I). This simplifies the classification of phase diagrams, and accordingly, we shall only consider phase diagrams in field space.

In this paper, we classify typical neighborhoods of phase diagrams by observing that phase diagrams seem to be homeomorphic to bifurcation sets of algebraic functions. We, therefore, posit that there exists a one-to-one correspondence between typical neighborhoods of phase diagrams and typical neighborhoods of bifurcation sets of smooth functions with a global minimum. Adding various transversality conditions gives a classification of acceptable phase diagrams and allows us to deduce various forms of the Gibbs phase rule.

Section I summarizes Griffiths's work and gives some of the mathematical definitions needed to understand it. Section II introduces additional mathematical terms and various examples of stratified sets. Section III is devoted to the important notion of bifurcation sets and gives a general description of the type of modeling we use. In Sec. IV, we specifically describe the model we have in mind and quote the results from singularity theory that we need. This section is very concise and will probably make extremely difficult reading for all but the most mathematically oriented. We thereby advise the

reader to glance quickly through this section and return to it for reference while reading the later sections. In Sec. V, the results of Sec. IV are applied to thermodynamics and we rephrase Griffiths's results in these terms. In Sec. VI a local classification of phase diagrams is given together with a powerful generalization of Gibbs phase rule. Section VII, which is more philosophical and speculative, suggests possible extensions of our results.

Our theory makes no predictions about critical-point exponents. However, extra assumptions can be incorporated to take care of this. Although we are presenting a phenomenological theory, the authors are convinced that an exact theory will ultimately be formulated along these lines. In particular, we feel that the generalized Morse lemma is the key to understanding how thermodynamic variables and phases arise from systems with a large number of degrees of freedom. In our opinion, the single greatest problem with phenomenological theories of phase transitions is not that they are inadequate regarding numerical predictions, but, rather, why they work at all. For example, in a fluid or magnetic system, it seems almost incredible that, given the enormous number of degrees of freedom of the system, the qualitative features of the phase transition can be described in terms of a polynomial in one order parameter. We feel that the theory we outline here is especially important in that it provides a mathematical explanation for this.

Our theory also gives rise to significant algebraicization of the mathematical techniques used in describing phases and allows particularly elegant formulations of the Gibbs phase rule and the conditions under which it will apply. We also sketch some of the ideas which may be used to discuss symmetry and symmetry breaking.

The mathematical ideas used in this paper are due mostly to Thom<sup>2</sup> and Arnol'd.<sup>3</sup> Recently, some of the applications of Thom's theory have come under attack. Although we feel that criticism of the more ex-

travagant claims is justified, the controversy should not be allowed to obscure the value of Thom's theory. We hope that this paper will convince physicists of the value of catastrophe-theory modeling and singularity theory.

I. BASIC DEFINITIONS

We first define the basic ideas employed in this paper. Readers who feel uncomfortable with the word *topological space* may substitute *subset of Euclidean space* with no harm to anything except mathematical generality. Recall that a homeomorphism of two topological spaces is a one-to-one continuous map between the spaces with a continuous inverse.

*Definition.* A pair of topological spaces  $(Y, Q)$  is a topological space,  $Y$ , together with some distinguished subspace  $Q \subseteq Y$ .

*Definition.* A homeomorphism  $h: (Y, Q) \rightarrow (Y', Q')$  of two pairs of topological spaces is a homeomorphism  $h: Y \rightarrow Y'$  such that  $h(Q) = Q'$ .

A homeomorphism of pairs of topological spaces is a *diffeomorphism* of pairs of topological spaces if  $Y$  and  $Y'$  are differentiable manifolds and  $h$  and  $h^{-1}$  are infinitely differentiable. Two pairs of topological spaces are *homeomorphic* (diffeomorphic) if there exists a homeomorphism (diffeomorphism) between them.

We remark that the assertion that  $(Y, Q)$  and  $(Y', Q')$  are homeomorphic as pairs is *stronger* than the assertion that  $Y$  is homeomorphic to  $Y'$  and  $Q$  is homeomorphic to  $Q'$ . For example, let  $Y = Y' = R^3$ , and let  $Q$  be the unit circle on  $xy$  plane and  $Q'$  a circle which is knotted (say a trefoil knot, cf. Fig 1). Then  $(Y, Q)$  and  $(Y', Q')$  are not homeomorphic as pairs, although  $Y$  is homeomorphic to  $Y'$  and  $Q$  is homeomorphic to  $Q'$ . It is intuitively clear that there is no way to unknot  $Q'$  in  $Y'$  without breaking it (for a formal proof see Crowell and Fox<sup>4</sup>).

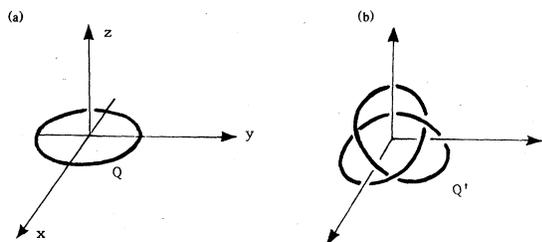


FIG. 1. (a)  $Q$  is the subset of  $R^3$  consisting of the points on unit circle in the  $xy$  plane. (b)  $Q' \in R^3$  is a trefoil knot. Then  $Q$  and  $Q'$  are homeomorphic, but the pairs  $(R^3, Q)$  and  $(R^3, Q')$  are not homeomorphic.

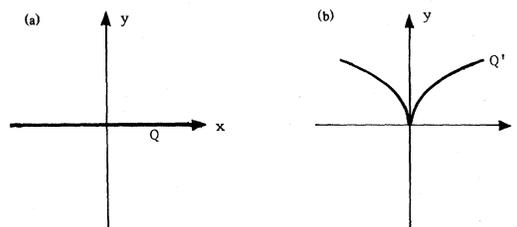


FIG. 2. (a)  $Q = \{(x, y) \in R^2 | y = 0\}$ . (b)  $Q' = \{(x, y) \in R^2 | x^2 = y^3\}$ .  $(R^2, Q)$  and  $(R^2, Q')$  are homeomorphic, but not diffeomorphic as pairs.

Note also that the condition that the pairs  $(Y, Q)$  and  $(Y', Q')$  be *diffeomorphic* is stronger than the condition that they be homeomorphic. For example, let  $Y = Y' = R^2$ ,  $Q = \{(x, y) : y = 0\}$ ,  $Q' = \{(x, y) : x^2 = y^3\}$  (see Fig. 2). It is easily seen that  $(Y, Q)$  and  $(Y', Q')$  are homeomorphic but not diffeomorphic as pairs. Since  $(Y, Q)$  and  $(Y', Q')$  would be physically two very different phase diagrams, this suggests that we consider two diagrams to be the same if and only if they are diffeomorphic as pairs.

However, it turns out that diffeomorphism is too strong a requirement. Consider the following example. Let  $Y = Y' = R^2$  and  $Q$  and  $Q'$  be subsets of  $R^2$  consisting of four lines through the origin with different cross ratios (see Fig. 3). We would certainly consider  $(Y, Q)$  and  $(Y', Q')$  to be qualitatively the same, and yet, even though they are homeomorphic as pairs, they are not diffeomorphic because diffeomorphisms preserve the cross ratios of our lines.

Hence, for physical purposes, the correct notion of equivalence of pairs of topological spaces would seem to lie somewhere between homeomorphism and diffeomorphism. In Sec. II, we shall propose a different definition of equivalence which seems to be suitable. Our strategy will be to classify pairs by diffeomorphism and then group together diffeomorphism classes which are qualitatively similar.

For the sake of clarity, we define what we mean by

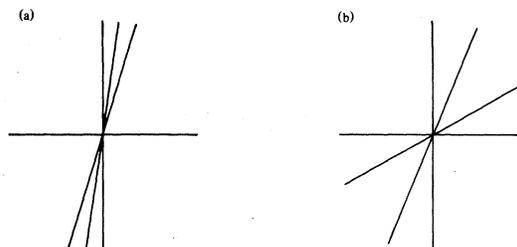


FIG. 3. There is no diffeomorphism of  $R^2$  carrying the four lines in (a) to the four lines in (b).

a phase diagram. Recall first, that a *field variable* is one which takes the same value in two coexisting phases. Examples are the temperature, pressure, and chemical potentials of the components (in fluid systems). It is always possible to pick a complete set of thermodynamic field variables.

Now, suppose  $Y$  is thermodynamic field space and  $Q$  is the subset consisting of all the points at which at least two phases coexist or coalesce. The pair of topological spaces  $(Y, Q)$  is called a *phase diagram*. We often call either  $Y$  or  $Q$  the phase diagram when the other member is clear from the context. Experiment and theory suggest that  $Q$  is not just any arbitrary subset of  $Y$ . Griffiths asks for topological conditions on  $(Y, Q)$  such that  $(Y, Q)$  be an "acceptable" phase diagram.

In order to discuss such conditions, Griffiths introduces the notions of *characteristic* and *typical* neighborhoods. These notions apply to any pair of topological spaces and we shall state their definitions at this level of generality. Let us agree that a *neighborhood* of a point  $y \in Y$  is a connected open subset of  $Y$  containing  $y$ . If  $Y$  is a metric space (i.e., distance is defined), then we may assume that a neighborhood of  $y \in Y$  is an open ball (i.e., the set of  $x \in Y$  such that the distance between  $x$  and  $y$  is less than some number  $r$ ).

*Definition.* In a pair of topological spaces  $(Y, Q)$  a *typical neighborhood*,  $N$ , of a point  $y \in Y$  is a neighborhood of  $y$  satisfying the property that if  $N'$  is any other neighborhood of  $y$  contained in  $N$ , then  $(N, N \cap Q)$  is homeomorphic to  $(N', N' \cap Q)$  (see Fig. 4).

Note that if  $N \cap Q = \emptyset$ , then we merely require that  $N$  be homeomorphic to  $N'$ . Hence, a typical neighborhood of a point  $y$  in  $Y$  which is not in  $Q$  is

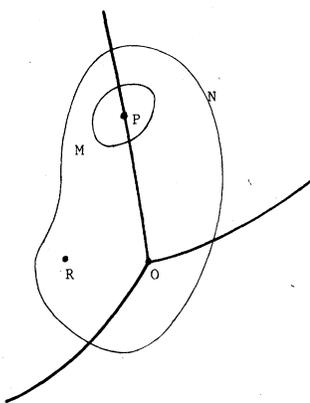


FIG. 4.  $N$  is a typical neighborhood of  $O$ , but not of  $P$  or of  $R$ .  $M$  is a typical neighborhood of  $P$ .  $N$  is also a characteristic neighborhood of  $O$ , while  $M$  is not a characteristic neighborhood of  $P$ .

any neighborhood of  $y$  which does not meet  $Q$ . In most cases, we shall only consider typical neighborhoods of points  $q \in Q$ . Typical neighborhoods are of two types. A particularly nice type is the following.

*Definition.* A *characteristic neighborhood* of a point  $q \in Q$  is a typical neighborhood  $N$  which satisfies the property that if  $N'$  is any other typical neighborhood of  $q$ , then any homeomorphism  $h: (N, N \cap Q) \rightarrow (N', N' \cap Q)$  is such that  $h(q) = q$ .

Whether a typical neighborhood of a point is a characteristic neighborhood depends on the dimension of the space  $Y$ . For example, any typical neighborhood of a triple point is a characteristic neighborhood when  $\dim Y = 2$ . This is not the case if  $\dim Y = 3$  (see Fig. 5). Now, one might conjecture that if a typical neighborhood of a point is not a characteristic neighborhood, then it can be derived by extending a characteristic neighborhood along a line, or a plane, or a higher-dimensional hyperplane. For example, if a triple point occurs in the case when  $\dim Y = 3$ , one observes a line of such points. That is, the typical neighborhood is just the Cartesian product of the characteristic neighborhood of a triple point with an open interval. This leads us to define another type of typical neighborhood.

*Definition.* A *characteristic cylinder* of a point  $q \in Q$  is a typical neighborhood  $N$  of  $q \in Q$  such that  $(N, N \cap Q)$  is homeomorphic to  $(W \times B, M \times B)$  where  $(W, M)$  is a characteristic neighborhood of a point in  $M$ , and  $B$  is homeomorphic to an open ball in  $R^m$  for some  $m < \dim Y$ .

Griffiths defines an *acceptable phase diagram*  $(Y, Q)$  as one such that (i) any point  $q \in Q$  has a typical neighborhood which is either a characteristic neighborhood or a characteristic cylinder; and (ii) any characteristic neighborhood is equivalent to one of a given list.

It is unclear, in Griffiths's paper, how the list mentioned in (ii) is constructed. He indicates that there are elementary and composite characteristic neighbor-

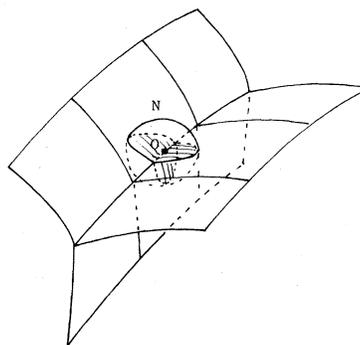


FIG. 5.  $N$  is a typical neighborhood of the triple point, which is a characteristic cylinder.

hoods and he gives a set of rules for constructing composite characteristic neighborhoods from elementary characteristic neighborhoods.

In Secs. II and III, we will give a method for constructing elementary characteristic neighborhoods and will conjecture that all elementary characteristic neighborhoods can be constructed in this fashion. By making use of the theory of Sergeraert, we are also able to get a set of rules for determining composite characteristic neighborhoods from elementary characteristic neighborhoods.

II. STRATIFIED SETS AND BIFURCATION SETS

In this section, we recall some standard mathematical terminology which we shall need. Experimental evidence indicates that in a phase diagram  $(Y, Q)$ ,  $Q$  is not a submanifold of field space  $Y$ . For, if it were, then in a small enough neighborhood,  $N$ , of any point  $q \in Q$ , there would have to exist local coordinates  $x_1, \dots, x_n$  on  $Y$  ( $\dim Y = n$ ) such that  $N \cap Q$  is given by  $x_1 = \dots = x_k = 0, k < n, q$  being the origin. Clearly, this condition is not satisfied in the neighborhood of a triple point (or critical point). However,  $Q$  is a union of submanifolds (of different dimensions) of field space,  $Y$ , which are arranged in a very definite fashion. For example, in the neighborhood of a triple point ( $\dim Y = 2$ ) we have three submanifolds of codimension 1, consisting of points of two-phase coexistence, and one submanifold of codimension 2, consisting of the single point that is the triple point. If  $\dim Y = 3$ , in a neighborhood,  $N$ , of a critical endpoint,  $N \cap Q$  is the union of two submanifolds of codimension 1, two submanifolds of codimension 2, and one submanifold of codimension 3 which is a single point (see Fig. 6). These are examples of stratified sets, the union of the submanifolds of the same codimension being considered as a single (unconnected) submanifold. The formal definition is as follows:

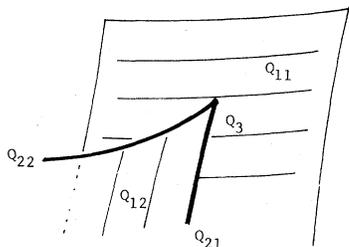


FIG. 6. A typical neighborhood of a critical endpoint (when  $\dim Y = 3$ ) showing the components of the natural stratification of the neighborhood.

*Definition.* Suppose  $Y$  is a differentiable manifold and  $Q \subseteq Y$  is a subset of  $Y$ . A stratification of  $Q$  is a partition of  $Q$  into disjoint subsets  $Q = Q_0 \cup \dots \cup Q_n$ , called strata, which satisfy the following conditions: (i)  $Q_i$  is an open submanifold of  $Y$  consisting of finitely-many connected components, each of which is a submanifold of the same codimension as  $Q_i$ . (ii) The codimension of  $Q_i$  is  $i$ . (iii)  $Q_{i+1} \subset \bar{Q}_i$ , where the bar denotes closure.

A subset  $Q \subseteq Y$  which admits a stratification is said to be stratified.

Returning to Fig. 6, a stratification of  $Q \subseteq Y$  in the neighborhood of a critical endpoint CE is given by  $Q_0 = \emptyset, Q_1 = Q_{11} \cup Q_{12}, Q_2 = Q_{21} \cup Q_{22}, Q_3 = \text{CE}$ . In general, for any stratification of a phase diagram  $(Y, Q)$  we will have  $Q_0 = \emptyset$ .

In the mathematical literature different definitions of a stratification are sometimes used. Various regularity conditions are often imposed as part of the definition. These subtleties will not concern us here. Later, when we mention stratifications of subsets of infinite-dimensional spaces, we shall allow a countable infinity of strata and waive the requirement that each stratum consist of finitely many components.

Acceptable phase diagrams always seem to have a "natural" stratification in the sense that it is clear, physically, how to define the strata. Each component of a stratum should be composed of points of the same type. We would, however, like a definition of natural stratification which is more geometric and rigorous. The following is an attempt at such a definition.

Suppose that we have two stratifications  $Q' = \bigcup_{i=0}^n Q'_i$  and  $Q'' = \bigcup_{i=0}^n Q''_i$  of the same underlying set. We say that the stratification  $Q''$  dominates  $Q'$ , written  $Q' < Q''$ , if

$$\bigcup_{i=j}^n Q'_i \subseteq \bigcup_{i=j}^n Q''_i \text{ for all } j, 0 \leq j \leq n.$$

The relation " $<$ " gives a partial ordering on the set of stratifications of a set. Intuitively, if  $Q' < Q''$  then  $Q''$  has larger strata than  $Q'$ . We say that  $Q = Q_0 \cup \dots \cup Q_n$  is a natural stratification of  $Q$  if (a)

$$\partial Q_i = \bar{Q}_i - Q_i = \bigcup_{j=i+1}^n Q_j$$

and (b) any other stratification  $Q' = Q'_0 \cup \dots \cup Q'_n$  of the set  $Q$  which satisfies (a), is such that  $Q' < Q$ .

For example, the stratification given above for the neighborhood of a critical endpoint (Fig. 6) is natural. The stratification

$$Q_0 = \emptyset, Q_1 = Q_{11} \cup Q_{12} \cup Q_{21}, Q_2 = Q_{22}, Q_3 = \text{CE}$$

is not natural, because (a) is not satisfied. On the

other hand, the stratification of the plane given by setting

$$Q_0 = \{(x,y) | xy \neq 0\} ,$$

$$Q_1 = \{(x,y) | xy = 0, (x,y) \neq (0,0)\} ,$$

$$Q_2 = \{(0,0)\} ,$$

satisfies condition (a), but is not natural (since  $Q_0$  is not maximal).

It is worth noting that not every stratified set admits a stratification satisfying (a). For example the subset  $Q$  of  $R^3$  consisting of the union of the  $xy$  plane and the  $z$  axis is clearly stratified. It is also clear that condition (a) can never be met.

If we allow that any "acceptable" phase diagram admits a natural stratification, then we can give a definition of equivalence of phase diagrams which overcomes the defects mentioned earlier in both the notions of topological and differentiable equivalence.

*Definition.* Two phase diagrams  $(Y, Q)$  and  $(Y', Q')$  will be said to be *equivalent* if there is a homeomorphism  $h: Y \rightarrow Y'$  which carries the natural stratification of  $Q$  onto the natural stratification of  $Q'$ .

That is, if  $Q = Q_1 \cup \dots \cup Q_n$  and  $Q' = Q'_1 \cup \dots \cup Q'_n$  are the natural stratifications of  $Q$  and  $Q'$  then  $h(Q_i) = Q'_i$ .

We remind the reader, that in an acceptable phase diagram,  $Q_0 = \emptyset$ . The above definition depends on the fact that every acceptable phase diagram admits a natural stratification. This is the case if our classification scheme is correct. A natural stratification is necessarily unique.

In addition, we could require that the restriction of  $h$  to  $Q_i$  be a diffeomorphism. Under this definition of equivalence, the two phase diagrams in Fig. 2 are not equivalent. We remark that the characteristic graphs of Griffiths are just a method for keeping track of the incidence relations between the components of the strata in the natural stratification of the phase diagram.

Stratified sets arise in a number of different ways in mathematics. The zero set of a polynomial function is a stratified set. For instance, the subset of  $R^3$ , considered above, consisting of the union of the  $xy$  plane and the  $z$  axis is the zero set of the polynomial  $(x^2 + y^2)z^2$ . Another way stratified sets arise is as the bifurcation set of algebraic or analytic functions. Since it is in this latter context that we envisage phase diagrams as arising, we pause to give some definitions.

### III. NOTION OF MODELS AND BIFURCATION SETS

In this paragraph, we introduce the notion of a bifurcation set. The definitions we present will be tailored to our purposes and the reader should be

aware that the mathematical definitions can be extended to many more general situations than presented here. However, although our definitions and results will be restricted to those cases which we actually need, we preface the formal (and narrow) definitions with a general philosophical discussion which hopefully will motivate and place in perspective the more technical discussion to follow.

Suppose that we are given a system which, microscopically, has an extremely large number of degrees of freedom, but which exhibits macroscopic behavior which seems to depend on relatively few macroscopic variables. This is the case for thermodynamic systems. One way of trying to handle this situation mathematically is to associate, to any microstate of the system, a mathematical object,  $f$ , belonging to some space,  $X$ , such that the macroscopic state of the system will be determined by some gross qualitative feature of  $f$ . We suppose that the object  $f_s$  varies continuously with a set of parameters  $s \in B$  (which are values taken by the macroscopic variables). By saying that  $f_s$  "determines" the macrostate of the system, we imply that, if the mathematical objects  $f_s$  and  $f_t$  are qualitatively the same (a situation which we denote by  $f_s \sim f_t$ ), then the corresponding states of the system are qualitatively the same.

The specific example we have in mind is where  $B = Y$  is thermodynamic field space. Then to each value of the pressure, temperature, chemical potentials, and so on, at which a phase transition does not occur, there corresponds a single phase (liquid, gas, or solid). However, at any such point in field space there are many possible microstates. Moreover, at two nearby points of field space the microstates may be different, but the phase of the system is the same. We want some way to pass from the set of microstates allowable at a fixed point in  $Y$  to the phase of the system at the same point. Thus, we would like to parametrize the set of microstates by a space  $X$ , the members of which have qualitative features which determine the phase. Clearly,  $X$  must be a large space. In our model, we take  $X$  to be a function space.

It may happen that, although  $f_s$  depends continuously on  $s$ , qualitative features of  $f_s$  may change discontinuously. The set of all points in  $X$  at which the qualitative features change will typically (but not necessarily) constitute a closed, nowhere-dense subset  $\Sigma_X$  of  $X$  called the bifurcation set in  $X$ . The subset  $\Sigma_B$  of  $B$  consisting of all points  $s$  for which  $f_s \in \Sigma_X$  will be called the *bifurcation set in  $B$*  or the *catastrophe set*. Of great interest is the pair of topological spaces  $(B, \Sigma_B)$ . It is this pair that we intend to identify with the phase diagram. Before doing so, let us formalize the above discussion somewhat.

*Definition:* A *model* will consist of a quadruple  $(X, B, \Phi, \sim)$  where (a)  $X$  is a topological space (the space of objects or microstates), (b)  $B$  is a topological

space (the space of macroscopic parameters), (c)  $\Phi: B \rightarrow X$  is a one-to-one continuous map [specifying how and what  $B$  parametrizes in  $X$ ; if  $s \in B$ , we often write  $\Phi(s) = f_s$ ], (d)  $\sim$  is an equivalence relation on  $X$  (which specifies when  $f, g \in X$  have the same qualitative features). In our model, the elements of  $X$  are functions.

In general, we try to choose  $\sim$  such that there exists a finite set  $f_1, \dots, f_n \in X$ , such that (i) the set  $\theta_i = \{g \in X \mid f_i \sim g\}$  is open in  $X$ , (ii)  $f_i \not\sim f_j$  if  $i \neq j$ , (iii)  $\bigcup_{i=1}^n \theta_i$  is dense in  $X$ . Then,  $\Sigma_X = X - (\bigcup_{i=1}^n \theta_i)$  and  $\Sigma_B = \Phi^{-1}(\Sigma_X)$  are the bifurcation sets in  $X$  and  $B$ , respectively. The map  $\Phi$  is called a *process* and the pair  $(B, \Sigma_B)$  the *morphology* of the process.

Hence in modeling a system as described above, we must specify four "things":  $X, B, \Phi, \sim$ . Frequently we know, or are trying to explain, the morphology  $(B, \Sigma_B)$ . We choose  $X$  and  $\sim$  to be "reasonable" in some sense. Specifying  $\Phi$  is difficult, if not impossible.

Thom discovered that, for many purposes, it is not necessary to strictly determine  $\Phi$ . More precisely, he found that for some classes of topological spaces  $X$ , and relations  $\sim$ , there exist very mild conditions on  $\Phi$  (which most models of physical interest seem to satisfy) which guarantee that locally the morphology  $(B, \Sigma_B)$  can only take finitely-many different topological types. Moreover, for low-dimensional spaces of parameters  $B$ , he explicitly listed all these topological types.

Rather than give examples here, we refer the reader to Thom's book.<sup>2</sup> The following two paragraphs will actually constitute an example of the above approach. Specific examples of computations will be restricted to those of interest for phase transitions.

#### IV. SPECIFIC MODEL

##### A. Basic notation

We shall take  $B$  to be thermodynamic field space and  $X$  to be  $C_*^\infty(R^m)$ , that is, the space of infinitely differentiable functions, with a global minimum, on  $R^m$ . To specify the relation  $\sim$ , we must pick out a gross distinguishing feature of the elements of  $X$  which determines the phase of the system. We choose the most obvious feature, namely, the structure of the absolute minima of the functions.

More precisely, we say that at a point  $y \in R^m$ , the function  $f \in C_*^\infty(R^m)$  is equivalent to a function  $g \in C_*^\infty(R^m)$  at the point  $z \in R^m$ , if there exists a diffeomorphism  $h$  of a neighborhood  $U$  of  $y$  with  $h(y) = z$  and a diffeomorphism  $k: R \rightarrow R$  such that  $h(x) = z + k(f(x))$  for all  $x \in U$ . We write  $f, y \sim g, z$ . Two functions  $f, g \in C_*^\infty(R^m)$  with isolated absolute minima  $y^1, \dots, y^r$  and  $z^1, \dots, z^s$ ,

respectively, will be said to be *equivalent*, written  $f \sim g$ , if (i)  $r = s$ , and (ii) there exists a permutation of the  $y^j$  such that

$$f, y^j \sim g, z^j \text{ for all } 1 \leq j \leq r.$$

The definition of  $\sim$  for functions with absolute minima which are not isolated is similar. We again examine neighborhoods  $U$  of points at which the function has an absolute minimum. Functions with nonisolated minima will turn out to be unimportant for what follows.

We have now specified  $B, X, \sim$ . To complete the description of our model, we need to say a few words about  $\Phi$ . In particular, we must describe the condition on  $\Phi$  under which the result of Thom, that we alluded to earlier, applies. It turns out that these conditions are intimately related to the structure of  $\Sigma_X$ . In fact, the conditions we impose on  $\Phi$  are exactly those necessary to guarantee that the structure of  $\Sigma_X$  determines the structure of  $\Sigma_B$ . Hence, we must also discuss the structure of  $\Sigma_X$ . We shall find it more convenient to discuss  $\Sigma_X$  before discussing the conditions on  $\Phi$ .

We shall find that  $\Sigma_X$  is an infinite-dimensional analog of a stratified set. In order to make this more precise, we introduce the notion of codimension of equivalence classes of functions. Although it is not necessary, it is easier to do this in terms of germs of functions and equivalence classes of germs, and this is the approach we take. These considerations occupy Secs. IV B–IV D. In Sec. IV E we discuss the conditions on  $\Phi$  and in Sec. IV F we describe how  $\Sigma_X$  determines  $\Sigma_B$ .

##### B. Germ of a function

Two functions  $f$  and  $g$  in  $C_*^\infty(R^m)$  will be said to have the *same germ at a point*  $y \in R^m$ , if there is a neighborhood  $N$  of  $y$  in  $R^m$  for which  $f(x) = g(x)$  for all  $x \in N$ . The *germ of  $f$  at the point*  $y \in R^m$  is the set (equivalence class) of all functions having the same germ as  $f$  at  $y$ . It is denoted by  $\langle f \rangle_y$  or simply  $\langle f \rangle$  if  $y$  is clear from context. Defining arithmetical operations on classes in the usual way, it becomes evident that  $\langle f + g \rangle = \langle f \rangle + \langle g \rangle$ ,  $\langle fg \rangle = \langle f \rangle \langle g \rangle$  and if  $g(y) \neq 0$ ,  $\langle g \rangle^{-1} = \langle g^{-1} \rangle$ . The set of germs of functions at  $y$ , which we denote by  $C_{y, \infty}(R^m)$ , is not only a vector space, but an algebra.

Two germs  $\langle f \rangle, \langle g \rangle \in C_{y, \infty}(R^m)$  are said to be *equivalent*, written  $\langle f \rangle \sim \langle g \rangle$ , if there are functions  $f, g$  with germs  $\langle f \rangle$  and  $\langle g \rangle$ , respectively, such that  $f, y \sim g, y$  with  $k = \text{identity}$  ( $k: R \rightarrow R$  as in the definition of " $\sim$ "). Note that we use the same symbol to denote equivalence of functions and equivalence of germs. This should not prove to be confusing, because it is evident from the definitions that if  $f$  and  $g$  are functions with a unique, isolated global minimum

at  $y \in R^n$ , then  $\langle f \rangle_y \sim \langle g \rangle_y \Rightarrow f \sim g$ . This observation, although trivial, allows us to make a drastic simplification of the problem. Namely, at least for functions with a single, isolated global minimum, we need only consider germs of functions. We will take care of the case where functions have more than one isolated, global minimum a little later. The procedure of replacing functions by germs and replacing  $C_*(R^m)$  by  $C_y(R^m)$  is an example of the mathematical procedure called *localization*. It is a very powerful technique.

C. Codimension of a germ

Given a germ,  $\langle f \rangle$ , of the function  $f$  at  $y$ , define the set  $\theta(\langle f \rangle)$ , called the *orbit* of  $\langle f \rangle$ , by

$$\theta(\langle f \rangle) = \{ \langle g \rangle \in C_y^\infty(R^m) \mid \langle f \rangle \sim \langle g \rangle \} .$$

Now  $\theta(\langle f \rangle)$  is a subset of  $C_y^\infty(R^m)$  and  $C_y^\infty(R^m)$  is an infinite dimensional vector space [e.g., the germs of functions,  $\langle 1 \rangle$ ,  $\langle x - y \rangle$ ,  $\langle (x - y)^2 \rangle$ ,  $\langle (x - y)^3 \rangle$ , . . . , are linearly independent over  $R$  in  $C_y^\infty(R^1)$ ]. It is natural to inquire as to whether  $\theta(\langle f \rangle)$  has some "nice" structure, perhaps as a submanifold of  $C_y^\infty(R^m)$ . To this end, we define a number  $\text{cod}_s[\theta(\langle f \rangle)]$  and then show that  $\theta(\langle f \rangle)$  can be thought of as a submanifold and  $\text{cod}_s[\theta(\langle f \rangle)]$  as its (smooth) codimension. Thus, without any further ado we set

$$\text{cod}_s(f, y) = \text{cod}_s(\langle f \rangle_y) = \dim \frac{C_y^\infty(R^m)}{\Delta_y(\langle f \rangle_y)} - 1 ,$$

where  $\Delta_y(\langle f \rangle_y)$  is the subspace of  $C_y(R^m)$  defined by

$$\Delta_y(\langle f \rangle_y) = \left\{ \langle g \rangle_1 \left\langle \frac{\partial f}{\partial x_1} \right\rangle + \cdots + \langle g \rangle_m \left\langle \frac{\partial f}{\partial x_m} \right\rangle \right\} ,$$

where  $\langle g \rangle_1, \dots, \langle g \rangle_m$  range over  $C_y^\infty(R^m)$  and  $\langle \partial f / \partial x_1 \rangle, \dots, \langle \partial f / \partial x_m \rangle$  are considered as germs at  $y$ .  $C_y^\infty(R^m) / \Delta_y(\langle f \rangle_y)$  denotes the quotient space of germs of functions at  $y$  modulo  $\Delta_y(\langle f \rangle_y)$ . That is, it is the space of all germs with two germs  $\langle g \rangle_1, \langle g \rangle_2$  being considered equal if there exists a  $\langle h \rangle \in \Delta_y(\langle f \rangle_y)$  such that  $\langle g \rangle_1 = \langle g \rangle_2 + \langle h \rangle$ . The codimension is said to be infinite if  $\dim C_y^\infty(R^m) / \Delta_y(\langle f \rangle_y)$  is not defined.

We give four examples. In all of them we take  $y$  to be the origin,  $\underline{0}$ , in  $R^m$  and we systematically drop the angle brackets  $\langle \ \rangle$ , it being understood that all functions are to be thought of as germs at  $\underline{0}$ . We write  $\Delta$  in place of  $\Delta_0$ .

(i)  $m = 1, f(x) = x^n, n > 1$ . Since  $\partial f / \partial x = nx^{n-1}$ ,

$$\Delta(f) = \{ hx^{n-1} \mid h \in C_0^\infty(R^1) \} .$$

If  $g \in \Delta(f)$  then  $x^{n-1}$  divides  $g$  and so  $C_0^\infty(R^m) /$

$\Delta(f)$  is spanned by  $1, x, x^2, \dots, x^{n-2}$  whence  $\dim C_0(R^1) / \Delta(f) = n - 1$  and  $\text{cod}_s(f) = n - 2$ .

(ii)  $m$  arbitrary,  $f(x) = x_1^2 + \cdots + x_m^2$ .

$$\Delta(f) = \{ h_1 x_1 + \cdots + h_n x_n \mid h_1, \dots, h_n \in C_0^\infty(R^m) \} .$$

But any nonconstant  $g \in C_0^\infty(R^m)$  can be written in the form

$$g(x) = x_1 g_1(x) + \cdots + x_m g_m(x) ,$$

where

$$g_i \in C_0^\infty(R^m) .$$

For

$$\begin{aligned} g(x) &= \int_0^1 \frac{d}{dt} g(tx) dt \\ &= \int_0^1 [ \partial_1 g(tx) x_1 + \cdots + \partial_m g(tx) x_m ] dt \\ &= x_1 \int_0^1 \partial_1 g(tx) dt + \cdots + x_m \int_0^1 \partial_m g(tx) dt . \end{aligned}$$

and we may set

$$g_i(x) = \int_0^1 \partial_i g(tx) dt .$$

Hence 1 spans  $C_0^\infty(R^m) / \Delta(f)$  and  $\text{cod}_s f = 0$ .

(iii)  $m = 2, f(x) = x_1^4 + x_2^4$ . Then  $\partial f / \partial x_1 = 4x_1^3, \partial f / \partial x_2 = 4x_2^3$ , and so

$$\Delta(f) = \{ h_1 x_1^3 + h_2 x_2^3 \mid h_1, h_2 \in C_0^\infty(R^2) \} .$$

Then an easy computation shows that

$$\{ 1, x_1, x_2, x_1^2, x_1 x_2, x_2^2, x_1 x_2^2, x_1^2 x_2, x_1^2 x_2^2 \}$$

spans  $C_0^\infty(R^2) / \Delta(f)$  (see for example, Raghavan<sup>5</sup>). Hence  $\text{cod}_s(f) = 9 - 1 = 8$ . We will return to this example later as it turns out that for different  $a, f(x) = x_1^4 + x_2^4 + ax_1^2 x_2^2$  are differentially inequivalent but may be topologically equivalent (see Godwin<sup>6</sup>), so that the topological codimension of  $f$  is equal to 7.

(iv) Suppose  $f \in C_0^\infty(R^m)$  and

$$g(x_{m+1}, \dots, x_{m+n}) = x_{m+1}^2 + \cdots + x_{m+n}^2 \in C_0^\infty(R^n) .$$

Let

$$\begin{aligned} h(x_1, \dots, x_{m+n}) &= f(x_1, \dots, x_m) \\ &\quad + g(x_{m+1}, \dots, x_{m+n}) \in C_0^\infty(R^{m+n}) . \end{aligned}$$

Then  $\text{cod}_s h = \text{cod}_s f$ .

The number  $\text{cod}_s(\langle f \rangle)$  is called the *smooth codimension* of the germ  $\langle f \rangle$ . Later we shall define the *topological codimension* of  $\langle f \rangle$ .

We now wish to explain in what sense  $\text{cod}_s$  is the codimension of  $\theta(\langle f \rangle)$ . Let  $y = (y_1, \dots, y_m)$  be a point of  $R^m$ . Since  $C_y^\infty(R^m)$  is infinite dimensional, a natural approach is to look at finite-dimensional

subspaces of it. Let  $\epsilon_y(R^m)$  be the subspace of  $C_y^\infty(R^m)$  consisting of all  $\langle f \rangle \in C_y^\infty(R^m)$  satisfying  $\langle f \rangle(y) = 0, d\langle f \rangle(y) = 0$  [i.e.,  $(\partial\langle f \rangle/\partial x_1)(y) = \dots = (\partial\langle f \rangle/\partial x_m)(y) = 0$ ]. Let  $R_y[x_1, \dots, x_m]_k^2$  denote the set of all polynomials in  $x_1 - y_1, \dots, x_m - y_m$  with degree less than or equal to  $k$  and no terms of degree less than 2. Define the projections

$$j_y^k: \epsilon_y(R^m) \rightarrow R_y[x_1, \dots, x_m]_k^2 \quad (k \geq 2)$$

by setting  $j^k\langle f \rangle = \{T(\langle f \rangle, y, k)\}$ , where  $T$  represents a Taylor series expansion of  $\langle f \rangle$  about  $y$  up to and including terms of order  $k$ .  $R_y[x_1, \dots, x_m]_k^2$  is a finite-dimensional vector space. It is easy to show that  $j_y^k(\theta(\langle f \rangle))$  is a submanifold of  $R_y[x_1, \dots, x_m]_k^2$ . Moreover, given  $\langle f \rangle$  of finite smooth codimension, there exists an integer  $N$ , such that for all  $k \geq N$ ,  $j_y^k(\theta(\langle f \rangle))$  is a submanifold of  $R_y[x_1, \dots, x_m]_k^2$  of codimension equal to  $\text{cod}_s(\langle f \rangle)$  (Trotman and Zeeman<sup>7</sup>). The reader may easily verify this for example (i) above. This result means that we can think of  $\theta(\langle f \rangle)$  as a "limit" of submanifolds of codimension  $\text{cod}_s(\langle f \rangle)$ .

D. Multigerms

We now have to consider functions,  $f$ , with  $n$  distinct isolated global minima  $y^1, \dots, y^n \in R^m, n > 1, y^i = (y_1^i, \dots, y_m^i), 1 \leq i \leq n$ . Then we are only interested in the  $n$  tuple of germs

$$\begin{aligned} \underline{\langle f \rangle} &= (\langle f \rangle_{y^1}, \dots, \langle f \rangle_{y^n}) \\ &\in C_{y^1}^\infty(R^m) \times \dots \times C_{y^n}^\infty(R^m) \end{aligned}$$

Sergeraert<sup>8</sup> has shown that if we set

$$\text{cod}_s(\underline{\langle f \rangle}) = \sum_{i=1}^n \dim \frac{C_{y^i}^\infty(R^m)}{\Delta_{y^i}(\langle f \rangle_{y^i})} - 1,$$

then  $\text{cod}_s(\underline{\langle f \rangle})$  has a geometric interpretation as a codimension in a manner exactly analogous to that given for functions with one absolute minimum. Henceforth, we will refer to this result as Sergeraert's theorem.

The  $n$  tuple  $\underline{\langle f \rangle} = (\langle f \rangle_{y^1}, \dots, \langle f \rangle_{y^n})$  of germs of a function,  $f$ , at its  $n$  isolated global minima  $y^1, \dots, y^n$  will be called the *multigerms* (or, more simply, germ) associated to  $f$ . If  $f$  has only isolated global minima we set  $\text{cod}_s f = \text{cod}_s(\underline{\langle f \rangle})$ . If  $f$  has nonisolated global minima we set  $\text{cod}_s f = \infty$ . Using these definitions and Sergeraert's theorem, we can now stratify  $\Sigma_{C^\infty(R^m)}$ . First note that  $f \notin \Sigma_{C^\infty(R^m)}$  if  $\text{cod}_s f = 0$ . This is equivalent to the following conditions: (i)  $f$  has a unique isolated, global minimum

say at  $y \in R^m$ ; (ii)

$$\det \parallel \frac{\partial^2}{\partial x_i \partial x_j} f(y) \parallel_{1 \leq i, j \leq m} \neq 0$$

(that is,  $y$  is a *nondegenerate critical point*). In fact, a theorem of Morse says that the above conditions hold if and only if

$$\langle f \rangle_y \sim f(y) + (x_1 - y_1)^2 + \dots + (x_m - y_m)^2,$$

where  $y = (y_1, \dots, y_m)$  and the right-hand side is understood as a germ at  $y$ .  $f \in \Sigma_{C_*^\infty(R^m)}$  is such that  $\text{cod}_s(f) = 1$  only if  $f$  has exactly two nondegenerate global minima. If  $\text{cod}_s(f) = 2$  then it can be shown that there are only two possibilities: either  $f$  has exactly three nondegenerate global minima or  $f$  has a single (isolated) minimum  $y$  and

$$\begin{aligned} \langle f \rangle_y &\sim f(y) + (x_1 - y_1)^4 \\ &\quad + (x_2 - y_2)^2 + \dots + (x_m - y_m)^2, \end{aligned}$$

where the right-hand side is to be interpreted as a germ.

In general, a stratum of  $\Sigma_{C^\infty(R^m)}$  of codimension  $n \geq 1$  will consist of the set of functions  $f \in \Sigma_{C^\infty(R^m)}$  such that  $\text{cod}_s(f) = n$ . If  $f \in \Sigma_{C^\infty(R^m)}$ , and  $\text{cod}_s(f) \leq 5$  then  $f$  will belong to one of finitely-many equivalence classes of functions. If  $\text{cod}_s(f) \geq 6$  then there are infinitely-many different possible equivalence classes to which  $f$  can belong. However, if we change our definition of equivalence  $\sim$  (given at the beginning of this paragraph), by allowing  $h$  in the definition of  $\sim$  to be a homeomorphism (instead of a diffeomorphism), then  $f$  will belong to one of only *finitely*-many different equivalence classes.

The above theory and what follows in Secs. IV E and IV F can be presented in a mathematically more elegant fashion by defining  $\text{cod}_s(f)$  without reference to germs and interpreting it as a codimension in the space  $C_*^\infty(R^m)$ . However, the definitions and concepts are more difficult in this case and for computation one needs to use germs. For an exposition of this more global approach see the excellent papers of Dubois, Dufour, and Stanek.<sup>9</sup> Very efficient methods for computing the codimension of a function have been developed. See, for example, Kushnirenko.<sup>10</sup>

E. Transversality conditions on  $\Phi$

We now must say a few words about  $\Phi$ . We suppose that  $\Phi$  is 1-1 and smooth. Both these assumptions could be weakened somewhat at the expense of clarity. According to the fundamental dogma of Thom,  $\Phi$  will be structurally stable. By this we mean that small variations in  $\Phi$  should result in maps

“essentially the same as  $\Phi$ ” and, hence, in the same morphologies. The justification for this is that no two experimental situations are exactly the same; that is,  $\Phi$  varies slightly from observation to observation. The fact that the results of various observations agree lends credence to the idea that the morphology should be independent of small perturbations of  $\Phi$ .

For thermodynamics there is another good reason why small variations in  $\Phi$  should not matter. Namely, to any fixed value of the thermodynamic field variables there correspond many possible microstates. (In fact, it is the statistical distribution of the possible microstates which is usually thought of as determining the macrostate). Hence there are likely to be many possible choices for  $\Phi$ . In general, small changes in  $\Phi$  should not change the morphology qualitatively.

There is one easy condition that mathematically sums up many phrases currently used by physicists, such as “lucky accidents don’t happen,” “in general,” etc. This is the notion of *transversality*. The notion of transversal intersection makes precise the feeling that it is “exceptional” for two lines in  $R^3$  to intersect or for two curves in  $R^2$  to be tangent at any point of intersection. The formal definition is as follows:

*Definition.* Let  $X, Y$  be manifolds and  $N \subseteq Y$  a submanifold. The map  $f: X \rightarrow Y$  is said to be *transversal to  $N$*  at  $x \in X$  if (i)

$$df_x(T_x X) + T_{f(x)} N = T_{f(x)} Y, \quad f(x) \in N,$$

or (ii)  $f(x) \notin N$ . Here  $df_x$  is the derivative of  $f$  at  $x$  and  $T_a$  denotes the tangent space to a manifold at the point  $a$ . We write  $f \perp N$ .  $f$  is *transversal to  $N$* ,  $f \perp N$ , if  $f \perp N$  for all  $x \in X$ . Finally, if  $N$  is a stratified set (and, hence, not necessarily a submanifold of  $Y$ ), then  $f$  is transversal to  $N$ , written  $f \perp N$ , if  $f$  is transversal to each stratum of  $N$ .

Two submanifolds  $N, M$  of  $X$  are said to *intersect transversally* if  $i: N \rightarrow X$  is transversal to  $M$  for all  $x \in N$ , where  $i$  denotes the inclusion map.

Intuitively, if we think of  $f(X)$  as a manifold of dimension  $\dim f(X)$  then,  $f$  transversal to  $N$  means that (i) if  $\dim f(X) < \text{cod} N$  then  $f(X)$  and  $N$  do not intersect (i.e., lucky accidents don’t happen); (ii)  $f(X)$  and  $N$  are not “tangent” in any sense. For more examples see Fig. 7. Note that if  $f$  is not transversal to  $N$ , any small perturbation of  $f$  will radically alter the nature of the intersection  $f(X) \cap N$ .

We have seen that  $\Sigma_{C_*(R^m)}$  is stratified. If  $\Phi$  is transversal to  $\Sigma_{C_*(R^m)}$  then we shall say that the system modeled is *generic*. [ $\Phi \perp \Sigma_{C_*(R^m)}$  means that there exists  $K$  such that  $\text{cod} \Phi(b) \leq K$  and  $j_y^k \Phi T_{b,j_y^k}(\Sigma_{C_*(R^m)}^\infty)$  for all  $b \in B$ ,  $k \geq K$ , and any  $y$  which is a global minimum of  $\Phi(b)$ ]. We believe that systems consisting of mixtures of pure fluids are gen-

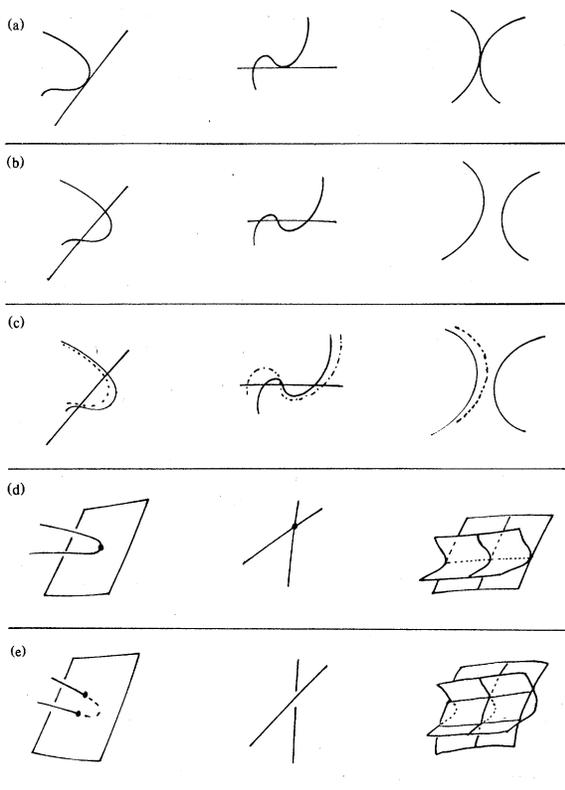


FIG. 7. (a) Examples of curves in  $R^2$  which do not meet transversally. (b) Curves in  $R^2$  which meet transversally. (c) A schematic indication that arbitrarily small perturbations preserve the transversal nature of the intersection. (d) Some nontransversal intersections in  $R^3$ . (e) Some transversal intersections in  $R^3$ .

eric. It is this case on which we shall concentrate in the next section.

Of course, not all systems are generic. It may happen that there are symmetries which are always obeyed and which force  $\Phi(B)$  to intersect strata with a higher codimension than  $\dim B$ . This seems to be the case for some magnetic systems.

### F. Determination of $\Sigma_B$ from $\Sigma_X$

It is clear that via  $\Phi^{-1}$  the bifurcation set  $\Sigma_B$  (phase diagram) is just a copy in some sense of the bifurcation set  $\Sigma_X$ . In particular, there should be some relation between the natural stratification of a phase diagram and the stratification of  $\Sigma_X$ . It was Thom who discovered the basic techniques for determining  $\Sigma_B$  from  $\Sigma_X$ . The work of others, notably Sergeraert, Dubois, and Dufour have provided us with a more complete picture. The key notion is that of the

universal unfolding of a function. We present the basic definitions.

*Definition.* If  $f \in C^\infty(R^m)$  then an *unfolding* of  $f$  is a function  $F \in C^\infty(R^{m+n})$  such that  $F(x, 0) = f(x)$  for all  $x \in R^m$ ,  $0 \in R^n$ . An unfolding  $F \in C^\infty(R^{m+n})$  is called *versal* if, as  $u$  varies in some neighborhood of  $0$  in  $R^n$ ,  $F(x, u) = f_u(x)$  describes all possible inequivalent functions into which  $f$  can be deformed by arbitrarily small perturbations. A versal unfolding  $F \in C^\infty(R^{m+n})$  of  $f$  is called *universal* if any other unfolding  $G \in C^\infty(R^{m+r})$ , where  $r < n$  fails to be versal.

The usual definitions given in the mathematical literature, are equivalent to those given above. What makes the above definition workable is the following theorem of Mather.<sup>11</sup>

*Theorem.* Let  $f \in C^\infty(R^m)$  have a unique global isolated minimum at  $0 \in R^m$ ,  $f(0) = 0$ . Then a universal unfolding  $F \in C^\infty(R^{m+n})$  is given by

$$F(x, y) = f(x) + u_1 g_1(x) + \dots + u_n g_n(x),$$

where  $g_1, \dots, g_n$  are functions in  $C^\infty(R^m)$  which are such that  $\langle 1 \rangle, \langle g_1 \rangle, \dots, \langle g_n \rangle$  are a basis for  $C_0^\infty(R^m)/\Delta_0(\langle f \rangle_0)$ . In particular,  $n = \text{cod}_s f$ . An immediate corollary is as follows.

*Corollary.* Let  $f \in C^\infty(R^m)$  have a unique isolated global minimum and be such that  $\text{cod}_s f = n$ . Then a versal unfolding  $F \in C^\infty(R^m \times R^r)$ ,  $r > n$ , is given by

$$F(x, y_1, \dots, y_r) = f(x) + y_1 g_1(x) + \dots + y_n g_n(x),$$

where  $g_1, \dots, g_n$  are as in the theorem above and the variables  $y_{n+1}, \dots, y_r$  play no role.

Mather's theorem is extremely useful. We shall use it throughout all that follows. For the moment, we use it to motivate the definition of topological codimension. Let  $f(x) \in C^\infty(R^m)$  have a unique isolated global minimum and let  $F(x, u) \in C^\infty(R^{m+n})$  be a universal unfolding of  $f(x)$ . From Mather's theorem we know that  $n = \text{cod}_s f$ . Let  $G(x, v) \in C^\infty \times (R^{m+r})$  be an unfolding of  $f(x) \in C^\infty(R^m)$  which has the property that as  $v$  varies in a neighborhood of  $0$  in  $R^r$ ,  $f_v(x) = G(x, v)$  runs through all possible topologically inequivalent functions into which  $f$  can be deformed by arbitrarily small perturbations. [Recall that two functions  $f_1, f_2 \in C^\infty(R^m)$  are topologically equivalent if they are equivalent in the sense of Sec. IV A with  $h$  and  $k$  allowed to be homeomorphisms.] If no other unfolding with fewer than  $r$  parameters satisfies the above condition, then  $r$  is called the *topological codimension* of  $f$ , written  $r = \text{cod } f$ . Clearly  $\text{cod } f \leq \text{cod}_s f$ . The number  $(\text{cod}_s f - \text{cod } f)$  is called the *modality* of  $f$ . Mather<sup>12</sup> has shown that there are only finitely many different topological equivalence classes of functions  $f \in C^\infty(R^m)$  with a given topological codimension.

As an example, let us consider  $f(x) \in C^\infty(R^2)$ ,

where  $f(x_1, x_2) = x_1^4 + x_2^4$ . Then by Mather's theorem and example (iii) of Sec. IV C a universal unfolding is given by  $F(x, u) \in C^\infty(R^{2+8})$  where

$$\begin{aligned} F(x_1, x_2, u_1, u_2, \dots, u_8) \\ = x_1^4 + x_2^4 + u_1 x_1^2 x_2^2 + u_2 x_1^2 x_2 + u_3 x_1 x_2^2 \\ + u_4 x_1^2 + u_5 x_1 x_2 + u_6 x_2^2 + u_7 x_1 + u_8 x_2. \end{aligned}$$

Now, we have mentioned that for small variations of  $\mu_1$  the topological type of  $f_u(x) = F(x, u)$  does not change. Hence,  $\text{cod}(f) = \text{cod}_s(f) - 1 = 7$ . For more on the question of modality and topological codimension, see Arnol'd.<sup>3</sup>

It is worth mentioning that there is a definition of equivalence of unfoldings, which we do not give (cf. Thom<sup>2</sup>), and that the universal unfolding is unique, up to this notion of equivalence. More importantly, if  $f, g \in C^\infty(R^m)$  and  $f \sim g$  then the universal unfoldings of  $f$  and  $g$  are equivalent. We shall only need the weaker, but nevertheless, remarkable results listed below.

*Definition.* Let  $F \in C^\infty(R^m \times R^n)$  be an unfolding of  $f \in C^\infty(R^m)$ . Define the *bifurcation set* of  $F$  in  $R^n$  as  $\Sigma_F = \{u \in R^n \mid \text{either (i) } f_u(x) = F(x, u) \text{ has a degenerate global minimum } y \in R^m, \text{ or (ii) } f_u \text{ has two or more global minima}\}$ .

*Theorem.* [Thom<sup>2</sup> and Dubois, Dufour, and Stanek (DDS)<sup>9</sup>]: Suppose  $F$  and  $G$  are universal unfoldings of  $f \in C^\infty(R^m)$ , then the pair  $(R^n, \Sigma_F)$  is diffeomorphic to the pair  $(R^n, \Sigma_G)$ .

*Theorem.* (Thom<sup>2</sup> and DDS<sup>9</sup>): If  $F, G \in C^\infty(R^{m+n})$  are universal unfoldings of  $f$  and  $g$ , respectively, and if  $f \sim g$  then the pair  $(R^n, \Sigma_F)$  is diffeomorphic to the pair  $(R^n, \Sigma_G)$ .

*Theorem.* (Thom<sup>2</sup> and DDS<sup>9</sup>): Suppose  $f \in C^\infty \times (R^m)$  and let  $F \in C^\infty(R^{m+n})$  be a versal unfolding of  $f$ . Suppose  $\Phi: B \rightarrow C^\infty(R^m)$  is one to one and transverse to  $\Sigma_{C^\infty(R^m)}$  and that  $\Phi(a) = f$ , where  $a \in B$ . Then there exists a neighborhood  $N$  of  $a$  in  $B$  and a neighborhood  $U$  of  $0$  in  $R^n$  for which the pair  $(N, \Sigma_B \cap N)$  is diffeomorphic to  $(U, \Sigma_F \cap U)$ .

Mather's theorem applies only to functions  $f \in C^\infty(R^m)$  with a single, isolated global minimum. How do we construct universal unfoldings of functions with more than one isolated global minimum? The answer has been supplied by Dubois, Dufour, and Stanek.

*Theorem.* (DDS<sup>9</sup>): Let  $f \in C^\infty(R^m)$  be a function with isolated absolute minima  $y^1, \dots, y^r$ . For each  $i$  such that  $1 \leq i \leq r$  choose two open balls  $U_i$  and  $V_i$  centered at  $y^i$  such that  $U_i \subset V_i$  and such that  $y^j \notin \bar{V}_i$  for any  $j \neq i$ . (Here  $\bar{V}_i$  denotes the closure of  $V_i$ , that is, the closed ball with the same radius as  $V_i$ .) Now, for each  $i$  choose a  $C^\infty$  function on  $R^m$ ,  $\epsilon_i(x)$ , the restriction of which is identically equal to 1 on  $U_i$  and 0 on  $R^m - V_i$ . [This is always possible; in fact, we may assume that  $\epsilon_i(x) \leq 1$  for all  $x \in R^m$ ; see

Golubitsky and Guillemin<sup>13</sup>.] For each  $i$ , let  $\text{cod}(f_{y^i}) = s_i$  and let

$$\begin{aligned} D_i(x, u^i) &\equiv D_i(x, u_1^i, u_2^i, \dots, u_{s_i}^i) \\ &= u_1^i g_1^i(x) + \dots + u_{s_i}^i g_{s_i}^i(x) \\ &= \sum_{k=1}^{s_i} u_k^i g_k^i, \end{aligned}$$

where

$$u^i = (u_1^i, \dots, u_{s_i}^i) \in R^{s_i}$$

and

$$g_1^i, \dots, g_{s_i}^i \in C^\infty(R^m)$$

are functions such that

$$\langle 1 \rangle, \langle \langle g_1^i \rangle \rangle_{y^i}, \dots, \langle \langle g_{s_i}^i \rangle \rangle_{y^i}$$

are a basis for  $C_{y^i}^\infty(R^m)/\Delta_{y^i}(\langle f \rangle_{y^i})$ . Then a universal unfolding of  $f$  is given by

$$F(x, u) = f(x) + \sum_{i=1}^{r-1} u_i \epsilon_i(x) + \sum_{i=1}^r \epsilon_i(x) D_i(x, u^i).$$

Here,

$$\begin{aligned} u &= (u_1, \dots, u_{r-1}, u_1^1, \dots, u_{s_1}^1, \dots, u_1^r, \dots, u_{s_r}^r) \\ &\in R^{r-1+s_1+\dots+s_r}, \end{aligned}$$

$$\text{cod}_s(f) = r - 1 + s_1 + \dots + s_r$$

(in agreement, with Sergeraert's theorem), and  $F \in C^\infty(R^{m+\text{cod}_s(f)})$ .

The above theorem is not as complicated as it looks. If we think of  $f + D_i$  as a "local" universal unfolding of  $f$  in a neighborhood of  $y^i$ , then the theorem says that a universal unfolding of  $f$  is given by combining the local universal unfoldings at each isolated absolute minimum and adding the term  $\sum_{i=1}^{r-1} u_i \epsilon_i(x)$  which has the effect of separating the values that  $f$  takes at each minimum. An example will be given in the next paragraph.

### V. GENERIC PHASE DIAGRAMS

We now draw some conclusions about phase diagrams subject to the assumption that the model outlined above is valid and that the system is generic. The first observation is that genericity implies that a point  $b \in Y$  of the phase diagram lies on a stratum of codimension equal to  $\text{cod}[\Phi(b)]$ . We shall classify points on the phase diagram by the topological type of the corresponding function  $\Phi(b)$ .

Let us elaborate on this statement a little. We envisage a global minimum of  $f \in C^\infty(R^m)$  as corresponding to a phase. If at a point  $b \in B$ ,  $\Phi(b) = f_b$  has codimension 0, then  $f_b$  will have exactly one nondegenerate minimum and  $b$  will be a point in  $Y - Q$ . If  $\Phi(b) = f_b$  has codimension 1, then  $f_b$  will have exactly two distinct, nondegenerate global minima and  $b$  will be a point of two-phase coexistence. Moreover,  $b$  will lie on the stratum of  $Q$  with codimension 1. Similarly, if  $\Phi(b) = f_b$  has three distinct absolute minima, then  $b$  is a point of three-phase coexistence and  $b$  will lie in the stratum of  $Q$  with codimension 2.

We say that the points  $b \in Q$  such that  $\Phi(b)$  has a unique minimum are *elementary*. If the minimum is degenerate, then  $b$  will be a critical point (possibly, a higher-order critical point). By the theorems in subsection F of the previous section, we can construct a characteristic neighborhood of  $b$  by considering a universal unfolding of  $\Phi(b)$ . For example, suppose that

$$\Phi(b)(x) \sim x_1^4 + x_2^2 + \dots + x_m^2.$$

In order to minimize confusion, we shall frequently denote the image of  $b$  under  $\Phi$ , which is a function in  $C^\infty(R^m)$  by  $\Phi_b$  instead of  $\Phi(b)$ . By Mather's theorem a universal unfolding of  $\Phi(b)$  is given by

$$\Phi_b(x_1, u_1, u_2) = x_1^4 + u_1 x_1^2 + u_2 x_1 + x_2^2 + \dots + x_m^2,$$

where  $x = (x_1, \dots, x_m)$  and  $u_1$  and  $u_2$  are coordinates in thermodynamic field space with  $b$  as the origin (in particular  $\dim Y = 2$ ). We find that  $\Sigma_{\Phi_b}$  is just the half line  $u_1 \leq 0, u_2 = 0$ . Hence, by the theorems of Thom quoted in Sec. IV F, a neighborhood of  $b$  in  $(Y, Q)$  is diffeomorphic to a neighborhood of 0 in  $(R^2, \Sigma_{\Phi_b})$  (see Fig. 8).

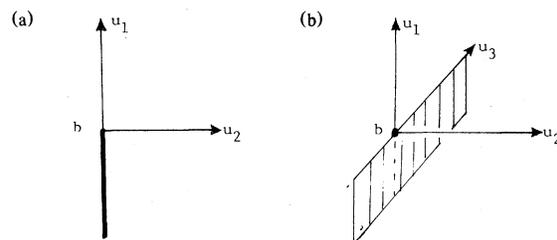


FIG. 8. (a) Bifurcation set of the universal unfolding of

$$\Phi(x_1, \dots, x_m) = x_1^4 + x_2^2 + \dots + x_m^2.$$

(b) The bifurcation set of a versal unfolding of  $\Phi$  with three parameters  $u_1, u_2, u_3$ .

In the case that  $\dim Y = n > 2$ , Mather's theorem tells us that

$$\Phi_b(x, u_1, \dots, u_n) = x^4 + u_1 x^2 + u_2 x_1 + x_2^2 + \dots + x_m^2$$

is a versal unfolding. Again, a neighborhood of  $b$  in  $(Y, Q)$  is diffeomorphic to a neighborhood of 0 in  $(R^n, \Sigma_{\Phi_b})$ . If  $n = 3$ ,  $\Sigma_{\Phi_b}$  is just the closed half plane  $(u_1 \leq 0, u_2 = 0, u_3 \text{ arbitrary})$  in  $R^3$ . We have sketched this situation in Fig. 8. In this case, we have constructed a characteristic cylinder. It is clear from the results of Sec. IV that, if  $b$  is an elementary point and if  $\text{cod } \Phi_b < \dim Y$ , then, in Griffiths's terms,  $b$  will lie on a characteristic cylinder of the entity corresponding to  $b$ . Moreover, our construction of the characteristic cylinder gives the same results as Griffiths's construction.

A point  $b \in Q$  such that  $\Phi_b$  has two or more distinct, isolated, global minima will be called a *composite point*. The characteristic neighborhood of  $b$  in  $(Y, Q)$  is diffeomorphic to a neighborhood of 0 in  $(R^n, \Sigma_{\Phi_b})$ , where  $\Phi_b$  is the universal unfolding of  $\Phi_b$ . This latter characteristic neighborhood is called a *composite entity*. As shown in Sec. IV F,  $\Phi_b$  can be regarded as having been constructed from the universal unfoldings of the germs of  $\Phi_b$  at each distinct global minimum of  $\Phi_b$ . In this sense, a composite entity may be regarded as made up of elementary entities.

We give an example. Suppose  $\Phi_b$  has two global isolated minima at  $y^0$  and  $y^1$  in  $R^m$ . Suppose further that

$$\Phi_{b, y^0} \sim x_1^4 + x_2^2 + \dots + x_m^2, \underline{0}$$

and

$$\Phi_{b, y^1} \sim (x_1 - 1)^2 + x_2^2 + \dots + x_m^2, \underline{a}$$

where  $\underline{a} = (1, 0, \dots, 0)$ . Then from the theorem of Dubois, Dufour, and Stanek, a universal unfolding  $\Phi_b$  of  $\Phi_b$  is given by

$$\begin{aligned} \Phi_b(x, u_1, u_2, u_3) &= \epsilon_0(x)(x_1^4 + u_1 x_1^2 + u_2 x_2 + u_3 + x_2^2 + \dots + x_m^2) \\ &+ \epsilon_a(x)[(x_1 - 1)^2 + x_2^2 + \dots + x_m^2] \end{aligned}$$

where  $\epsilon_0(x)$  is a  $C^\infty$  function which is identically equal to 1 on a small open ball,  $U$ , centered at  $\underline{0} = (0, \dots, 0)$  and identically equal to 0 on  $R^m - V$  where  $V$  is an open ball centered at  $\underline{0}$  containing  $U$  but not  $\underline{a}$ . We can take  $\epsilon_a(x) = 1 - \epsilon_0(x)$ . Computing  $\Sigma_{\Phi_b}$ , we find that it has the shape sketched in Fig. 9. The computations are given in DDS.<sup>9</sup> Hence,  $b$  has a typical neighborhood in  $(Y, Q)$  ( $\dim Y = 3$ ) diffeomorphic to  $(R^3, \Sigma_{\Phi_b})$ .

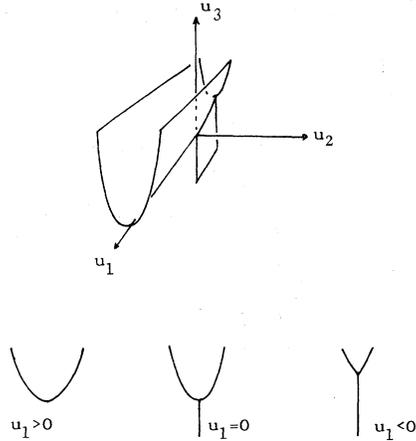


FIG. 9. Typical neighborhood of the bifurcation set of a function with two global minima, one nondegenerate and the other having codimension 2.

Sergeraert's theorem gives us the codimension of a composite point in terms of the codimension of the elementary entities which comprise it. In fact, it shows that Griffiths's conjecture regarding the codimension of a composite entity is correct. Sergeraert's theorem also gives a general form of the Gibbs phase rule. We shall return to this point later.

It is clear from the above remarks and the theorems of the last paragraph that, in order to get a complete local classification of phase diagrams, we need only produce a list of inequivalent functions with a single global minimum. In fact, it clearly suffices to produce a list of inequivalent germs of functions,  $f$ , which have an absolute minimum at  $\underline{0} \in R^m$  and satisfy  $f(\underline{0}) = 0$ . This classification has been carried out by Arnold for all functions of codimension less than or equal to 16. We will state the required definitions and results below.

## VI. CLASSIFICATION

According to the remarks made at the end of Sec. V, the classification of pairs of topological spaces  $(U, U \cap Q)$  where  $U$  is a sufficiently small neighborhood of  $b \in Q \subseteq Y$  in a phase diagram  $(Y, Q)$  reduces to the classification of elementary points and, hence, to the classification of functions  $f \in C_*^\infty(R^m)$  with a single isolated, global minimum. By a translation in  $R^m$  we may assume that the minimum is the origin  $\underline{0} \in R^m$ . Moreover, by translating coordinates in  $R$  we may assume that  $f(\underline{0}) = 0$ . In this paragraph, we give the classification of such functions and use it to get a generalized version of the Gibbs phase rule. We start with a definition:

*Definition.* Let  $f \in C_*^\infty(R^m)$ ,  $f(\underline{0}) = 0$  a minimum of  $f$  at  $\underline{0}$ . The *corank* of  $f$  at 0 is the number  $m - r$

where  $r$  is the rank of the matrix of second derivatives of  $f$  evaluated at  $\underline{0}$

$$r = rk \left\| \frac{\partial^2 f}{\partial x_i \partial x_j} \right\|_{\underline{x}=\underline{0}}$$

Notice that  $\underline{0}$  is a nondegenerate minimum of  $f$  if and only if  $\text{corank } f = 0$ . A very basic theorem, which generalizes the theorem of Morse mentioned in Sec. IV D, is the following:

*Theorem.* (Generalized Morse lemma): Let  $f \in C_*^\infty(R^m)$ ,  $f(\underline{0}) = 0$  a minimum of  $f$ . Suppose  $\text{corank } f = p$ . Then

$$f, \underline{0} \sim g(x_1, \dots, x_p) + x_{p+1}^2 + \dots + x_m^2, \underline{0},$$

where  $g$  contains no terms of degree less than 4 (that is,  $j^3 \langle g \rangle_0 = 0$ ).

The variables  $x_1, \dots, x_p$  are often called the *essential variables* of  $f$ . It is important to realize that they are only defined with respect to a given coordinate system. The generalized Morse lemma is also referred to as the theorem of the residual singularity.

Notice that  $\text{cod}_s \langle f \rangle_0 = \text{cod}_s \langle g \rangle_0$  [example (iv), Sec. IV C]. It is, in fact, true that  $\text{cod} \langle f \rangle_0 = \text{cod} \langle g \rangle_0$  (see Arnol'd<sup>3</sup>). We can get an estimate on the codimension of  $f$  in terms of the corank of  $f$  as follows. If the corank of  $f$  at 0 is equal to  $p \geq 0$  and  $g$  is as above, then  $\text{cod}_s f \geq \{N_1\} + \{N_2\} + \{N_3\}$ , where the  $N$ 's represent the number of missing linear, quadratic, and cubic terms in  $\Delta_0(\langle g \rangle_0)$ , respectively. Thus

$$\begin{aligned} \text{cod}_s f &\geq p + \frac{1}{2}p(p+1) + \frac{1}{6}p(p+1)(p+2) \\ &= \frac{1}{6}(p^3 + 6p^2 + 11p) \end{aligned}$$

With a little more work we can get an estimate on  $\text{cod } f$  in terms of  $p$ . The corank of  $f$  has a simple physical interpretation. It equals the number of order parameters needed to describe the phase transition. Before discussing this, we give the classification theorem:

*Theorem (Arnol'd).* Let  $f \in C_*^\infty(R^m)$  have a minimum at  $\underline{0} \in R^m$ ,  $f(\underline{0}) = 0$ . Suppose  $\text{cod}_s f \leq 10$ .

Then

$$f(x), \underline{0} \sim g(x_1, x_2) + x_3^2 + \dots + x_m^2, \underline{0},$$

where  $g(x_1, x_2)$  is one of the functions listed in Table I.

To determine the characteristic neighborhood corresponding to any type of function listed in Table I, we merely find the bifurcation set of the universal unfolding of the function in the question. This is constructed, using Mather's theorem, from the list of monomials given in the last column of the table.

To list all composite singularities and their codimensions we use Sergeraert's theorem. In an obvious notation,  $A_1^3 A_3 X_9$  refers to a function with five isolated absolute minima, three of which are nondegenerate (of type  $A_1$ ), one of which is of type  $A_3$ , and one of which is of type  $X_9$ . By Sergeraert's theorem applied repeatedly:

$$\begin{aligned} \text{cod}_s(A_1^3 A_3 X_9) &= 3 \text{cod}_s(A_1) + \text{cod}_s(A_3) \\ &\quad + \text{cod}_s(X_9) + 4 = 2 + 8 + 4 = 14 \end{aligned}$$

and

$$\text{cod}(A_1^3 A_3 X_9) = 13$$

In view of the above, we propose the following system for classifying points on a generic phase diagram  $(Y, Q)$ . If  $b \in Q$ , we say that the type of  $b$  is the type of  $\Phi_b$ . We set  $\text{cod } b = \text{cod } \Phi_b$ . The Gibbs phase rule now takes the form:

*Gibbs phase rule.* Let  $(Y, Q)$  be a generic phase diagram. Then  $b \in Q$  only if  $\text{cod } b \leq \dim Y$ . If  $\text{cod } b = r$  and  $b \in Q$ , then  $b$  lies on a submanifold of  $Y$  of codimension  $r$  which consists entirely of points of the same type as  $b$ .

The above follows from the properties of bifurcation sets of versal unfoldings. This version of the phase rule easily implies the usual Gibbs phase rule, where  $(\dim Y) - r$  is the number of thermodynamic degrees of freedom.

As we have already mentioned, the corank of  $\Phi_b$  equals the number of order parameters needed to describe the transition. Since we have an estimate for  $\text{cod } \Phi_b$  in terms of the corank, we get an estimate

TABLE I. A list of representatives,  $g(x, y) \in C_*^\infty(R^2)$ , of all inequivalent functions having a unique global minimum at  $0 \in R^2$  of smooth codimension less than or equal to 10.

Type	$g(x, y)$	$\text{cod}_s g$	$\text{cod } g$	Monomials needed to construct universal unfolding
$A_{2k-1}$	$x^{2k} + y^2$ ( $k \geq 1$ )	$2k - 2$	$2k - 2$	$x, x^2, \dots, x^{2k-2}$
$X_9$	$x^4 + ax^2y^2 + y^4$ , $ a  \leq 2$	8	7	$x, x^2, y, y^2, xy, x^2y, xy^2, x^2y^2$
$X_{11}$	$x^4 + x^2y^2 + ay^6$ , $a > 0$	10	9	$x, x^2, x^3, y, y^2, \dots, y^5, xy, x^2y^2$

TABLE II. A list of representatives,  $g(x,y) \in C_*^\infty(R^2)$ , of all inequivalent functions having a unique global minimum at  $0 \in R^2$  with finite codimension (functions listed in Table I are not repeated).

Type	$g(x,y)$	$\text{cod}_s g$	$\text{cod } g$
$Y_{2r,2s}^1$	$x^{4+2r} + ax^2y^2 + y^{4+2s}$ $0 < a < 2$	$8 + 2r + 2s$	$7 + 2r + 2s$
$Y_{2r,2s}^k$	$\{[x + (a_0 + \dots + a_{k-2}y^{k-2})y^k]^2$ $+ (b_0 + \dots + b_{2k-2}y^{k-2})y^{2(k+s)}\}$ $\times (x^2 + y^{2(k+r)})$ $1 \leq 2s \leq 2r,$ $a_0 \neq 0, b_0 > 0, k > 1$	$12k - 4 + 2(r+s)$  $12 + 4q$	$9k - 2 + 2(r+3)$  $10 + 4q$
$W_{1,4q-2}$	$(x^2 + y^3)^2 + (a_0 + a_1y)x^2y^{2+2q}$ $q > 0, a_0 > 0$		

on the number of thermodynamic parameters needed to observe a transition with any given number of order parameters. This number increases sharply with the corank.

Arnol'd has, in fact, classified all germs of functions with finite codimension having corank less than or equal to 2. A complete list of those with a global minimum at the origin can be culled from Arnol'd's list.<sup>3</sup> Table II together with Table I gives a complete list of all  $g \in C^\infty(R^2)$  such that  $f(x) \in C_*^\infty(R^m)$  has a minimum at  $0 \in R^m$ ,  $f(0) = 0$ , and

$$f(x), 0 \sim g(x_1, x_2) + x_3^2 + \dots + x_m^2, 0.$$

Finally, we remark that the characteristic graph of an entity (in the sense of Griffiths) can be calculated by looking at a neighborhood in  $C_*^\infty(R^m)$  of the function corresponding to the entity and checking the incidence relations of the various components of the strata of the stratification of  $C_*^\infty(R^m)$ . These incidence relations have been largely worked out by Arnol'd.<sup>3</sup> Using this observation and some elementary Morse theory, Raghavan<sup>5</sup> works out the characteristic graph of the entity  $X_9(D_2)$  in Griffiths's notation).

VII. FURTHER REMARKS, NONGENERIC SYSTEMS, AND ALTERNATIVE MODELS

(i) The generalized Morse lemma, quoted in Sec. VI, is an important conceptual result. It states that even if the number of microscopic variables is large, we can change variables, so that the nature of the singularity is entirely described by very few variables. We believe that this is the ultimate explanation of the fact that frequently few macroscopic parameters suffice to describe a system which depends on a very

large number of microscopic parameters.

It is worth noting that the essential variables need not be related diffeomorphically to the order parameters, in fact there is no reason to assume that such a relationship holds. Hence our model makes no predictions with regard to critical-point exponents. This has been emphasized by Schulman<sup>14</sup> and O'Shea.<sup>15</sup> See, however, Vendrik.<sup>16</sup> Of course, if we knew the map  $\Phi$  precisely and exactly how  $C_*^\infty(R^m)$  parametrizes the microstates of the system we would be in a strong position to make definite predictions.

(ii) A complete phenomenological theory would also have to take account of nongeneric systems. Such systems can arise when some symmetry forces the image of  $\Phi$  to meet strata of codimension greater than  $\dim B$ . One way of incorporating this into our model would be to express the symmetry in terms of a group operating on the space of microstates. We would then posit that the image of  $\Phi$  be restricted to functions which are invariant under the symmetry group, and so, would replace  $C_*^\infty(R^m)$  by the space of such functions. We could then consider unfoldings invariant under the action of the group. Developing a theory of bifurcation of such unfoldings would then give a classification of phase diagrams with various symmetries. Recently, efforts to develop such a theory of unfoldings have been made by several mathematicians, notably Golubitsky and Schaeffer.<sup>17</sup>

(iii) In our model, the theorems of Thom imply that, for critical-point behavior at a point  $b \in B$ , the two most important factors are the dimension of the parameter space,  $B$ , and the corank of  $\Phi_b$  (that is, the number of order parameters). This is strongly reminiscent of the hypothesis of critical-point universality. All this suggests that the techniques of differential topology, some of which we have introduced here, could be highly useful, or even indispensable,

for an understanding of critical-point phenomena.

While we are speculating, let us note that quantum electrodynamics seems to require 32 order parameters. Modeling this as we have suggested would require that the image of  $\Phi$  meet strata of codimension greater than 6544. Such a system would be highly nongeneric.

(iv) We chose the space  $X = C^\infty(R^m)$  and relation  $\sim$  in our model for two main reasons: (a) the results give good agreement with experiment, and (b) the space  $C^\infty(R^m)$  under the relation  $\sim$  is relatively well-understood mathematically. Such reasons are, of course, not definitive. It would be a major achievement if someone explicitly associated such a model with an exactly soluble system, such as the Ising model. That is, if to each microstate (or statistical distribution of microstates) one managed to associate an element of  $C^\infty(R^m)$  such that a global minimum of the element determines the phase. We do not have a great deal of confidence that this can

be done. We do, however, believe that there might well be some topological space  $X$  with an equivalence relation  $\sim$ , which would provide an exact model.

The analogs of the Thom and Morse theorems in this setting would then provide a link between the microscopic and macroscopic worlds.

In the general context of this type of modeling, Thom has suggested various candidates for the space  $X$  and relation  $\sim$  which might serve to specify a macrostate. Among them are  $X$  equal to the space of smooth vector fields on a manifold  $M$ , with  $\sim$  referring to the topological equivalence of attractors. For further details, see Thom.<sup>2</sup>

(v) The classification we have achieved is purely local. It would be nice to have a theory which yielded some global rules. For example, if we let  $Y$  be the space of all realizable (in principle) values of the thermodynamic field variables, we would like to be able to deduce that  $Q$  is connected and  $\partial Y \cap \partial Q$  is not empty.

<sup>1</sup>R. B. Griffiths, Phys. Rev. B 12, 345 (1975).

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<sup>3</sup>V. I. Arnol'd, Russ. Math. Surveys 30, 1 (1975) [Uspekhi Mat. Nauk 30, 3 (1975)].

<sup>4</sup>R. H. Crowell and R. H. Fox, *Introduction to Knot Theory* (Ginn, New York, 1963).

<sup>5</sup>R. Raghavan, J. Phys. A 11, 731 (1978).

<sup>6</sup>A. N. Godwin, Proc. Cambridge Philos. Soc. 77, 293 (1975).

<sup>7</sup>D. J. A. Trotman and E. C. Zeeman, in *Structural Stability, the Theory of Catastrophes, and Applications in the Sciences*, edited by P. Hilton (Springer, New York, 1976).

<sup>8</sup>F. Sergeraert, Ann. Sci. Ec. Norm. Sup. 5, 599 (1972).

<sup>9</sup>J. G. Dubois, J.-P. Dufour, and O. Stanek, Ann. Inst. Henri Poincaré A 24, 261 (1976).

<sup>10</sup>A. G. Kushnirenko, Invent. Math. 32, 1 (1976).

<sup>11</sup>J. N. Mather, Publ. Math. I.H.E.S. 35, 279 (1968).

<sup>12</sup>J. N. Mather, Notes on Topological Stability (these are a set of lecture notes available from Harvard University Math Department).

<sup>13</sup>M. Golubitsky and V. Guillemin, *Stable Mappings and Their Singularities* (Springer, New York, 1974).

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