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# Critical exponents of n th-order phase transitions derived from catastrophe theory on fractal lattices

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**Abstract.** A general and unifying theory of *n*th-order phase transitions is developed by combining catastrophe theory with self-similar fractal lattices. The scaling laws governing the latter imply the relation  $D = (c+2)(2-\eta)/c$  between the dimension D of the fractal lattice and the codimension c = 2n-2 of the free energy topological normal forms characterising isolated *n*th-order transitions. This together with the Euclidean dimension of the real system yields numerical values for bicritical, tricritical and tetracritical exponents which are in very good agreement with experiment and those of solvable models. The results are independent of the details of the interaction because *n*th-order phase transitions are essentially topological phenomena.

## 1. Introduction

This paper is a direct continuation and extension of a preceding one (Keller 1981, hereafter referred to as I; further references may be found in this paper) in which a lattice model with non-integer (fractional) dimensionality and the cusp singularity of catastrophe theory were combined with scaling principles to describe second-order phase transitions in a fluid. The model led to critical exponents within experimental accuracy. As announced in I, we generalise this model in the present paper to *n*th-order critical phenomena, i.e. to *n*-critical phase transitions. Adopting the notation of I and Griffiths' terminology (Griffiths and Wheeler 1970, Griffiths 1973, Griffiths and Widom 1973, Widom 1973, Griffiths 1974), we call an *n*-critical phase transition bicritical if n = 2, tricritical if n = 3, tetracritical if n = 4, and so forth. Characteristic for an *n*-critical phase transition is a special set of values, the *n*-critical exponents. The objective of our analysis is to calculate numerical values for the corresponding bicritical, tricritical and tetracritical exponents. The results are in very good agreement with both experiment and exact model solutions and independent of the details of the interaction.

The motivation for using catastrophe theory on a fractal lattice to derive critical exponents of equilibrium phase transitions was explained in I. A general physical interpretation is given in § 6. The idea is to classify the singularities and bifurcation properties of the free energy corresponding to a fractal lattice Hamiltonian (on spaces with non-integral dimension D) in terms of the Thom-Arnol'd topological normal forms of singularities of maps and using the scaling laws governing the self-similarity of fractals (Mandelbrot 1977). Combining catastrophe theory with fractional

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dimensionality is imperative because (i) equilibrium phase transitions are structurally stable phenomena, (ii) order parameters of three-dimensional and two-dimensional Ising models cannot be diffeomorphically related to each other, (iii) the dimensionality of tetracritical and higher-order transitions is a non-integer even in the Landau limit unless two order parameters are introduced, and (iv) long-range interaction is induced by nearest-neighbour interaction in systems with intrinsic fractional dimension. In a sense, the non-diffeomorphic relation between physical and formal parameters is induced by the fractal dimensionality of the lattice model.

In §2 we set up the lattice model. A closed physical system can be covered completely by N samples at time  $\ell_0$ . We assume that for each sample m physical quantities, i.e. micro-observables, have been measured. The result is a set of N state vectors  $w_i \in \mathbb{R}^m$  ( $1 \le i \le N$ ). We assign each vector to precisely one site  $z_i$  of a lattice L with spacing  $l_0$  and dimension  $D \in \mathbb{R}_+$ . D needs not to be an integer. The lattice L defines a complete static model of the physical system at time  $\ell_0$  iff the set of measurements is complete. In general, for  $\ell > \ell_0$ ,  $w_i(\ell) \neq w_i(\ell_0)$   $(1 \le i \le N)$  because of the real interaction between the samples in the physical system. To simulate this time behaviour of  $w_i(\ell)$  in the lattice model we use a Hamiltonian with only nearestneighbour interaction. This gives rise to a partition function and a free energy F. The system automatically acquires long-range interaction by virtue of the model's fractional dimensionality (cf § 6 and Güttinger and Keller 1982). The next step is to define unit volumes whose lateral extension l is of the order of the correlation length  $\xi$  and so contain many samples  $(l \gg l_0)$ , at least near an *n*-critical phase transition of the system. If  $\vec{F}$ , the free energy per unit volume, is either smooth or at least continuous on a compact connected set  $S \in \mathbb{R}^{m}$ , we can classify the possible singularities of  $\tilde{F}$  at an n-critical isolated point in phase space in terms of the Thom-Arnol'd polynomial normal forms (Thom 1975).

In §3 some elementary physical consequences will be drawn concerning the macroscopic stable states of the model. The Maxwell convention (Fowler 1972, Thom 1975) will be deduced and the connection between Gibbs' phase rule and the codimension of the normal forms of catastrophe theory will be established. In §4, we determine the Hausdorff-Besicovitch dimension D of the lattice by changing the size of the unit volumes through scaling. It is found that D depends essentially on the codimension c(n) of the normal forms and weakly on a small additional parameter  $\eta$ . Furthermore, the relation between the mathematical parameters of the normal forms and measurable quantities of the physical system will be derived using scaling arguments.

Critical, tricritical and tetracritical exponents will be calculated in § 5. These exponents turn out to depend strongly on the dimension D of the fractal lattice and on the Euclidean dimension  $\overline{D}$  of the physical system, and weakly on another small parameter  $\overline{\eta}$ . The two free parameters  $\eta$  and  $\overline{\eta}$  could not be derived from basic properties of the model but are necessarily small,  $0 \le |\eta| \le 0.1$ ,  $0 \le |\overline{\eta}| \le 0.1$ . For  $\eta = 0$  the dimension D is determined by the order n of the phase transition and  $\overline{D} = 3$  for a real physical system. The *n*-critical exponents calculated with  $\eta = 0$  and  $\overline{\eta} = 0$  yield realistic improvements over Landau exponents but do not give exactly the experimental mean values. However, a small deviation of  $\eta$  and  $\overline{\eta}$  from zero yields a very good fit with experimental data. Furthermore, small variations of  $\eta$ ,  $\overline{\eta}$  allows us to reproduce the *n*th-order critical exponents of various theories in the following way. We replace the physical system by a  $\overline{D}$ -dimensional model system. If  $\overline{\eta}$  is known in that model

we insert its value in our formulae for the *n*-critical exponents. If it is not, we have to choose  $\eta$ ,  $\bar{\eta}$  in an appropriate way. This enables us to derive numerical values for bicritical, tricritical and tetracritical exponents which are within experimental accuracy and also the exponents known from Landau theory, Ising model theories, Heisenberg models and Schofield's equation of state. Finally, in § 6, we summarise our findings, interpret the results and sketch related further developments.

#### 2. Lattice model for *n*th-order phase transitions

We consider a thermodynamic system of given extension which undergoes a phase transition of *n*th order (cf e.g. Griffiths and Wheeler 1970, Stanley 1971, Blume 1972, Griffiths and Widom 1973, Widom 1973, Keller *et al* 1979). The system may represent a real physical one with integer dimension  $\overline{D} = 3$  or a theoretical model system. The system's behaviour is macroscopically controlled by a set of control variables  $\tilde{\boldsymbol{u}} = (\tilde{\boldsymbol{u}}_1, \ldots, \tilde{\boldsymbol{u}}_k)$ , representing temperature, magnetic field, chemical potentials, pressure, etc, which form a control space  $U = \mathbb{R}^k$  of integer dimension k. Since some of the control variables may be unknown or not accessible experimentally, k is a priori not determined by the order n of the transition. We assume that the phase transition occurs at the value  $\tilde{\boldsymbol{u}} = \tilde{\boldsymbol{u}}_0$  and define reduced variables  $\tilde{\boldsymbol{u}}$  by  $\tilde{\boldsymbol{u}}_j = (\tilde{\boldsymbol{u}}_j - \tilde{\boldsymbol{u}}_{j0})/\tilde{\boldsymbol{u}}_{j0}$ .

The different phases or macroscopic states of the system are distinguished by the average values of m micro-observables w which are defined by a set of m independent measurements made at an arbitrary microscopic sample. The set of micro-observables forms a vector  $w \in E \subset \mathbb{R}^m$  where E is the space of internal state variables. For example, in the case of a magnetic system, a micro-observable may be the magnetic moment per atom or molecule or groups of these. For a mixture such as CH<sub>3</sub>OH-H<sub>2</sub>O-CO<sub>2</sub>, the micro-observables may represent the set  $(n_1, n_2, n_3)$ , where  $n_1$ ,  $n_2$  and  $n_3$  denote the number of CH<sub>3</sub>OH, H<sub>2</sub>O and CO<sub>2</sub> molecules in a small volume v (of the order of, say, 100 Å), respectively.

The spatial closure of the thermodynamic system in a  $\overline{D}$ -dimensional Euclidean space implies that the system can be covered completely by a finite number N of samples. Consequently, at each time the system is described by a set of N state vectors,  $w_j = w_j(\ell)$   $(1 \le j \le N)$ . Since  $w_j$  is time dependent the samples interact mutually. We assign each vector  $w_j(\ell)$  precisely to one lattice site  $z_j$  of a D-dimensional abstract lattice with lattice spacing  $l_0$ . This lattice dimension D (not to be confused with  $\overline{D}$ ) may take any positive real value and the lattice will therefore be called a fractal lattice. The need for using fractal dimensions in phase transitions has been emphasised by Keller (I) and Gefen *et al* (1980) and will be discussed by us in the more general context of critical and universal phenomena in a forthcoming paper. Neighbouring samples do not necessarily correspond to neighbouring lattice sites because if  $D \neq \overline{D}$  such a correspondence is quite impossible to establish (cf § 6).

Interaction in the fractal lattice model is defined by introducing a Hamiltonian H representing nearest-neighbour interaction of the vectors  $w_i$   $(1 \le j \le N)$ ,

$$H(\tilde{u}, w) = J(\tilde{u}) \sum_{\ll z_j, z_i \gg} \{ w(z_j, \ell) \cdot w(z_i, \ell) \}$$
(2.1)

where  $w(z_i, \ell) \equiv w_i(\ell)$  and  $\ll z_i, z_i \gg$  denotes summation over nearest meighbours only. The dot in the braces in (2.1) may either be understood as denoting the scalar product  $w_i \cdot w_i^{\mathrm{T}}$  or as some other product, e.g.  $(w_i \cdot w_i^{\mathrm{T}}) \cdot (w_i/|w_i|)$ . The constant J in (2.1) does not necessarily represent a physical coupling constant because such a physical coupling is difficult to define if, e.g.,  $w = (n_1, n_2, n_3)$  as in the case of a ternary mixture. However, not the details but only the type of the interaction plays a significant role in the proposed theory, which reflects its universality.

The Hamiltonian gives rise to the partition function

$$Z = \sum_{w(z_j)}^{*} \exp[-\beta H(\hat{\boldsymbol{u}}, \boldsymbol{w})].$$
(2.2)

Here, the asterisk indicates that summation goes over the possible configurations and  $\beta = 1/kT$ , where k is the Boltzmann constant and T the temperature. The free energy  $\mathscr{F}$  is given by

$$\mathscr{F} = -\beta^{-1} \ln(Z). \tag{2.3}$$

The macroscopic order parameter  $\tilde{y}$  is defined as the ensemble average of the microscopic order parameter w,

$$\tilde{\mathbf{y}} = \langle \mathbf{w} \rangle = (1/Z) \sum_{\mathbf{w}_i}^* \mathbf{w}_i \exp[-\beta H(\tilde{\mathbf{u}}, \mathbf{w})].$$
(2.4)

Although, by definition, w is a measurable quantity, this is not necessarily the case for  $\tilde{y}$  because the ensemble averages are calculated for a *D*-dimensional and not a  $\overline{D} = 3$ -dimensional system. But  $\tilde{y}$  is a function of a measurable macroscopic order parameter which depends on w, too. Equations (2.3) and (2.4) tell us that the free energy depends on  $\tilde{u}$  and  $\tilde{y}$ , although one cannot solve equations (2.3) and (2.4) explicitly for  $F(\tilde{y}, \tilde{u})$  except for very special cases. To be able to apply scaling arguments in §4 we divide the total lattice into unit volumes  $\mathcal{V}$  or blocks. The extension *l* of each block is assumed to be large compared with  $l_0$  but much smaller than the total extension *L* of the system. Since near a critical point the correlation length  $\xi$  satisfies this condition, we choose *l* to be of the order of  $\xi$ , say,  $l = \xi$ . Then

$$\dot{F} = \mathscr{F}/\mathscr{V} \tag{2.5}$$

is the free energy per unit volume. Since the quantities Z,  $\beta$  and  $\mathcal{V}$  are real scalars,  $\tilde{F}: E \times \tilde{U} \rightarrow \mathbb{R}$  is a real-valued potential function. Let  $\tilde{y}_c$  be the critical value of the macroscopic order parameter  $\tilde{y}$  and let us introduce the reduced order parameter  $y = (\tilde{y} - \tilde{y}_c)/\tilde{y}_c$ . The potential function  $\tilde{F}(y, \tilde{u})$  must be globally bounded below in Efor otherwise the partition sum would diverge. Hence, F(y, u) is even in y, i.e. in each component of y.

At this stage we can apply catastrophe theory (Thom 1975, Güttinger and Eikemeier 1979, I) to predict the physical behaviour of the system. Let us choose a compact and connected subset  $\tilde{E}$  of E. The only assumption we need is that  $\tilde{F}$  is at least continuous on  $\tilde{E}$ . Then  $\tilde{F}$  can be approximated by another potential function  $F_u(y) = F(y, u)$  to any degree of accuracy where F is a polynomial in y of order  $\leq q'$ , and  $|\tilde{F} - F| < \varepsilon(q') \rightarrow 0$  as  $q' \rightarrow \infty$ . In F a new parameter  $u \in \mathbb{R}^{q'}$  appears which depends on  $\tilde{u}$ , though in general not in a diffeomorphic way. F is even in y as is  $\tilde{F}$ , and smooth. The coalescence of phases, i.e. of macroscopic states, at an *n*-critical phase transition point implies that  $\tilde{F}$  and, therefore, F is a singularity (see, e.g. Stewart 1981 and I for definitions), i.e.,  $F_{u_0}(y)$  is a singular member of the family  $F_u(y)$ . Singularities can be classified in terms of the Thom-Arnol'd topological normal forms of codimension  $c := \operatorname{codim} F$  (see e.g. Stewart 1981, Güttinger and Keller 1982), where the

codimension is a measure for the degree of degeneracy of the singularity. Normal forms which are odd in y are excluded because  $F_{u_0}(y)$  is even in y.

By their very definition, bicritical, tricritical, tetracritical, pentacritical, ... transition phenomena possess codimension c = 2, 4, 6, 8, ..., respectively, and comparing c with the order n = 2, 3, 4, 5... of the phase transitions one sees at once that

$$c = 2n - 2 \tag{2.6}$$

Consequently, for an *n*-critical phase transition we obtain near  $u_0$ 

$$F(\mathbf{y}, \mathbf{u}) \underset{C^{\infty}}{\propto} V_{2n-2}(\mathbf{x}, \mathbf{a}) + Q_{2n-2}(\mathbf{x}', \mathbf{a}')$$
(2.7)

where for  $n \ge 4 x$  may possess two components. In (2.7)  $V_{2n-2}(x, a)$  is the standard Thom-Arnol'd catastrophe polynomial of codim c = 2n - 2 and corank  $\le 2$ , while  $Q_c$  are quadratic (Morse) forms in x' which obviously do not influence critical behaviour. The dimension of the space of x' is m-1 if x is a scalar and m-2 if x has two components. The dimension of  $\{a'\}$  is q'-k. The relation between (x, x', a, a') and (y, u) is diffeomorphic.

#### 3. Physical consequences

In virtue of the splitting lemma, equation (2.7) shows that the multicomponent order parameter splits into two parts x, x' with the number of components of x restricted to at most two, no matter how large the number m of micro-observables w and, furthermore, that the space U of relevant control variables is made up of at most 2n-2 independent variables, n being the order of the transition. Therefore, at most 2n-2 variables can be varied in any experiment to reach an isolated nth-order critical point, and if there are no unknown fixed variables or physical symmetries involved, then exactly 2n-2 control variables must be varied (cf also Schulman 1973, Keller *et al* 1979).

Next, let us focus on the so-called 'Maxwell convention' introduced by Thom (1975) to discriminate between competing minima of  $V_{c}$ . This convention states that for a given a the thermodynamic stable states are those with absolute lowest minima. As pointed out by Schulman (Schulman and Revzen 1973), Vendrik (1979) and Keller (1979) (cf also Coleman and O'Shea 1981) this convention follows from the partition function Z because maxima of Z correspond to minima of F and Z has a sharply peaked probability distribution (e.g. Kittel 1969). Q possesses only one minimum with respect to x' and therefore does not contribute to a phase transition (a change between two different states,  $x_1, x_2$ ). We therefore call x the relevant order parameter and disregard Q in the following. Then, in a neighbourhood of  $u_{0}$ ,

$$F(\boldsymbol{u},\boldsymbol{y}) \propto V_{2n-2}(\boldsymbol{x},\boldsymbol{a}) = V_c(\boldsymbol{x},\boldsymbol{a}) \quad (3.1)$$

where the symbol  $\propto$  denotes  $C^{\infty}$ -equivalence up to quadratic remainders Q. Since the coordinates in F and  $V_c$  are related diffeomorphically, the minima of  $V_c$  with respect to x are minima of F with respect to  $y(x) \propto x + \ldots$ . Therefore, the lowest minima of  $V_c$  in x determine the most probable macroscopically stable states. The space of macroscopically stable states is therefore given by the set

$$\Sigma(V_c) = \{(\mathbf{x}, \mathbf{a}) | \partial V_c(\mathbf{x}, \mathbf{a}) / \partial \mathbf{x} = \mathbf{0} \text{ and } | \partial^2 V_c / \partial \mathbf{x}^2 | \ge 0 \}$$
(3.2)

where  $\partial V_c/\partial x$  denotes the gradient of  $V_c$  and  $|\partial^2 V_c/\partial x^2|$  the Hessian. A phase transition of the first kind occurs if, for a given a, two or more minima of  $V_c$  have the same absolute lowest value,  $V_c(x_1, a) = \ldots = V_c(x_r, a)$ . The set of such points (x, a), the Maxwell set, will be denoted by  $\omega'$  and its projection onto U will be called  $\omega$ . Higher-order phase transitions occur if p minima of  $V_c$ ,  $(2 \le p \le n)$  coalesce. This set of coalescence will be denoted by  $\Gamma'$  and its projection onto U by  $\Gamma$  (cf Keller *et al* 1979). It is easily seen that the above sets satisfy the familiar stability criteria for phase transitions of kth order  $(k = 1, 2, \ldots, n)$ .

We conclude this section with a remark about Gibbs' phase rule. Assume that an *r*-component mixture coexists in *p* phases  $(1 \le p \le n)$ . Then, according to Gibbs' phase rule, the number *f* of independent variables is

$$f = r + 2 - p. \tag{3.3}$$

In our model the values of the order parameter follow once the value of a in the control space is prescribed. Therefore, the maximum number of independent variables equals  $f_{\max} = \dim U = c = 2n - 2$ . Coexistence of p phases implies p - 1 additional conditions for the independent variables. The number of degrees of freedom is, therefore,

$$f = f_{\max} - (p-1)$$

or

$$f = (f_{\max} - 1) + 2 - p. \tag{3.4}$$

Comparing (3.4) with (3.3), we see that the number of components of the mixture is given by (cf also, Keller *et al* 1979)

$$r = f_{\max} - 1 = 2n - 3 = c - 1. \tag{3.5}$$

Consequently, an isolated phase transition point of n th order occurs only in mixtures consisting of an odd number of chemical components. This means that single-component mixtures possess one isolated bicritical point, ternary mixtures possess one isolated tricritical point, and so on. Binary mixtures or alloys exhibit an infinite line of bicritical points, quaternary mixtures are characterised by an infinite line of tricritical point and so forth. In order to observe an isolated nth-order critical point for these mixtures (r even) and to apply the catastrophe theoretic classification scheme, it must therefore be possible to fix one thermodynamical variable.

#### 4. Scaling and transformation laws

When a critical point is approached, the correlation length diverges with the reduced temperature t as

$$\xi \simeq |t|^{-\nu}$$
 if  $t > 0$  and  $\xi \simeq |t|^{-\nu'}$  if  $t < 0$ . (4.1)

Let us, for simplicity, assume that  $\nu = \nu'$ . To keep the size of the unit volumes constant we have to change the fractal's intrinsic length scale  $l_0$  by a factor

 $s = |t|^{\nu}.\tag{4.2}$ 

By this procedure more and more lattice points will move into one unit volume and contribute to  $\tilde{F}$ . Then, either the fractal lattice shrinks or one has to consider samples

of increasingly smaller size. To avoid such trouble, either we assume that t varies only very near the critical point (without reaching it), or else, as in the fluid case (I), we assume that the fractal lattice is infinitely extended, which is justified because  $L \gg l$ .

Because of the fractal's inherent self-similarity, changing the length scale transforms a volume  $\mathcal{V}_1$  according to

$$\mathcal{V}_s = s^{-D} \mathcal{V}_1. \tag{4.3}$$

The total free energy remains constant under length scaling and therefore (2.5) and (4.3) yield

$$\tilde{F}_s = s^D \tilde{F}_1$$

and the same transformation law holds for F and the normal polynomials  $V_c(x, a)$ (c = 2n - 2). Let us confine ourselves to the cuspoids with dim $\{x\} = 1$ , i.e. to a single scalar order parameter x. Then

$$V_c(x, \boldsymbol{a}) = x^{2n}/2n + \sum_{k=1}^{2n-2} a_k x^k / k, \qquad (4.4)$$

and  $(V_c)_s = s^D (V_{2n})_1$  yields

$$x \propto s^{D/2n},$$

$$a_{2n-2} \propto s^{D/n},$$

$$\vdots$$

$$a_1 \propto s^{D(2n-1)/2n}.$$
(4.5)

To eliminate the fractal dimension D in (4.5), we use the scaling law for the correlation function G(k) (cf e.g. I). This is the only ingredient of renormalisation group theory one needs. On the one hand  $y = \langle (w - w_c) / |w_c| \rangle \rightarrow s^q \langle (w - w_c) / w_c \rangle$  leads to

$$G(s\mathbf{k}) \propto s^{2q-D} \tag{4.6}$$

while, on the other hand, one knows (Stanley 1971, Ma 1976) that

$$G(s\boldsymbol{k}) \propto s^{-2+\eta} \tag{4.7}$$

where  $\eta$  is the critical-point exponent. Comparing (4.6) with (4.7) yields

$$q = (D - 2 + \eta)/2. \tag{4.8}$$

Now,  $(x, x') \underset{C^{\infty}}{\propto} y$  and because of the  $C^{\infty}$ -equivalence it follows with (4.5) and (4.8) that

$$D/2n = (D-2+\eta)/2,$$

i.e. by virtue of (2.6), the fractal lattice dimension is given by

$$D = n(2-\eta)/(n-1) = (c+2)(2-\eta)/c.$$
(4.9)

From experiment one knows that the parameter  $\eta$  appearing in (4.7) and (4.9) is very small,  $0 \le \eta_{exp} \le 0.1$ . Therefore, we see that the dimension D of the fractal lattice governing the model depends strongly on the order n of the phase transition and very weakly on the critical-point exponent  $\eta$ .

Next we establish a relation between the variables of the fractal lattice and the measurable variables of the thermodynamical system under consideration. Let  $\overline{F}$  be

the 'true' thermodynamic potential per unit volume  $\bar{\mathcal{V}}$  of the system with Euclidean dimension  $\bar{D}$ . Suppose that in  $\bar{\mathcal{V}}$  there are as many samples as there are lattice points in  $\mathcal{V}$ . Then  $\bar{\mathcal{V}} = \bar{l}^{\bar{D}}$ . Since  $\bar{F}_s = \tilde{F}_s$  if  $\bar{F}_1 = \tilde{F}_1$  (i.e. equality of free energies per unit volume in system and fractal model holds before and after length scaling) we have that

$$s^D = \bar{s}^{\bar{D}}$$

so that with  $s \propto |t|^{\nu}$ 

$$\bar{s} \propto |t|^{\nu D/\bar{D}}, \qquad \bar{s} \propto |t|^{\bar{\nu}}$$

$$(4.10)$$

where

$$\bar{\nu} = \nu D / \bar{D}. \tag{4.11}$$

Since  $w_i$  is the measured micro-observable for the *j*th sample one can define a reduced density m of micro-observables in  $\overline{D}$ -dimensional space. Then the same argument used for the correlation function above leads to

$$m \propto \bar{s}^{\bar{a}}$$
 (4.12)

and

$$\bar{q} = (\bar{D} - 2 + \bar{\eta})/2.$$
 (4.13)

Combining equations (4.12), (4.10) and (4.5) yields  $m \propto |t|^{\bar{q}\nu D/\bar{D}} \propto y^{2n\bar{q}/\bar{D}}$ . For the essential component *m* of *m* we therefore obtain the relation

$$x(m) \propto m^{\theta} \tag{4.14}$$

with

$$\theta = \bar{D}/2n\bar{q} = \bar{D}/n(\bar{D}-2+\bar{\eta}). \tag{4.15}$$

The line  $K = \{(x, a) | a_2 < 0, a_1 = 0, a_3 = ... = a_{n-2} = 0\}$  describes the coexistence of two phases, i.e. a line of phase transitions of the first kind. From equations (4.2) and (4.5) one concludes that

$$a_2(t) \propto |t|^{\lambda_2} \tag{4.16}$$

with

$$\lambda_2 = \nu D(n-1)/n. \tag{4.17}$$

Similarly one obtains the general result that

$$a_{2k}(t) \propto |t|^{\lambda_{2k}}$$
 (4.18)

where

$$\lambda_{2k} = \nu D(n-k)/n. \tag{4.19}$$

W is the field conjugate to m and  $a_1$  the conjugate to x. Therefore

$$W \propto a_1 \partial x / \partial m. \tag{4.20}$$

The relations between catastrophe variables and measurable variables of the thermodynamic system are given by (4.14), (4.18). These relations are diffeomorphic only in very exceptional cases. But, as we have seen, a diffeomorphic relation is not necessary in applying catastrophe theory because this theory also works for free energies defined on spaces with non-integral dimensionality, nor is such a diffeomorphic relation physically possible. The essential point is that the non-diffeomorphic properties are induced by the fractal dimensionality of the lattice. We note that the order parameter x(m) depends on the Euclidean dimension D, whereas the unfolding parameters  $a_{2_k}$  depend on the fractal dimension D and interrelate through (4.11).

## 5. Calculation of critical exponents for *n*th-order phase transitions

In this section we calculate the critical exponents for *n*th-order phase transitions for  $n \le 4$ . It will be seen that the computed exponents agree with the observed values within experimental accuracy independent of interaction details.

## 5.1. Bicritical exponents

5.1.1. General results. According to (2.7), for a second-order transition (n = 2) the singularity of the fractal lattice free energy is equivalent to the cusp normal form (cf also I)

$$V_2(x, a) = x^4/4 + a_2 x^2/2 + a_1 x.$$
(5.1)

The dimensionality of the fractal lattice is given by equation (4.9) with n = 2, i.e. by

$$D = 4 - 2\eta. \tag{5.2}$$

The transformation laws reduce to

$$x(m) \propto m^{\theta}, \qquad a_2(t) \propto t^{\lambda_2}$$
 (5.3)

where, by virtue of (4.15) and (4.17),

$$\theta = \overline{D} / [2(\overline{D} - 2 + \overline{\eta})], \qquad \lambda_2 = \nu D / 2. \tag{5.4a, b}$$

The equation of state is

$$\Sigma(V_2) = \{(x, a_1, a_2) | x^3 + a_2 x + a_1 = 0 \text{ and } 3x^2 + a_2 \ge 0\}.$$
(5.5)

The Maxwell set consists of a single line, the coexistence line  $\omega = \{(a_1, a_2) | a_1 = 0, a_2 \le 0\}$ . On this line we have by virtue of (5.5)  $x^3 + a_2x = 0$  or  $x^2 = -a_2$ , and inserting (5.3) it follows that

$$m \propto (-t)^{\lambda_2/2\theta}.$$
(5.6)

Therefore, the critical exponent  $\beta$  is given by

$$\boldsymbol{\beta} = \lambda_2 / 2\boldsymbol{\theta} = \nu (2 - \eta) (\bar{\boldsymbol{D}} - 2 + \tilde{\eta}) / \bar{\boldsymbol{D}}.$$
(5.7)

On the critical isotherm  $t \equiv 0$ , we have  $a_2 \equiv 0$  and  $a_1 = -x^3$ . Hence, with (4.20), it follows that

$$W \propto m^{3\theta} m^{\theta-1} = m^{4\theta-1}. \tag{5.8}$$

The critical exponent  $\delta$  is given by

$$\delta = 4\theta - 1. \tag{5.9}$$

The exponent  $\alpha$  describes the change of the specific heat  $c_m(t)$  if the critical point is approached along the line m = 0, W = 0 and t > 0. Generally, the specific heat for constant order parameter m is given by  $c_m = -T(\partial S/\partial T)_m$ , and  $S = \partial F/\partial T$  leads to

$$c_m = -(1+t)(1/T_c)^2 (\partial^2 \vec{F} / \partial t^2)_m \propto -(1+t)(\partial^2 V_2 / \partial t^2)_x / T_c^2.$$
(5.10)

Since both W and m should vanish we insert (4.4) for  $V_2$  and obtain with (5.10)

$$c_m \propto (1+t)t^{\nu D-2}$$
 (5.11)

and because the exponent  $\alpha$  is defined by  $c_m \sim t^{-\alpha}$  we see that

$$\alpha = 2 - \nu D. \tag{5.12}$$

The exponent  $\alpha'$  describes the specific heat's change when the critical point is approached along the coexistence line  $\omega$ . There  $x^2 \propto t^{\lambda_2}$  and  $V_2 \propto t^{2\lambda_2}$  and by virtue of (5.10)

$$c_m \sim (1+t)t^{2\lambda_2 - 2},$$
 (5.13)

i.e. with (5.4b) and (5.2)

$$\alpha' = 2 - 2\lambda_2 = 2 - \nu D. \tag{5.14}$$

The generalised susceptibility is defined by  $\chi = (M_c/W_c)(\partial m/\partial W)_t$  and the critical exponents  $\gamma$ ,  $\gamma'$  give the change of  $\chi^{-1}$  with  $t \ge 0$ , respectively  $t \le 0$ ,

$$\chi^{-1} \propto \begin{cases} t^{\gamma} & (t \ge 0) \\ (-t)^{\gamma} & (t \le 0). \end{cases}$$
(5.15)

On  $\Sigma(V_2)$  we have  $a_1(W) = -x^3(m) - a_2(t)x(m)$  and with (5.3)

$$a_1(W) = -m^{3\theta} - t^{\lambda_2} m^{\beta}.$$
(5.16)

On the critical isotherm (t = 0),  $a_1(W) \propto m^{3\theta}$  and with (5.8) we obtain the relation

$$a_1(W) \propto W^{\lambda_1} \tag{5.17}$$

where

$$\lambda_1 = 3\theta/(4\theta - 1). \tag{5.18}$$

Solving equations (5.17) and (5.16) for W yields

$$W \propto (-t^{\lambda_2} m^{\theta} - m^{3\theta})^{1/\lambda_1}$$
 (5.19)

and, therefore,

$$\chi^{-1} \propto (-t^{\lambda_2} m^{\theta} - m^{3\theta})^{(1/\lambda_1 - 1)} (-\theta t^{\lambda_2} m^{\theta - 1} - 3\theta m^{3\theta - 1}).$$
 (5.20)

For the change of m with  $t \to 0_+$  we insert  $m \propto t^{\nu D/4\theta}$  given by (4.5) into (5.20). This yields with  $\lambda_2 \approx \nu D/2$  for  $t \ge 0$  the result

$$\chi^{-1} \propto (-2t^{3\nu D/4})^{(\theta-1)/3\theta} (-\theta t^{\nu D/2 + \nu D(\theta-1)/4\theta} - 3\theta t^{\nu D(3\theta-1)/4\theta})$$

and, therefore,

$$\chi^{-1} \propto t^{\nu D(2\theta-1)/2\theta}.$$
 (5.21)

We have previously assumed  $\nu = \nu'$  and, therefore,  $m \propto t^{\nu'D/4\theta} \equiv t^{\nu D/4\theta}$  if  $t \to 0_-$ . Consequently,

$$\gamma = \gamma' = \nu D(2\theta - 1)/2\theta = \beta(\delta - 1). \tag{5.22}$$

# 5.1.2. Specification of $\eta$ , $\bar{\eta}$ and $\bar{D}$ for various models.

#### (i) The two-dimensional Ising model

In this case we have  $\overline{D} = 2$  and  $\overline{\eta} = 0.25$ . The only free parameter  $\eta$  will be set equal to zero. From the general formulae derived above, it follows then that D = 4 and  $\nu = 0.5 \ \theta = 4$ ,  $\lambda_2 = 1$ ,  $\lambda_1 = 4/5$ , and the critical exponents of the two-dimensional Ising

model predicted by the fractal lattice model (with D=4) are  $\alpha = \alpha' = 0$ ,  $\beta = 1/8$ ,  $\gamma = \gamma' = 7/4$ ,  $\delta = 15$ ,  $\bar{\nu} = 1$ . These values agree with those obtained by solving the Ising model exactly (Stanley 1971).

(ii) The three-dimensional Heisenberg model with infinite spin

Here  $\overline{D} = 3$  and  $\overline{\eta} = 0$ . As above we set  $\eta = 0$ . In that case the fractal lattice again possesses dimension D = 4 and the transformation powers are  $\theta = 3/2$ ,  $\lambda_2 = 1$ ,  $\lambda_1 = 9/10$ . The critical exponents derived with these values are  $\alpha = \alpha' = 0$ ,  $\beta = 1/3$ ,  $\gamma = \gamma' = 4/3$ ,  $\delta = 5$ ,  $\overline{\nu} = 2/3$ , in agreement with the exponents given by Benguigui and Schulman (1973) for the approximate solution of the Heisenberg model.

(*iii*) The three-dimensional Ising model

Here  $\bar{D} = 3$  but  $\bar{\eta}$  is unknown. We are free to choose  $\bar{\eta} = 0$  and  $\eta = 0.12$ . The dimension of the fractal lattice model is then D = 3.76. The critical exponents derived from the fractal lattice are easily computed to be  $\alpha = \alpha' = 0.12$ ,  $\beta = 0.31$ ,  $\gamma = \gamma' = 1.25$ ,  $\delta = 5$ ,  $\bar{\nu} = 0.63$ . For comparison, the critical exponents calculated by solving the model approximately (Ma 1976) are  $\alpha = 0.13 \pm 0.01$ ,  $\beta = 0.312^{+0.002}_{-0.005}$ ,  $\gamma = 1.25 \pm 0.002$ ,  $\delta = 5 \pm 0.05$ ,  $\nu = 0.638^{+0.002}_{-0.001}$ , and (Stanley 1971)  $\alpha = \alpha' = 0.125$ ,  $\beta = 0.312$ ,  $\gamma = \gamma' = 1.25$ ,  $\delta = 5$ ,  $\bar{\nu} = 0.638$ ,  $\bar{\eta} = 0.04$ .

(iv) The three-dimensional Heisenberg model with two spins ( $s = \pm 1/2$ ) Here  $\overline{D} = 3$  is prescribed. We choose  $\eta = -0.2$  and  $\overline{\eta} = 0.05$ . This choice gives D = 4.4,  $\theta = 1.43$  and  $\lambda_2 = 1.1$  and the critical exponents turn out to be  $\alpha = \alpha' = -0.24$ ,  $\beta = 0.38$ ,  $\gamma = \gamma' = 1.42$ ,  $\nu = \overline{\nu} = 0.78$ ,  $\delta = 4.72$ . This result is to be compared with the one quoted by Ma (1976), namely  $\alpha = \alpha' = -0.20 \pm 0.08$ ,  $\gamma = 1.43 \pm 0.01$ ,  $\nu = \nu' = 0.70 \pm 0.03$ .

(v) The three-dimensional Heisenberg model with arbitrary spin in three-dimensional space

 $\overline{D} = 3$  as above, but we may choose  $\eta = -0.14$  and  $\overline{\eta} = 0.6$ . The result is then D = 4.28and  $\theta = 1.41$ ,  $\lambda_2 = 1.07$  which yields the exponents  $\alpha = \alpha' = -0.14$ ,  $\beta = 0.38$ ,  $\gamma = \gamma' = 1.38$ ,  $\delta = 4.64$ ,  $\nu = 0.71$  for our model. Ma (1976) gives the exponents  $\alpha = -0.14 \pm 0.06$ ,  $\beta = 0.38 \pm 0.03$ ,  $\gamma = 1.375^{+0.020}_{-0.010}$ ,  $\nu = 0.703 \pm 0.010$  which agree quite well with our results. However, the value for  $\overline{\eta}$  necessary in our theory is very large.

(vi) The Landau theory

Let  $D = \overline{D}$  and  $\eta = \overline{\eta} = 0$ . Then we get the exponents  $\alpha = \alpha' = 0$ ,  $\gamma = \gamma' = 1$ ,  $\beta = 0.5$ ,  $\delta = 3$ ,  $\nu = \nu' = 0.5$  of the Landau theory. The dimension of the fractal lattice is D = 4 and the relation between catastrophe theory variables and Landau theory variables is diffeomorphic as  $\theta = 1$ ,  $\lambda_2 = 1$  indicates.

(vii) The real three-dimensional thermodynamical systems

As above, small variations of  $\eta$ ,  $\bar{\eta}$ , will yield slightly different exponents like those found in experimental investigations (compare tables 1-3).

Table 1. Measured critical exponents for some ferromagnetic systems (Kittel 1969).

Material	γ	β	$T_{\rm c}$ in K
Fe	$1.33 \pm 0.015$	$0.34 \pm 0.04$	1043
Co	$1.21 \pm 0.04$	-	1388
Ni	$1.35 \pm 0.02$	$0.42 \pm 0.07$	627.2
Gd	$1.30 \pm 0.10$	_	292.5
CrO <sub>2</sub>	$1.63 \pm 0.02$	_	386.5
CrBr <sub>3</sub>	$1.21 \pm 0.02$	$0.37 \pm 0.01$	32.6
EuS		$0.33 \pm 0.02$	16.5

Critical points	Material		$T_{\rm e}\left({ m K} ight)$	$\alpha, \alpha'$	β	γ, γ΄	δ
Antiferro- magnetic	CoCl <sub>2</sub> ·6H <sub>2</sub> O	Uniaxial	2.29	$\alpha < 0.11$ $\alpha' < 0.19$	$0.23 \pm 0.02$		
0	FeF <sub>2</sub>	Uniaxial	78.26	$\alpha = \alpha'$ = 0.112 +0.044			
	RbMnF <sub>3</sub>	Isotropic	83.05	$\alpha = \alpha'$ = -0.139 +0.007	0.316± 0.008	$\begin{array}{c} \gamma = 1.397 \\ \pm 0.034 \end{array}$	
Liquid- gas	CO <sub>2</sub>	<i>n</i> = 1	304.16	$\alpha \simeq 1/8$	$0.3447 \pm 0.0007$	$\begin{array}{l} \gamma = \gamma' \\ = 1.20 \\ \pm 0.02 \end{array}$	4.2
	Xe		289.74	$\alpha = \alpha' = 0.08 \pm 0.02$	0.344 ± 0.003	$\begin{array}{l} \gamma = \gamma' \\ = 1.203 \\ \pm 0.002 \end{array}$	$4.4 \pm 0.4$
	He <sup>3</sup>		3.3105	$\alpha < 0.3$ $\alpha' < 0.2$	0.361± 0.001	$\begin{array}{l} \gamma = \gamma' \\ = 1.15 \\ \pm 0.03 \end{array}$	
	He⁴		5.1885	$\begin{array}{l} \alpha = 0.127 \\ \alpha' = 0.159 \end{array}$	$0.3554 \pm 0.0028$	$\gamma = \gamma'$ = 1.17 +0.0005	
γ	He <sup>4</sup>		1.8-2.1	$-0.04 < \alpha = \alpha' < 0$			
Binary mixture	$CCl_4-C_7F_{14}$	<i>n</i> = 1	301.78		0.335± 0.02	$\gamma = 1.2$	≃4
Binary alloy	Co-Zn	<i>n</i> = 1	739		0.305± 0.005	$\begin{array}{l} \gamma = 1.25 \\ \pm 0.02 \end{array}$	
Ferro electric	Triglycine sulphate	<i>n</i> = 1	322.6			$\begin{array}{l} \gamma = \gamma' \\ = 1.00 \\ \pm 0.05 \end{array}$	

Table 2. Critical exponents for different systems (Ma 1976).

Table 3. Measured critical exponents for selected systems (Stanley 1971).

System	System $T < T_0$		$T = T_0$		$T > T_0$				
	α'	β	γ'	ν'	δ	η	α	γ	ν
Fluids									
$CO_2$	~0.1	0.34	~1.0		4.2		$\sim 0.1$	1.35	_
Xe	< 0.2	0.35	~1.2	0.57	4.4			1.3	
Magnets									
Ni	$\alpha'_{s} = -0.3$	0.42		_	4.22		0	1.35	
EuS	$\alpha'_{s} = -0.15$	0.33				—	0.05		
CrBr <sub>2</sub>	-	0.368			4.3			1.215	

We choose  $\eta$ ,  $\bar{\eta}$  to get the best fit for the mean values from tables 1-3. This is achieved by  $\eta = 0.04$  and  $\bar{\eta} = 0.08$ , because then D = 3.92 and  $\theta = 1.38$ ,  $\lambda_2 = 0.98$  gives for the fractal lattice model the exponents

$$\alpha = \alpha' = 0.04, \ \beta = 0.35, \ \gamma = \gamma' = 1.25, \ \delta = 4.52, \ \bar{\nu} = 0.65$$

which should be compared with the mean values from tables 1-3, i.e. with  $\alpha = 0.05 \pm 0.08$ ,  $\alpha' = 0.03 \pm 0.16$ ,  $\beta = 0.34 \pm 0.04$ ,  $\gamma = 1.27 \pm 0.13$ ,  $\gamma' = 1.13 \pm 0.09$ ,  $\delta = 4.25 \pm 0.14$ ,  $\bar{\nu} = 0.60 \pm 0.03$ .

#### 5.2. Tricritical exponents

5.2.1. General results. According to (2.7) the singularity of the fractal lattice free energy for third-order phenomena is determined by the butterfly catastrophe normal form

$$V(x, a) = x^{6}/6 + a_{1}x + a_{2}x^{2}/2 + a_{3}x^{3}/3 + a_{4}x^{4}/4.$$
 (5.23)

The fractal dimension is  $D = 3(2 - \eta)/2$ , i.e.  $D \approx 3$  since  $\eta$  is small. A variety of examples—ternary mixtures, ferroelectrics and ferromagnetics, superfluid helium etc—(cf Keller *et al* 1979) fall into this class.

In analogy with § 5.1 we find

$$\theta = \overline{D}[3(\overline{D} - 2 + \overline{\eta})], \tag{5.24}$$

$$\lambda_2 = 2\nu D/3. \tag{5.25}$$

The tricritical exponents depend strongly on the path along which the tricritical point is approached (Riedel and Wegener 1974, Vohrer and Brezin 1976, Griffiths 1973, Yelon 1973), and logarithmic corrections to the power laws appear in some models.

Pure exponents can be defined only in some domains of the control space. Between these, in the crossover regions, one has concurrent behaviour between the critical and the tricritical fixed points. Only effective exponents are measurable. Pure tricritical exponents are obtained when the tricritical point is approached within a small cone whose axis is identical with  $a_2$ . Then, following the same lines of reasoning as above, we obtain by virtue of  $\lambda_4 = \lambda_2/2$  and with  $a_1 = a_3 = 0$  on the coexistence areas  $E_1$  and  $E_2$  (see Keller *et al* (1979) for the explicit equations for  $E_1$  and  $E_2$ ) the general tricritical exponents

$$\alpha = 2 - 3\lambda_2/2, \qquad \beta = \lambda_2/4\theta, \qquad \gamma = \gamma' = \beta(\delta - 1), \qquad \delta = 6\theta - 1,$$
  
$$\alpha' = 2 - 2\lambda_2. \qquad (5.26)$$

It should be observed that  $\alpha \neq \alpha'$  in contrast with the bicritical case.

# 5.2.2. Specification of $\eta$ , $\bar{\eta}$ and $\bar{D}$

(i) The Landau case

Here we have again  $D = \overline{D}$  and  $\eta = \overline{\eta} = 0$ . Equations (5.24), (5.25) and (5.26) yield then: D = 3,  $\theta = 1$ ,  $\lambda_2 = 1$  iff  $\nu = 1/2$ . The tricritical exponents derived from the fractal model are  $\alpha = 0.5$ ,  $\alpha' = 0$ ,  $\beta = 0.25$ ,  $\gamma = \gamma' = 1$ ,  $\delta = 5$ ,  $\overline{\nu} = 0.5$  and coincide with those of the Landau theory (e.g. Benguigui 1972).

(ii) Let us choose  $\eta = 0.09$ ,  $\bar{\eta} = -0.27$ . Then D = 2.86, whence (with  $\nu = 0.5$  as usual) we get  $\theta = 1.37$  and  $\lambda_2 = 0.96$  and therefore  $\alpha = 0.56$ ,  $\alpha' = 0.08$ ,  $\beta = 0.18$ ,  $\gamma = \gamma' = 1.09$ ,  $\delta = 7.22$ ,  $\bar{\nu} = 0.48$ .

With the exception of  $\alpha'$ , the above exponents agree quite well with those determined by Kortman (1972) from Schofield's equation of state (Schofield 1969): Kortman obtains  $\alpha = \alpha' = 0.57$ ,  $\beta = 0.17$ ,  $\gamma = 1.13$ ,  $\gamma' = 1.06$ ,  $\delta = 7.25$ . In table 4 we quote some experimentally measured tricritical exponents and their mean values. The value  $\beta = 0.16$  (\*) in table 4 was neglected in calculating the latter because the point investigated by Benepe and Reese (1967) is probably tetracritical.

**Table 4.** Experimental tricritical values for selected systems: (1) Jahn and Neumann (1973) for  $NH_4Cl_xBr_{1-x}$ , (2) Strukov *et al* (1968) for  $KH_2PO_4$ , (3) Yelon (1973) for  $ND_4Cl$ , (4) Egert *et al* (1971) for  $NH_4Br$ , (5) Benepe and Reese (1967) for  $KH_2PO_4$ .

	α'	α	γ	$\gamma'$	δ	β
(1)						≈0.25
(2)		$0.51 \pm 0.01$			≥5	≤0.25
(3)		0.59	$1.05 \pm 0.2$			$0.18 \pm 0.01$
(4)						$0.25 \pm 0.02$
(5)		0.5-0.66	≃1	≃1		0.16 (*)
Mean values	0(?)	$0.56 \pm 0.07$	$1.02 \pm 0.03$	~1	≥5	$0.23 \pm 0.03$

The best fit to the mean values is obtained with  $\eta = 0.09$ ,  $\bar{\eta} = -0.06$ . This implies D = 2.86 and  $\theta = 1.06$ ,  $\lambda = 0.96$ . The exponents derived from (5.26) are  $\alpha' = 0.08$ ,  $\alpha = 0.56$ ,  $\beta = 0.23$ ,  $\gamma = \gamma' = 1.21$ ,  $\delta = 5.26$  and  $\bar{\nu} = 0.42$  in excellent agreement with the experimental results.

5.2.3. Bicritical exponents from the parameters for best fit ( $\eta = 0.09$ ,  $\bar{\eta} = -0.06$ ). The semiaxis  $a_4 \ge 0$  is a line of critical points and so (0, 0, 0, 1) is a critical point in phase space ((0, 0, 0, 0) being the tricritical point). On the coexistence set  $E_1$  (Keller *et al* 1979) we approach this point along the line  $\ell = \{(0, a_2, 0, 1) | a_2 \le 0\}$ . Then  $V_4(x, a) = x^6/6 + x^4/4 + a_2x^2/2$  is the free energy along this line. On this line the terms  $x^6$  and  $x^4$  cannot scale equally. Hence, to apply scaling arguments we have to neglect one of those terms, either  $x^4$  if  $x \gg 1$  or  $x^6$  if  $x \ll 1$ . Since x = 0 at the critical point (0, 0, 0, 1) we neglect the  $x^6$  term and obtain  $V_4(x, a) \approx x^4/4 + a_2x^2/2$ . Since  $a_2(t)$  scales as  $a_2 \propto t^{2\nu D/3}$  for tricritical phenomena (cf (5.26)) but  $a_2 \propto t^{\nu D/2}$  for bicritical phenomena (cf (4.16) with n = 2, k = 1), we conclude that  $\tilde{\nu} = 4\nu/3$  and  $\tilde{\nu} = 4D\nu/3 = 0.635$ . The transformation exponent  $\lambda$  remains unchanged ( $\lambda_2 = 0.96$ ), but in the step leading from (4.13) to (4.14) we have to replace  $\nu$  by  $\tilde{\nu}$  and obtain  $\theta_{bc} = 4\theta_{tc}/3 = 1.41$ . These values for  $\lambda_2$ ,  $\theta_{bc}$  inserted in the equations for critical exponents derived from  $V_4(x, a)$  yield (cf (5.12), (5.14), (5.7), (5.22) and (5.9))  $\alpha = \alpha' = 0.08, \beta = 0.34, \gamma = \gamma' = 1.24, \delta = 4.64, \bar{\nu} = 0.635$  in good agreement with § 5.1.2 (vii).

#### 5.3. Tetracritical exponents using one order parameter

5.3.1. General results. A tetracritical phenomenon is governed by the star catastrophe normal polynomial  $V_6$  if a single order parameter is used:

$$V_6(x, a) = x^8/8 + \sum_{k=1}^6 a_k x^k/k.$$
 (5.27)

The dimension of the fractal lattice follows from equation (4.9):

$$D = 4(2 - \eta)/3. \tag{5.28}$$

It is obvious that the tetracritical exponents depend even more sensitively than the

tricritical ones on the path in the phase diagram along which the tetracritical point is approached. We approach the tetracritical point along the  $a_2$  axis or in a small cone around this axis. Following the lines pursued in § 5.1, we obtain the following general formulae for the tetracritical exponents:

$$\alpha = 2 - 4\lambda_2/3, \qquad \alpha' = 2 - 2\lambda_2, \qquad \beta = \lambda_2/6\theta,$$
  
$$\gamma = \gamma' = \beta(\delta - 1), \qquad \delta = 8\theta - 1, \qquad \bar{\nu} = D/2\bar{D} \qquad (5.29)$$

where

$$\theta = \bar{D}/[4(\bar{D}-2+\bar{\eta})], \qquad \lambda_2 = 3\nu D/4.$$
 (5.30)

## 5.3.2. Specification of $\eta$ , $\bar{\eta}$ and $\bar{D}$

(i) To reproduce the Landau theory we set  $D = \overline{D}$  and  $\eta = \overline{\eta} = 0$ . This yields  $D = 8/3 \approx 2.67$  for the dimension of the fractal lattice. The resulting transformation exponents are  $\theta = 1$  and  $\lambda_2 = 1$  and lead to  $\alpha = 2/3$ ,  $\alpha' = 0$ ,  $\beta = 1/6$ ,  $\gamma = \gamma' = 1$ ,  $\delta = 7$ ,  $\overline{\nu} = 1/2$  in agreement with the Landau exponents of KH<sub>2</sub>PO<sub>4</sub> calculated by Benguigui (1972).

(ii) Only very few experimental data are known to us for tetracritical phenomena. For ND<sub>4</sub>Cl one has  $\beta = 0.15$  (Yelon 1973) and  $0.5 \le \alpha \le 0.66$ ,  $\beta = 0.16$ ,  $\gamma = \gamma' \simeq 1$  quoted by Benepe and Reese (1967) for KH<sub>2</sub>PO<sub>4</sub> indicate tetracritical behaviour, too. We have computed the exponents from equation (5.30) for various choices of  $\eta$ ,  $\bar{\eta}$ . The results for  $0 \le |\eta| \le 0.1$  and  $0 \le |\tilde{\eta}| \le 0.1$  are altogether very close, but the best choice is  $\eta = 0.1$  and  $\bar{\eta} = -0.1$ , namely D = 2.53,  $\theta = 0.83$ ,  $\lambda_2 = 0.95$  whence  $\alpha = 0.73$ ,  $\alpha' = 0.10$ ,  $\beta = 0.19$ ,  $\gamma = \gamma' = 0.88$ ,  $\delta = 5.64$ ,  $\bar{\nu} = 0.42$ .

#### 6. Interpretation and conclusion

We have constructed and analysed a general model for *n*th-order phase transitions by assigning *m* measurements made at a microsample, i.e. an *m*-vector, to a lattice point of a *D*-dimensional fractal lattice. Without making any special assumptions about details of the interaction and without evaluating the partition sum of the fractal lattice explicitly, a wealth of numerical data and information about critical exponents was readily obtained by classifying the lattice free energy *F* by means of the topological normal forms of catastrophe and singularity theory. This classification is possible if *F* is smooth or at least continuous on a proper compact and connected subset in the space of measurement variables. Qualitative topological features of phase diagrams and their bifurcation properties follow immediately without any specific physical assumptions or knowledge of the dimensionality *D*. The reason for this universality is that by virtue of their structural stability, *n*th-order phase transitions are essentially a topological phenomenon (cf also Keller *et al* and Rasetti in Güttinger and Eikemeier (1979) and Stewart (1981)).

Changing the fractal's length scale led to scaling of the free energy per unit volume and determined (via the correlation function) the dimension  $D = n(2-\eta)/(n-1)$  of the fractal lattice. As a test of the model bicritical, tricritical and tetracritical exponents have been calculated. These exponents turned out to depend via  $\lambda_2$  on the fractal dimension D and via  $\theta$  on the Euclidean dimension  $\overline{D}$  and the small parameter  $\overline{\eta}$ . If  $\overline{D} = D$  and  $\eta = \overline{\eta} = 0$  the *n*-critical exponents of the Landau theory follow from our model. If  $\overline{D} = 3$  and  $\eta = \overline{\eta} = 0$ , improved *n*-critical exponents are found. If  $\eta, \overline{\eta}$  are chosen slightly different from zero, or equivalently, D is chosen slightly different from  $D_0 = 2n/(n-1)$  and  $\bar{\eta}$  slightly different from zero, it turns out that most of the experimental and theoretical exponents can be reproduced with good accuracy. In table 5 we compare the values of the parameters governing Landau exponents with those reproducing experimental mean exponents.

	Lattice free energy	Order n	Landau		Experiment	
Transition			$D \ (\tilde{D} = D)$	$ar\eta$	D $(\tilde{D}=3)$	$ar\eta$
Bicritical	Cusp	2	4	0	3.92	0.08
Tricritical	Butterfly	3	3	0	2.86	-0.06
Tetracritical	Star	4	8/3	0	2.53	-0.10
Pentacritical	• • •	5	5/2	0	• • •	
				• • •		• • •

**Table 5.** Choice of D,  $\hat{\eta}$  for Landau and experimental exponents.

For small *n* the influence of  $\eta$  on *D* is very small and for critical behaviour *D* is determined almost completely by *n*. But for n = 4 the dimension D = 2.53 of the fractal lattice governing the experimental exponents is almost the same as D = 2.50which models Landau pentacritical behaviour. Furthermore, the difference between *n*-critical and (n + 1)-critical exponents becomes smaller the larger *n* and the qualitative behaviour of  $V_c$ , which depends alone on the codimension c = 2n - 2, dominates the transitions completely whatever the exact values of  $\eta$ ,  $\bar{\eta}$ , provided the latter remain small as experiments indicate  $(0 \le \eta \le 0.1)$ . At the elementary level of our model a deduction of the free parameters  $\eta$  and  $\bar{\eta}$  is not possible. It is conjectured that  $\eta$ ,  $\bar{\eta}$  are related to the detailed physical structure of the interaction.

As the order *n* of criticality of the phase transition increases so does the degree of degeneracy, i.e. the singularity, of  $V_c$  and the fractal lattice dimension decreases,  $D \rightarrow 2 - \eta$ . Since, as we shall indicate below, *D* may be interpreted as a measure for the effective interaction between the subsystems or samples which make up the real system, this implies that the 'degree' of interaction decreases with the order of criticality. For  $\eta = 0$ , the dimension D = 2n/(n-1), i.e.  $D = 4, 3, 2.67, 2.5, \ldots$ , reflects the result of the renormalisation group theory that for each successive *D* a new direction of instability appears in parameter space with the order of the potential function in the Hamiltonian for the fixed point increasing by 2.

We have confined our discussion to a single order parameter, i.e. to cuspoid normal forms acting as organising centres (cf. e.g. Stewart (1981) for the terminology) for singularities in the family of free energies depending on one essential order parameter. However, it should be pointed out that cuspoids of a given order can be generated from cuspoids of lower order by a Legendre transformation with respect to x (Sewell 1978, Keller 1979). Therefore, other thermodynamic potentials (related to the free energy by a Legendre transformation) can be classified by means of catastrophe theory, too (Güttinger and Keller 1982).

The corank-1 cuspoid geometry makes the introduction of a fractal dimension D < 3 imperative for tetracritical and higher-order phenomena, even in the Landau limit. However, if D is smaller than the dimension of the real system one runs into interpretational problems. For, D < 3 implies that each lattice site of the fractal interacts with fewer than the six other sites surrounding it. This means that each

subsystem interacts with fewer subsystems than its nearest spatial neighbours. This, in turn, implies that at least for tetracritical and higher-order critical-but possibly also for tricritical-phenomena the real interaction in three dimensions must be anisotropic with respect to long-range forces. This strongly indicates that two order parameters  $(x_1, x_2)$  should be introduced (Keller 1979). The cuspoid 'star' normal form, therefore, can be expected to give only an incomplete picture of real tetracritical behaviour although the tetracritical exponents came out quite well. Incomplete means here that the order parameter relation x(m) remains true, but that the physical order parameter m may be some function of two underlying physical order parameters  $m_1$ ,  $m_2$  giving rise to relations  $x_1(m_1), x_2(m_2)$ , whence a relation  $x(x_1, x_2)$  must hold. On the other hand, one may assume as well that tetracritical behaviour is governed by the unimodal family  $X_9$  (in Arnol'd's notation), i.e. by the unfolding of the double cusp  $x_1^4 + a^2 x_1^2 x_2^2 + x_2^4$ . The reason is that  $X_9$  is the simplest corank-2 singularity which is bounded below.  $X_9$  has been used by Keller (1979) to analyse tetracritical behaviour and by Keller et al (in Güttinger and Eikemeier 1979) to model ferroelectricferromagnetic, crystalline-superfluid etc systems and binary mixtures in a qualitative way. Triple junctions in caustic networks exhibiting hexagons are described by  $X_{9}$ , too (Berry and Nye 1977, Berry and Upstill 1980). Moreover, the double cusp  $X_{2}$ apparently also governs nucleation and percolation clustering (Dukek 1981). Since these phenomena play an increasing role in phase transitions of various kinds (equilibrium critical phenomena (Gefen et al 1980), non-equilibrium problems such as chaos (Ott 1981), transitions from hadronic to nuclear and to quark condensates (Satz et al 1981)), and seem altogether to be describable in terms of catastrophe and singularity theory on fractal lattices, we shall explore these questions in a forthcoming paper (Güttinger and Keller 1982) which will also shed some light on the role played by symmetries and imperfections in critical phenomena (Golubitsky and Schaeffer 1979, Sattinger 1980, Armbruster et al 1981).

We have shown that *n*th-order equilibrium phase transitions are topological phenomena determined completely by the codimension and corank of the topological normal form of the free energy. Consequently, critical-point universality is a consequence of the principle of structural stability rather than a hypothesis. The prediction of critical exponents which agree with experiment and those of exactly or approximately solvable models was a consequence of the scaling laws resulting from the internal fractal dimensionality D of the system. While structural stability, or persistence of a phenomenon under slight perturbations, is a well established first principle of nature, the meaning and physical significance of a fractal dimension remains still some sort of mystery. The following observations serve to clarify the situation. The integer Euclidean dimension  $\overline{D} = 0$  (a point), = 1 (a line), = 2 (a plane) and so forth, which we are intuitively used to, is nothing but a similarity dimension. To see this, divide each side of a  $\overline{D} = 2$ -dimensional Euclidean rectangle into l equal parts. This gives  $N = l^2$ self-similar rectangles, with affine diminution ratio  $r(N) = 1/l = N^{-1/2}$ . More generally, for an Euclidean  $\overline{D}$ -dimensional parallelepipoid one finds that  $r(N) = 1/N^{1/\overline{D}}$ , i.e.  $\vec{D} = \log N(r) / \log (1/r)$ . Generalising this to  $\vec{D} \rightarrow D$  non-integer and passing to the limit yields the Hausdorff-Besicovitch fractal dimension  $D = \lim_{r \to 0} \log N(r) / \log (1/r)$ of a compact metric space M by covering it with N(r) D-dimensional spheres of radius r. Thus D is a similarity dimension as is  $\overline{D}$  because every l divides the fractal into  $N = l^D$  similar parts, and  $N(r) \propto r^{-D}$ .

The scaling law  $N(ar) = a^{-D}N(r)$  is an immediate consequence of the definition of D and the self-similarity of the fractal. Since  $D \in \mathbb{R}_+$ , the integer Euclidean dimension  $\overline{D}$  is an exception rather than the rule. Fractals are geometric objects with

hierarchical structure down to arbitrarily small scales whose macroscopic forms are self-similar to their microscopic parts, i.e. objects with no length scale at all, physics permitting. Every fractal can be embedded into an Euclidean space and when looked at from this, its points appear totally inhomogeneously distributed. But when looked at within its own fractal dimension, the fractal object is completely homogeneous. If there is an inherent minimum unit length defined in a fractal, the resulting object forms a fractal lattice and the number s of nearest neighbours of a given lattice site is  $s = 2^{D}$  as in the Euclidean case. We have assumed a Hamiltonian with nearestneighbour interaction. Since each lattice site corresponds to precisely one sample of the real physical system, the dimension D describes the real effective interaction between the samples and, as we have seen, this interaction decreases with increasing criticality. D > 3 corresponds to an effective long-range interaction, D < 3 indicates an asymmetry in the interaction that points to the introduction of two order parameters. This may be understood in geometric terms. A  $\overline{D}$ -dimensional system,  $\overline{D}$  an integer, made up of short-range interacting subsystems, will exhibit long-range interaction between its constituents when it is folded indefinitely in  $(\overline{D} + 1)$ -dimensional space. For example, by folding an infinite one-dimensional spin chain with only nearestneighbour interaction in a two-dimensional plane, spins from far distant chain segments come close enough to interact via the second dimension without being near neighbours in the one-dimensional chain. Since, however, no folding whatsoever of a line can fill or create even an infinitesimal area of a plane, the folded chain represents an object with fractional dimension D, 1 < D < 2. Similarly, to implement a threedimensional lattice with long-range interaction, a three-dimensional lattice with shortrange interaction between the subsystems occupying its sites must be folded indefinitely in four-dimensional space until it models a three-dimensional one with long-range interaction. The folded object thereby acquires a fractional dimensionality D with 3 < D < 4. Folding, therefore, creates long-range out of short-range interaction by allowing the physical forces to thrust from  $\bar{D}$ -towards  $(\bar{D}+1)$ -dimensional space. By folding, the object acquires non-integral dimensionality because, being non-smooth, it consists of infinitely more points than the  $\vec{D}$ -dimensional smooth one but possesses infinitely fewer points than the  $(\overline{D}+1)$ -dimensional one. The folded object possesses short-range interaction in D-dimensional space whereas the three-dimensional object to be modelled exhibits long-range interaction. The fractal dimension D is closely related to the entropy definition of Pontryagin (1932) and Hawkes (1974) because of the covering (i.e. measurement) procedure we have used. This is probably also at the root of chaotic regimes governed by fractional dimensional strange attractors. Furthermore, the tantalising analogies between fractal-lattice singularity theory of critical phenomena and the theory of waves encountering a random structure (Berry 1977, 1978, 1979) lead one to conjecture that critical behaviour as the reduced temperature tends to zero may correspond to the short-wavelength limit of optics and that the correct behaviour is embodied in a series of universal exponents. These are fascinating questions which we hope to explore in a forthcoming paper.

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