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SINGULARITIES AND PHASES IN THE STAR POTENTIAL*

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Densities and responses of one of the catastrophe potentials, the star potential, were calculated as the second part of Classical Calculations on the Phase Transition. For values of coefficients in certain ranges, there appears an intermediate ordered phase. Variations of the singular behavior of densities and responses at transition points were calculated.

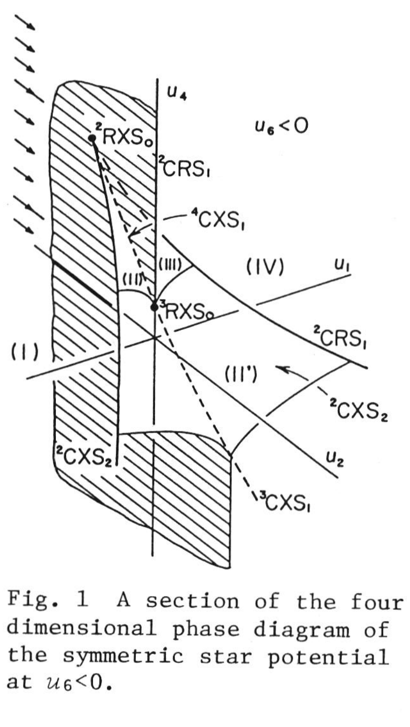

Fig. 1 A section of the four dimensional phase diagram of the symmetric star potential at $u_6<0$.

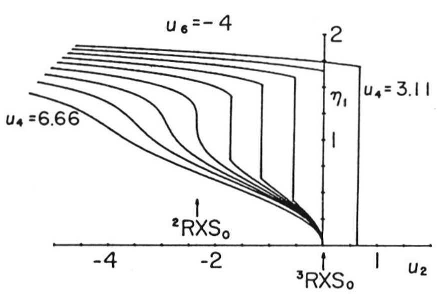

Fig. 2 Density η_1 (polarization) for $u_1=0$, $u_6=-4$ at various values of u_4. (refer to Fig. 3)

1. INTRODUCTION

In the catastrophe theory, the structure of singularities (critical spaces CRS and coexistence spaces CXS) in the phase diagram of any structurally stable potential, with one essential behavior variable and a number of control variables, is equivalent to that of a cuspoid potential. This potential has the same form as that of the Landau expansion. However, between the standard forms of catastrophe potentials and Landau expansions there is an essential difference, i.e. higher order terms in the former are transformed away and those in the latter are neglected away.[1] The standard form of the catastrophe potential gives all of the topological aspects of any phase transition with one order parameter.

We consider one of the cuspoids, the star potential,

$$V(x,u_i)=\sum_{i=1}^{6}\frac{1}{i}u_i x^i+\frac{1}{8}x^8 \tag{1}$$

This potential contains all singularities of lower order cuspoids (fold, cusp, swallowtail, butterfly, and wigwam catastrophes) and experimentally detectable singularities. Physical field variables like electric field, magnetic field, temperature, and pressure are mapped to controls $\{u_i\}$, and the order parameter to the behavior x with $\{u_i\}$ as parameters, by diffeomorphisms. Eliminating x from eq.(1) and the stability condition

$$\partial V/\partial x = 0 \tag{2}$$

we obtain the potential of the stationary state $U(u_i)$ as a function of the controls.

Here we define the density vector and the response tensor by the negative gradient and the negative Hessian respectively, and we obtain easily from eqs. (1) and (2),

density vector: $\eta_i = -\dfrac{\partial U}{\partial u_i} = -\dfrac{1}{i}x^i$, (3)

response tensor: $\chi_{ij} = -\dfrac{\partial^2 U}{\partial u_i \partial u_j} = x^{i+j-2}/W$, (4)

where

$$W = u_2+2u_3x+3u_4x^2+4u_5x^3+5u_6x^4+7x^6 \ . \tag{5}$$

If we put $u_3=u_5=0$, the phase diagram is symmetric with respect to the u_1-axis. Detailed considerations of the phase diagram, complex singularities called critical coexistence spaces, and anomalous hysteresis loops of the symmetric star potential,

$$V = u_1x + \frac{1}{2}u_2x^2+ \frac{1}{4}u_4x^4+ \frac{1}{6}u_6x^6+ \frac{1}{8}x^8 \tag{6}$$

were given in the previous paper (part I).[2] The phase diagram of the star potential has been briefly discussed also in ref.[3].

In this paper (part II) we give the results of densities and responses of the symmetric star potential, eq.(6). In the Landau expansion, u_1 stands for negative field and u_2 for temperature difference from a fixed temperarure. In the case of a ferroelectric, for example, η_1 is polarization, η_2 entropy, χ_{11} susceptibility, χ_{12} pyroelectric coefficient, and χ_{22} specific heat.

2. DENSITY

Topological aspects of the phase diagram of the potential eq.(6) for $u_6 \geqq 0$ are the same as those of the symmetric butterfly (up to the sixth power), except that the origin of the control space is a critical point of order four $^4CRS_0$ when $u_6=0$. The case of $u_6<0$ is our main subject, and the phase diagram has been discussed in part I. It is reproduced in Fig. 1. We have three coexistence surfaces $^2CXS_2$, a vertical plane and two wing surfaces. The dashed line shows a triple line $^3CXS_1$ at $u_2>0$ and a quadruple line $^4CXS_1$ at $u_2<0$. The two fringe lines of wing surfaces are critical lines $^2CRS_1$, which intersect at $^2RXS_0$. At the critical coexistence point (bicritical end point [4]) $^2RXS_0$, two critical phases (I)/(II) and (III)/(IV) coexist. The u_4-axis is another

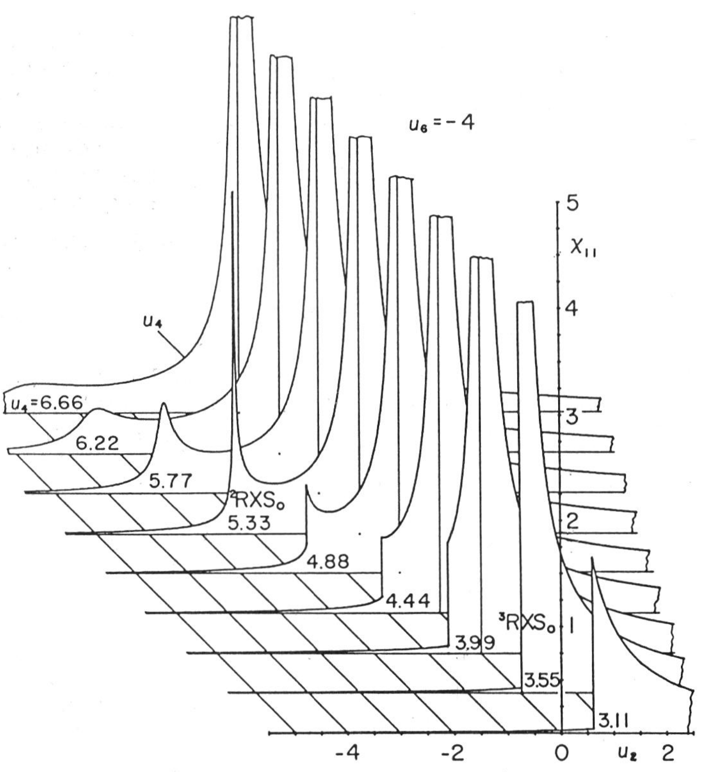

Fig. 3 Response χ_{11} (susceptibility) corresponding to Fig.2.

critical line $^2CRS_1$ ending at $^3RXS_0$. At the critical coexistence point (critical end point [4]) $^3RXS_0$, the critical phase (II)/(III) coexists with two regular phases (I) and (IV).

Figure 2 shows variations of the density $\eta_1=-x$ in the case of $u_6=-4$, along lines parallel to the u_2-axis indicated by small arrows in Fig. 1. This may correspond to the zero field polarization. For large values of u_4 we have one singularity at $u_2=0$. (on the u_4-axis $^2CRS_1$). For $u_4=5.33$ there appeares the second singularity at $^2RXS_0$. In this case, we have two critical points in η_1 vs. u_2 (polarization vs. temperature) at $u_2=0$ and $^2RXS_0$, of which critical exponents are $\beta=1/2$ and 1/3 respectively. Taking smaller values of u_4, the second singularity changes to a first-order transition at the crossing point with $^4CXS_1$. At $u_4=3.55$ we have only a discontinuity, a first-order transition, at $^3RXS_0$. The criticality at $^3RXS_0$ does not show itself in the η_1 vs. u_2 curve. When $u_4<3.55$, it gives the ordinary behavior of the first-order transition.

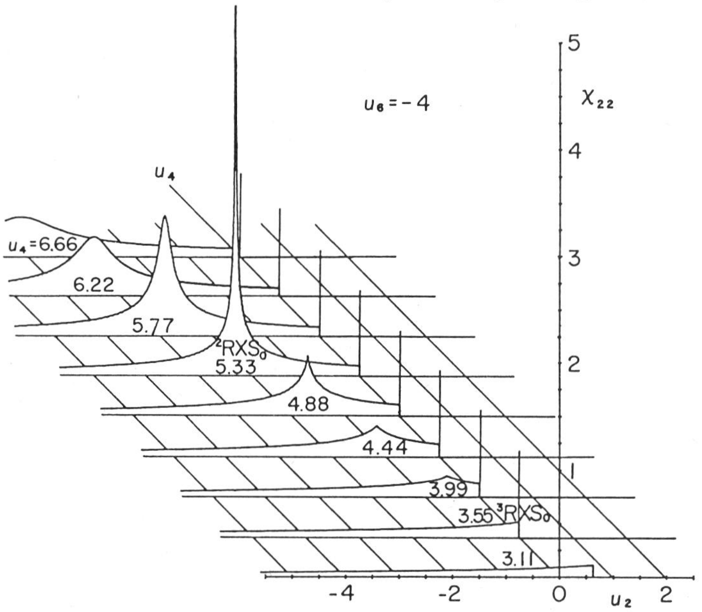

Fig. 4 Response χ_{22} (specific heat) corresponding to Fig.2.

3. RESPONSE

We calculated responses χ_{11}, χ_{22} and χ_{12}. First, Fig. 3 shows χ_{11}, which is susceptibility in the Landau analogue, in the same subspaces to those of Fig. 2. Along the line $u_4=5.33$ through $^2RXS_0$, it gives two divergences at two critical points. It looks similar to the relation of dielectric constant vs. temperature in rochelle salt with two Curie points, but it is not the case. One divergence changes itself to a discontinuous jump at $^4CXS_1$, for smaller values of u_4. After its collapsing at the second divergent peak at $u_2=0$, we have only one singularity, a discontinuous jump.

Secondly, χ_{22} is seen in Fig. 4. There is a peak at lower u_2

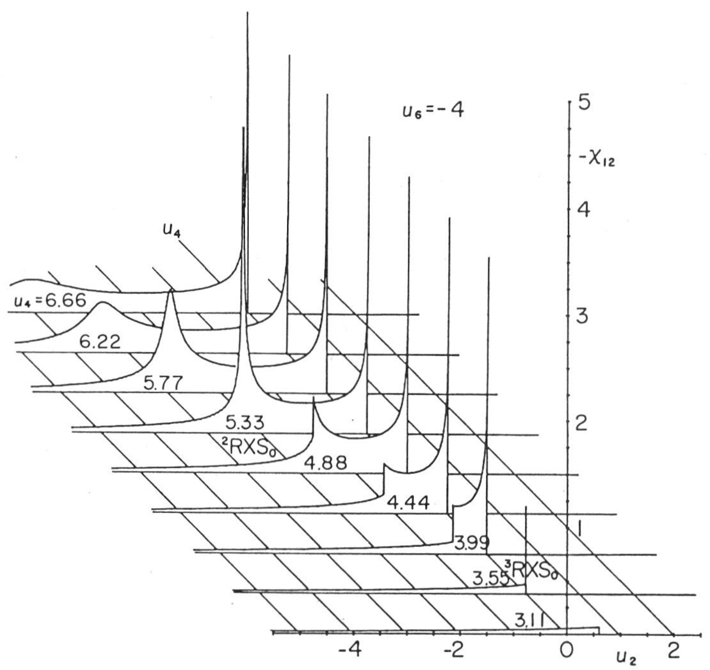

Fig. 5 Response χ_{12} (pyroelectric coefficient) corresponding to Fig.2.

and a discontinuity at $u_2=0$. The latter is the usual discontinuous specific heat in the Landau approximation. The complex singular point $^2RXS_0$ is the intersection point of two $^2CRS_1$. However, there appears an infinite peak in specific heat at $^2RXS_0$, in contrast to $^2CRS_1$ at $u_2=0$. This comes from the fact that the direction of differentiation (u_2-axis) makes an angle with the hidden coexistence line. (the strong direction [5]) This is clearly shown in Fig. 7A in part I. Singular behavior of responses depends upon the direction of differentiation relative to the direction of the coexistence line.[5] It also changes by the direction of the approaching path to the critical point. These dependencies in the cuspoid potential will be investigated in part III. For the value of $5.33>u_4>3.55$, the lower singularity assumes a cusp-type peak. Although it is a first-order transition point, the discontinuity disappears owing to the symmetry of the curve. It has a latent heat because of a discontinuity in entropy.

The response $-\chi_{12}$ shows similar behavior to that of χ_{11} except for $u_2>0$ as illustrated in Fig. 5.

4. DISCUSSION

One of the standard forms of the catastrophe potential eq.(6) has four stable phases at most. These are shown as (I), (II), (III), and (IV) in Fig. 1. The phase (II') is a degenerate phase resulting from being indistinguishable of phases (II) and (III), which is the paraelectric or the non-polar phase in ferroelectric analogue. Along a typical scanning path parallel to u_2 with $u_1=0$ and $u_6<0$, we calculated the critical behavior of densities and responses. There appears an intermediate phase between successive phase transitions. Owing to the intermediate phases (II) and (III), we can expect new transition schemes. For example, when the system is scanned by u_1, a triple hysteresis loop results. (part I) This theory, however, predicts nothing about the structure of the intermediate ordered phase.

We have shown only η_i and χ_{ij} with $i,j=1,2$. It is easy to get other quantities and their classical exponents from eqs.(3), (4), and (5).

Let the diffeomorphic mappings be

$$f_n \mapsto u_i:\ u_i = u_i(f_n),$$

$$y \mapsto x:\ x = x(y, f_n).$$

The physical densities d_n and physical responses K_{nm} can be calculated by

$$d_n = \sum_i \eta_i(f)\frac{\partial u_i}{\partial f_n}$$

$$K_{nm} = \sum_i [\eta_i(f)\frac{\partial^2 u_i}{\partial f_n \partial f_m} + \sum_j \chi_{ij}(f)\frac{\partial u_i}{\partial f_n}\frac{\partial u_j}{\partial f_m}]$$

When above diffeomorphisms are linear, physical densities and responses are linear combinations of η_i and χ_{ij} respectively, with the Landau expression as the simplest case. The dominant terms of them give critical exponents of those quantities.

* This paper stands for Part II of the preceding paper, ref. [2]. ** Dpto. de Optica, Universidad Autonoma de Madrid, Madrid, Spain.

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