The Mandelbrot Set in a Model for Phase Transitions *) Heinz-Otto Peitgen and Peter H. Richter **)

INTRODUCTION

According to D. Ruelle [18] "... the main problem of equilibrium statistical mechanics is to understand the nature of phases and phase transitions ...". A remarkable observation of B. Derrida, L. De Seze and C. Itzykson [4] has put these problems of theoretical physics into a new perspective: For a very particular model (the hierarchical q-state Potts model on a hierarchical lattice) they indicated that the Julia set of the corresponding renormalization group transformation is the zero set of the partition function in the classical theory of C. N. Yang and T. D. Lee [22]. The Yang-Lee theory describes a physical phase as a domain of analyticity for the free energy, viewed as a function of complex temperature. The boundaries of these domains are given by the zeroes of the partition function. Carrying on these ideas we show a connection with a discovery of B. Mandelbrot [13]. More precisely, in a discussion of the morphology of the above zero sets we discover a structure which is related to the Mandelbrot set (see [15]) attached to the one-parameter family $\mathbb{C} \ni z \rightarrow z^2 + c$, $c \in \mathbb{C}$ a fixed constant. For this we exploit recent results of D. Sullivan [21] which classify the stable regions of rational maps on $\overline{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$. Though the physical meaning of the hierarchical Potts model is certainly very questionable it seems that the classical (see G. Julia [12] and P. Fatou [8]) and recent (see A. Douady and J. Hubbard [5,6,7], D. Sullivan [21], M. Herman [11]) theory of complex dynamical systems may produce a major step towards a deeper understanding of the nature of phase transitions. Besides the hierarchical Potts model we have analyzed 1- and 2-dimensional Ising models with and without an external magnetic field and have found that the theory of Julia sets and

^{*)} This paper surveys the recent interaction between the theory of phase transitions in statistical mechanics and the theory of complex dynamical systems.

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their typical fractal properties play a very significant role in the interaction between the Yang-Lee theory and the renormalization group approach. None of these and the findings in [15] would have been possible without the aid of extensive computer graphical studies and experiments.

PRELIMINARIES AND NOTATION

The hierarchical Potts model is associated with a very particular and physically unrealistic lattice construction which we introduce schematically in fig. 1.



Figure 1. The diamond hierarchical lattice with $n = n(k) = 4 + 2(4^{k-1} - 4)/3$ atoms (dotts) and 4^{k-1} bonds (line segments) for $k \ge 1$.

For this particular lattice and nearest neighbor coupling an explicit form of the renormalization group transformation is known and that is why it is valuable here. On each lattice site i we assume a spin with $q \in \mathbf{N}$ possible states

The partition function $Z_k(T)$ is the sum of Boltzmann factors extended over all configurations

 $\{\sigma : \{1,\ldots,n\} \rightarrow \{1,\ldots,q\}\}$, n = # of lattice points,

(1)
$$Z_{k}(T) = \sum_{\sigma} \exp \left(-\frac{1}{k_{B}T} E(\sigma)\right),$$

where $E(\sigma)$ is the potential energy of the configuration σ . Assuming that the interaction of different lattice sites is restricted to nearest neighbors only, i.e. only across a bond indicated by a line segment in figure 1, the energy across such a bond for a fixed configuration σ is:

(2)
$$E(i,j) = \begin{cases} -U, & \text{if } \sigma_i = \sigma \\ 0, & \text{else.} \end{cases}$$

Hence,

(3)
$$E(\sigma) = \sum_{bonds} E(i,j)$$
.

For convenience we introduce new variables

(4)
$$x = \exp(\frac{U}{k_{B}} \cdot T)$$

so that $Z_n(x)$ becomes a polynomial in x with integer coefficients. The coupling constant U is characteristic for the material, U > 0 for ferromagnetic, and U < 0 for antiferromagnetic coupling. From Z_{ν} one derives the free energy per atom

(5)
$$f_n = -\frac{k_B T}{n} \ln Z_k$$
, $n = n(k)$.

Thus, zeroes of Z_k correspond to logarithmic singularities of f_n and are reasonable candidates for phase transitions. Note, however, that $Z_k(x) \neq 0$ for any finite lattice with n = n(k) points and for all x > 0, which is the physically meaningful temperature range.

THE YANG-LEE MODEL OF PHASE TRANSITIONS

In essence the idea of C. N. Yang and T. D. Lee [22], which had a substantial impact on the forthcoming attempts to solve phase transition problems, is as follows:

Let

(6)
$$N_k = \{x \in \mathbb{C}, Z_k (x) = 0\},\$$

i.e. one embeds the partition function in a complex temperature plane. To make boundary effects negligable one has to pass to the *thermodyna-mic limit*, i.e. one lets $n \to \infty$. It is not obvious, of course, that such a limit makes sense and exists. If, however, the potential energy E admits an appropriate growth condition and the range of the interaction is sufficiently small, which is trivially satisfied in our case, then (see [18]) the limit exists and we denote by N_{∞} the zero-set of the partition function Z_{∞} in the thermodynamic limit. Now Yang and Lee postulated that N_{∞} would distinguish a unique point $x_{c} > 0$,

$$N_{\infty} \cap \mathbf{I} \mathbf{R}_{+} = \{\mathbf{x}_{C}\},$$

so that T $_{\rm C}$, x $_{\rm C}$ = exp($^{U\!/}\,{\rm k}_{\rm B}^{}\cdot{\rm T}_{\rm C}^{})$, is the phase transition point (see fig. 2).



Figure 2. Note that $T = \infty$ corresponds to x = 1.

Thus to find and characterize T_c it remains to find x_c and interprete N_{∞} in the neighborhood of x_c . For example the critical index α , which characterizes the singularity of the *specific heat*,

$$(8) C \sim | T - T_{\alpha} |^{-\alpha}$$

can be obtained from the density of the zeroes in the thermodynamic limit near x_{c} (see [9]).

THE RENORMALIZATION GROUP APPROACH

In general the partition function Z_k is not only a function of temperature x but also of other variables like for example an external magnetic field H. In essence the idea of the renormalization group approach is to relate

$$z_{k-1}$$
 with z_k , i.e.

(9)
$$\begin{cases} Z_{k}(x,H,\ldots) = Z_{k-1}(\overline{x},\overline{H},\ldots) & \phi(x,H,\ldots) \\ (\overline{x},\overline{H},\ldots) = R(x,H,\ldots) & . \end{cases}$$

Thus, up to a trivial factor φ the partition function of step k is obtained by that of step k-1 modulo an appropriate adaption of the variables (x,H, ...). This determines a map R, the *renormalization* transformation.

In our specific hierarchial q-states Potts model Z_k is only a function of x, the temperature variable. However, Z_k depends on the material constant q. An elementary calculation shows that (see [4], [15])

(10)
$$\begin{cases} Z_{k}(x) = Z_{k-1}(\overline{x}) \cdot \varphi(x) , k > 2 \\ R(x) = \overline{x} = \left(\frac{x^{2}+q-1}{2x+q-2}\right)^{2} \\ Z_{1}(x) = q(x+q-1) \\ \varphi(x) = (2x+q-2)^{2+4} \\ \end{cases}$$

Thus, the renormalization transformation is a rational map of degree 4. Actually, as we let q vary in c we obtain a 1-parameter family $R = R_{\alpha}$. For any q we have that

(11)
$$\begin{cases} R_{q}(1) = 1 \text{ and } R'_{q}(1) = 0 \\ R_{q}(\infty) = \infty \text{ and } R'_{q}(\infty) = 0 , \end{cases}$$

i.e. 1 and ∞ are superstable attractors. Their basins of attraction are defined by ($\overline{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$)

(12)
$$\begin{cases} A_q(1) = \{ x \in \overline{\mathbb{C}} : R_q^n(x) \to 1 \text{ as } n \to \infty \} \\ A_q(\infty) = \{ x \in \overline{\mathbb{C}} : R_q^n(x) \to \infty \text{ as } n \to \infty \} \end{cases}$$

As a consequence of the classical theory of G. Julia [12] and P. Fatou [8] on the interation of rational functions in \mathfrak{C} we have that

(13)
$$\partial A_q(1) = J_q = \partial A_q(\infty)$$

is the Julia set of R_{α} .

JULIA SETS AND PHASE TRANSITIONS

We are now in a position to discuss the Yang-Lee model in terms of the renormalization approach from the point of view of the theory of Julia sets. We begin by listing a few interesting conjectures and problems:

CONJECTURE 1.1.

$$N_{\infty} = J_{q}$$
 , i.e.

 $A_q(1)$ (resp. $A_q(\infty)$) corresponds to the nonmagnetic (resp. magnetic) phase.

To discuss this crucial conjecture the following immediate observation from (10) is of importance:

Note that $Z_{k-1}(R_q(x)) = \frac{\eta(x)}{\phi(x)}$ for some $\eta(x)$ and therefore

(14) $N_k = \{x \in \overline{\mathbb{C}} : R_q^{k-1}(x) = 1 - q\}$.

Moreover, the free energy in the thermodynamic limit f_{∞} satisfies the functional equation (15) as a consequence of (5) and (10):

(15)
$$\begin{cases} f_{\infty}(x) = \frac{1}{4}f_{\infty}(R_{q}(x)) + g(x), & \text{with} \\ g(x) = \frac{1}{2}\ln(2x+q-2). \end{cases}$$

PROBLEM 1.2.

- (a) In what sense is $N_k \rightarrow N_\infty$ as $k \rightarrow \infty$?
- (b) For which $q \in \mathbb{C}$ is $N_{\infty} = J_{\alpha}$?
- (c) For which $q \in \mathbb{C}$ does R_q admit further attractors, other than 1 and ∞ ?

If R_q admits a further attractor other than 1 and ∞ then its corresponding basin of attraction may characterize a third magnetic phase such as for example the *antiferromagnetic phase*.

In view of (14) and (15) conjecture (1.1) means that the singularities of f_{∞} , the phase transitions points, are given by points from J_q , and this is intimately related to an understanding of the forward and backward orbit

(16) $R_{q}^{i}(1-q) \}_{i \in Z}$

for $q\in {\mathbb C}$. Thus, the question which remains is: Is $(1-q)\in J_q$ or in which component of $\overline{{\mathbb C}}\smallsetminus J_q$ is it?

THE CLASSIFICATION OF STABLE REGIONS

This leads us directly into one of the most celebrated recent results in the theory of complex dynamical systems: The classification of stable regions of D. Sullivan [14,21]. Let f be an analytic endomorphism of $\overline{\mathbf{C}}$. A point $\mathbf{x} \in \overline{\mathbf{C}}$ is *stable* for f if on some neighborhood of x the family of iterates f, f^2, f^3, \ldots is an equicontinuous family of mappings of that neighborhood into \mathbf{C} . Note that when x is not stable, i.e *unstable*, for any neighborhood the union of images of iterates must cover $\overline{\mathbf{C}}$ except for two points at most. The set of unstable points for f is the Julia set J of f. It is the closure of the expanding periodic points. The open set of stable points $\overline{\mathbf{C}} \setminus \mathbf{J}$ consists of countably many connected components, the *stable regions* of f, which are transformed among themselves by f. The following three theorems of D. Sullivan [21] and P. Fatou [8] are crucial for conjecture 1.1 and problem 1.2. Let f be a rational mapping with d = deg(f) > 2.

THEOREM 1.3. (Sullivan) Each stable region is eventually cyclic. (For any component $C \subset \overline{\mathbb{C}} \smallsetminus J$ there is $n \in \mathbb{N}$ such that $D = f^{n}(C)$ is cyclic, i.e. $f^{k}(D) = D$ for some $k \in \mathbb{N}$.) THEOREM 1.4. (Sullivan) The cycles of stable regions D are classified into five types: (a) An attractive basin D arises from an attractive periodic cycle γ with non zero derivative of modulus less than one, $\gamma = \{z, f(z), \dots, f^{n-1}(z)\}, f^{n}(z) = z, 0 < |(f^{n})'(z)| < 1,$ and D consists of components of $\bigcup_{\mathbf{x}\in\mathbf{y}} \{\mathbf{y}: \lim_{n\to\infty} \text{distance } (\mathbf{f}^{n}(\mathbf{y}), \mathbf{f}^{n}(\mathbf{x})) = 0\}$ containing points of γ . (b) A parabolic basin D arises from a non-hyperbolic periodic cycle γ with derivative a root of unity, $\gamma = \{z, f(z), \dots, f^{n-1}(z)\}, f^{n}(z) = z, ((f^{n})'(z))^{m} = 1,$ γ is contained in the boundary of D , and each compact in Dconverges to γ under forward iteration of f. (c) A superattractive basin D is defined just like an attractive basin but now $(f^n)'(z) = 0$.

(d) A Siegel disk D is a stable region which is cyclic and on which the appropriate power of f is analytically conjugate to an irrational ratotion of the standard unit disk.

(C.L. Siegel [19] proved these occur near a non-hyperbolic fixed point if the argument α of its derivative satisfies the following diophantine condition: there exists c > 0 and $\nu > 2$ such that

$$|\alpha - p/q| > c/q^{\nu}$$

for all relatively prime integers p and q.)

(e) A Herman ring D is a stable region similar to a Siegel disk. Now we have a periodic cycle of annuli and a power of f which restricted to any of these annuli is analytically equivalent to an irrational rotation of the standard annulus.

(For appropriate Θ and a M. Herman [10] found such regions for the map:

$$x \xrightarrow{e^{i\Theta}} \left(\frac{x-a}{1-\overline{a}x} \right)^2$$
)

The fate of critical points $\{c : f'(c) = 0\}$ is crucial in connection with theorem (1.4).

THEOREM 1.5. (Fatou)

- (a) If D is an attractive or parabolic basin then D contains at least one critical point of f.
- (b) If D is a Siegel disk or Herman ring then ∂D is contained in the ω -limit sets of critical points.

Thus f can have only finitely many cyclic stable regions. But it is still an open problem whether 2d-2 (d > 2 the degree of f) is a sharp upper bound. Another open problem is whether a Siegel disk always has a critical point on its boundary. M. Herman [11] in a remarkable paper proved this conjecture recently for $f(z) = z^2 + \lambda$.

Note that theorem 1.5 and theorem 1.4 provide an excellent basis for computer experiments. For the detection and characterization of all cyclic stable regions of a map f one simply has to follow the forward orbits of all critical points. The following example illustrates the strength of these results:

EXAMPLE 1.6.
$$f(x) = \left(\frac{x-2}{x}\right)^2$$
, $J = \overline{c}$.

The critical points are: 2,0. Observe that $2 \mapsto 0 \mapsto \infty \mapsto 1 \mapsto 1$ and f'(1) = -4. Thus $\overline{\mathbf{c}} \smallsetminus \mathbf{J} = \emptyset$, because none of the cases (a), (b) in theorem 1.5 is possible. The critical points of the renormalization map ${\rm R}_{\rm q}$ and a morphology of ${\rm N}_{\rm \infty}$

Our map

$$R_{q}(x) = \left(\frac{x^{2}+q-1}{2x+q-2}\right)^{2}$$

has the six critical points:

(

1,
$$\infty$$
, 1-q, $\pm \sqrt{1-q}$, $(2-q)/2$.

Since 1 and ∞ are attractive fixed points and since $(2-q)/2 \mapsto \infty$, $\pm \sqrt{1-q} \mapsto 0$ it suffices to examine the orbits of 1-q and 0 only. We do this in the spirit of B. Mandelbrot's history making experiment: Let

(17)
$$A_{1} := \{q \in \mathbb{C} : \mathbb{R}_{q}^{n}(1-q) \rightarrow 1 , n \rightarrow \infty \}$$
$$A_{\infty} := \{q \in \mathbb{C} : \mathbb{R}_{q}^{n}(1-q) \rightarrow \infty , n \rightarrow \infty \}$$
$$M_{R} := \mathbb{C} \smallsetminus (A_{1} \cup A_{\infty})$$

Figures 3,4 and 5 show A_1 , A_{∞} and M_R . Figure 6 shows a blow up of a detail of figure 5. Surprisingly it displays a structure which looks like a copy of the original Mandelbrot set [13]. I.e. it is exactly similar to the bifurcation set of the quadratic family $x \rightarrow x^2 + c$, $c \in \mathbf{C}$. It is obvious that any q such that |q| >> 1 is in A_{∞} , thus A_1 and M_R are bounded. Experimentally it turned out that the fate of the two crucial orbits of (1-q) and 0 were related, i.e. whenever

(18)
$$\begin{cases} R_q^n(1-q) \to 1 \quad \text{then} \quad R_q^n(0) \to \infty \text{, as } n \to \infty \\ R_q^n(1-q) \to \infty \quad \text{then} \quad R_q^n(0) \to 1 \text{, as } n \to \infty \end{cases}$$





<u>Figure 3</u>. A_1 in black



Figure 4. A_{∞} in black



<u>Figure 6</u>. Detail in M_{R}



Detail of $M^{}_{\rm R}$ (see figure 6) in black surrounded by $A^{}_1$ in yellow and $A^{}_\infty$ in green.



The Mandelbrot set M in black together with its electrostatic potential given by the Douady-Hubbard conformal homeomorphism $C \to C M$.



Figure 6. (continued) Detail of M_R A_1 and M_R in black

where

(20)
$$\begin{cases} \Psi_{q}(x) = \frac{x+q-1}{x-1} \\ and \\ S_{q}(x) = \frac{x^{2}+q-1}{x^{2}-1} \end{cases}$$

This means that

(21)
$$\begin{cases} R_{q}(x) = (\Psi_{q} \circ S_{q} \circ \Psi_{q})^{2}(x) = D_{q}^{2}(x) , \\ \text{with} \\ D_{q}(x) = \left(\frac{x+q-1}{x-1}\right)^{2} . \end{cases}$$

Thus, Ψ_q exchanges the *hot* phase (x=1) with the cold phase (x= ∞) and the two crucial critical orbits of (1-q) and 0.

Figures 3-6 are explained and described in greater detail in [15]. In particular problem 1.2 (c) is answered. Roughly speaking the main body of M_R and each of its buds as well as the main body of the detail in figure 6 and each of its buds identify parameters q for which there is a periodic attractor. Their basins of attraction establish a third magnetic phase and the boundary of these basins, which is the Julia set of R_q , being also the boundary of $A_q(1)$ and $A_q(\infty)$, is a candidate for a formal locus of phase transitions. Note, however, that even though N_{∞} may be given by J_q , the Julia set of R_q , its points may not be singularities of the free energy f_{∞} in the thermodynamic limit. This seems to contradict (5), but note that in the thermodynamic limit the free energy may simply allow an analytic continuation.

In summary our experiments leed to the following interesting conjectures:

CONJECTURE 1.7.

- (1) M_{R} is connected.
- (2) The subset of $M_{\rm R}$ shown in figure 6 is homeomorphic (quasi conformally) to the Mandelbrot set M , where

$$\begin{cases} M = \{c \in \mathbb{C} : f_c^n(0) \not \to \infty , as n \to \infty \} \\ f_c(x) = x^2 + c . \end{cases}$$

$$(3) \quad N_{\infty} = J_q \quad \text{for any} \quad q \in (\overline{\mathbb{C}} \sim M_q) \cup \mathring{M}_q . \end{cases}$$

Note that according to [5] the Mandelbrot set M is connected. Actually, Douady and Hubbard showed that $\mathbb{C} \setminus M$ and $\mathbb{C} \setminus D$, $D = \{x \in \mathbb{C} : |x| < 1\}$, are homeomorphic subject to a conformal mapping. Sullivan [21] gave an alternative proof which may apply also to our case. To indicate the idea we briefly survey another remarkable result of J. Curry, L. Garnett and D. Sullivan [3]:

NEWTON'S METHOD AND THE MANDELBROT SET

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Consider the one-parameter family of rational maps

(22)
$$\begin{cases} g_{\lambda}(x) = x - p_{\lambda}(x)/p_{\lambda}'(x) , & \text{where} \\ p_{\lambda}(x) = x^{3} + (\lambda - 1)x - \lambda . \end{cases}$$

Note that Newton's method for any cubic is equivalent by a linear change of variables to at least one of the g_{λ} 's. The 4 critical points of g_{λ} are the 3 roots of p_{λ} and the distinguished point 0, which in view of theorem 1.5 is the only non-trivial critical point. The black regions in the complex λ -plane in figures 7, 8 and 9 were determined by the condition of the forward orbit of 0 converging to the root 1 of $p_{\lambda}(x)$. Let

(23)
$$M_g = \{\lambda \in \overline{\mathbb{C}} : g_{\lambda}^n(0) \not\rightarrow \text{ root of } p_{\lambda}, \text{ as } n \rightarrow \infty \}$$
.

Then Sullivan [21] argues that the components in $\overline{\mathbb{C}} \sim M_{g}$ correspond to quasi-conformal conjugacy classes which are analytically just punctured disks. Hence, M_{g} is connected. The subset of M_{g} shown in figure 9 is actually homeomorphic to the Mandelbrot set M, as A. Douady and J. H. Hubbard show in [6]. Arguments similar to those in



-2.25

1.75

Figure 7. { $\lambda \in \mathbb{C}$: $g_{\lambda}^{n}(0) \rightarrow 1$, $n \rightarrow \infty$ } = black



Figure 8. (a) Detail of figure 7.





Figure 9. (a) Detail of figure 8a.



 $\{\lambda \in \mathbb{C} : g_{\lambda}^{n}(0) \not\rightarrow \text{ root of } p_{\lambda}, n \rightarrow \infty\}$

[6] and [21] should suffice to establish conjecture 1.7 (1), (2).

We add in passing that figure 9 gives some insight into a completely different set of questions: Given a polynomial, describe the set of initial values in \mathbb{R} for which Newton's method converges towards a root. It is known, that for a polynomial with real coefficients and real roots this set is \mathbb{R} except for a set of Lebesgue measure zero (see [1,20]). Now figure 9 teaches us that this remarkable result does not extend to \mathbb{C} , because for any λ in the Mandelbrot-like set (see figure 9) Newton's method allows a periodic attractor with an open basin of attraction.

Conjecture 1.7(3) is meant to contribute to problem 1.2 (a) and (b). Note that if one knew that

(24)
$$M_{R}^{2} = hyp (M_{R})$$
, (= hyperbolic part of M_{R})

i.e. for any $q \in \mathring{M}_{R}$ the orbit of (1-q) converges towards a periodic attractor of R_{q} , then conjecture 1.7 (3) could be established from classical theory. Note, however, that an identity corresponding to (24) is not even known for the much more fundamental Mandelbrot set M. On the other hand it is known that if M were locally connected then $\mathring{M} = hyp$ (M) (see [7]). For a good visual impression of the difficulties with regard to the last questions we refer to the pictures and experiments in [16].

SOME JULIA SETS FOR R

Finally we discuss some Julia sets of R_q for the physically meaningful choices q = 2,3,4; see figure 10. Firstly, one shows that

$$2 \in A_1$$
, $3 \in A_1$, $4 \in A_\infty$.

Furthermore, for q = 4 one has that $A_q^*(1) = A_q(1)$ and $A_q^*(\infty) = A_q(\infty)$, where A* denotes the immediate basin of attraction, i.e. the component which contains the attractor. Hence, it follows from [2] that the Julia set J_q , q = 4, is a Jordan curve, which, due to the symmetry with respect to conjugation, must intersect \mathbb{R}_+ in a unique point x_c , the ferromagnetic transition point.



Figure 10. The Julia set J $_{
m q}$ of R $_{
m q}$ for six values of q .





Remarkably, also the Julia sets for q < 4 in figure 10 distinguish a unique phase transition on \mathbb{R}_{\perp} .

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