PHASE TRANSITIONS ON STRANGE SETS

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Abstract: The "thermodynamic" formalism provides a very general division of strange (Cantor, fractal) sets into two classes; those which do exhibit phase transitions, and those which do not.

The "thermodynamic formalism"^{1,2,3,4}) is based on the observation that the sum used in determining the Hausdorff dimension of a strange (fractal, Cantor) set

$$\sum_{i=1}^{N} \ell_{i}^{-\tau}$$

resembles a partition sum over "configurations" i, with τ playing the role of "temperature", and covering interval sizes playing the role of "Boltzmann weights".

The "thermodynamic" functions extracted from the above partition sum exhibit a phenomenon that might have gone unnoticed were it not for the thermodynamic formalism. They can undergo "phase transitions". These phase transitions can be visualized in the following way: the exponent τ acts as a "magnifying lens" which blows up some of the covering intervals, and (relatively), shrinks the others. For negative τ , the fat intervals are expanded, and the thin ones are made even thinner. For positive τ , the thin intervals are (relatively) blown up. Below the phase transition, the sum is dominated by a few fat intervals. Visually, the cover consists of a few

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black blocks and vanishing amount of fine "dust". Above the phase transition, the large number of thin intervals overwhelms the few fat ones; visually, the strange set looks gray. All known examples $^{5-12}$ are of first order; at the transition the average segment width jumps discontinuously, by a finite amount.

An important (conjectured) example of such system is the Hénon attractor. In the "hyperbolic" phase, the attractor is well described as a hyperbolic set, composed of sheets whose scale can be determined from the associated unstable cycles^{13,14}. In the other phase, the "thermodynamics" is dominated by the "turnbacks".⁸⁾

In physics existence of a phase transition is a dramatic effect--a liquid freezes into a solid--and a realization that a certain strange set undergoes a phase transition is (potentially) of greater import than knowing that its Hausdorff dimension equals .8701....

In this way the "thermodynamics" offers a broad classification of all strange sets into those which exhibit phase transitions, and those which do not. Examples of the first class are the Hénon attractor and the set of irrational windings for critical circle maps;^{5,6}) examples of the second class are the period doubling attractor and hyperbolic (axiom A) sets.

r in the partition sum is a mathematical invention, not a physical temperature. There is no "heat bath" that an experimentalist can dip a strange set into. If you thus find varying r objectionable, you should probably think of the above classification as a division of strange sets into those with smooth measures (axiom A) and those with measures that are not smooth. In the "thermodynamic" language, the first class has smooth scaling spectra (f(α) functions); the second does not. Scaling spectra are accessible directly, by binning the experimental data, but in practice the results are very noisy, and introduction of an "artificial temperature" r is the preferred technique in searches for phase transitions.

From the experimental point of view, phase transitions are elusive. The problem is that the experiments are limited by noise to extraction of a few hundred intervals ("thermodynamic configurations"), and are very far from the thermodynamic

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limit. In such small systems phase transitions signal their presence by a further slowdown in convergence, and can be extracted only by finite scaling techniques.

A warning: strange sets, unlike physical systems, often have no unique "thermodynamics"; the weights associated with different pieces of the set might reflect mathematical prejudices⁶⁾ rather than physical imperatives.

1. THERMODYNAMIC DESCRIPTION OF STRANGE SETS

Given a strange set⁺ on an interval (for example, the period doubling attractor), and limited patience, one tries to pin down the set by partitioning the interval into a finite number of segments. i-th segment is either "empty (a "hole" Δ_i), or it contains a piece of the strange set (a "cover" ℓ_i). This partition is not unique, and as a sloppy cover can make a strange set appear fatter than it actually is, one needs to insure that the cover is "optimal". The simplest approach is to cut up the interval into equal size segments and discard the holes. This is the blind man's approach to strange sets, oblivious both to the actual layout of the set and its internal systematics. A better cover is obtained by poking holes of maximal size (with a point of the set at both ends), and with labels which reflect the structure of the set.

What is the typical size of a covering interval? Intuitively, if the cover is good, and there are N covering intervals, each covering interval is smaller than 1/N. We can sharpen this intuition by reminding ourselves how Cantor sets are generated by dynamical systems. Typically they arise by dynamical stretching and squeezing, with a "mother" interval at time t giving rise to several "daughter" intervals at time t+At

$$\ell_{\rm d} = \sigma_{\rm dm} \ell_{\rm m} \tag{1}$$

The <u>scaling function</u> $\sigma_{\rm dm}$ is related to the contraction rate of the system. If $\sigma_{\rm dm}$ is on average of size σ , and the average number of daughters is α , than after k time steps $\ell \simeq \sigma^{\rm k}$, $N \simeq \alpha^{\rm k}$, and $\ell n \ \ell \simeq \ell n \ N$. Clearly, instead of using $\ell_{\rm i}$ (which

⁺A definition: compact, perfect, totally disconnected set.

shrink to zero as we refine the cover), we should define the <u>scaling exponents</u>

$$\mu_{i} - \frac{1}{t} \ln \ell_{i}$$

$$t - \ln N$$
(2)

For "good" covers the covering intervals do not vary too widely in size, and μ_i are bounded.

<u>Exercise 1</u>. A two-scale Cantor set is generated by recursively replacing each interval ℓ_m by a "fat" subinterval $\ell_{mo} = \sigma_0 \ell_m$ and a "thin" subinterval $\ell_{m1} = \sigma_1 \ell_m$, $o < \sigma_1 < \sigma_0 < 1$, $\sigma_0 + \sigma_1 < 1$. Show that

 $\mu_{\min} = - \frac{\ln \sigma_o}{\ln 2} \ , \ \mu_{\max} = - \frac{\ln \sigma_1}{\ln 2} \ .$

A theory of a strange set should yield a good labeling scheme for the covering intervals of the set (the "symbolic dynamics") and predict the scale associated with each interval (the "scaling function"). An experiment yields a finite cover for the set. How are we to efficiently compare the two?

A robust procedure for averaging the experimental data is called for. The first temptation is to extract the "size" of the set from the N experimental covering intervals ℓ_i by forming the sum

$$Z_{N} = \sum_{i=1}^{N} \ell_{i} \qquad (3)$$

As the set is dense with holes, this sum tends to vanish, in step with refinement of the cover. Our intuitive estimates (2) of ℓ_i tell us that it vanishes exponentially. We can compensate for the exponential shrinkage by introducing exponent τ :

$$Z_{N}(\tau) = \sum_{i=1}^{N} \ell_{i}^{\tau}$$
(4)

For a deftly chosen value $\tau = -D$, the blown-up segments fill up the entire interval, no matter how fine the refinement:

$$\lim_{N \to \infty} Z_N(-D) =$$

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For an optimal cover D equals D_{H} , the Hausdorff dimension: a sloppy cover yields an upper bound on D_{H} .

<u>Exercise 2</u>. If a set is of dimension D, it can be covered with $n(e) \propto l^{-D}$ balls of diameter l. Check that (5) conforms to this notion of dimension by taking equal size covering intervals.

Eq. (4) enables us to extract much more information about the strange set than just its Hausdorff dimension. The parameter τ can be used to extract different scales in the set. For $\tau \to -\infty$ the fattest intervals dominate, and $Z_N(\tau) \to \exp(t\tau \mu_{\min})$. For $\tau=0$, $Z_N(0) = N$, and for $\tau \to +\infty$ the thinnest intervals dominate, $Z_N(\tau) \to \exp(t\tau \mu_{\max})$. The sum grows exponentially with $t = \ln N$ for the entire range of τ , so the object that has a finite limit as $N \to \infty$ is

$$q_{t}(\tau) = \frac{1}{t} \ln Z_{N}(\tau) = \frac{1}{t} \ln \sum_{i=1}^{N} e^{t\tau \mu_{i}} \rightarrow q(\tau)$$
(6)

This function grows monotonically with τ . By our normalization convention

$$q_t(o) = 1 \tag{7}$$

The Hausdorff dimension condition (5) can now be restated in terms of a quantity finite in the $N \rightarrow \infty$ limit:

$$q(-D_{o}) = 0 \tag{8}$$

In practice, $q(\tau)$ is a rather boring function, and the distribution of the scales is displayed more effectively by the mean scaling exponent

$$\frac{\mathrm{dq}_{t}(\tau)}{\mathrm{d}\tau} = \frac{1}{\mathrm{Z}_{\mathrm{N}}(\tau)} \sum_{i=1}^{\mathrm{N}} \mu_{i} e^{t\mu_{i}\tau} = \mu(\tau)$$
(9)

and the higher moments such as

$$\frac{d^2 q_t(\tau)}{d\tau^2} = t\{<\mu_1^2>_{\tau} - \mu(\tau)^2\}$$
(10)

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 $q''(\tau)$ is strictly positive. $\mu(\tau)$ grows monotonically from $\mu(-\infty) = \mu_{\min}$ to $\mu(\infty) = \mu_{\max}$.

Exercise 3. Show that for the two-scale Cantor set introduced in exercise 1 the asymptotic q(r) is given by

$$q(\tau) = \frac{\ln\left(\sigma_{o}^{-\tau} + \sigma_{1}^{-\tau}\right)}{\ln 2}$$

(hint: use binomial theorem). Show that for finite N, $q_t(\tau) = q(\tau) - \tau/t \ln \ell$, where ℓ is the size of the single covering interval at the top level. How can such finite N contributions be eliminated? Plot $q(\tau)$, $\mu(\tau)$ and $q''(\tau)$.

Actually, as we know the $\tau \rightarrow \pm \infty$ behaviour of $q(\tau)$, we might just as well subtract it out, and plot the result as the function of μ :

$$S_{t}(\mu) = q_{t}(\tau) - \tau \mu(\tau)$$
(11)

We recognize (11), together with (9) and

$$\tau = -\frac{\mathrm{dS}_{\mathrm{t}}(\mu)}{\mathrm{d}\mu} \tag{12}$$

to be a Legendre transformation. In practice it is performed by evaluating (6), (9) and plotting $\mu(\tau)$, $S_t(\mu(\tau))$ pairs for a range of τ .

 $S_t(\mu)$ function has almost always compact support $\mu_{\min} \le \mu \le \mu_{\max}$, is positive (by strict positivity of q''(τ)), is convex by (12), and bounded by 1 (by normalization convention (7)), so it fits nicely on a piece of graph paper.

Exercise 4. Plot $S(\mu)$ for the 2-scale Cantor set. How does $S_t(\mu)$ depend on the finite t?

 $S(\mu)$ is called the <u>scaling spectrum</u> and is the most succint summary of all information obtainable from averages over the covering interval lengths. In order to elucidate its physical significance, reconsider the defining sum (4). The sum depends only on the interval sizes and not on the way in which set was generated (reflected in the label i in the sum (4)). Therefore it can be written as

$$Z_{N}(\tau) = \int_{\ell_{\min}}^{\ell_{\max}} d\ell N(\ell) \ell^{-\tau}$$
(13)

where N(l)dl is the number of intervals whose size falls into range [l,dl]. N(l) grows with, and is bounded by N, the total number of intervals. We extract the rate of growth by defining

$$s_{t}(\mu) = \frac{1}{t} \ln(\ell N(\ell))$$
(14)

The sum (4) now takes form

$$Z_{N}(\tau) = e^{tq_{t}(\tau)} = e^{t(S_{t}(\mu) + \tau\mu)} = t \int_{\mu_{min}}^{\mu_{max}} d\mu e^{t(S_{t}(\mu) + \tau\mu)}$$
(15)

In the t $\rightarrow \infty$ limit a saddle point evaluation yields (11) and (12), with identification $s(\mu) = S(\mu)$, so the scaling spectrum $S(\mu)$ indicates how <u>numerous is scaling exponent μ </u>. The saddle point estimate picks out the global maximum of $s(\mu)+\tau\mu$, and it can jump discontinously in μ . As we show in the next section, this implies that $S(\mu)$ is actually the convex envelope of $s(\mu)$. $S(\mu)$ is smooth and easy to obtain numerically; counting involved in constructing $s(\mu)$ requires a detailed understanding of the strange set.

- <u>Exercise 5</u>. Evaluate $N(\ell)$ and $s(\mu)$ for the 2-scale Cantor set. Estimate $q(\tau)$, $S(\mu)$ by a saddle-point evaluation of the integral (15). (Hint: use the Stirling approximation for k!).
- <u>Exercise 6</u>. Consider scaling functions (1) which depend on finite memory (the preceeding few symbols in the mother interval label in Exercise 1). Relate q(r) to the eigenvalues of the matrix σ_{dm} .

Remark 1: falfas

A strange set is usually highly inhomogenous; some covering intervals can contain most of the set, and others

practically nothing. The inhomogeneity of the cover can be taken into account by replacing (2) by a weighted sum $^{3,15,8)}$

$$1 = \sum_{i=1}^{N} \frac{p_i^{q}}{\ell_i^{\tau}}$$
(16)

For dynamically built-up strange sets (such as the Hénon attractor) p_i are determined by a unique "natural" measure: p_i is the fraction of the points of the set which land in the i-th covering interval:

$$P_{i} = \frac{N_{i}}{N}$$
(17)

For many other strange sets (such as the set of all irrational winding parameter values of critical circle maps⁶) there is no "natural" choice of p_i , other than the uniform probability $p_i = 1/N$. If the probability is uniform,(16) reduces to (4).

However, in analysis of experimental data it is sometimes easier to fix $l_i = l = \text{const}$, and measure the p_i in (16). In this case it is r(q), rather than q(r), that is extracted from the data;

$$r(q) = -\frac{\ln \sum_{i=1}^{N} p_{i}^{q}}{\ln \ell} .$$
 (18)

Instead of the scaling exponent μ_i , one now defines³⁾ the "pointwise dimension"

$$\alpha_{i} = \frac{\ln p_{i}}{\ln \ell_{i}}$$
(19)

Intuitively, the pointwise dimension should be the same regardless of whether we compute it by choosing balls of the same radius or the same probability. If we chose uniform probability, we see from (2) that the pointwise dimension and the scaling exponent are related by

$$\alpha_i = 1/\mu_i \tag{20}$$

Following the same line of reasoning that led to the scaling spectrum (11) one now arrives at the "f of alpha" function $^{3)}$

$$f(\alpha) = -\tau(q) + q\alpha(q)$$

$$f(\alpha) = S(\mu)/\mu .$$
(21)

The scaling spectrum and $f(\alpha)$ are the same function, up to coordinate redefinitions.

<u>Exercise 7</u>. Prove that the scaling spectrum $S(\mu)$ is independent of the choice of covering intervals ℓ_i , as long as the probabilities p_i arise from the same measure.

Remark 2: previously defined dimensions

The function $\tau(q)$ of (18) is related to the generalized dimensions $^{16-19}$ by

$$D_{q} = \frac{\tau}{q-1}$$
(22)

 D_o is the Hausdorff dimension (8). By (11) and (12), D_o is the slope of the tangent to $S(\mu)$ at $\mu_H = \mu(-D_o)$ which satisfies

$$D_{o} = \frac{dS(\mu_{H})}{d\mu} = \frac{S(\mu_{H})}{\mu_{H}}$$
(23)

The information dimension is the dimension of the most numerous interval length, with scaling exponent $\mu_{\tau} = \mu(o)$:

$$D_{1} = \frac{d\tau(q)}{dq} \Big|_{q=1} = \frac{1}{\frac{dq(r)}{dr}} \Big|_{\tau=0} = 1/\mu(0) \quad . \tag{24}$$

For $\tau \to \pm \infty$ we obtain

$$D_{\infty} = 1/\mu_{\max}, \ D_{-\infty} = 1/\mu_{\min}$$
 (25)

Remark 3: scale invariance

The sum (4) has an obvious flaw; nothing defines the units in which the lengths ℓ_i are to be measured. Under change of scale $\ell_i \rightarrow e^{-\beta}\ell_i$, the value of $Z_N(\tau)$ scales as $Z_N(\tau) \rightarrow e^{\tau\beta}Z_N(\tau)$, and the $q_t(\tau)$ function picks up a correction of $O(t^{-1})$:

$$q_{+}(\tau) \rightarrow q_{+}(\tau) + \beta \tau / t$$
, $\mu(\tau) \rightarrow \mu(\tau) + \beta / t$.

This is a 1/lnN correction, and in practice large. It is usually eliminated by computing $q(\tau)$ from ratios of $Z_N's$:

$$q_{t-t}'(r) = \frac{1}{t-t}, \ ln \frac{Z_N(r)}{Z_N(r)}$$
 (25)

The scaling spectrum $S(\mu)$, and $q''(\tau)$ are invariant under the change of scale

<u>Exercise 8</u>. Argue that $q(\tau)$ and the functions derived from it are invariant under the smooth deformations of the strange set.

Remark 4: Scaling spectrum vs. scaling function

Note that a Cantor set with only 2 scales has a continuous spectrum, so infinity of the scaling exponents does not imply an infinity of generating scales.

Remark 5: true thermodynamics

In our evaluation of the partition sum (4) we have assumed something that we can rarely afford in statistical mechanics: that the Boltzmann weight for each and every of the N "configurations" i is explicitely given. The price we pay for this is slow lnN convergence of the thermodynamic functions $q_t(\tau)$, $S_t(\mu)$ toward the asymptic $t \rightarrow \infty$ limits $q(\tau)$, $S(\mu)$. It would be more in the spirit of statistical mechanics to estimate the $q(\tau)$ by computing a few l_i for high N, and explore the "configuration" space by the Monte Carlo methods.

<u>Exercise 9</u>. Estimate the thermodynamic functions for Hénon attractor from a subset of l_i computed from very long unstable cycles.

<u>Remark 6:</u> l_i for asymptotic N can be computed only by renormalization methods, ie. recursive rescalings of local neighborhoods, such that l_i at n-th level is of order of unity.

2. PHASE TRANSITIONS

Determining that there is a phase transition on basis of a finite covering of a strange set can be tricky. Here we describe

three methods: finite size scaling, convexity of the scaling spectrum, and hysteresis.

Approximate the partition sum (15) by two scaling exponents μ_1, μ_2

$$Z_{N}(\tau) = e^{t(s_{1}+\mu_{1}\tau)} + e^{t(s_{2}+\mu_{2}\tau)}.$$
 (26)

In the N $\rightarrow \infty$ limit the sum is dominated either by the first or by the second term, and $q(\tau)$ goes through a first order phase transition (here we assume $\mu_1 < \mu_2$)

$$q(\tau) = \begin{cases} s_1^{+\mu_1 \tau} & \tau < \tau_c \\ s_2^{+\mu_2 \tau} & \tau > \tau_c \end{cases},$$
(27)

where the critical τ is determined by the condition that the two terms in (26) contribute equally

$$\tau_{\rm c} = -\frac{{\rm s}_2^{-{\rm s}}1}{\mu_2^{-\mu_1}} \quad . \tag{28}$$

This simple model teaches us how to diagnose the existence of a first order phase transition, and estimate the critical τ and the gap in μ from the finite N effects. At the phase transition we have

$$q_{t}(\tau_{c}) = q(\tau_{c}) + \frac{\ln 2}{t}$$

$$\dot{q}_{t}(\tau_{c}) = \mu_{t}(\tau_{c}) = \mu(\tau_{c}) = \frac{\mu_{1} + \mu_{2}}{2}$$

$$q_{t}'(\tau_{c}) = t \left(\frac{\mu_{2} - \mu_{1}}{2}\right)^{2}$$
(29)

This is illustrated in Fig. 1



Fig. 1. Thermodynamic functions for the 2-scale model (26), with t = 1,2,...,10 (t=10 corresponds to about 22,000 covering intervals). The asymptotic limits are indicated by the dotted lines.

It is hard to appreciate how slow 1/lnN convergence is before you actually try to beat it⁵⁾. The problem is not that experimental N is of order hundred; the problem is that no super-computer can bludgen such creeping convergence into submission, unless the nature of convergence is well understood.

If the phase transition is indeed of form (27), than s_1, s_2 , μ_1, μ_2 , t and r_c can be extracted by fitting the finite N thermodynamic curves. However, in practice both s_i and μ_i are also N-dependent, and one is forced to resort to unreliable numerical acceleration techniques.⁶⁾

The second method for diagnosing existence of a phase transition is based on comparison of $s(\mu)$, the detailed interval counting (14), with $S(\mu)$ from (11), extracted from the global average (4). The two functions differ if $s(\mu)$ is not convex. To see why $S_t(\mu)$ must be convex, consider a three scaling exponent $(\mu_1 < \mu_2 < \mu_3)$ approximation to the sum (15)

$$\begin{array}{c} t(s_1 + \mu_1 \tau) & t(s_2 + \mu_2 \tau) & t(s_3 + \mu_3 \tau) \\ Z_N(\tau) = e & + e & + e \end{array}$$
(30)

 $q(\tau)$ is given by the upper boundary of the union of rays $q = s_i^{+\mu} t_i^{-\tau}$, see Fig. 2. In this sum, the second term contributes only if the ray $q = s_2^{+\mu} t_2^{-\tau}$ crosses the intersection of the two rays from above. The critical s_2 is given by the coalescence condition for the three intersections:



Fig. 2. The second term in (30) contributes to $q(\tau)$, S(μ) only if s(μ_2) falls above the dotted line (case 2). In case 2' S(μ) and s(μ) differ; $\mu(\tau)$ jumps from μ_1 to μ_2 without detecting the μ_2 scale.

$$\frac{s_2^{-s_1}}{\mu_2^{-\mu_1}} = \frac{s_3^{-s_2}}{\mu_3^{-\mu_2}}$$
(31)

This is the condition that three $s(\mu)$ points lie on a line. If $s(\mu_2)$ for $\mu_1 < \mu_2 < \mu_3$ falls below this line, $\mu(\tau)$ jumps from μ_1 to μ_3 as τ goes through τ_c given by (28) and $s(\mu_2)$ does not contribute to $S(\mu)$. The critical τ is given by the slope of the straight section of $S(\mu)$ (see 12)). In other words, if the scale counting function $s(\mu)$ has a concave dimple, the system exhibits a first order phase transition. In practice one evaluates $s'(\mu_c)$, which requires counting only in the neighborhood of μ_c . If $s'(\mu_c)$ falls below a convexity bound imposed by known $S(\mu)$ values, $s(\mu)$ is concave.

Exercise 10. Generalize the above arguments to continuous $s(\mu)$. (Hint; estimate (15) by saddle point methods)

Unfortunately, I do not know of anything as simple as the 2-scale Cantor set (exercise 3) with a non-trivial concave $s(\mu)$ segment. The best I can offer here is a rather artificial set which arises in the study of circle maps⁶: at n-th level, there are N = 2ⁿ intervals, labelled by all distinct strings of n 0's and 1's. If there are k 1's, the covering interval is given by

$$l_{\rm k} = \sigma({\rm x})^{-2{\rm n}{\rm x}}$$
, ${\rm x} = {\rm k/n}$
 $\sigma({\rm x}) = (1+\sqrt{1+4{\rm x}^2})/(2{\rm x})$
(32)

 $\sigma(x)$ here is in an estimate of the scaling factor associated with an average string of 0's. n/k = 1/x is the average length of 0-string, if there are k 1's. For this set, the thermodynamic functions are plotted in Fig. 3.



Fig. 3. The first order transition for the covering intervals defined by (32), as seen in the average scaling exponent $\mu(\tau)$, and in the difference between the counting function $s(\mu)$ and its convex envelope, the scaling spectrum $S(\mu)$.

<u>Exercise 11</u>. Show that interval ℓ_k occurs $\binom{n}{k}$ times, and that

$$Z_{N}(\tau) = \int_{0}^{1} dx e^{t(f(x) + \tau \mu(x))}$$

 $f(x) = -\frac{x \ln x + (1-x) \ln(1-x)}{\ln 2} , \quad \mu(x) = \frac{2x \ln \sigma(x)}{\ln 2}$ Plot s(μ), S(μ). Estimate τ_c . (Hint; use the Stirling approximation. $\tau_c = -0.80318...$.)

<u>Remark 7: Hysteresis</u>. The "true thermodynamics" offers a third way to establish a phase transition; metastability around $r_{\rm c}$ makes it difficult for Monte Carlo updates to discover the true "ground state". Hence hysteresis is expected.

To summarize: determination of phase transitions on (finite size) strange sets is a non-trivial task. If the transition is of first order, finite size scaling, convexity of $S(\mu)$ and hysteresis can offer the essential clues. Transitions of higher order, to best of my knowledge, are not known in this context.

The thermodynamics formalism is an effective tool for extracting average scale information from experimental data; it is theoretically elegant (through its connection to scaling functions^{2,4)}; and it leads to the phenomenon of strange set phase transitions.

The thermodynamic formalism views a strange set as a static, given object. It is blind to the dynamics of the system, the detailed layout and ordering of its various parts, to dynamic correlations. It is simply an averaging technique; understanding a strange set requires a detailed study of its symbolic and scaling dynamics.

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