Appendix K

Statistical mechanics recycled

(R. Mainieri)

A spin system with long-range interactions can be converted into a chaotic dynamical system that is differentiable and low-dimensional. The thermodynamic limit quantities of the spin system are then equivalent to long time averages of the dynamical system. In this way the spin system averages can be recast as the cycle expansions. If the resulting dynamical system is analytic, the convergence to the thermodynamic limit is faster than with the standard transfer matrix techniques.

K.1 The thermodynamic limit

There are two motivations to recycle statistical mechanics: one gets better control over the thermodynamic limit and one gets detailed information on how one is converging to it. From this information, most other quantities of physical interst can be computed.

In statistical mechanics one computes the averages of observables. These are functions that return a number for every state of the system; they are an abstraction of the process of measuring the pressure or temperature of a gas. The average of an observable is computed in the thermodynamic limit — the limit of system with an arbitrarily large number of particles. The thermodynamic limit is an essential step in the computation of averages, as it is only then that one observes the bulk properties of matter.

Without the thermodynamic limit many of the thermodynamic properties of matter could not be derived within the framework of statistical mechanics. There would be no extensive quantities, no equivalence of ensembles, and no phase transitions. From experiments it is known that certain quantities are extensive, that is, they are proportional to the size of the system. This is not true for an interacting set of particles. If two systems interacting via pairwise potentials are brought close together, work will be required to

join them, and the final total energy will not be the sum of the energies of each of the parts. To avoid the conflict between the experiments and the theory of Hamiltonian systems, one needs systems with an infinite number of particles. In the canonical ensemble the probability of a state is given by the Boltzman factor which does not impose the conservation of energy; in the microcanonical ensemble energy is conserved but the Boltzmann factor is no longer exact. The equality between the ensembles only appears in the limit of the number of particles going to infinity at constant density. The phase transitions are interpreted as points of non-analyticity of the free energy in the thermodynamic limit. For a finite system the partition function cannot have a zero as a function of the inverse temperature β, as it is a finite sum of positive terms.

The thermodynamic limit is also of central importance in the study of field theories. A field theory can be first defined on a lattice and then the lattice spacing is taken to zero as the correlation length is kept fixed. This continuum limit corresponds to the thermodynamic limit. In lattice spacing units the correlation length is going to infinity, and the interacting field theory can be thought of as a statistical mechanics model at a phase transition.

For general systems the convergence towards the thermodynamic limit is slow. If the thermodynamic limit exists for an interaction, the convergence of the free energy per unit volume f is as an inverse power in the linear dimension of the system.

$$f(\beta) \to \frac{1}{n} \tag{K.1}$$

where n is proportional to $V^{1/d}$, with V the volume of the d-dimensional system. Much better results can be obtained if the system can be described by a transfer matrix. A transfer matrix is concocted so that the trace of its nth power is exactly the partition function of the system with one of the dimensions proportional to n. When the system is described by a transfer matrix then the convergence is exponential,

$$f(\beta) \to e^{-\alpha n} \tag{K.2}$$

and may only be faster than that if all long-range correlations of the system are zero — that is, when there are no interactions. The coefficient α depends only on the inverse correlation length of the system.

One of the difficulties in using the transfer matrix techniques is that they seem at first limited to systems with finite range interactions. Phase transitions can happen only when the interaction is long range. One can try to approximate the long range interaction with a series of finite range interactions that have an ever increasing range. The problem with this approach is that in a formally defined transfer matrix, not all the eigenvalues of the matrix correspond to eigenvalues of the system (in the sense that the rate of decay of correlations is not the ratio of eigenvalues).

Knowledge of the correlations used in conjunction with finite size scaling to obtain accurate estimates of the parameters of systems with phase transitions. (Accurate critical exponents are obtained by series expansions or transfer matrices, and seldomly by renormalization group arguments or Monte Carlo.) In a phase transition the coefficient α of the exponential convergence goes to zero and the convergence to the thermodynamic limit is power-law.

The computation of the partition function is an example of a functional integral. For most interactions these integrals are ill-defined and require some form of normalization. In the spin models case the functional integral is very simple, as "space" has only two points and only "time" being infinite has to be dealt with. The same problem occurs in the computation of the trace of transfer matrices of systems with infinite range interactions. If one tries to compute the partition function Z_n

$$Z_n = \mathrm{tr}\, T^n$$

when T is an infinite matrix, the result may be infinite for any n. This is not to say that Z_n is infinite, but that the relation between the trace of an operator and the partition function breaks down. We could try regularizing the expression, but as we shall see below, that is not necessary, as there is a better physical solution to this problem.

What will described here solves both of these problems in a limited context: it regularizes the transfer operator in a physically meaningful way, and as a a consequence, it allows for the faster than exponential convergence to the thermodynamic limit and complete determination of the spectrum. The steps to achieve this are:

- Redefine the transfer operator so that there are no limits involved except for the thermodynamic limit.
- Note that the divergences of this operator come from the fact that it acts on a very large space. All that is needed is the smallest subspace containing the eigenvector corresponding to the largest eigenvalue (the Gibbs state).
- Rewrite all observables as depending on a local effective field. The eigenvector is like that, and the operator restricted to this space is trace-class.
- Compute the spectrum of the transfer operator and observe the magic.

K.2 Ising models

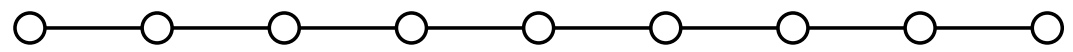
The Ising model is a simple model to study the cooperative effects of many small interacting magnetic dipoles. The dipoles are placed on a lattice and

their interaction is greatly simplified. There can also be a field that includes the effects of an external magnetic field and the average effect of the dipoles among themselves. We will define a general class of Ising models (also called spin systems) where the dipoles can be in one of many possible states and the interactions extend beyond the nearest neighboring sites of the lattice. But before we extend the Ising model, we will examine the simplest model in that class.

K.2.1 Ising model

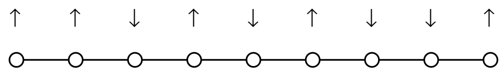
One of the simplest models in statistical mechanics is the Ising model. One imagines that one has a one-dimensional lattice with small magnets at each site that can point either up or down.

Each little magnet interacts only with its neighbors. If they both point in the same direction, then they contribute an energy $-J$ to the total energy of the system; and if they point in opposite directions, then they contribute $+J$. The signs are chsen so that they prefer to be aligned. Let us suppose that we have n small magnets arranged in a line: A line is drawn between two sites to indicate that there is an interaction between the small magnets that are located on that site



. (K.3)

(This figure can be thought of as a graph, with sites being vertices and interacting magnets indicated by edges.) To each of the sites we associate a variable, that we call a spin, that can be in either of two states: up ($\uparrow$) or down ($\downarrow$). This represents the two states of the small magnet on that site, and in general we will use the notation Σ_0 to represent the set of possible values of a spin at any site; all sites assume the same set of values. A configuration consists of assigning a value to the spin at each site; a typical configuration is



. (K.4)

The set of all configurations for a lattice with n sites is called Ω_0^n and is formed by the Cartesian product $\Omega_0 \times \Omega_0 \cdots \times \Omega_0$, the product repeated n times. Each configuration $\sigma \in \Omega^n$ is a string of n spins

$$\sigma = \{\sigma_0, \sigma_1, \dots \sigma_n\}\,, \tag{K.5}$$

In the example configuration (K.4) there are two pairs of spins that have the same orientation and six that have the opposite orientation. Therefore the total energy H of the configuration is $J \times 6 - J \times 2 = 4J$. In general we can associate an energy H to every configuration

$$H(\sigma) = \sum_i J\delta(\sigma_i, \sigma_{i+1}) , \tag{K.6}$$

where

$$\delta(\sigma_1, \sigma_2) = \begin{cases} +1 & \text{if } \sigma_1 = \sigma_2 \\ -1 & \text{if } \sigma_1 \neq \sigma_2 \end{cases} . \tag{K.7}$$

One of the problems that was avoided when computing the energy was what to do at the boundaries of the one-dimensional chain. Notice that as written, (K.6) requires the interaction of spin n with spin $n+1$. In the absence of phase transitions the boundaries do not matter much to the thermodynamic limit and we will connect the first site to the last, implementing periodic boundary conditions.

Thermodynamic quantities are computed from the partition function $Z^{(n)}$ as the size n of the system becomes very large. For example, the free energy per site f at inverse temperature β is given by

$$-\beta f(\beta) = \lim_{n\to\infty} \frac{1}{n} \ln Z^{(n)} . \tag{K.8}$$

The partition function $Z^{(n)}$ is computed by a sum that runs over all the possible configurations on the one-dimensional chain. Each configuration contributes with its Gibbs factor $\exp(-\beta H(\sigma))$ and the partition function $Z^{(n)}$ is

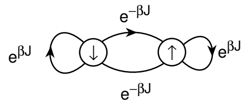
$$Z^{(n)}(\beta) = \sum_{\sigma \in \Omega_0^n} e^{-\beta H(\sigma)} . \tag{K.9}$$

The partition function can be computed using transfer matrices. This is a method that generalizes to other models. At first, it is a little mysterious that matrices show up in the study of a sum. To see where they come from, we can try and build a configuration on the lattice site by site. The frst thing to do is to expand out the sum for the energy of the configuration

$$Z^{(n)}(\beta) = \sum_{\sigma \in \Omega^n} e^{\beta J\delta(\sigma_1,\sigma_2)} e^{\beta J\delta(\sigma_2,\sigma_3)} \cdots e^{\beta J\delta(\sigma_n,\sigma_1)} . \tag{K.10}$$

Let us use the configuration in (K.4). The first site is $\sigma_1 = \uparrow$. As the second site is $\uparrow$, we know that the first term in (K.10) is a term $e^{\beta J}$. The third

spin is $\downarrow$, so the second term in (K.10) is $e^{-\beta J}$. If the third spin had been $\uparrow$, then the term would have been $e^{\beta J}$ but it would not depend on the value of the first spin σ_1. This means that the configuration can be built site by site and that to compute the Gibbs factor for the configuration just requires knowing the last spin added. We can then think of the configuration as being a weighted random walk where each step of the walk contributes according to the last spin added. The random walk take place on the Markov graph



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Choose one of the two sites as a starting point. Walk along any allowed edge making your choices randomly and keep track of the accumulated weight as you perform the n steps. To implement the periodic boundary conditions make sure that you return to the starting node of the Markov graph. If the walk is carried out in all possible 2^n ways then the sum of all the weights is the partition function. To perform the sum we consider the matrix

$$T(\beta) = \begin{bmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{bmatrix} . \tag{K.11}$$

As in chapter 10 the sum of all closed walks is given by the trace of powers of the matrix. These powers can easily be re-expressed in terms of the two eigenvalues λ_1 and λ_2 of the transfer matrix:

$$Z^{(n)}(\beta) = \operatorname{tr} T^n(\beta) = \lambda_1(\beta)^n + \lambda_2(\beta)^n . \tag{K.12}$$

K.2.2 Averages of observables

Averages of observables can be re-expressed in terms of the eigenvectors of the transfer matrix. Alternatively, one can introduce a modified transfer matrix and compute the averages through derivatives. Sounds familiar?

K.2.3 General spin models

The more general version of the Ising model — the spin models — will be defined on a regular lattice, $\mathbb{Z}^D$. At each lattice site there will be a spin variable that can assumes a finite number of states identified by the set Ω_0.

The transfer operator $\mathcal{T}$ was introduced by Kramers and Wannier [K.12] to study the Ising model on a strip and concocted so that the trace of its nth power is the partition function Z_n of system when one of its dimensions is n. The method can be generalized to deal with any finite-range interaction. If the range of the interaction is L, then $\mathcal{T}$ is a matrix of size $2^L \times 2^L$. The longer the range, the larger the matrix.

K.3 Fisher droplet model

In a series of articles [K.20], Fisher introduced the droplet model. It is a model for a system containing two phases: gas and liquid. At high temperatures, the typical state of the system consists of droplets of all sizes floating in the gas phase. As the temperature is lowered, the droplets coalesce, forming larger droplets, until at the transition temperature, all droplets form one large one. This is a first order phase transition.

Although Fisher formulated the model in three-dimensions, the analytic solution of the model shows that it is equivalent to a one-dimensional lattice gas model with long range interactions. Here we will show how the model can be solved for an arbitrary interaction, as the solution only depends on the asymptotic behavior of the interaction.

The interest of the model for the study of cycle expansions is its relation to intermittency. By having an interaction that behaves asymptotically as the scaling function for intermittency, one expects that the analytic structure (poles and cuts) will be same.

Fisher used the droplet model to study a first order phase transition [K.20]. Gallavotti [K.21] used it to show that the zeta functions cannot in general be extended to a meromorphic functions of the entire complex plane. The droplet model has also been used in dynamical systems to explain features of mode locking, see Artuso [K.22]. In computing the zeta function for the droplet model we will discover that at low temperatures the cycle expansion has a limited radius of convergence, but it is possible to factorize the expansion into the product of two functions, each of them with a better understood radius of convergence.

K.3.1 Solution

The droplet model is a one-dimensional lattice gas where each site can have two states: empty or occupied. We will represent the empty state by 0 and the occupied state by 1. The configurations of the model in this notation are then strings of zeros and ones. Each configuration can be viewed as groups of contiguous ones separated by one or more zeros. The contiguous ones represent the droplets in the model. The droplets do not interact with each other, but the individual particles within each droplet do.

To determine the thermodynamics of the system we must assign an energy to every configuration. At very high temperatures we would expect

a gaseous phase where there are many small droplets, and as we decrease the temperature the droplets would be expected to coalesce into larger ones until at some point there is a phase transition and the configuration is dominated by one large drop. To construct a solvable model and yet one with a phase transition we need long range interaction among all the particles of a droplet. One choice is to assign a fixed energy θ_n for the interactions of the particles of a cluster of size n. In a given droplet one has to consider all the possible clusters formed by contiguous particles. Consider for example the configuration 0111010. It has two droplets, one of size three and another of size one. The droplet of size one has only one cluster of size one and therefore contributes to the energy of the configuration with θ_1. The cluster of size three has one cluster of size three, two clusters of size two, and three clusters of size one; each cluster contributing a θ_n term to the energy. The total energy of the configuration is then

$$H(0111010) = 4\theta_1 + 2\theta_2 + 1\theta_3 \,. \tag{K.13}$$

If there where more zeros around the droplets in the above configuration the energy would still be the same. The interaction of one site with the others is assumed to be finite, even in the ground state consisting of a single droplet, so there is a restriction on the sum of the cluster energies given by

$$a = \sum_{n>0} \theta_n < \infty \,. \tag{K.14}$$

The configuration with all zeros does not contribute to the energy.

Once we specify the function θ_n we can computed the energy of any configuration, and from that determine the thermodynamics. Here we will evaluate the cycle expansion for the model by first computing the generating function

$$G(z,\beta) = \sum_{n>0} z^n \frac{Z_n(\beta)}{n} \tag{K.15}$$

and then considering its exponential, the cycle expansion. Each partition function Z_n must be evaluated with periodic boundary conditions. So if we were computing Z_3 we must consider all eight binary sequences of three bits, and when computing the energy of a configuration, say 011, we should determine the energy per three sites of the long chain

$$\ldots 011011011011 \ldots$$

In this case the energy would be $\theta_2 + 2\theta_1$. If instead of 011 we had considered one of its rotated shifts, 110 or 101, the energy of the configuration would have been the same. To compute the partition function we only need to consider one of the configurations and multiply by the length of the configuration to obtain the contribution of all its rotated shifts. The factor $1/n$ in the generating function cancels this multiplicative factor. This reduction will not hold if the configuration has a symmetry, as for example 0101 which has only two rotated shift configurations. To compensate this we replace the $1/n$ factor by a symmetry factor $1/s(b)$ for each configuration b. The evaluation of G is now reduced to summing over all configurations that are not rotated shift equivalent, and we call these the basic configurations and the set of all of them B. We now need to evaluate

$$G(z,\beta)=\sum_{b\in B}\frac{z^{|b|}}{s(b)}e^{-\beta H(b)}\,. \tag{K.16}$$

The notation $|\cdot|$ represents the cardinality of the set.

Any basic configuration can be built by considering the set of droplets that form it. The smallest building block has size two, as we must also put a zero next to the one so that when two different blocks get put next to each other they do not coalesce. The first few building blocks are

$$\begin{array}{ll} \text{size} & \quad\text{droplets} \\ 2 & 01 \\ 3 & 001\ \ 011 \\ 4 & 0001\ \ 0011\ \ 0111 \end{array} \tag{K.17}$$

Each droplet of size n contributes with energy

$$W_n=\sum_{1\le k\le n}(n-k+1)\theta_k\,. \tag{K.18}$$

So if we consider the sum

$$\sum_{n\ge1}\frac{1}{n}\Big(z^2e^{-\beta H(01)}+z^3(e^{-\beta H(001)}+e^{-\beta H(011)})+ \\ +z^4(e^{-\beta H(0001)}+e^{-\beta H(0011)}+e^{-\beta H(0111)})+\cdots\Big)^n \tag{K.19}$$

then the power in n will generate all the configurations that are made from many droplets, while the z will keep track of the size of the configuration. The factor $1/n$ is there to avoid the over-counting, as we only want the basic configurations and not its rotated shifts. The $1/n$ factor also gives the correct symmetry factor in the case the configuration has a symmetry. The sum can be simplified by noticing that it is a logarithmic series

$$-\ln\Big(1-(z^2e^{-\beta W_1}+z^3(e^{-\beta W_1}+e^{-\beta W_2})+\cdots\Big)\,, \tag{K.20}$$

where the $H(b)$ factors have been evaluated in terms of the droplet energies W_n. A proof of the equality of (K.19) and (K.20) can be given , but we there was not enough space on the margin to write it down. The series that is subtracted from one can be written as a product of two series and the logarithm written as

$$-\ln\Big(1-(z^1+z^2+z^3+\cdots)(ze^{-\beta W_1}+z^2e^{-\beta W_2}+\cdots)\Big) \tag{K.21}$$

The product of the two series can be directly interpreted as the generating function for sequences of droplets. The first series adds one or more zeros to a configuration and the second series add a droplet.

There is a whole class of configurations that is not included in the above sum: the configurations formed from a single droplet and the vacuum configuration. The vacuum is the easiest, as it has zero energy it only contributes a z. The sum of all the null configurations of all sizes is

$$\sum_{n>0}\frac{z^n}{n}\,. \tag{K.22}$$

The factor $1/n$ is here because the original G had them and the null configurations have no rotated shifts. The single droplet configurations also do not have rotated shifts so their sum is

$$\sum_{n>0}\frac{z^ne^{-\beta H(\overbrace{11\ldots11}^{n})}}{n}\,. \tag{K.23}$$

Because there are no zeros in the above configuration clusters of all size exist and the energy of the configuration is $n\sum\theta_k$ which we denote by na.

From the three sums (K.21), (K.22), and (K.23) we can evaluate the generating function G to be

$$G(z,\beta)=-\ln(1-z)-\ln(1-ze^{-\beta a})-\ln(1-\frac{z}{1-z}\sum_{n\ge1}z^ne^{-\beta W_n})\,. \tag{K.24}$$

The cycle expansion $\zeta^{-1}(z,\beta)$ is given by the exponential of the generating function e^{-G} and we obtain

$$\zeta^{-1}(z,\beta)=(1-ze^{-\beta a})(1-z(1+\sum_{n\ge1}z^ne^{-\beta W_n})) \tag{K.25}$$

To pursue this model further we need to have some assumptions about the interaction strengths θ_n. We will assume that the interaction strength decreases with the inverse square of the size of the cluster, that is, $\theta_n = -1/n^2$. With this we can estimate that the energy of a droplet of size n is asymptotically

$$W_n \sim -n + \ln n + \mathcal{O}(\frac{1}{n})\,. \tag{K.26}$$

If the power chosen for the polynomially decaying interaction had been other than inverse square we would still have the droplet term proportional to n, but there would be no logarithmic term, and the $\mathcal{O}$ term would be of a different power. The term proportional to n survives even if the interactions falls off exponentially, and in this case the correction is exponentially small in the asymptotic formula. To simplify the calculations we are going to assume that the droplet energies are exactly

$$W_n = -n + \ln n \tag{K.27}$$

in a system of units where the dimensional constants are one. To evaluate the cycle expansion (K.25) we need to evaluate the constant a, the sum of all the θ_n. One can write a recursion for the θ_n

$$\theta_n = W_n - \sum_{1\leq k<n} (n-k+1)\theta_k \tag{K.28}$$

and with an initial choice for θ_1 evaluate all the others. It can be verified that independent of the choice of θ_1 the constant a is equal to the number that multiplies the n term in (K.27). In the units used

$$a = -1\,. \tag{K.29}$$

For the choice of droplet energy (K.27) the sum in the cycle expansion can be expressed in terms of a special function: the Lerch transcendental ϕ_L. It is defined by

$$\phi_L(z,s,c) = \sum_{n\geq 0} \frac{z^n}{(n+c)^s}\,, \tag{K.30}$$

excluding from the sum any term that has a zero denominator. The Lerch function converges for $|z|<1$. The series can be analytically continued to the complex plane and it will have a branch point at $z=1$ with a cut chosen along the positive real axis. In terms of Lerch transcendental function we can write the cycle expansion (K.25) using (K.27) as

$$\zeta^{-1}(z,\beta) = \left(1 - ze^{\beta}\right)\left(1 - z(1+\phi_L(ze^{\beta},\beta,1))\right) \tag{K.31}$$

This serves as an example of a zeta function that cannot be extended to a meromorphic function of the complex plane as one could conjecture.

The thermodynamics for the droplet model comes from the smallest root of (K.31). The root can come from any of the two factors. For large value of β (low temperatures) the smallest root is determined from the $(1 - ze^{\beta})$ factor, which gave the contribution of a single large drop. For small β (large temperatures) the root is determined by the zero of the other factor, and it corresponds to the contribution from the gas phase of the droplet model. The transition occurs when the smallest root of each of the factors become numerically equal. This determines the critical temperature β_c through the equation

$$1 - e^{-\beta_c}(1 + \zeta_R(\beta_c)) = 0 \tag{K.32}$$

which can be solved numerically. One finds that $\beta_c = 1.40495$. The phase transition occurs because the roots from two different factors get swapped in their roles as the smallest root. This in general leads to a first order phase transition. For large β the Lerch transcendental is being evaluated at the branch point, and therefore the cycle expansion cannot be an analytic function at low temperatures. For large temperatures the smallest root is within the radius of convergence of the series for the Lerch transcendental, and the cycle expansion has a domain of analyticity containing the smallest root.

As we approach the phase transition point as a function of β the smallest root and the branch point get closer together until at exactly the phase transition they collide. This is a sufficient condition for the existence of a first order phase transitions. In the literature of zeta functions [K.23] there have been speculations on how to characterize a phase transition within the formalism. The solution of the Fisher droplet model suggests that for first order phase transitions the factorized cycle expansion will have its smallest root within the radius of convergence of one of the series except at the phase transition when the root collides with a singularity. This does not seem to be the case for second order phase transitions.

The analyticity of the cycle expansion can be restored if we consider separate cycle expansions for each of the phases of the system. If we separate the two terms of ζ^{-1} in (K.31), each of them is an analytic function and contains the smallest root within the radius of convergence of the series for the relevant β values.

K.4 Scaling functions

> "Clouds are not spheres, mountains are not cones, coastlines are not circles and bark is not smooth, nor does lightning travel in straight line."
> —B.B. Mandelbrot

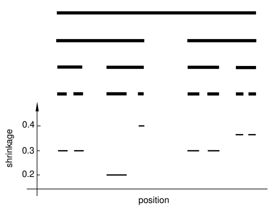

Figure K.1: Construction of the steps of the scaling function from a Cantor set. From one level to the next in the construction of the Cantor set the covers are shrunk, each parent segment into two children segments. The shrinkage of the last level of the construction is plotted and by removing the gaps one has an approximation to the scaling function of the Cantor set.

There is a relation between general spin models and dynamical system. If one thinks of the boxes of the Markov partition of a hyperbolic system as the states of a spin system, then computing averages in the dynamical system is carrying out a sum over all possible states. One can even construct the natural measure of the dynamical system from a translational invariant "interaction function" call the scaling function.

There are many routes that lead to an explanation of what a scaling function is and how to compute it. The shortest is by breaking away from the historical development and considering first the presentation function of a fractal. The presentation function is a simple chaotic dynamical system (hyperbolic, unlike the circle map) that generates the fractal and is closely related to the definition of fractals of Hutchinson [K.24] and the iterated dynamical systems introduced by Barnsley and collaborators [G.19]. From the presentation function one can derive the scaling function, but we will not do it in the most elegant fashion, rather we will develop the formalism in a form that is directly applicable to the experimental data.

In the upper part of figure K.1 we have the successive steps of the construction similar to the middle third Cantor set. The construction is done in levels, each level being formed by a collection of segments. From one level to the next, each "parent" segment produces smaller "children" segments by removing the middle section. As the construction proceeds, the segments better approximate the Cantor set. In the figure not all the segments are the same size, some are larger and some are smaller, as is the case with multifractals. In the middle third Cantor set, the ratio between a segment and the one it was generated from is exactly 1/3, but in the case shown in the figure the ratios differ from 1/3. If we went through the last level of the construction and made a plot of the segment number and its ratio to its parent segment we would have a scaling function, as indicated in the figure. A function giving the ratios in the construction of a fractal is the basic idea for a scaling function. Much of the formalism that we will introduce is to be able to give precise names to every segments and to arrange the "lineage" of segments so that the children segments have the correct parent. If we do not take these precautions, the scaling function would be a "wild function", varying rapidly and not approximated easily by simple functions.

To describe the formalism we will use a variation on the quadratic map that appears in the theory of period doubling. This is because the

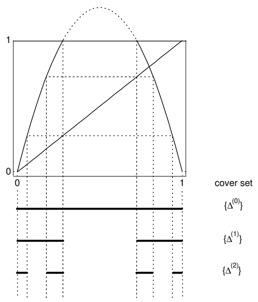

Figure K.2: A Cantor set presentation function. The Cantor set is the set of all points that under iteration do not leave the interval $[0, 1]$. This set can be found by backwards iterating the gap between the two branches of the map. The dotted lines can be used to find these backward images. At each step of the construction one is left with a set of segments that form a cover of the Cantor set.

combinatorial manipulations are much simpler for this map than they are for the circle map. The scaling function will be described for a one dimensional map F as shown in figure K.2. Drawn is the map

$$F(x) = 5x(1-x) \tag{K.33}$$

restricted to the unit interval. We will see that this map is also a presentation function.

It has two branches separated by a gap: one over the left portion of the unit interval and one over the right. If we choose a point x at random in the unit interval and iterate it under the action of the map F, (K.33), it will hop between the branches and eventually get mapped to minus infinity. An orbit point is guaranteed to go to minus infinity if it lands in the gap. The hopping of the point defines the orbit of the initial point x: $x \mapsto x_1 \mapsto x_2 \mapsto \cdots$. For each orbit of the map F we can associate a symbolic code. The code for this map is formed from 0s and 1s and is found from the orbit by associating a 0 if $x_t < 1/2$ and a 1 if $x_t > 1/2$, with $t = 0, 1, 2, \ldots$.

Most initial points will end up in the gap region between the two branches. We then say that the orbit point has escaped the unit interval. The points that do not escape form a Cantor set $\mathcal{C}$ (or Cantor dust) and remain trapped in the unit interval for all iterations. In the process of describing all the points that do not escape, the map F can be used as a presentation of the Cantor set $\mathcal{C}$, and has been called a presentation function by Feigenbaum [27.13].

How does the map F "present" the Cantor set? The presentation is done in steps. First, we determine the points that do not escape the unit interval in one iteration of the map. These are the points that are not part of the gap. These points determine two segments, which are an approximation to the Cantor set. In the next step we determine the points that do not escape in two iterations. These are the points that get mapped into the gap in one iteration, as in the next iteration they will escape; these points form the two segments $\Delta_0^{(1)}$ and $\Delta_1^{(1)}$ at level 1 in figure K.2. The processes can be continued for any number of iterations. If we observe carefully what is being done, we discover that at each step the pre-images of the gap (backward iterates) are being removed from the unit interval. As the map has two branches, every point in the gap has two pre-images, and therefore the whole gap has two pre-images in the form of two smaller gaps. To generate all the gaps in the Cantor set one just has to iterate the gap backwards. Each iteration of the gap defines a set of segments, with the nth iterate defining the segments $\Delta_k^{(n)}$ at level n. For this map there will be 2^n segments at level n, with the first few drawn in figure K.2. As $n \to \infty$ the segments that remain for at least n iterates converge to the Cantor set $\mathcal{C}$.

The segments at one level form a cover for the Cantor set and it is from a cover that all the invariant information about the set is extracted (the cover generated from the backward iterates of the gap form a Markov partition for the map as a dynamical system). The segments $\{\Delta_k^{(n)}\}$ at level n are a refinement of the cover formed by segments at level $n-1$. From successive covers we can compute the trajectory scaling function, the spectrum of scalings $f(\alpha)$, and the generalized dimensions.

To define the scaling function we must give labels (names) to the segments. The labels are chosen so that the definition of the scaling function allows for simple approximations. As each segment is generated from an inverse image of the unit interval, we will consider the inverse of the presentation function F. Because F does not have a unique inverse, we have to consider restrictions of F. Its restriction to the first half of the segment, from 0 to 1/2, has a unique inverse, which we will call F_0^{-1}, and its restriction to the second half, from 1/2 to 1, also has a unique inverse, which we will call F_1^{-1}. For example, the segment labeled $\Delta^{(2)}(0,1)$ in figure K.2 is formed from the inverse image of the unit interval by mapping $\Delta^{(0)}$, the unit interval, with F_1^{-1} and then F_0^{-1}, so that the segment

$$\Delta^{(2)}(0,1) = F_0^{-1}\left(F_1^{-1}\left(\Delta^{(0)}\right)\right) . \tag{K.34}$$

The mapping of the unit interval into a smaller interval is what determines its label. The sequence of the labels of the inverse maps is the label of the segment:

$$\Delta^{(n)}(\epsilon_1, \epsilon_2, \ldots, \epsilon_n) = F_{\epsilon_1}^{-1} \circ F_{\epsilon_2}^{-1} \circ \cdots F_{\epsilon_n}^{-1}\left(\Delta^{(0)}\right) .$$

The scaling function is formed from a set of ratios of segments length. We use $|\cdot|$ around a segment $\Delta^{(n)}(\epsilon)$ to denote its size (length), and define

$$\sigma^{(n)}(\epsilon_1, \epsilon_2, \ldots, \epsilon_n) = \frac{|\Delta^{(n)}(\epsilon_1, \epsilon_2, \ldots, \epsilon_n)|}{|\Delta^{(n-1)}(\epsilon_2, \ldots, \epsilon_n)|} .$$

We can then arrange the ratios $\sigma^{(n)}(\epsilon_1, \epsilon_2, \ldots, \epsilon_n)$ next to each other as piecewise constant segments in increasing order of their binary label $\epsilon_1, \epsilon_2, \ldots, \epsilon_n$ so that the collection of steps scan the unit interval. As $n \to \infty$ this collection of steps will converge to the scaling function.

K.5 Geometrization

The $\mathcal{L}$ operator is a generalization of the transfer matrix. It gets more by considering less of the matrix: instead of considering the whole matrix it is possible to consider just one of the rows of the matrix. The $\mathcal{L}$ operator also makes explicit the vector space in which it acts: that of the observable functions. Observables are functions that to each configuration of the system associate a number: the energy, the average magnetization, the correlation between two sites. It is in the average of observables that one is interested in. Like the transfer matrix, the $\mathcal{L}$ operator considers only semi-infinite systems, that is, only the part of the interaction between spins to the right is taken into account. This may sound un-symmetric, but it is a simple way to count each interaction only once, even in cases where the interaction includes three or more spin couplings. To define the $\mathcal{L}$ operator one needs the interaction energy between one spin and all the rest to its right, which is given by the function ϕ. The $\mathcal{L}$ operators defined as

$$\mathcal{L}g(\sigma) = \sum_{\sigma_0 \in \Omega_0} g(\sigma_0\sigma) e^{-\beta\phi(\sigma_0\sigma)} .$$

To each possible value in Ω_0 that the spin σ_0 can assume, an average of the observable g is computed weighed by the Boltzmann factor $e^{-\beta\phi}$. The formal relations that stem from this definition are its relation to the free energy when applied to the observable ι that returns one for any configuration:

$$-\beta f(\beta) = \lim_{n\to\infty} \frac{1}{n} \ln \|\mathcal{L}^n \iota\|$$

and the thermodynamic average of an observable

$$\langle g \rangle = \lim_{n\to\infty} \frac{\|\mathcal{L}^n g\|}{\|\mathcal{L}^n \iota\|} .$$

Both relations hold for almost all configurations. These relations are part of theorem of Ruelle that enlarges the domain of the Perron-Frobenius theorem and sharpens its results. The theorem shows that just as the transfer matrix, the largest eigenvalue of the $\mathcal{L}$ operator is related to the free-energy of the spin system. It also hows that there is a formula for the eigenvector related to the largest eigenvalue. This eigenvector $|\rho\rangle$ (or the corresponding one for the adjoint $\mathcal{L}^*$ of $\mathcal{L}$) is the Gibbs state of the system. From it all averages of interest in statistical mechanics can be computed from the formula

$$\langle g \rangle = \langle \rho | g | \rho \rangle .$$

The Gibbs state can be expressed in an explicit form in terms of the interactions, but it is of little computational value as it involves the Gibbs state for a related spin system. Even then it does have an enormous theoretical value. Later we will see how the formula can be used to manipulate the space of observables into a more convenient space.

The geometrization of a spin system converts the shift dynamics (necessary to define the Ruelle operator) into a smooth dynamics. This is equivalent to the mathematical problem in ergodic theory of finding a smooth embedding for a given Bernoulli map.

The basic idea for the dynamics is to establish the a set of maps F_{σ_k} such that

$$F_{\sigma_k}(0) = 0$$

and

$$F_{\sigma_1} \circ F_{\sigma_2} \circ \cdots \circ F_{\sigma_n}(0) = \phi(+, \sigma_1, \sigma_2, \ldots, \sigma_n, -, -, \ldots)\,.$$

This is a formal relation that expresses how the interaction is to be converted into a dynamical systems. In most examples F_{σ_k} is a collection of maps from a subset of R^D to itself.

If the interaction is complicated, then the dimension of the set of maps may be infinite. If the resulting dynamical system is infinite have we gained anything from the transformation? The gain in this case is not in terms of added speed of convergence to the thermodynamic limit, but in the fact that the Ruelle operator is of trace-class and all eigenvalues are related to the spin system and not artifacts of the computation.

The construction of the higher dimensional system is done by borrowing the state space reconstruction technique from dynamical systems. State space reconstruction can be done in several ways: by using delay coordinates, by using derivatives of the position, or by considering the value of several independent observables of the system. All these may be used in the construction of the equivalent dynamics. Just as in the study of dynamical systems, the exact method does not matter for the determination of the thermodynamics ($f(\alpha)$ spectra, generalized dimension), also in the construction of the equivalent dynamics the exact choice of observable does not matter.

We will only consider configurations for the half line. This is bescause for translational invariant interactions the thermodynamic limit on half line is the same as in the whole line. One can prove this by considering the difference in a thermodynamic average in the line and in the semiline and compare the two as the size of the system goes to infinity.

When the interactions are long range in principle one has to specify the boundary conditions to be able to compute the interaction energy of a configuration in a finite box. If there are no phase transitions for the interaction, then which boundary conditions are chosen is irrelevant in

the thermodynamic limit. When computing quantities with the transfer matrix, the long rrange interaction is truncated at some finite range and the truncated interaction is then use to evaluate the transfer matrix. With the Ruelle operator the interaction is never truncated, and the boundary must be specified.

The interaction $\phi(\sigma)$ is any function that returns a number on a configuration. In general it is formed from pairwise spin interactions

$$\phi(\sigma) = \sum_{n>0} \delta_{\sigma_0,\sigma_n} J(n)$$

with different choices of $J(n)$ leading to differnt models. If $J(n) = 1$ only if $n = 1$ and) otherwise, then one has the nearest neighbor Ising model. If $J(n) = n^{-2}$, then one has the inverse square model relevant in the study of the Kondo problem.

Let us say that each site of the lattice can assume two values $+, -$ and the set of all possible configurations of the semiline is the set Ω. Then an observable g is a function from the set of configurations Ω to the reals. Each configuration is indexed by the integers from 0 up, and it is useful to think of the configuration as a string of spins. One can append a spin η_0 to its begining, $\eta \vee \sigma$, in which case η is at site 0, ω_0 at site 1, and so on.

The Ruelle operator $\mathcal{L}$ is defined as

$$\mathcal{L}g(\eta) = \sum_{\omega_0 \in \Omega_0} g(\omega_0 \vee \eta) e^{-\beta\phi(\omega_0 \vee \eta)}\,.$$

This is a positive and bounded operator over the space of bounded observables. There is a generalization of the Perron-Frobenius theorem by Ruelle that establishes that the largest eigenvalue of $\mathcal{L}$ is isolated from the rest of the spectrum and gives the thermodynamics of the spin system just as the largest eigenvalue of the transfer matrix does. Ruelle alos gave a formula for the eigenvector related to the largest eigenvalue.

The difficulty with it is that the relation between the partition function and the trace of its nth power, $\mathrm{tr}\,\mathcal{L}^n = Z_n$ no longer holds. The reason is that the trace of the Ruelle operator is ill-defined, it is infinite.

We now introduce a special set of observables $\{x_1(\sigma), \ldots, x_1(\sigma)\}$. The idea is to choose the observables in such a way that from their values on a particular configuration σ the configuration can be reconstructed. We also introduce the interaction observables h_{σ_0}

To geometrize spin systems, the interactions are assumed to be translationally invariant. The spins σ_k will only assume a finite number of values. For simplicity, we will take the interaction ϕ among the spins to depend only on pairwise interactions,

$$\phi(\sigma) = \phi(\sigma_0, \sigma_1, \sigma_2, \ldots) = J_0\sigma_0 + \sum_{n>0} \delta_{\sigma_0,\sigma_n} J_1(n) \,, \tag{K.35}$$

and limit σ_k to be in $\{+, -\}$. For the one-dimensional Ising model, J_0 is the external magnetic field and $J_1(n) = 1$ if $n = 1$ and 0 otherwise. For an exponentially decaying interaction $J_1(n) = e^{-\alpha n}$. Two- and three-dimensional models can be considered in this framework. For example, a strip of spins of $L \times \infty$ with helical boundary conditions is modeled by the potential $J_1(n) = \delta_{n,1} + \delta_{n,L}$.

The transfer operator $\mathcal{T}$ was introduced by Kramers and Wannier [K.12] to study the Ising model on a strip and concocted so that the trace of its nth power is the partition function Z_n of system when one of its dimensions is n. The method can be generalized to deal with any finite-range interaction. If the range of the interaction is L, then $\mathcal{T}$ is a matrix of size $2^L \times 2^L$. The longer the range, the larger the matrix. When the range of the interaction is infinite one has to define the $\mathcal{T}$ operator by its action on an observable g. Just as the observables in quantum mechanics, g is a function that associates a number to every state (configuration of spins). The energy density and the average magnetization are examples of observables. From this equivalent definition one can recover the usual transfer matrix by making all quantities finite range. For a semi-infinite configuration $\sigma = \{\sigma_0, \sigma_1, \ldots\}$:

$$\mathcal{T} g(\sigma) = g(+ \vee \sigma) e^{-\beta\phi(+\vee\sigma)} + g(- \vee \sigma) e^{-\beta\phi(-\vee\sigma)} \,. \tag{K.36}$$

By $+ \vee \sigma$ we mean the configuration obtained by prepending $+$ to the beginning of σ resulting in the configuration $\{+, \sigma_0, \sigma_1, \ldots\}$. When the range becomes infinite, $\mathrm{tr}\, \mathcal{T}^n$ is infinite and there is no longer a connection between the trace and the partition function for a system of size n (this is a case where matrices give the wrong intuition). Ruelle [K.13] generalized the Perron-Frobenius theorem and showed that even in the case of infinite range interactions the largest eigenvalue of the $\mathcal{T}$ operator is related to the free-energy of the spin system and the corresponding eigenvector is related to the Gibbs state. By applying $\mathcal{T}$ to the constant observable u, which returns 1 for any configuration, the free energy per site f is computed as

$$-\beta f(\beta) = \lim_{n\to\infty} \frac{1}{n} \ln \|\mathcal{T}^n u\| \,. \tag{K.37}$$

To construct a smooth dynamical system that reproduces the properties of $\mathcal{T}$, one uses the phase space reconstruction technique of Packard *et al.* [K.6] and Takens [K.7], and introduces a vector of state observables $x(\sigma) = \{x_1(\sigma), \ldots, x_D(\sigma)\}$. To avoid complicated notation we will limit the discussion to the example $x(\sigma) = \{x_+(\sigma), x_-(\sigma)\}$, with $x_+(\sigma) = \phi(+ \vee \sigma)$

and $x_-(\sigma) = \phi(- \vee \sigma)$; the more general case is similar and used in a later example. The observables are restricted to those g for which, for all configurations σ, there exist an analytic function G such that $G(x_1(\sigma), \ldots, x_D(\sigma)) = g(\sigma)$. This at first seems a severe restriction as it may exclude the eigenvector corresponding to the Gibbs state. It can be checked that this is not the case by using the formula given by Ruelle [K.14] for this eigenvector. A simple example where this formalism can be carried out is for the interaction $\phi(\sigma)$ with pairwise exponentially decaying potential $J_1(n) = a^n$ (with $|a| < 1$). In this case $\phi(\sigma) = \sum_{n>0} \delta_{\sigma_0,\sigma_n} a^n$ and the state observables are $x_+(\sigma) = \sum_{n>0} \delta_{+,\sigma_n} a^n$ and $x_-(\sigma) = \sum_{n>0} \delta_{-,\sigma_n} a^n$. In this case the observable x_+ gives the energy of $+$ spin at the origin, and x_- the energy of a $-$ spin.

Using the observables x_+ and x_-, the transfer operator can be re-expressed as

$$\mathcal{T} G\left(x(\sigma)\right) = \sum_{\eta\in\{+,-\}} G\left(x_+\left(\eta \vee \sigma\right), x_-\left(\eta \vee \sigma\right)\right) e^{-\beta x_\eta(\sigma)} \,. \tag{K.38}$$

In this equation the only reference to the configuration σ is when computing the new observable values $x_+(\eta \vee \sigma)$ and $x_-(\eta \vee \sigma)$. The iteration of the function that gives these values in terms of $x_+(\sigma)$ and $x_-(\sigma)$ is the dynamical system that will reproduce the properties of the spin system. For the simple exponentially decaying potential this is given by two maps, F_+ and F_-. The map F_+ takes $\{x_+(\sigma), x_+(\sigma)\}$ into $\{x_+(+\vee\sigma), x_-(+\vee\sigma)\}$ which is $\{a(1+x_+), a x_-\}$ and the map F_- takes $\{x_+, x_-\}$ into $\{a x_+, a(1+x_-)\}$. In a more general case we have maps F_η that take $x(\sigma)$ to $x(\eta \vee \sigma)$.

We can now define a new operator $\mathcal{L}$

$$\mathcal{L} G\left(x\right) \stackrel{\text{def}}{=} \mathcal{T} G(x(\sigma)) = \sum_{\eta\in\{+,-\}} G\left(F_\eta(x)\right) e^{-\beta x_\eta} \,, \tag{K.39}$$

where all dependencies on σ have disappeared — if we know the value of the state observables x, the action of $\mathcal{L}$ on G can be computed.

A dynamical system is formed out of the maps F_η. They are chosen so that one of the state variables is the interaction energy. One can consider the two maps F_+ and F_- as the inverse branches of a hyperbolic map f, that is, $f^{-1}(x) = \{F_+(x), F_-(x)\}$. Studying the thermodynamics of the interaction ϕ is equivalent to studying the long term behavior of the orbits of the map f, achieving the transformation of the spin system into a dynamical system.

Unlike the original transfer operator, the $\mathcal{L}$ operator — acting in the space of observables that depend only on the state variables — is of trace-class (its trace is finite). The finite trace gives us a chance to relate the trace of $\mathcal{L}^n$ to the partition function of a system of size n. We can do better.

As most properties of interest (thermodynamics, fall-off of correlations) are determined directly from its spectrum, we can study instead the zeros of the Fredholm determinant $\det(1-z\mathcal{L})$ by the technique of cycle expansions developed for dynamical systems [18.2]. A cycle expansion consists of finding a power series expansion for the determinant by writing $\det(1-z\mathcal{L}) = \exp(\mathrm{tr}\,\ln(1-z\mathcal{L}))$. The logarithm is expanded into a power series and one is left with terms of the form $\mathrm{tr}\,\mathcal{L}^n$ to evaluate. For evaluating the trace, the $\mathcal{L}$ operator is equivalent to

$$\mathcal{L}G(x) = \int_{\mathbf{R}^D} dy\,\delta(y-f(x))e^{-\beta y}G(y) \tag{K.40}$$

from which the trace can be computed:

$$\mathrm{tr}\,\mathcal{L}^n = \sum_{x=f^{(\circ n)}(x)} \frac{e^{-\beta H(x)}}{\left|\det\left(1-\partial_x f^{(\circ n)}(x)\right)\right|} \tag{K.41}$$

with the sum running over all the fixed points of $f^{(\circ n)}$ (all spin configurations of a given length). Here $f^{(\circ n)}$ is f composed with itself n times, and $H(x)$ is the energy of the configuration associated with the point x. In practice the map f is never constructed and the energies are obtained directly from the spin configurations.

To compute the value of $\mathrm{tr}\,\mathcal{L}^n$ we must compute the value of $\partial_x f^{(\circ n)}$; this involves a functional derivative. To any degree of accuracy a number x in the range of possible interaction energies can be represented by a finite string of spins ϵ, such as $x = \phi(+,\epsilon_0,\epsilon_1,\ldots,-,-,\ldots)$. By choosing the sequence ϵ to have a large sequence of spins $-$, the number x can be made as small as needed, so in particular we can represent a small variation by $\phi(\eta)$. As $x_+(\epsilon) = \phi(+\vee\epsilon)$, from the definition of a derivative we have:

$$\partial_x f(x) = \lim_{m\to\infty} \frac{\phi(\epsilon\vee\eta^{(m)})-\phi(\epsilon)}{\phi(\eta^{(m)})}, \tag{K.42}$$

where $\eta^{(m)}$ is a sequence of spin strings that make $\phi(\eta^{(m)})$ smaller and smaller. By substituting the definition of ϕ in terms of its pairwise interaction $J(n) = n^s a^{n^\gamma}$ and taking the limit for the sequences $\eta^{(m)} = \{+,-,-,\ldots,\eta_{m+1},\eta_{m+2},\ldots\}$ one computes that the limit is a if $\gamma=1$, 1 if $\gamma<1$, and 0 if $\gamma>1$. It does not depend on the positive value of s. When $\gamma<1$ the resulting dynamical system is not hyperbolic and the construction for the operator $\mathcal{L}$ fails, so one cannot apply it to potentials such as $(1/2)^{\sqrt{n}}$. One may solve this problem by investigating the behavior of the formal dynamical system as $\gamma\to 0$.

The manipulations have up to now assumed that the map f is smooth. If the dimension D of the embedding space is too small, f may not be smooth. Determining under which conditions the embedding is smooth is a

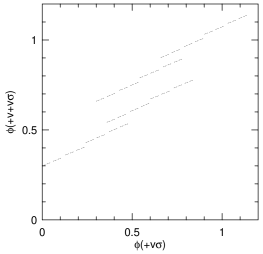

Figure K.3: The spin adding map F_+ for the potential $J(n) = \sum n^2 a^{\alpha n}$. The action of the map takes the value of the interaction energy between $+$ and the semi-infinite configuration $\{\sigma_1,\sigma_2,\sigma_3,\ldots\}$ and returns the interaction energy between $+$ and the configuration $\{+,\sigma_1,\sigma_2,\sigma_3,\ldots\}$.

complicated question [K.15]. But in the case of spin systems with pairwise interactions it is possible to give a simple rule. If the interaction is of the form

$$\phi(\sigma) = \sum_{n\geq 1}\delta_{\sigma_0,\sigma_n}\sum_k p_k(n)a_k^{n^\gamma} \tag{K.43}$$

where p_k are polynomials and $|a_k|<1$, then the state observables to use are $x_{s,k}(\sigma) = \sum \delta_{+,\sigma_n} n^s a_k^n$. For each k one uses $x_{0,k}, x_{1,k},\ldots$ up to the largest power in the polynomial p_k. An example is the interaction with $J_1(n) = n^2(3/10)^n$. It leads to a 3-dimensional system with variables $x_{0,0}$, $x_{1,0}$, and $x_{2,0}$. The action of the map F_+ for this interaction is illustrated figure K.3. Plotted are the pairs $\{\phi(+\vee\sigma),\phi(+\vee+\vee\sigma)\}$. This can be seen as the strange attractor of a chaotic system for which the variables $x_{0,0}$, $x_{1,0}$, and $x_{2,0}$ provide a good (analytic) embedding.

The added smoothness and trace-class of the $\mathcal{L}$ operator translates into faster convergence towards the thermodynamic limit. As the reconstructed dynamics is analytic, the convergence towards the thermodynamic limit is faster than exponential [2.17, K.16]. We will illustrate this with the polynomial-exponential interactions (K.43) with $\gamma=1$, as the convergence is certainly faster than exponential if $\gamma>1$, and the case of a^n has been studied in terms of another Fredholm determinant by Gutzwiller [K.17]. The convergence is illustrated in figure K.4 for the interaction $n^2(3/10)^n$. Plotted in the graph, to illustrate the transfer matrix convergence, are the number of decimal digits that remain unchanged as the range of the interaction is increased. Also in the graph are the number of decimal digits that remain unchanged as the largest power of $\mathrm{tr}\,\mathcal{L}^n$ considered. The plot is effectively a logarithmic plot and straight lines indicate exponentially fast convergence. The curvature indicates that the convergence is faster than exponential. By fitting, one can verify that the free energy is converging to its limiting value as $\exp(-n^{(4/3)})$. Cvitanović [2.17] has estimated that the Fredholm determinant of a map on a D dimensional space should converge as $\exp(-n^{(1+1/D)})$, which is confirmed by these numerical simulations.

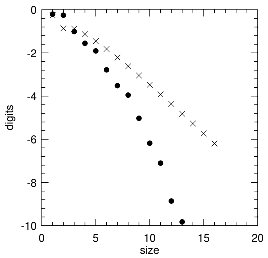

Figure K.4: Number of digits for the Fredholm method (•) and the transfer function method (×). The size refers to the largest cycle considered in the Fredholm expansions, and the truncation length in the case of the transfer matrix.

Commentary

Remark K.1 Presentation functions. The best place to read about Feigenbaum's work is in his review article published in *Los Alamos Science* (reproduced in various reprint collections and conference proceedings, such as ref. [18.5]). Feigenbaum's *Journal of Statistical Physics* article [27.13] is the easiest place to learn about presentation functions.

Remark K.2 Interactions are smooth In most computational schemes for thermodynamic quantities the translation invariance and the smoothness of the basic interaction are never used. In Monte Carlo schemes, aside from the periodic boundary conditions, the interaction can be arbitrary. In principle for each configuration it could be possible to have a different energy. Schemes such as the Sweneson-Wang cluster flipping algorithm use the fact that interaction is local and are able to obtain dramatic speed-ups in the equilibration time for the dynamical Monte Carlo simulation. In the geometrization program for spin systems, the interactions are assumed translation invariant and smooth. The smoothness means that any interaction can be decomposed into a series of terms that depend only on the spin arrangement and the distance between spins:

$$\phi(\sigma_0, \sigma_1, \sigma_2, \ldots) = J_0\sigma_0 + \sum \delta(\sigma_0, \sigma_n) J_1(n) + \sum \delta(\sigma_0, \sigma_{n_1}, \sigma_{n_2}) J_2(n_1, n_2) + \cdots$$

where the J_k are symmetric functions of their arguments and the δ are arbitrary discrete functions. This includes external constant fields (J_0), but it excludes site dependent fields such as a random external magnetic field.

Résumé

The geometrization of spin systems strengthens the connection between statistical mechanics and dynamical systems. It also further establishes the value of the Fredholm determinant of the $\mathcal{L}$ operator as a practical computational tool with applications to chaotic dynamics, spin systems, and semiclassical mechanics. The example above emphasizes the high accuracy that can be obtained: by computing the shortest 14 periodic orbits of period 5 or less it is possible to obtain three digit accuracy for

the free energy. For the same accuracy with a transfer matrix one has to consider a 256×256 matrix. This make the method of cycle expansions practical for analytic calculations.

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