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Lyapunov Exponents of Stochastic Dynamical Systems

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It is shown that stochastic equations can have stable solutions. In particular, there exists stochastic dynamics for which the motion is both ergodic and stable, so that all trajectories merge with time. We discuss this in the context of Monte Carlo-type dynamics, and study the convergence of nearby trajectories as the number of degrees of freedom goes to infinity and as a critical point is approached. A connection with critical slowdown is suggested.

KEY WORDS: Stochastic dynamics; chaos; Lyapunov exponents; Monte Carlo; critical phenomena.

1. INTRODUCTION

There has been much interest in the past few years in the onset of instabilities in dynamical systems.[1] Chaotic behavior arises because of sensitive dependence on initial conditions. This can be characterized by a Lyapunov exponent. The effects of a small amount of noise have been investigated and are now well understood.[2] The noise in physical systems is usually due to thermal fluctuations, but it is also sometimes useful to view some of the internal degrees of freedom as generating noise for the modes of interest. A familiar equation which describes the effects of thermal noise is the Langevin equation. It leads to Brownian motion, and is in fact a stochastic equation. The noise it models can be thought of as being very large. Our purpose is to understand the existence of instabilities in the large noise limit, so we will study the stability of the solutions to stochastic equations. It was realized some time ago that Lyapunov exponents could

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be used to characterize the stability of stochastic as well as ordinary differential equations.[3] We present here both numerical and analytical results for Lyapunov exponents of these systems.

For the stochastic equations of motion we consider, standard theorems show that the trajectories generated are ergodic, that is, any trajectory fills configuration space densely. The ergodicity however does not require the motion to be sensitive to perturbations or initial conditions. It is in fact very easy to find ergodic stochastic dynamics where all initial conditions converge exponentially in time to a unique trajectory.

Our emphasis is on Monte Carlo dynamics of thermodynamical systems. The stability of the motion thus depends both on the volume and the temperature. The discussion is as follows.

Sections 2 and 3 review some necessary notions of Lyapunov exponents and Monte Carlo dynamics. Section 4 gives examples of stochastic dynamics for which the Lyapunov exponents exist and such that all trajectories merge with time. Section 5 discusses properties of the Lyapunov exponents as the number of degrees of freedom is increased, and as one approaches a second order phase transition. It is argued that the exponent for critical slowdown "z" determines how the maximum Lyapunov exponent scales as $\beta \to \beta c$. These points are illustrated with a simulation of the $O(3)$ model.

2. STABILITY AND LYAPUNOV EXPONENTS OF A DYNAMICAL SYSTEM

Consider a set of first-order equations for an N-component vector:

$$\dot{X}_i = F_i(X, t), \qquad i = 1, N \tag{1}$$

where one allows an explicit time dependence in F. The motion is asymptotically stable if a small change $\delta X(0)$ in the initial position does not affect the long-time behavior of the trajectory, $X(t)$. Sufficiently close trajectories then converge with time. Consider a nearby trajectory, $X(t) + \delta X(t)$. To lowest order in δX. we have

$$\delta \dot{X}(t) = \frac{\partial F}{\partial X} \delta X(t) = J(X, t)\, \delta X(t) \tag{2}$$

The asymptotic stability of the trajectory is assured if

$$\delta X(t) \to 0 \qquad \text{as} \quad t \to \infty \tag{3}$$

It may happen that the quantity

$$\lambda^1 = \lim_{t \to \infty} \frac{1}{t} \ln \frac{\|\delta X(t)\|}{\|\delta X(0)\|} \tag{4}$$

exists for almost all initial vectors $\delta X(0)$. The existence of this limit has been proved only for a limited class of dynamics,[4] but it seems to exist for many dynamical systems.[5] Then, from Eq. (4), one sees that two trajectories on average converge or diverge exponentially in time. λ^1 is called the one-dimensional Lyapunov exponent. A sufficient condition for the motion to be stable is that λ^1 be strictly negative.

One can also consider the evolution of an infinitesimal k-dimensional parallelepiped. Its volume on average increases or decreases exponentially at a rate given by the kth dimensional Lyapunov exponent. From these exponents, one defines the Lyapunov spectrum which describes how the various directions δX grow or shrink exponentially with time.

The above equations can be extended to discrete time maps in a straightforward way. Analogously to Eqs. (1) and (2), one has

$$\begin{aligned} X(n+1) &= F(X(n), n) \\ \delta X(n+1) &= \frac{\partial F}{\partial X} \delta X(n) = J(X(n), n)\, \delta X(n) \end{aligned} \tag{5}$$

One can similarly discuss the stability of the motion and consider the Lyapunov exponent

$$\lambda^1 = \lim_{n \to \infty} \frac{1}{n} \ln \frac{\|\delta X(n)\|}{\|\delta X(0)\|} \tag{6}$$

as well as the Lyapunov spectrum.

This formalism will be applied to stochastic differential equations and stochastic maps in Section 4. Next, we describe Monte Carlo dynamics which is an example of a stochastic map.

3. MONTE CARLO DYNAMICS

Monte Carlo simulations are widely used for determining properties of statistical systems, and in particular for measuring critical exponents. Consider a thermodynamical system which has an energy function H defined on a space of N variables. The Monte Carlo generates a sequence of points $X(n)$ in this N-dimensional space such that the long-time behavior of the distribution of these points is Boltzmannian, i.e., the points have relative probabilities $\exp[-\beta H(X)]$, where β is the inverse temperature of the system. At each time step n, one "updates" $X(n)$, the current value of X: a new vector $X(n+1)$ is chosen with probability $T(X(n), X(n+1))$, making $X(n+1)$ a stochastic function of $X(n)$. T is called the transition matrix, and defines a Markov process. T is chosen so that the sequence $X(n)$ is ergodic. Ensemble averages can then be replaced by time averages. In practice, the choice of $X(n+1)$ is obtained by taking $X(n+1) = F(X(n), R(n))$ where $R(n)$ is a random number or vector, and F is a function chosen so that $X(n+1)$ has the right probability distribution. For a fixed sequence $R(n)$, one can consider the Monte Carlo dynamics $X(n+1) = F(X(n), n)$ as a time dependent (deterministic) map. The formalism of Section 2 thus applies.

Note that the statics (i.e., H) of a statistical mechanical model do not specify T uniquely. Different choices of T lead to different dynamics and thus to different Monte Carlo methods: metropolis, heat bath, etc.... It is important to observe that T does not uniquely specify F either: the probability distribution of $X(n+1)$ is unchanged if one substitutes for $R(n)$ another random number $h(X(n), R(n))$ as long as h preserves the probability distribution of the random number. The function h thus does not affect the statistical properties of the Markov chain, but it will affect the Lyapunov exponents as discussed in Section 4.

When do these discrete time dynamics have Lyapunov exponents? In the standard Metropolis method, the Jacobian matrix J is singular, so one does not expect λ^1 to exist. Many other Monte Carlo dynamics though have analytic Jacobians. In such cases, as long as the Markov chain has only short term memory and is ergodic, it is natural to expect that λ^1 and possibly the whole Lyapunov spectrum exists.

Since the motion depends on the sequence of random numbers $R(n)$, the Lyapunov exponents may *a priori* depend on the choice of $R(n)$. However, the exponents are defined in the infinite time limit. They thus depends on the statistical properties of the tail of the sequence, and so should be constant for almost all sequences $R(n)$.[3]

4. EXAMPLES OF ERGODIC DYNAMICS WITH NEGATIVE LYAPUNOV EXPONENTS

4.1. Langevin Dynamics

The Langevin equations are first-order, continuous-time stochastic equations which describe the brownian motion of interacting particles in contact with a thermal bath at inverse temperature β. For an energy function $H(X)$, the equations of motion are (in vector notation)

$$X(t) = -\beta \frac{\partial H}{\partial X} + \eta(t) \tag{7}$$

where the η's are independent Gaussian random variables. It can be shown that time averages using these equations lead to the correct ensemble averages, i.e., the trajectory is ergodic with probability one and reproduces the Boltzmann distribution. The equations of motion for a difference vector are simply

$$\delta\dot{X}(t) = -\beta \frac{\partial^2 H}{\partial X \partial X} \delta X(t). \tag{8}$$

Consider first a single particle in a harmonic potential so that $\partial^2 H/\partial X \partial X$ is constant and positive. Then λ^1 exists and the motion is absolutely stable: $\delta X(t) \to 0$; all initial conditions converge exponentially in time to the same trajectory. The same result holds for a system of coupled harmonic oscillators describing free fields on a lattice: the Lyapunov exponents are all negative, the maximum exponent being the negative of the mass squared. For general H, a sufficient condition for the stability of the motion of Eq. (7) is $\partial^2 H/\partial X \partial X > 0$. This is satisfied for massive free fields and also for a class of interacting field theories.(6)

4.2. The Heat Bath Method

In the Monte Carlo method, time is discrete. A simple way to ensure Boltzmann distribution is to update the components of X one at a time while satisfying detailed balance. At the time step n, only the component $j(n)$ of $X(n)$ is changed:

$$X_i(n+1) = \delta_{i,j(n)} F_{j(n)}(X(n), n, \beta) + (1 - \delta_{i,j(n)})\, X_i(n) \tag{9}$$

In the heat bath method, F is chosen so that $X_{j(n)}$ has a Boltzmann distribution. For our purposes, the various components i of X will be variables on a lattice. These variables can be updated in a random or in an orderly fashion. To keep the discussion as simple as possible, we shall consider the latter kind of update only, so one can introduce the notion of a sweep. After one sweep, all the variables on the lattice have been updated exactly once. Denoting by s the sweep number, we have

$$X(s+1) = G(X(s), R(s), \beta) \tag{10}$$

where $R(s)$ denotes the random numbers used in the sweep. If F (and thus G) is differentiable, the behavior of an infinitesimal difference vector is given by

$$\delta X(s+1) = J_G(X(s), R(s), \beta)\, \delta X(s) \tag{11}$$

as in Eq. (5).

If $\|J_G\| < 1$ for all (X, R), then necessarily the motion is stable:

$$\lim_{\delta \to \infty} \delta X(s) = 0 \tag{12}$$

This does not even require λ^1 to exist. Now we will show that for the heat bath algorithm, one can find an F such that $\|J\| \sim \beta$ as $\beta \to 0$. Thus, at least at high temperatures, there exist dynamics such that all trajectories merge with time: the motion is absolutely stable.

In the heat bath algorithm, the updated variable has a Boltzmann distribution. At $\beta = 0$, this distribution is "flat," so one can take an F such that $X(n+1) = F(X(n), R(n), \beta = 0)$ is completely independent of $X(n)$. Then $\|J\| = 0$ at $\beta = 0$. If F is taken to be differentiable (this is possible if H is differentiable), one has $\|J\| \ll 1$ for $\beta \ll 1$. The motion is then both stable at high temperatures and ergodic. In non stochastic maps, the stability decreases with increasing noise (temperature), and here it is the opposite. This can be understood easily: in the first case, one is perturbing about an orbit with no noise (deterministic). In the second case, the orbit at high temperature is determined mainly by the sequence of random numbers, and it is the "deterministic" piece which generates the instability or perturbation. If λ^1 exists, one has $\lambda^1 \sim \ln \beta \ll 0$. We will now give numerical evidence that λ^1 does indeed exist for certain choices of F.

We considered the $O(3)$ model which is a two-dimensional spin model. The spin variables are normalized three-component vectors which live on the lattice sites. We took several differentiable choices of F corresponding to a heat bath on each site, and considered both sequential and checkerboard updates. (See the Appendix for details.) We used the algorithm of Ref. 5 to calculate the exponents, and observed that they converged to their limits statistically. There is thus good numerical evidence that the Lyapunov spectrum exists. Fig. 1 shows a summary of the values of λ^1 as a function of β. The main features are (i) certain choices of F lead to $\lambda^1 \sim \ln \beta$ as argued above; it is not difficult to have ergodic and stable motion at small β; (ii) as β increases, λ^1 tends to increase, sometimes becoming positive at low enough temperatures.

What limits the stability of the motion, and in particular, when does the motion have to become unstable? Given the possibility of stability at

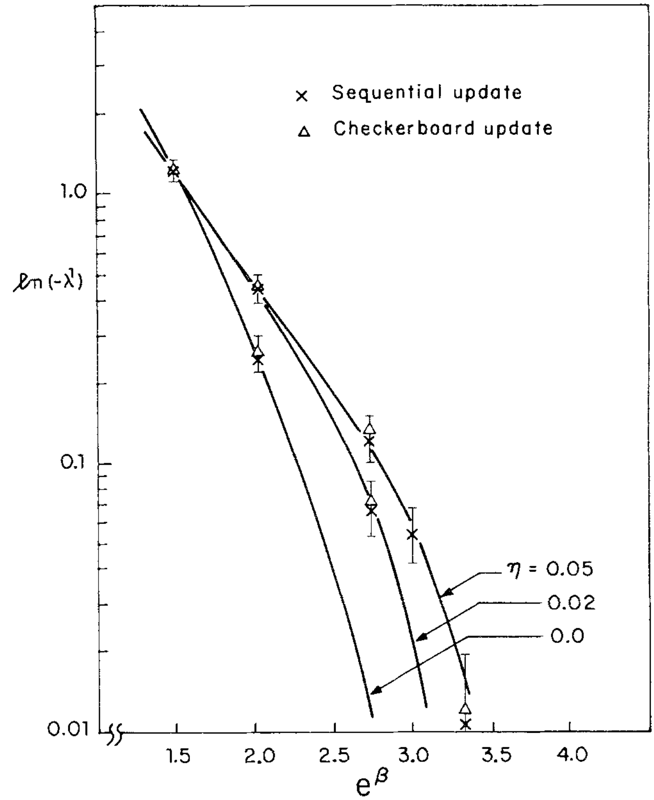

Fig. 1. The one-dimensional Lyapunov exponent for a one-parameter family of F's in a heat bath simulation of the $O(3)$ model.

high temperature for our choice of the transition matrix T, there should be a critical value of the inverse temperature, $\beta_c(T)$, above which all choices of F lead to unstable motion.

4.3. Condition for the Negativity of λ^1

Here, we make use of a connection between stability and a source method which can be used to extract correlation functions.[6,7] Consider a persistent perturbation of an absolutely stable motion. If the perturbation is small enough, the distance between the perturbed and unperturbed trajectories remains bounded in time.[8] Apply this to a lattice system where the metric on configuration space is given by the norm $\|X\| = \sum_j |X_j|$. Suppose there is a choice of F such that the motion is absolutely stable. Now add a perturbation εX_{i_0} to the energy function H. It is not difficult to see that the difference of the perturbed and unperturbed trajectories satisfies

$$\langle \delta X(t) \rangle_t = \langle X(\varepsilon, t) - X(\varepsilon = 0, t) \rangle_t \underset{\varepsilon \to 0}{\simeq} \varepsilon \langle X_{i_0} X \rangle^c \tag{13}$$

where $\langle \ \rangle_t$ denotes a time average. The rightmost average is an ensemble one, and leads to a connected correlation function. Taking norms, one has

$$\langle \| \delta X(t) \| \rangle_t \geqslant \varepsilon \sum_j \langle X_{i_0} X_j \rangle^c \tag{14}$$

By hypothesis, this is bounded. If the lattice model under consideration is in a massless phase where the correlation length is infinite, correlation functions fall off as a power:

$$\langle X_i X_j \rangle^c \sim |i - j|^{-(d-2+\eta)}, \qquad \eta > 0 \tag{15}$$

d being the dimension of the system. Then the sum in Eq. (14) diverges in the infinite-volume limit, violating the inequality. This shows that generically, no choice of F can lead to absolute stability in the infinite-volume limit unless the correlation length is finite. Conversely, it may be that there exists a choice of F which leads to absolutely stable motion as long as correlation functions fall off exponentially. The critical inverse temperature of H then coincides with the onset of instability, $\beta_c(T)$. This seems to be the case for the $O(3)$ heat bath for sequential and checkerboard updates. For this model, spin-spin correlation functions fall off exponentially with distance at all β. Our results for λ^1 are displayed in Fig. 1. For all β, we have been able to find F's so that $\lambda^1 < 0$, though this becomes more and more difficult with increasing β. We thus suspect that for our choice of T (the heat bath), $\beta_c(T) = \beta_c$.

5. SCALING PROPERTIES OF THE LYAPUNOV EXPONENTS

5.1. The Infinite-Volume Limit

Consider a system of N uncoupled nonautonomous differential equations, and suppose that each equation has a one dimensional exponent. To find the exponents of the system of equations, take a difference vector δX with only one nonzero component: the Lyapunov spectrum of the total system is simply given by the set of exponents of the equations. Now imagine turning on a coupling between the equations and increasing N while keeping the coupling fixed at some value which is not too small. The difference vector obeys

$$\delta \dot{X}_i = \sum_j J_{ij}(X)\, \delta X_j \tag{16}$$

If all the variables are directly coupled to each other, the matrix $J(X)$ will have a largest eigenvalue which typically grows like N. This will happen for instance if $J_{ij} > 0$ for all (i, j), but slower growth can be expected if the J_{ij} are more random. λ^1 should have this same N dependence, so that in the above example, $\lambda^1 \sim N$. This has been seen numerically for a system with long-range interactions.(9) If, however, the number of variables which are coupled to any given one is fixed, the spectrum of $J(X)$ is bounded from above and below, independently of N, so one should have

$$\lambda^1 \to \text{const} \qquad \text{as} \quad N \to \infty \tag{17}$$

and one can argue similarly for the smallest exponent. Then the Lyapunov spectrum is bounded, and remains so as $N \to \infty$. This will be the case hereafter.

Similar arguments hold for discrete-time equations. From now on, we shall consider Monte Carlo lattice simulations to be specific. To keep the analogy with the continuous-time equations as close as possible, time will be measured in sweep units. Usually the interaction energy is of short range. The number of degrees of freedom directly coupled to each other is independent of N, so λ^1 should have a limit as the volume $N \to \infty$. However, for sequential updates, if $\|J\| > 1$, the limit may be infinity since a disturbance can propagate throughout the whole lattice in one sweep. A checkerboard update does not have this bad property and should have a smooth infinite-volume limit, converging as $N \to \infty$. In practice, we found that as long as $\lambda^1 < 0$, the sequential update had a finite $N \to \infty$ limit also.

As $N \to \infty$, all N exponents are restricted to a finite interval, $[a, b]$. There is thus an increasing density of exponents, and this density should grow linearly with N. This points to the existence of a function $\rho(\lambda)$ such that the number of exponents in an interval $d\lambda$ is given by $N\rho(\lambda)\, d\lambda$ as $N \to \infty$. This is to be contrasted with systems with a continuum of degrees of freedom,(10) where the density became independent of N and the spectrum became unbounded from below. In Fig. 2, the approach to the infinite volume is shown for the heat bath dynamics studied. The density of exponents shows a linear growth with N. This property can also be checked for free fields for both heat bath and Langevin dynamics.

What is the dependence of the maximum exponent λ^1 on the volume? The equilibrium distribution of the lattice at finite N has corrections to the

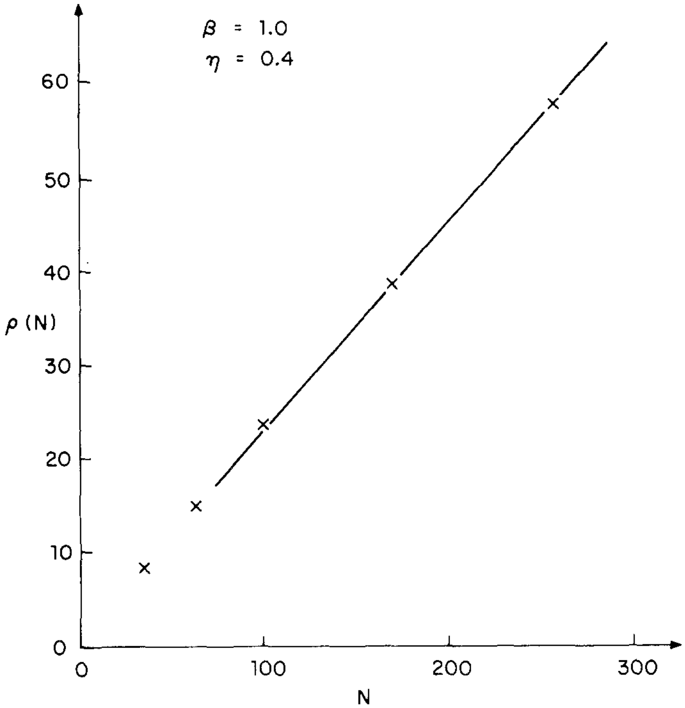

Fig. 2. Density of Lyapunov exponents at $\lambda = \lambda^1$ as a function of the lattice volume. $\beta = 1.0$; $\eta = 0.4$.

infinite-volume limit which are of order $\exp(-L/\xi)$, where ξ is the correlation length and L is the linear size of the lattice. (In our simulations, $L^2 = N$.) λ^1 should have similar corrections as confirmed by Fig. 3. In the case of a sequential update, one can expect in addition $\exp(\lambda^1 L)$ corrections. Note that these are responsible for the bad $N \to \infty$ limit when $\lambda^1 > 0$.

5.2. Temperature Dependence and Scaling

Let us assume as the numerical results suggest that λ^1 can be negative throughout the entire massive phase. It is evident from Fig. 1 that as the critical point $\beta = \infty$ of the $O(3)$ model is approached, the lower bound over F of λ^1 goes to 0. It is natural to expect a critical behavior of the form

$$\min_F \lambda^1 \sim \xi^{-y} \tag{18}$$

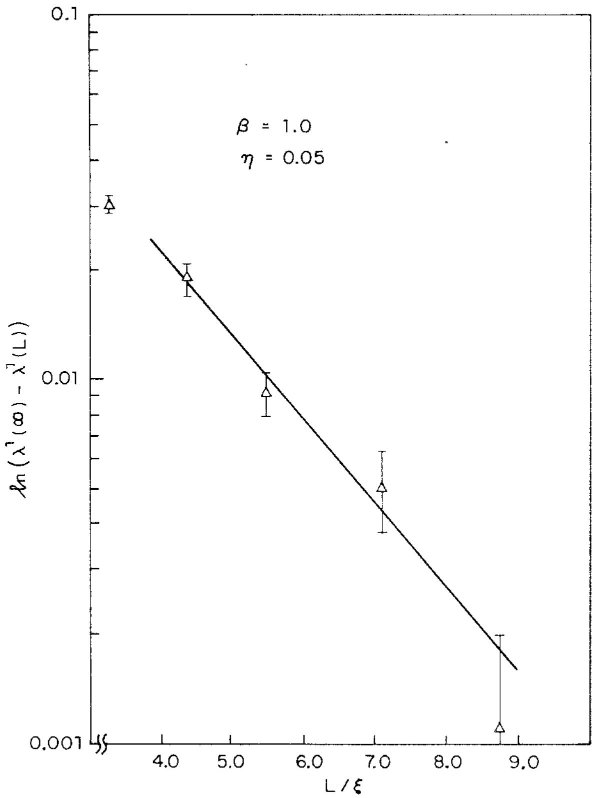

Fig. 3. Convergence of λ^1 to the infinite volume limit as a function of L/ξ for a checkerboard update. $\beta = 1.0$; $\eta = 0.05$.

where ξ is the correlation length and y is a new critical exponent. This scaling law can be checked in the case of free fields for heat bath and Langevin dynamics.

Is y related to known critical exponents? It is well known that the dynamics slow down at a critical point: there are modes which become static as $\beta \to \beta_c$. This critical slow down is characterized by a diverging autocorrelation time τ:

$$\tau \sim \xi^z \tag{19}$$

τ is the natural time scale of the dynamics. If no other time scale is involved in the problem, y and z should be identical. This is indeed the case for free fields, but more generally, it may be that only $y \geqslant z$. Numerical experiments can only set a bound on y as it is difficult in practice to do a thorough minimization over F. We have not considered the most general form for F, but our numerical results are certainly in agreement with the above inequality.

6. CONCLUSIONS

We have considered the stability of stochastic dynamics. There is a very large class of such dynamics which are ergodic and yet have all trajectories merge with time. The trajectories are then completely insensitive to initial conditions. We focused on equilibrium thermodynamic systems, and showed that the equations of motions can be very stable at high temperature (large thermal noise). We proved that a necessary condition for stability is that the correlation length be finite. It was argued that the number of Lyapunov exponents per degree of freedom should have a thermodynamical limit, and we discussed the finite-volume corrections to this limit. Finally, the maximum Lyapunov exponent has a critical behavior at the onset of the instability which can probably be related to usual critical properties.

APPENDIX

The partition function of the $O(3)$ model is

$$Z = \int \prod dS \exp\left(\beta \sum_{x,\mu} S_x S_{x+\mu}\right) \tag{A1}$$

where β is the inverse temperature, and S is a three-component spin of unit magnitude. The spins live on the sites x of a two-dimensional lattice, and are coupled by a nearest-neighbor spin–spin interaction. For heat bath dynamics, the updated spin has a probability distribution

$$dP(S_i) = C \exp\left(\beta S_i \sum_{J\mu} S_{i+\mu}\right) d\Omega \tag{A2}$$

where $d\Omega$ is the solid angle. The spin S_i thus has a Boltzmann distribution in an external field of direction $w = \sum_{\pm\mu} S_{i+\mu}/|\sum_{\pm\mu} S_{i+\mu}|$. To generate S_i, start with a random spin R on the sphere with a flat distribution. Let α be the angle between R and w. We choose F so that S_i is in the (R, w) plane, and makes an angle θ with w, where

$$\cos(\theta) = \ln[e^{\tilde\beta} + (\cos\alpha - 1)\sinh(\alpha)]/\tilde\beta$$
$$\tilde\beta = \beta\left|\sum_{\pm\mu} S_{i+\mu}\right| \tag{A3}$$

With this choice of F, λ^1 exists, and $\lambda^1 \sim \ln(\beta/2)$ as $\beta \to 0$. However at $\beta \sim 1.1$, λ^1 becomes positive. Any relabeling of R which preserves its (flat) distribution gives another possible F. A simple class of such relabelings is the set of continuous maps from the sphere to the sphere which are area preserving. In practice, this is a much too large space to explore, so we have restricted ourselves to a one-parameter family of rotations of the sphere. These rotations take the z axis into

$$w = \left(z + \eta \sum_{\pm\mu} S_{i+\mu} \right) \Bigg/ \left| z + \eta \sum_{\pm\mu} S_{i+\mu} \right| \tag{A4}$$

η is a real number parametrizing these rotations. The first choice of F is obtained for $\eta = \infty$. Figure 1 shows the values of λ^1 for a range of η's.

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