

Ergodicity properties of energy conserving single spin flip dynamics in the XY model

Abhishek Dhar

Theoretical Physics Group, Tata Institute of Fundamental Research, Homi Bhabha Road, Bombay 400005, India.

e-mail : abhi@theory.tifr.res.in

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A single spin flip stochastic energy conserving dynamics for the XY model is considered. We study the ergodicity properties of the dynamics. It is shown that phase space trajectories densely fill the geometrically connected parts of the energy surface. We also show that while the dynamics is discrete and the phase point jumps around, it cannot make transitions between closed disconnected parts of the energy surface. Thus the number of distinct sectors depends on the number of geometrically disconnected parts of the energy surface. Information on the connectivity of the surfaces is obtained by studying the critical points of the energy function. We study in detail the case of two spins and find that the number of sectors can be either one or two, depending on the external fields and the energy. For a periodic lattice in d dimensions, we find regions in phase space where the dynamics is non-ergodic and obtain a lower bound on the number of disconnected sectors. We provide some numerical evidence which suggests that such regions might be of small measure so that the dynamics is effectively ergodic.

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I. INTRODUCTION

A much studied problem in non-equilibrium statistical mechanics is the problem of heat conduction. Here one is interested in obtaining the steady state of a system whose two ends are kept at different temperatures. Some of the important problems are to see if local thermal equilibrium is achieved in the steady state, to calculate the temperature profile inside the system and to check the validity of linear response laws relating heat current and temperature gradient (Fourier Heat Law). In this context models with both deterministic and stochastic dynamics have been studied. Rieder et al exactly solved the problem of heat conduction in harmonic chains [1]. They found a constant temperature distribution inside the system and a heat current that was independent of system size. Since then, various authors have studied the effect of impurity and nonlinearity in one and two dimensional systems of interacting atoms evolving via deterministic Newtonian dynamics [2–4]. Numerical studies show that with some kinds of interaction one gets realistic temperature profiles and heat currents proportional to inverse of system size [4]. For the Lorenz gas in the Boltzmann-Grad limit, it has been proved that the linear Boltzmann equation holds and in this case too one gets the Fourier Law [5]. There are however not too many studies on heat conduction in stochastic models. Connor and Lebowitz studied the random reflection model in which particles moving on a line are reflected with some probability from randomly spaced scatterers [3]. Streater has studied heat conduction in a lattice model with finite degrees of freedom [6].

In this paper we are interested in stochastic lattice models of heat conduction. Specifically we look at classical spin systems with some kind of imposed dynamics. In studying spin systems one typically uses dynamics such as Glauber where each point of the lattice is kept in contact with heat baths at given temperature. In this case the spin flip rates are assumed to satisfy detailed balance condition, with the rates depending on the heat bath temperature. For equilibrium studies the same temperature is imposed at all points and the steady state is the canonical distribution. However, in studying heat conduction, the temperature distribution in the steady state is not known beforehand and should come out of the dynamics. Since the temperature is space dependent and not known in the beginning, one cannot specify the relaxation rates for energy raising and energy lowering transitions. The only simple choice is to make such rates zero. Thus we use dynamics where there is no exchange of heat with external reservoirs (except at the two ends) and there is local conservation of energy. However, in this case the dynamics becomes highly constrained, and it is not clear that it wont get stuck. A requirement of correct phenomenological description is that the system should relax to a state of local thermal equilibrium. In order that this occurs, we expect that the isolated system should reach thermal equilibrium, that is the dynamics should be ergodic and lead to a microcanonical distribution. In this paper we address this problem only. We study heat conduction in our model in a future paper.

It is easy to show that the Ising model with single spin flip energy conserving dynamics is non-ergodic in dimensions higher than one. For example, suppose we take a d -dimensional hypercubic lattice of N sites, and consider the spin configuration of one single up-spin in a sea of down-spins. If we take periodic boundary conditions then there are

N degenerate energy configurations corresponding to the N places where the single up-spin can be located. The dynamics does not connect these states. For other energies too one can show that there is no ergodicity. In order to do microcanonical simulations for the Ising model it is thus necessary to couple it to other degrees of freedom with which it can exchange energy. This has been studied by Bhanot et al [7]. Heat conduction in the Ising model (with additional degrees of freedom) was studied by Creutz [8].

One can ask what happens if we replace the Ising spins by continuous spins. Microcanonical simulations of the XY model have earlier been done by introducing additional degrees of freedom. This include the molecular dynamics study by Kogut and Polonyi who introduce momentum variables and use a continuous time Hamiltonian dynamics [9]. A microcanonical simulation using the Creutz algorithm was done by Ota et al [10].

In this paper we consider an energy conserving single spin flip dynamics for the XY model, with no additional degrees of freedom, and look at its ergodicity properties. We first study the instructive case of two spins interacting with each other and with external fields. This case is still non-trivial but can be worked out in full detail. We show that for generic values of external fields, the phase space trajectories (note that the trajectory is not continuous and is formed by the random iterates of a phase point) densely fill the geometrically connected parts of the constant energy contours. Thus whenever the energy contours are fully connected we have ergodicity. On the other hand, even though the dynamics is discontinuous, we show that jumps between closed disconnected parts of the energy contours are not allowed. Thus in such cases we have non-ergodic behavior and we have as many sectors as disconnected energy parts, within each of which the dynamics is ergodic. Thus ergodicity is related to nature of the constant energy contours. Information regarding the nature of the energy contours can be obtained from a study of the critical points. These are points at which the derivative of the energy w.r.t all angles vanish. For instance, if there are two or more stable critical points (these correspond to fixed points of the dynamics) with the same energy values then we will have closed energy contours around each of them, which are disconnected. We find that the nature of energy contours depend on the external fields. For some fields there are only single sectors at all energies while for other field values there are one or two sectors depending on the energy.

Next we study the case of $N > 2$ spins. Using the two spin results, we prove that even for the general case of N interacting spins, the phase space trajectory densely covers the geometrically connected parts of the constant energy surface. Thus ergodicity is related to the connectivity properties of the energy surfaces. As in the two-spin case, some information can be obtained by looking at the critical points. As an illustrative example, we study a system of three spins interacting with each other and with external fields. We show that the energy surfaces can be constructed by studying the critical points. In this case all energy surfaces are connected and phase space trajectories densely fill the surfaces. Finally we study spins on hypercubic lattices in d dimensions. In this case we are not able to obtain a full characterization of the energy surfaces. However we explicitly construct a large number of spin configurations which correspond to critical points, both stable and hyperbolic, and which span the entire energy spectrum of the system. The presence of degenerate stable points implies disconnected energy surfaces around the neighborhood of these points. Thus in such cases we get non-ergodic behavior. However we find some numerical evidence which suggests that such regions where the dynamics is non-ergodic are of small measure. For example, we find from simulations using the energy conserving dynamics that long time averages of correlation functions are the same as that obtained from a canonical simulation (which can be shown to be ergodic) whenever the initial conditions are chosen randomly. For initial conditions close to stable points the correlation functions can be calculated exactly and differ from the canonical averages. On the other hand if we start with initial conditions close to hyperbolic points we get from simulations results close to the canonical ones.

The paper is organized as follows. In section II we define the model and the dynamics. In section III the two spin case is first studied. The general case of $N > 2$ spin case is studied in section IV.

II. DEFINITION OF MODEL

In the XY model each spin is a two-component unit vector specified by the angle θ that it makes with some fixed axis. Equivalently every spin can be denoted by the complex number $z = e^{i\theta}$. The interaction energy for spins on a lattice is given by

$$\mathcal{H} = - \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) \quad (1)$$

where the sum is over all nearest neighbors. The dynamics is the following: during an infinitesimal time dt each spin undergoes an energy conserving flip with a probability dt . For discrete time evolution, as would be required for a computer implementation of the dynamics, this is equivalent to choosing a spin randomly at every time step and flipping it. Let $h = \sum_{i \in n.n} z_i$ be the net magnetic field at a site due to all the other nearest neighbor sites. Then the spin flip is given by the map

$$z' = hz^*/h^*. \quad (2)$$

which corresponds to a reflection of the spin z about the direction h .

For ergodic behavior it is necessary that starting from a generic initial condition it should be possible to access all other points on the constant energy surface. The detailed balance condition then ensures that a uniform probability distribution over the energy surface is the stationary distribution.

We note that a generalization of the above dynamics to the n -vector model can be made. For the Ising model ($n = 1$) a flip can only occur if a spin has equal number of up and down neighbors. For the XY model ($n = 2$) there is always a unique flipped state. For higher n the spin can flip to a continuum of values.

III. ERGODICITY IN TWO SPIN SYSTEMS

Consider two spins z_1 and z_2 coupled to each other by the xy-interaction and also interacting with constant external fields of magnitude h_1 and h_2 and directions given by the angles ϕ_1 and ϕ_2 . The fields h_1 and h_2 could be the effect of other spins held fixed in a bigger system. The energy of the system is given by

$$\mathcal{H} = -h_1 \cos(\theta_1 - \phi_1) - h_2 \cos(\theta_2 - \phi_2) - \cos(\theta_1 - \theta_2).$$

Here θ_1 and θ_2 are the angles of the two spins. We can choose the reference axis such that $\phi_1 = 0$ and $\phi_2 = \phi$. If we are interested only in finding the region that is accessed by the system, then for the two spin case, we may as well flip the spins successively. This is sufficient since flipping a spin twice successively leaves it unchanged. Thus we study the deterministic maps

$$z'_1 = \frac{h_1 + z_2}{h_1 + 1/z_2} 1/z_1, \quad z'_2 = \frac{h_2 e^{i\phi} + z'_1}{h_2 e^{-i\phi} + 1/z'_1} 1/z_2 \quad (3)$$

We first note the following points. In general any constant θ_i line will intersect the constant energy contour given by $\mathcal{H} = \epsilon$ at two points only. These correspond to the two equal energy configurations of a spin in a net magnetic field. The energy contours can thus be of the forms shown in fig. 1. In (a) the contours are connected while in (b) and (c) they are disconnected. However it is clear that the dynamics allows transitions between the disconnected parts in (b) but not so in case (c). This is because, at every step of the dynamics, only one spin can change. But moving between the disconnected parts of the energy contours in (c) requires two spins to change simultaneously. Thus whenever there are closed disconnected contours, that are non-spanning, there can be no transitions from one to the other.

We now show that for generic fields and initial conditions the trajectories are non-periodic and densely fill the constant energy contours. The proof consists of the following observations:

(i) Considered as a map in the θ_1, θ_2 plane, (3) is area preserving, i.e it has jacobian of modulus one. This is easily proved by writing eqns. (3) in the form $\theta'_1 = -\theta_1 + f(\theta_2), \theta'_2 = -\theta_2 + g(\theta'_1)$, where f and g are given functions. Thus the map can have no attractive periodic points.

(ii) The map (3) is equivalent to a smooth invertible map on the circle. Since there can be no attracting set of points, two kinds of behavior of the trajectories is possible. Either all trajectories are periodic with the same period or else trajectories are aperiodic and densely fill the circle.

(iii) For periodic orbits of order n we must have $z_1^{(n)} = z_1$ and $z_2^{(n)} = z_2$. For generic values of the fields, these equations will have a finite number of solutions, and therefore it follows that all points cannot belong to periodic orbits. Hence, because of (ii), all trajectories are aperiodic and fill the energy contours densely. It is however possible that at some special value of the fields the above eqns for periodic orbits are satisfied identically for some n . In that case all trajectories are periodic orbits of order n . Thus, as an example, for $h_1 = h_2 = 1$, the equations $z_1^{(3)} = z_1, z_2^{(3)} = z_2$ are identically satisfied. All points are then periodic of order 3 and there is no ergodicity. However if we change h_2 by an infinitesimal amount then the trajectories become dense. This can be seen in fig. 2 where we plot phase space trajectories for different initial conditions for $h_1 = 1.0, h_2 = 1.001$.

For the two spin case the nature of the constant energy contours can be completely determined by studying the critical points of the energy function $\mathcal{H} = -h_1 \cos(\theta_1) - h_2 \cos(\theta_2 - \phi) - \cos(\theta_1 - \theta_2)$. The critical points are obtained by setting the first derivatives of \mathcal{H} w.r.t θ_1 and θ_2 to zero. Thus we get:

$$\begin{aligned}\frac{\partial \mathcal{H}}{\partial \theta_1} &= h_1 \sin(\theta_1) + \sin(\theta_1 - \theta_2) = 0 \\ \frac{\partial \mathcal{H}}{\partial \theta_2} &= h_2 \sin(\theta_2 - \phi) - \sin(\theta_1 - \theta_2) = 0\end{aligned}\tag{4}$$

These equations can be written in the more transparent form:

$$\begin{aligned}z_1^2 &= \frac{h_1 + z_2}{h_1 + 1/z_2} \\ z_2^2 &= \frac{h_2 e^{i\phi} + z_1}{h_2 e^{-i\phi} + 1/z_1}.\end{aligned}\tag{5}$$

This form also follows from eqns (3) and imply that at the critical points either the field at any site vanishes or is parallel to the spin at that site. If the field does not vanish at both the sites then the critical point will be a fixed point of the dynamics. The nature of the critical points can be found by finding the eigenvalues of the matrix $M_{kl} = \partial^2 \mathcal{H} / \partial \theta_k \partial \theta_l$ evaluated at the critical points. We are interested in finding the phase diagram in the (h_1, h_2, ϕ) space showing regions where the energy contours are connected and the regions where they are disconnected. As we shall show now this can be obtained by studying solutions of eqn. (5). First we note certain symmetries of eqn. (5). It is left unchanged by the following transformations: (1) $h_1 \rightarrow -h_1, z_2 \rightarrow -z_2$; (2) $h_2 \rightarrow -h_2, z_1 \rightarrow -z_1$; (3) $z_1 \rightarrow 1/z_1, z_2 \rightarrow 1/z_2, \phi \rightarrow -\phi$; (4) $\phi \rightarrow \pi - \phi, z_1 \rightarrow -1/z_1, z_2 \rightarrow 1/z_2$; (5) $h_1 \rightarrow h_2, h_2 \rightarrow h_1, z_1 \rightarrow e^{i\phi}/z_2, z_2 \rightarrow e^{i\phi}/z_1$. It can also be shown that the equations determining the nature of the critical points are also invariant under the above transformations. Because of these symmetries it is sufficient to consider the subspace given by $h_1 > h_2 > 0, 0 < \phi < \pi/2$.

From eqn (5) we get the following equation for z_1

$$\begin{aligned}h_1^2 h_2 e^{-i\phi} z_1^6 + (h_1^2 h_2^2 + h_1^2 - h_2^2 e^{-i2\phi}) z_1^5 + (h_1^2 h_2 e^{i\phi} - 2h_1^2 h_2 e^{-i\phi}) z_1^4 + (-2h_1^2 h_2^2 - 2h_1^2 + 2h_2^2) z_1^3 + \\ (h_1^2 h_2 e^{-i\phi} - 2h_1^2 h_2 e^{i\phi}) z_1^2 + (h_1^2 h_2^2 + h_1^2 - h_2^2 e^{i2\phi}) z_1 + h_1^2 h_2 e^{i\phi} = 0\end{aligned}\tag{6}$$

For every solution z_1 of (6), z_2 is uniquely determined through the equation:

$$z_2 = \frac{h_2 z_1 (e^{i\phi} - e^{-i\phi} z_1^2)}{h_1 (z_1^2 - 1) (h_2 e^{-i\phi} z_1 + 1)}$$

Thus in general we obtain six sets of solutions to (5). The solutions for which z_1 and z_2 have modulus one correspond to the physically relevant solutions.

Let us first consider the case $\phi = 0$, for which (6) can be solved for z_1 . We obtain the following six solutions: $(z_1, z_2) = (1, 1), (1, -1), (-1, 1), (-1, -1), (e^{i\theta_1}, e^{-i\theta_2})$ and $(e^{-i\theta_1}, e^{i\theta_2})$ where $\cos(\theta_1) = (h_2^2 - h_1^2 - h_1^2 h_2^2) / 2h_1^2 h_2$ and $\cos(\theta_2) = (h_1^2 - h_2^2 - h_1^2 h_2^2) / 2h_2^2 h_1$. We see that two of the critical points merge and disappear as the lines $h_2 = h_1 / (h_1 \pm 1), h_2 = h_1 / (1 - h_1)$ are crossed. In fig. 3 we plot the phase diagram which shows the nature of the critical points in different regions in the h_1, h_2 plane. The important point to note is that in the region enclosed by the three curves, where we have three stable fixed points, we get disconnected energy contours. This is because of the following reason. Consider what happens as we move along some constant h_1 line as shown in fig. 3. At point A just below the phase boundary we have two stable critical points; $(1, 1)$, which is a energy minima and $(-1, 1)$ which is a maxima. The other two points $(-1, -1)$ and $(1, -1)$ are hyperbolic points. As we cross the line to point B, $(-1, 1)$ becomes unstable and at the same time, two new stable points, degenerate in energy appear from this point. The separatrix passing through $(-1, 1)$ encloses both the stable points. This at once implies that there will be disconnected closed energy contours of identical energies around the two stable points. In fact for all energy values greater than the separatrix energy, we get disconnected sectors, while for lower energies there are only single sectors. Similarly as we cross from the point D to E in fig. 3, the two degenerate stable maxima merge with the unstable point $(-1, -1)$ to give rise to a single stable point. Hence at E and all points above this we have only connected energy contours for all energy values. To illustrate the above point we plot in fig. 4 the energy contours for field values corresponding

to the points A, B, C, D and E . The energy contours were obtained by starting from different initial conditions and evolving through the map (3).

For $\phi \neq 0$, we can no longer solve eqn (6) explicitly. However we can still obtain the phase diagram. In this case for fixed h_1 suppose we increase the h_2 value starting from zero. Initially we have two stable critical points, one of which is a minima and the other a maxima, and two hyperbolic points. As we increase h_2 a pair of critical points, one stable and the other hyperbolic, appears in the region around the maxima. The separatrix passing through this new hyperbolic point encloses both the maxima and the new stable point which is also a maxima. The two maxima may not be degenerate but clearly, for a range of energy values greater than the separatrix energy and less than the energy of the smaller maxima, we will have disconnected energy contours. Since the extra pair of critical points emerge from a single point, the phase diagram can be obtained by finding the condition for two roots of eqn (6) to be identical. The equation that we thus get can be solved numerically and we obtain the phase diagram shown in fig. 5. This shows various constant ϕ sections of the phase diagram. In fig. 6 we plot constant energy contours for non zero ϕ and for field values on the two sides of the phase boundary. The plot illustrates the appearance of critical points and associated with it the disconnected energy contours.

To summarize the results obtained so far, we have shown that for a two spin system, for generic values of external fields, the dynamics is ergodic on the geometrically connected parts of energy contours. There are as many sectors as disconnected parts. Studying the critical points enables us to obtain full information on the number of sectors as a function of the fields and energy.

IV. ERGODICITY IN AN N SPIN SYSTEM

We now give some results that are valid for any number of spins. In this case too, if there are closed disconnected surfaces with the same energy, the dynamics does not allow transitions between them. This simply follows from the fact that any line, along which only θ_k varies, will intersect a closed energy surface at two points. Since we allow single flips only, at every time step, one can move only between these two points on the same surface.

It can also be shown that for the many spins case, phase space trajectories obtained for generic initial conditions densely fill the connected parts of the constant energy surface. This is an important result since it implies ergodicity within sectors. Consider any point $P(\theta_1, \theta_2, \dots, \theta_N)$ on the energy surface. Suppose we take any two nearest neighbor spins θ_k and θ_l and flip them successively while keeping all other spins fixed. The fixed spins in this case act as external fields. We know from the two spin case that for almost every value of the external fields, which in this case means for almost any configuration of the fixed spins, the trajectory will be dense in the restricted phase space. The restricted phase space is the intersection between the energy surface and the θ_k - θ_l plane. By choosing different nearest neighbor pairs of spins, we can have $(N - 1)$ independent directions emerging from the point P on the $(N - 1)$ dimensional energy surface, along each of which there exists a dense orbit. This in turn means that, for every point there exists a neighborhood such that all points of the neighborhood can be reached by the dynamics. Hence the trajectory obtained by evolving any initial condition cannot have a boundary and so has to fill all of the connected part of the energy surface.

Finally to obtain information on the connectivity of the energy surfaces, one can study the critical points. However unlike the two spin case, for more number of spins, we are not able to do this in full detail.

In the following subsections, first as an illustrative example, we treat the case of three spins in external fields. Then we consider spins on general hypercubic lattices.

A. Ergodicity in Three-spin case

For an open chain of three spins interacting with each other and with external fields, the energy function is given by

$$\mathcal{H} = -h_1 \cos(\theta_1 - \phi_1) - h_2 \cos(\theta_2) - h_3 \cos(\theta_3 - \phi_3) - \cos(\theta_1 - \theta_2) - \cos(\theta_2 - \theta_3)$$

In this case depending on the the sequence in which the spins are flipped we get different maps in the three dimensional phase space. Here we look at the stochastic map in which any one spin is chosen with equal probability and flipped. Thus if we represent the three spins by complex numbers z_1, z_2 and z_3 then at every time step we choose one of the following maps:

$$\begin{aligned}
z_1' &= \frac{h_1 e^{i\phi_1} + z_2}{h_1 e^{-i\phi_1} + 1/z_2} 1/z_1 \\
z_2' &= \frac{h_2 + z_1 + z_3}{h_2 + 1/z_1 + 1/z_3} 1/z_2 \\
z_3' &= \frac{h_3 e^{i\phi_3} + z_2}{h_3 e^{-i\phi_3} + 1/z_2} 1/z_3
\end{aligned} \tag{7}$$

Let us study this dynamics for the special case of fields given by: $h_1 = h_2 = h_3 = 1.0$ and $\phi_1 = \phi_3 = 0.0$. We first look at the nature of the constant energy surfaces. For this we study the critical points.

The critical points are obtained by setting to zero the first derivatives of \mathcal{H} w.r.t θ_1, θ_2 and θ_3 . This is equivalent to the condition that at every site the net field is either parallel to the spin at that site or it vanishes. Thus from (7) we get:

$$\begin{aligned}
z_1^2 &= \frac{1 + z_2}{1 + 1/z_2} \\
z_2^2 &= \frac{1 + z_1 + z_3}{1 + 1/z_1 + 1/z_3} \\
z_3^2 &= \frac{1 + z_2}{1 + 1/z_2}.
\end{aligned} \tag{8}$$

Solving the above equations we obtain the following critical points: $P_1(1, 1, 1)$, $P_2(-1, 1, -1)$, $P_3(1, 1, -1)$, $P_4(-1, 1, 1)$, $P_5(z_1, -1, 1/z_1)$, $P_6(z_1, -1, -z_1)$. In fig. 7, we show the locations of these critical points in the $(\theta_1, \theta_2, \theta_3)$ phase space.

By expanding \mathcal{H} around the critical points it can be shown that P_1 is a minimum of the energy with $\epsilon = -5$ while P_2 is a maximum with $\epsilon = 3$. The points P_3 and P_4 are hyperbolic points with $\epsilon = -1$. The lines P_5 and P_6 consist of hyperbolic points and correspond to $\epsilon = 1$. Knowing the nature of all the critical points and by carefully looking at the energy function, we construct the following picture of the energy surfaces: The point P_1 is the lowest energy state corresponding to all spins aligned along the field direction. For $\epsilon \approx -5$, the constant energy surfaces are ellipsoidal, enclosing the point P_1 . In fact for $-5 < \epsilon < -1$ the energy surfaces are all closed deformed ellipses. At $\epsilon = -1$ the energy surface passes through the two unstable points P_3 and P_4 . For $-1 < \epsilon < 1$ we get spanning surfaces. The $\epsilon = 1$ surface is again closed and passes through the critical lines P_5 and P_6 . Finally for $1 < \epsilon < 3$, the surfaces are closed around the other stable point at P_2 . We note that in all cases the energy surfaces are connected.

Let us now look at the numerically obtained phase space trajectories for different energy values. These are shown in fig. 8. For every energy value the trajectory was obtained by evolving a single initial condition. In all cases the dynamics appears to be ergodic. The energy values were chosen so that all the different types of surfaces discussed above are generated. For example it can be seen that at $\epsilon = -0.832$ we get a spanning surface while for $\epsilon > 1$ the surfaces are closed. The surface in fig. 8c is a spanning surface topologically equivalent to the one in fig. 8d. To further verify the ergodic nature of the trajectories we plot in fig. 9 constant θ_2 sections of the phase space trajectory for the energy value $\epsilon = -0.832$. It is easy to understand the form of the contours if we rewrite the energy in the following way

$$\mathcal{H} = 2 \cos(\theta_2/2)(\cos(\theta_1 - \theta_2/2) + \cos(\theta_3 - \theta_2/2)) + \cos(\theta_2).$$

For other values of energy we get results similar to those in fig. 9.

Thus in this three spin system we find that all energy surfaces are connected and the phase space trajectories densely fill the energy surfaces. Hence we have complete ergodicity.

B. Spins on a lattice

On a general hypercubic lattice consisting of N sites the equations for the critical points is

$$z_i = \frac{\sum_{j \in \langle i \rangle} z_j}{\sum_{j \in \langle i \rangle} 1/z_j} 1/z_i \quad i = 1, 2, \dots, N. \tag{9}$$

The sum over j is over nearest neighbors of i . In all cases we assume periodic boundary conditions. We have not been able to obtain the full set of solutions of these equations and analyze their structure. We have done this for a class of solutions and this is described below. The one dimensional case is a special case and we first describe it.

(i) One dimensional lattice

First we note that in this case, if we set all the coupling constants strictly to one then the dynamics is not ergodic even within sectors. The proof of ergodicity in III breaks down. This is because fixing all spins except two nearest neighbors now corresponds to the special case $h_1 = h_2 = 1.0$ mentioned in section III, which was shown to be periodic. However it was seen that if we make the couplings different from one by arbitrarily small amounts, then we get ergodicity (within sectors). Assuming this has been done we can still determine the phase space structure with the couplings set equal to one.

The set of eqns. (9) can be written in the following equivalent form:

$$z_k^2 = z_{k-1}z_{k+1} \quad \text{or} \quad z_{k-1} + z_{k+1} = 0 \quad k = 1, 2, \dots, N. \quad (10)$$

Due to periodic boundary condition we have $z_0 = z_N$ and $z_{N+1} = z_1$. Thus we have 2^N sets of equations whose solution would give us the critical points. It is easy to see that the only stable solutions (stable in all directions except for a uniform rotation) are obtained from the set of equations

$$z_k^2 = z_{k-1}z_{k+1} \quad k = 1, 2, \dots, N. \quad (11)$$

Every other of the 2^N sets gives saddle points since there are one or more sites where the field vanishes and at those sites one can freely rotate the spins without changing the energy. For this set since the fields don't vanish at any site they also correspond to fixed points of the dynamics. That the above set is stable is proved by explicitly solving for the fixed points and analyzing their nature. We get N solutions given by $z_k(n) = e^{2\pi i k n / N} z_1$ with n going from 1 to N . The factor z_1 signifies the fact that the direction of one of the spins can be fixed arbitrarily. We now look at the matrix $M_{kl} = \partial^2 \mathcal{H} / \partial \theta_k \partial \theta_l$ evaluated at the fixed points. The non-vanishing matrix elements thus obtained are $M_{kk}(n) = -2 \cos(2\pi n / N)$, $M_{kk-1} = M_{kk+1} = \cos(2\pi n / N)$. Here n refers to the n th fixed point. This can be easily diagonalised and gives the eigenvalues

$$\lambda_q(n) = -2 \cos(2\pi n / N)(1 - \cos(2\pi q / N)) \quad q = 0, 1, \dots, N - 1.$$

Except the first eigenvalue $q = 0$ which corresponds to a uniform rotation, all other eigenvalues are non-vanishing and have the same signs. Thus all fixed points are stable and the energy surfaces around them are elliptical. For the case when N is a multiple of 4, a special case arises for the $n = (N/4)$ th fixed point. In this case all eigenvalues vanish. This is because in this case the field at every site vanishes and spins can rotate freely.

The energy of the n th fixed point is given by $\epsilon = N \cos(2\pi n / N)$ and we note that every fixed point except those corresponding to the lowest and highest energies are doubly degenerate (for even N). The energy surfaces around these fixed points thus consist of two disconnected parts each of which is closed.

Another set of solutions of eqns.(10) is obtained by choosing any arbitrary direction and aligning every spin either along or opposite to it. The all up and the alternating up and down configurations have already been generated in the previous set of solutions. All the other solutions are saddles and it is easy to see that the degenerate points are all connected. The degeneracy of each solution is given by the number of configurations with a fixed number of bad bonds.

In summary, for the one dimensional lattice, we have obtained all the fixed points and shown that they are stable and doubly degenerate.

(ii) General case of d -dimensional hypercubic lattice of length L

In higher dimension, eqns. (9) are highly nonlinear and classifying all solutions is a difficult task. However we obtain by inspection a set of solutions corresponding to spin-waves. These are of the form

$$z_{\bar{k}}(\bar{n}) = e^{2\pi i \bar{k} \cdot \bar{n} / L} z \quad (12)$$

where the vector \bar{k} denotes points on the d -dimensional lattice with integral coordinates (k_1, k_2, \dots, k_d) and $\bar{n} = (n_1, n_2, \dots, n_d)$ denotes one of the L^d solutions. The indices k_i and n_i take values $1, 2, \dots, L$. As before the solutions contain an arbitrary constant phase factor z .

To understand the nature of the critical points we again look at the eigenvalues of the matrix $M_{\bar{k}\bar{l}} = \partial^2 \mathcal{H} / \partial \theta_{\bar{k}} \partial \theta_{\bar{l}}$, evaluated at the critical points. The non-vanishing matrix elements are in general given by $M_{\bar{k}\bar{k}} = -\sum_{\bar{l} \in \langle \bar{k} \rangle} \cos(\theta_{\bar{k}} - \theta_{\bar{l}})$ and $M_{\bar{k}\bar{k}_p} = \cos(\theta_{\bar{k}} - \theta_{\bar{k}_p})$. Here \bar{k}_p denotes the nearest neighbors along the p th axis, namely the points $(k_1, k_2, \dots, k_p \pm 1, \dots, k_d)$. In our case the matrix elements at the critical point \bar{n} are $M_{\bar{k}\bar{k}}(\bar{n}) = -2 \sum_{p=1}^d \cos(2\pi n_p / L)$ and $M_{\bar{k}\bar{k}_p}(\bar{n}) = \cos(2\pi n_p / L)$. It is easy to show that the eigenvalues of this matrix are

$$\lambda_{\bar{q}}(\bar{n}) = - \sum_{p=1}^d 2 \cos(2\pi n_p/L) (1 - \cos(2\pi q_p/L)) \quad q_p = 0, \dots, N-1. \quad (13)$$

Unlike in the one-dimensional case eigenvalues corresponding to a critical point can have opposite signs. In fact the only stable critical points are those for which $\cos(2\pi n_p/L)$ has the same sign for all p . To show this suppose there exists in the set (n_1, n_2, \dots, n_d) two values n_a and n_b for which $\cos(2\pi n_a/L)$ and $\cos(2\pi n_b/L)$ have the opposite signs. Then the eigenvalues for $\bar{q} = (0, 0, \dots, q_a, 0, \dots, 0)$ and $\bar{q} = (0, 0, \dots, q_b, 0, \dots, 0)$ have opposite signs. To find whether the critical points correspond to fixed points we look at the fields at each site. This is given by $H_{\bar{k}}(\bar{n}) = \sum_{\bar{k}_p} z_{\bar{k}_p}(\bar{n}) = 2e^{2\pi i \bar{k} \cdot \bar{n}} \sum_{p=1}^d \cos(2\pi n_p/L)$. Thus except for the small subset of points satisfying $\sum_{p=1}^d \cos(2\pi n_p/L) = 0$, all other critical points are fixed points. Unlike the one dimensional case, here we may have other fixed points corresponding to other solutions of eqns.(9).

The energy of the critical point \bar{n} is $\epsilon = N \sum_{p=1}^d \cos(2\pi n_p/L)$. We note that the spectrum of energies spans the entire allowed energy range. If d_g is the number of non-zero coordinate values in the set \bar{n} , then there is a degeneracy of 2^{d_g} associated with the corresponding energy value since we can flip the signs of n_i without affecting the energies.

The fact that there exist degenerate stable fixed points implies that there are disconnected energy surfaces corresponding to the neighborhoods of these points. This proves that the dynamics is non-ergodic for certain energies. It is however possible that we can get ergodicity for energies corresponding to unstable points and their neighborhood. The following numerical simulations address this question.

We took a 20×20 square lattice and computed 1st, 2nd, 3rd and 4th nearest neighbor correlation functions $(c(1), c(2), c(3), c(4))$ using monte-carlo simulation. We study the two cases when the initial data is chosen close to a stable or close to an unstable point. In each case we compare the results with those obtained from randomly chosen initial configuration. Close to a stable fixed point the correlation function $\langle \cos(\theta_{\bar{k}} - \theta_{\bar{k}+\bar{R}}) \rangle$ can be calculated exactly. At the fixed point \bar{n} this is simply $\cos(2\pi \bar{R} \cdot \bar{n}/L)$. The correlation $c(r)$ evaluated in the simulations corresponds to $(\cos(2\pi r n_1) + \cos(2\pi r n_2))/2$. The following table gives the numerical data and also the exact values at the stable points:

Initial Condition	$\epsilon/2 = c(1)$	$c(2)$	$c(3)$	$c(4)$
$\bar{n} \approx (2, 6)/\text{Unstable}$	0.24855	0.06646	0.01861	0.00524
Random	0.24855	0.06647	0.01898	0.00574
$\bar{n} \approx (3, 4)/\text{Stable}$	0.44640	-0.55508	-0.87305	-0.24811
Random	0.44640	0.23264	0.13246	0.07996
Exact	0.44840	-0.55902	-0.88004	-0.25

As expected for the stable case we get results totally different from the random case. On the other hand at the unstable points we get the same correlations as with random initial conditions. Thus as far as correlation functions are concerned there seems to be no dependence on initial conditions provided we don't start from near stable points.

Next we show that the correlation functions obtained with randomly chosen initial conditions are the same as those obtained from a canonical simulation. In fig. 10 we plot the correlations $c(2)$, $c(3)$ and $c(4)$ against the average energy given by $c(1)$ for data obtained from the energy conserving dynamics and from a canonical simulation. In the canonical simulation each spin is coupled to a heat bath at some temperature and clearly we have ergodicity. For the energy conserving dynamics we started with a high energy configuration of spins pointing in random directions. Subsequently the energy was decreased by choosing spins randomly and aligning them along the local field direction. For each configuration obtained in this way we calculated the correlation functions. The data from the two approaches seem to match closely.

The above numerical results suggest that:

- (1) the set of stable points and the sectors associated with them seem to have a small measure.
- (2) the unstable points with the same energies are either all connected by the dynamics or correlation functions in each sector are the same.

A more complete study of the phase space structure is needed in order to understand the above results.

Finally we note that as in the one dimensional case, another class of solutions of the critical point equations can be written. These are the solutions for which every spin points either along or opposite to a fixed direction. These critical points may be either stable or unstable. For example consider the spin configuration of a single up-spin in a sea of down-spins. This is an unstable fixed point. The different fixed points, corresponding to the N different locations of the single up-spin, are all connected. To show this suppose we start from a configuration which is arbitrarily close to such a fixed point. Now we fix all spins except for the single up-spin and any one of its down neighbors. The results

in section III imply that by flipping these two spins successively we can reach the configuration in which the two spins have interchanged their orientations. Repeating this for different nearest neighbor spin pairs, we can reach all the N fixed points. This is different from the Ising model with similar dynamics where the system would remain stuck in one of the fixed points. The above procedure can be used to prove hyperbolicity of other fixed points also.

In conclusion, we have studied a stochastic energy conserving single spin flip dynamics of the XY model. We find that phase space trajectories fill connected parts of the energy surface and there is loss of ergodicity whenever the energy surface consists of closed disconnected parts. We also show that one can obtain information about the nature of the energy surfaces by studying the critical points of the energy function. This can be done in full detail for a two-spin system. For spins on hypercubic lattices we have proved that the dynamics is not ergodic for all energies and time averages of physical quantities depend on choice of initial conditions. However, the total weight of non-typical initial conditions appears to be small and the dynamics is effectively ergodic.

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Figure Captions

FIG. 1. Schematic picture of constant energy contours for two spin case.

FIG. 2. Phase space trajectories of the map (3) for $h_1 = 1, h_2 = 1.001$, and $\phi = 0$.

FIG. 3. Phase diagram for $\phi = 0$, showing nature of critical points for different field values. In regions R_1, R_2 and R_3 there are four critical points of which two are hyperbolic, one a maxima and the other a minima. In region R_4 there are six critical points. Three of them are hyperbolic, two are maxima and one is a minima.

FIG. 4. Constant energy contours obtained by iteration of the map (3) starting from different initial conditions. The figures (a)-(e) are for five different field values corresponding to the points A-E in fig. 3. In all cases, some of the initial conditions were chosen close to the hyperbolic points, so that the separatrices can be seen.

FIG. 5. Phase diagram for different values of ϕ . In every case, for field values in the region bounded by the three curves, there is a range of energy where there are two sectors.

FIG. 6. Constant energy contours for $\phi = \pi/16$. The field strengths h_1 and h_2 were chosen to lie on two sides of the phase boundary shown in fig. 5. In (a) $h_1 = 1.25, h_2 = 0.77$ while in (b) $h_1 = 1.25, h_2 = 0.89$.

FIG. 7. Position of critical points of three spin energy function in the $(\theta_1, \theta_2, \theta_3)$ phase space. The value of θ ranges from $-\pi$ to π along each of the axes.

FIG. 8. Three dimensional phase space trajectories for field values $h_1 = h_2 = h_3 = 1.0$. Each of the 5 figures was obtained by iterating different initial conditions corresponding to different energy values.

FIG. 9. Constant θ_2 sections of the phase space trajectories for the energy value $\epsilon = -0.832$.

FIG. 10. Correlation functions $c(2), c(3)$ and $c(4)$ plotted against $c(1)$ for data obtained using energy conserving and non-conserving dynamics. In each case the averages were taken over 10^5 monte-carlo steps.

Fig. 2

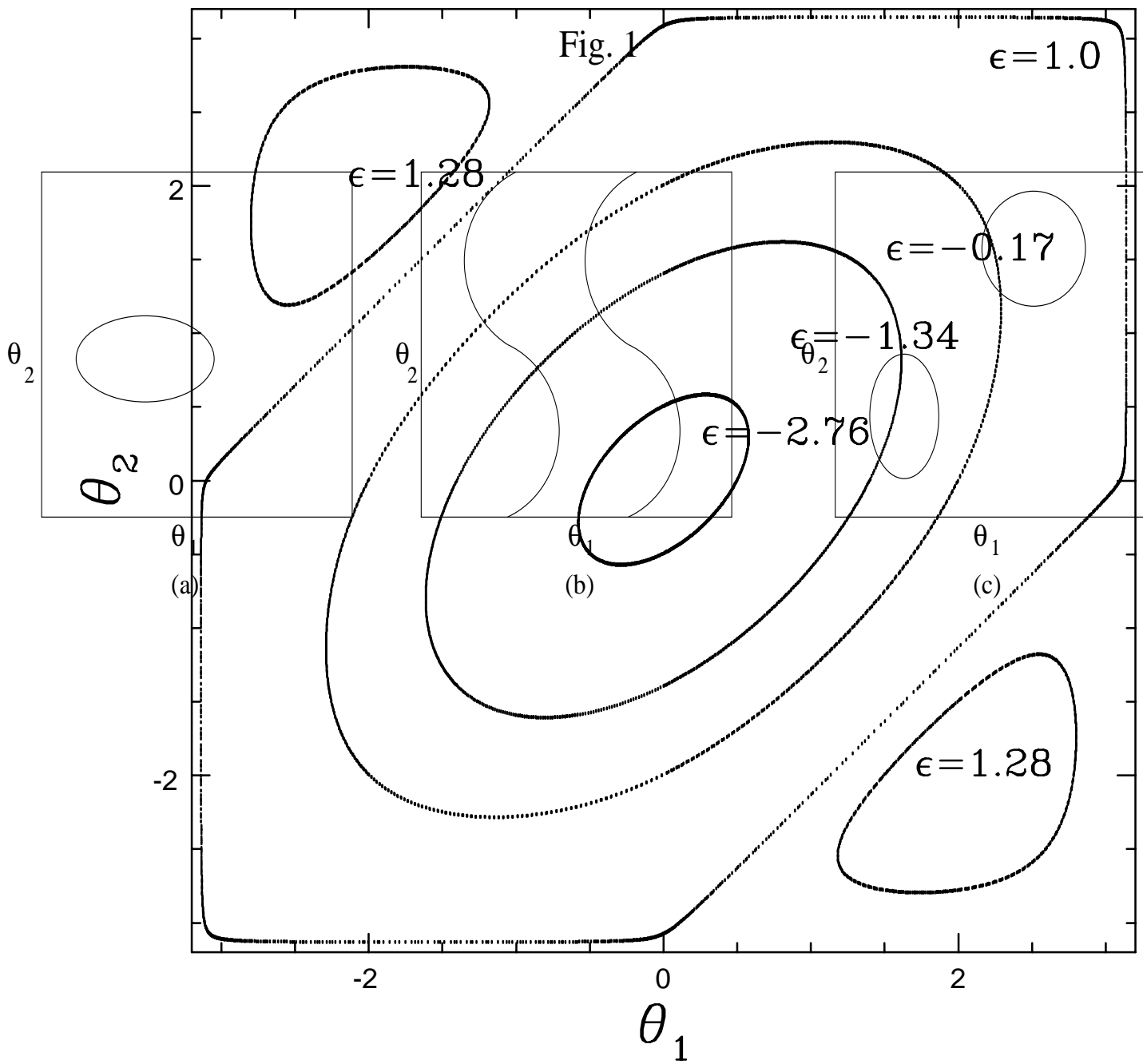


Fig. 3

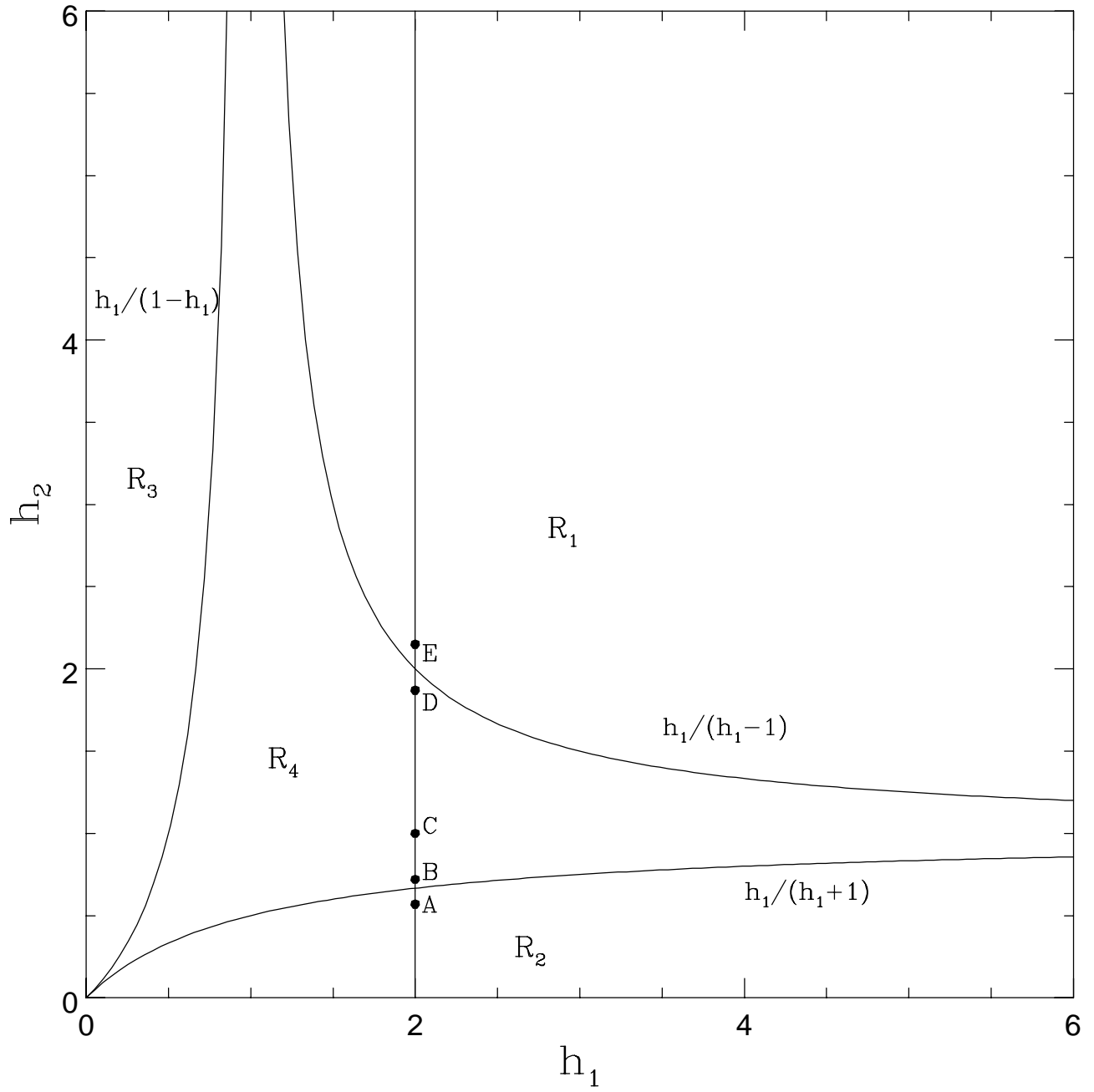


Fig. 4a

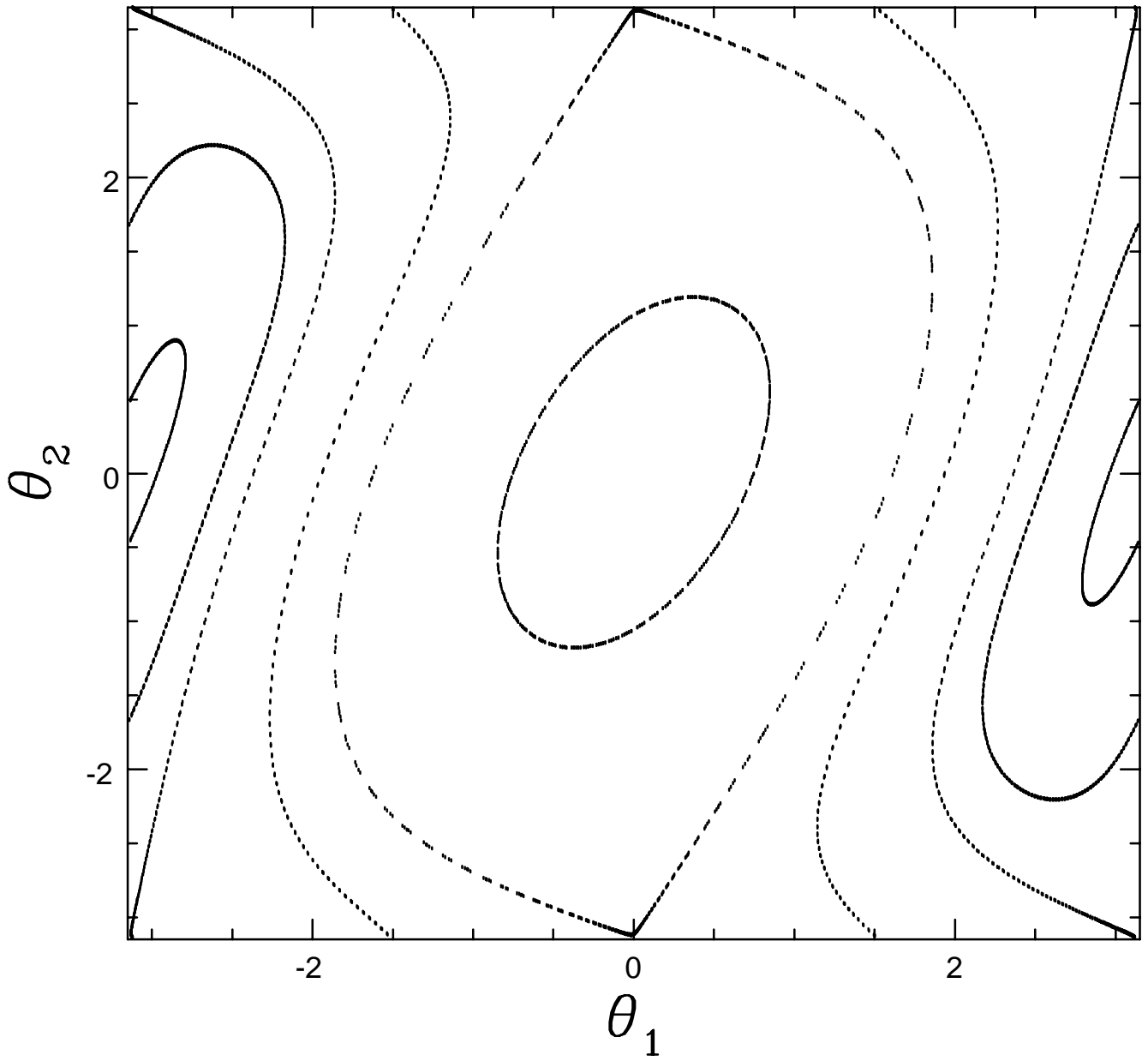


Fig. 4b

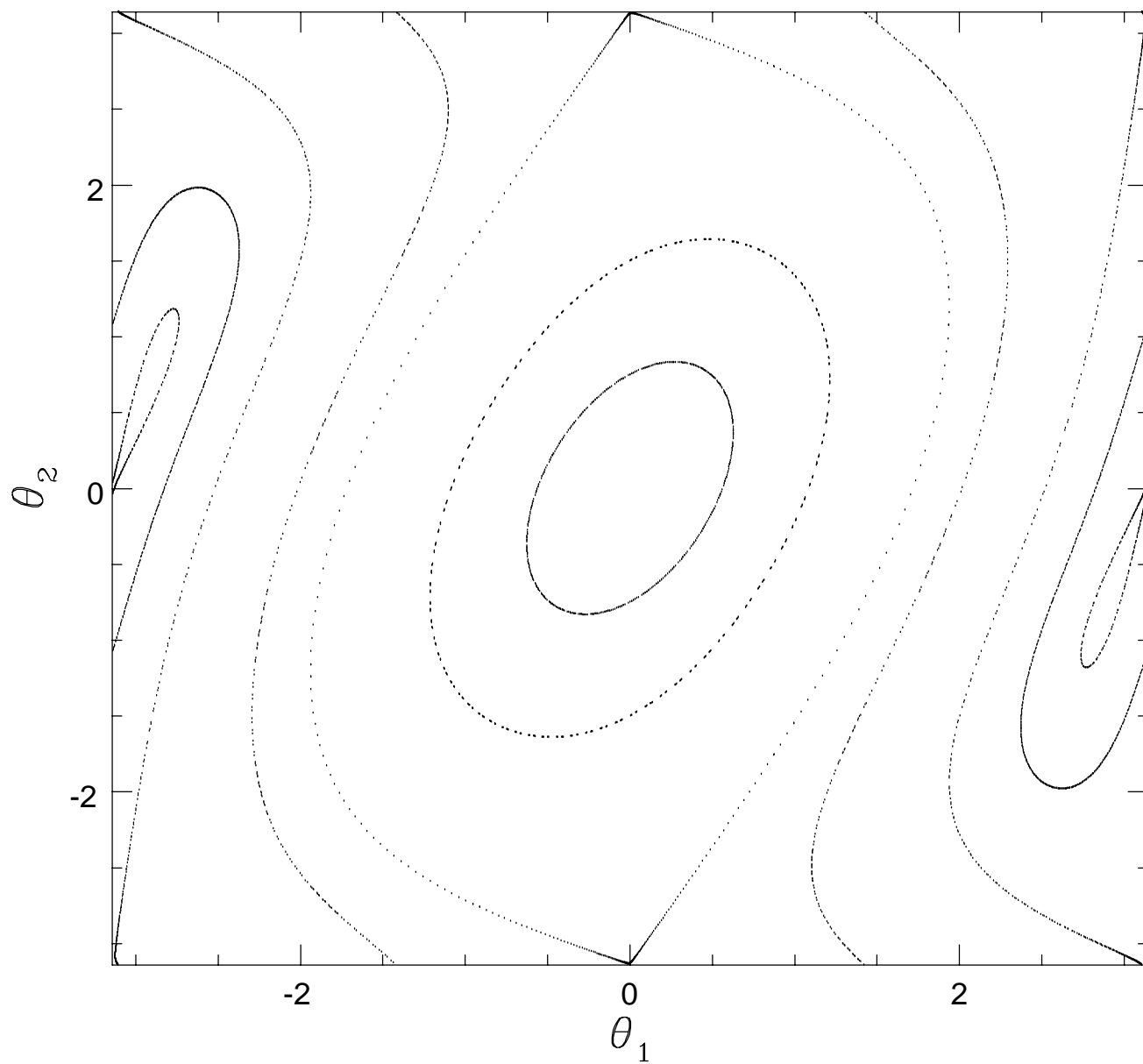


Fig. 4c

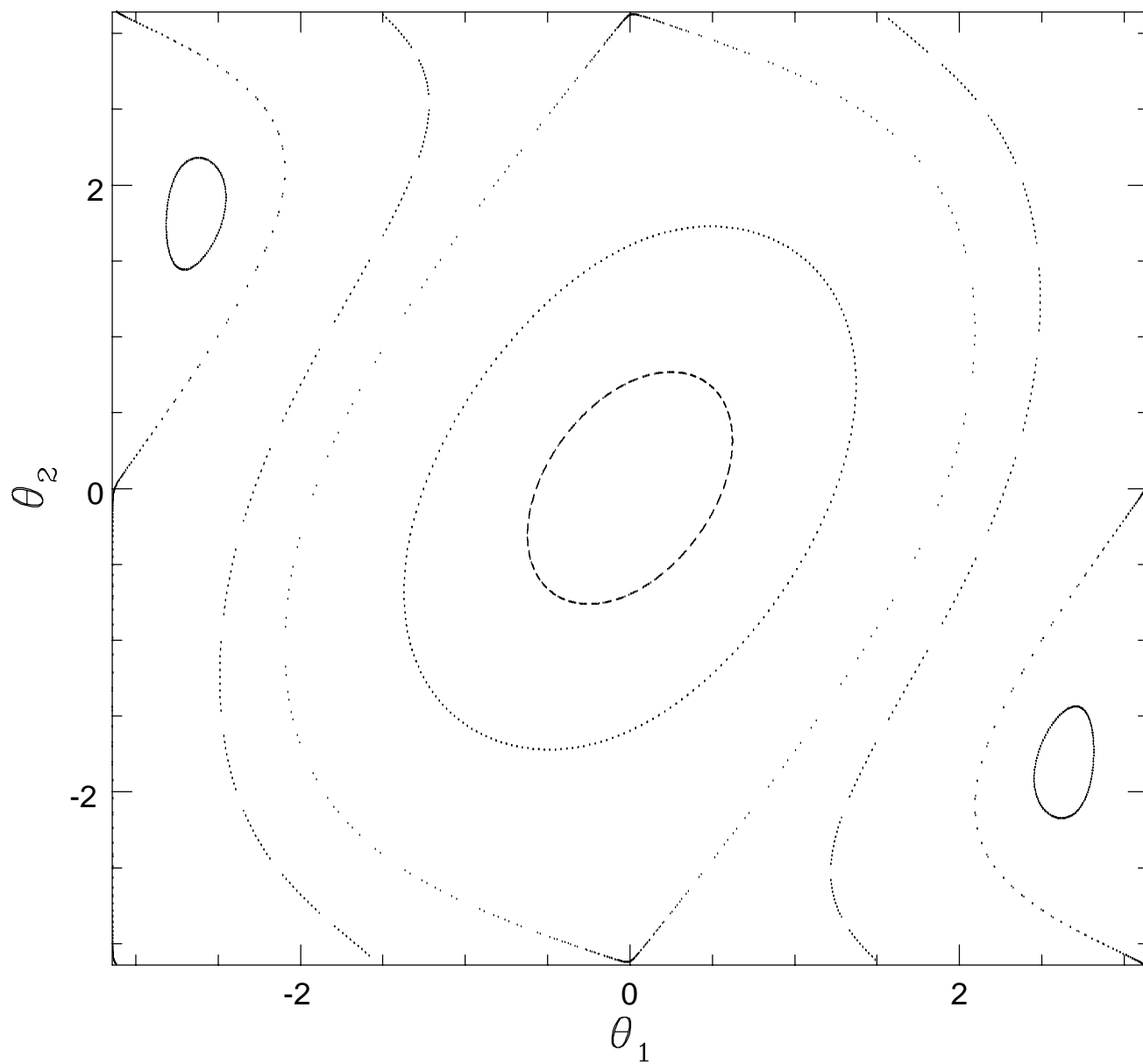


Fig. 4d

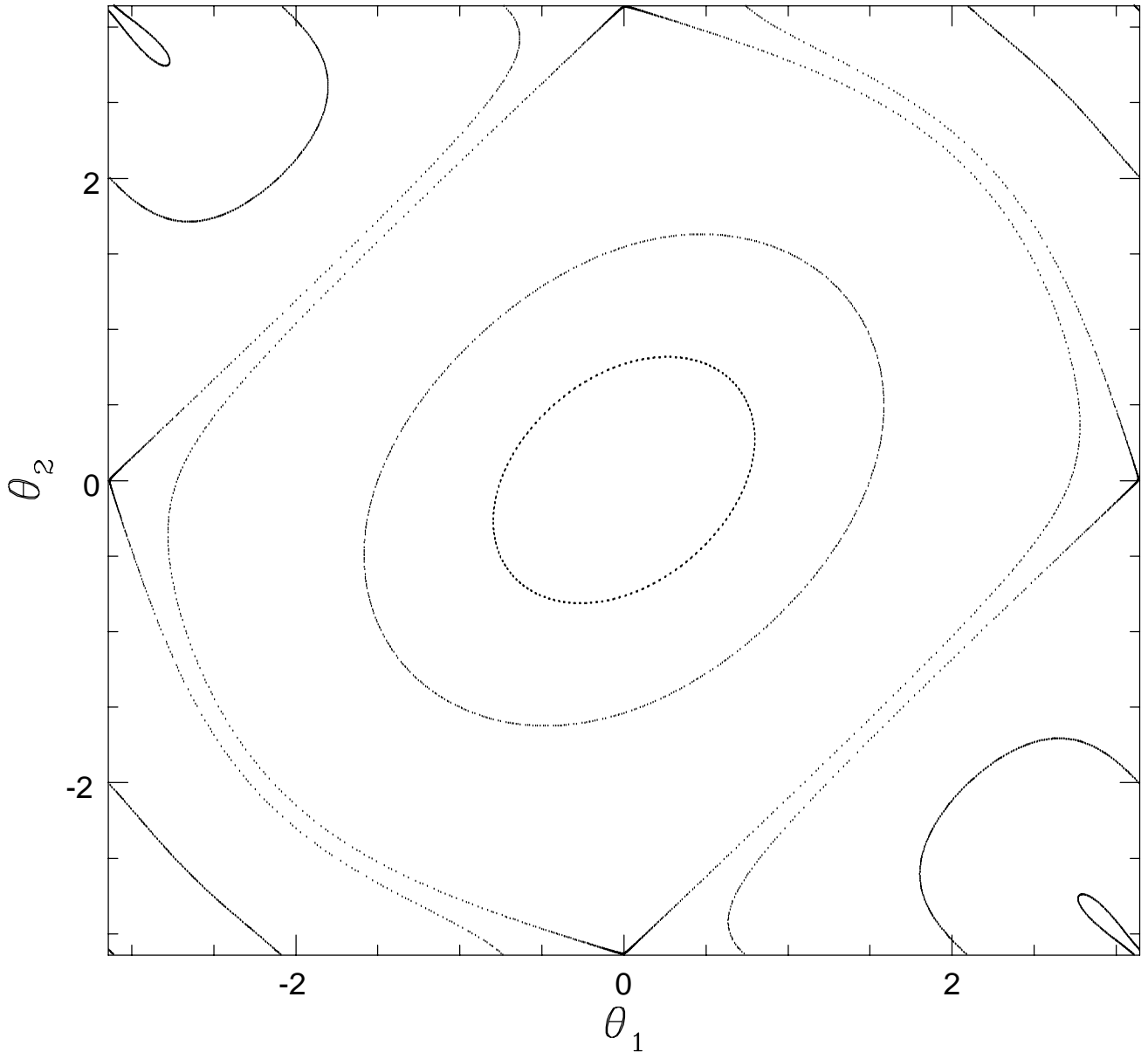


Fig. 4e

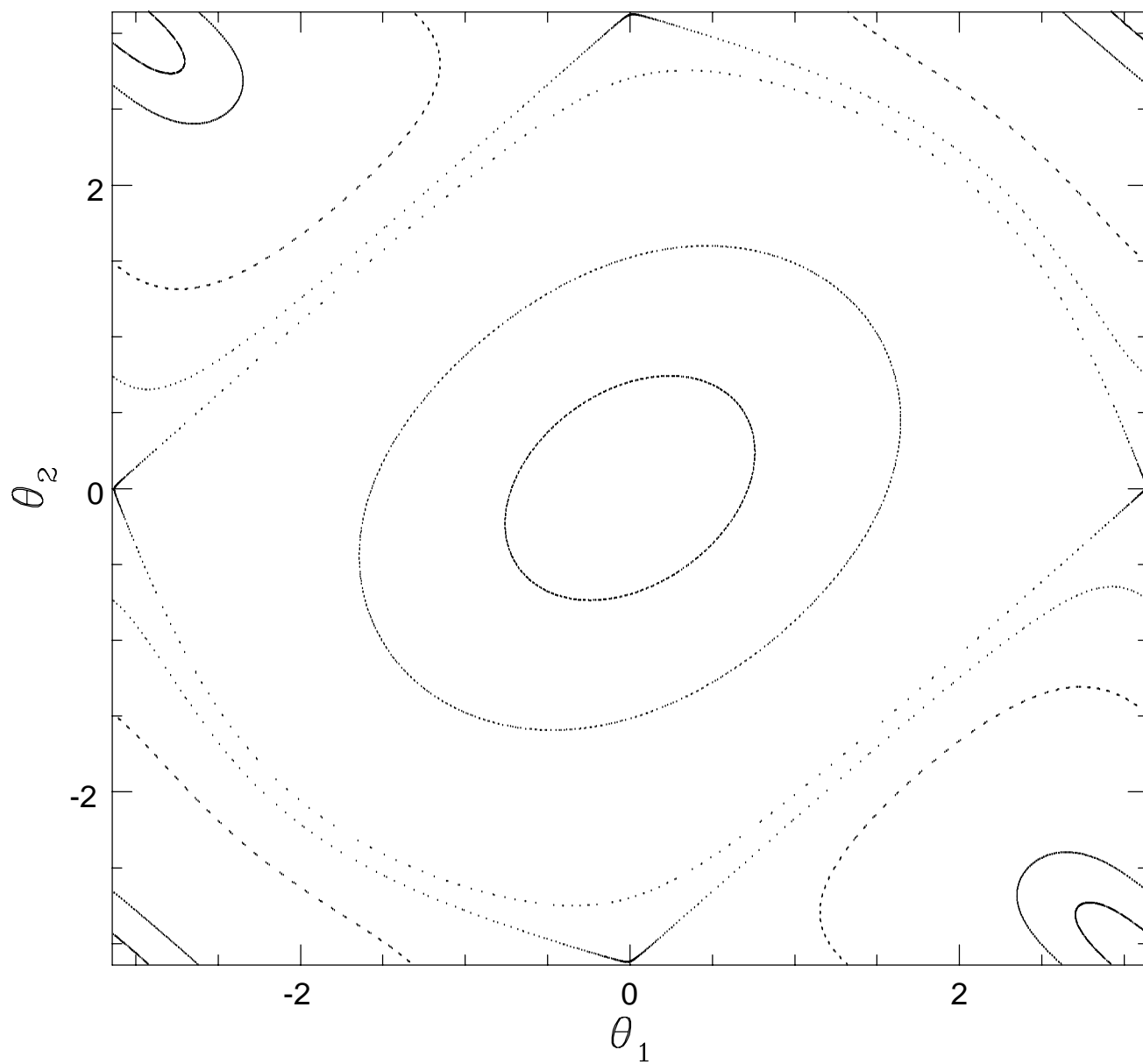


Fig. 5

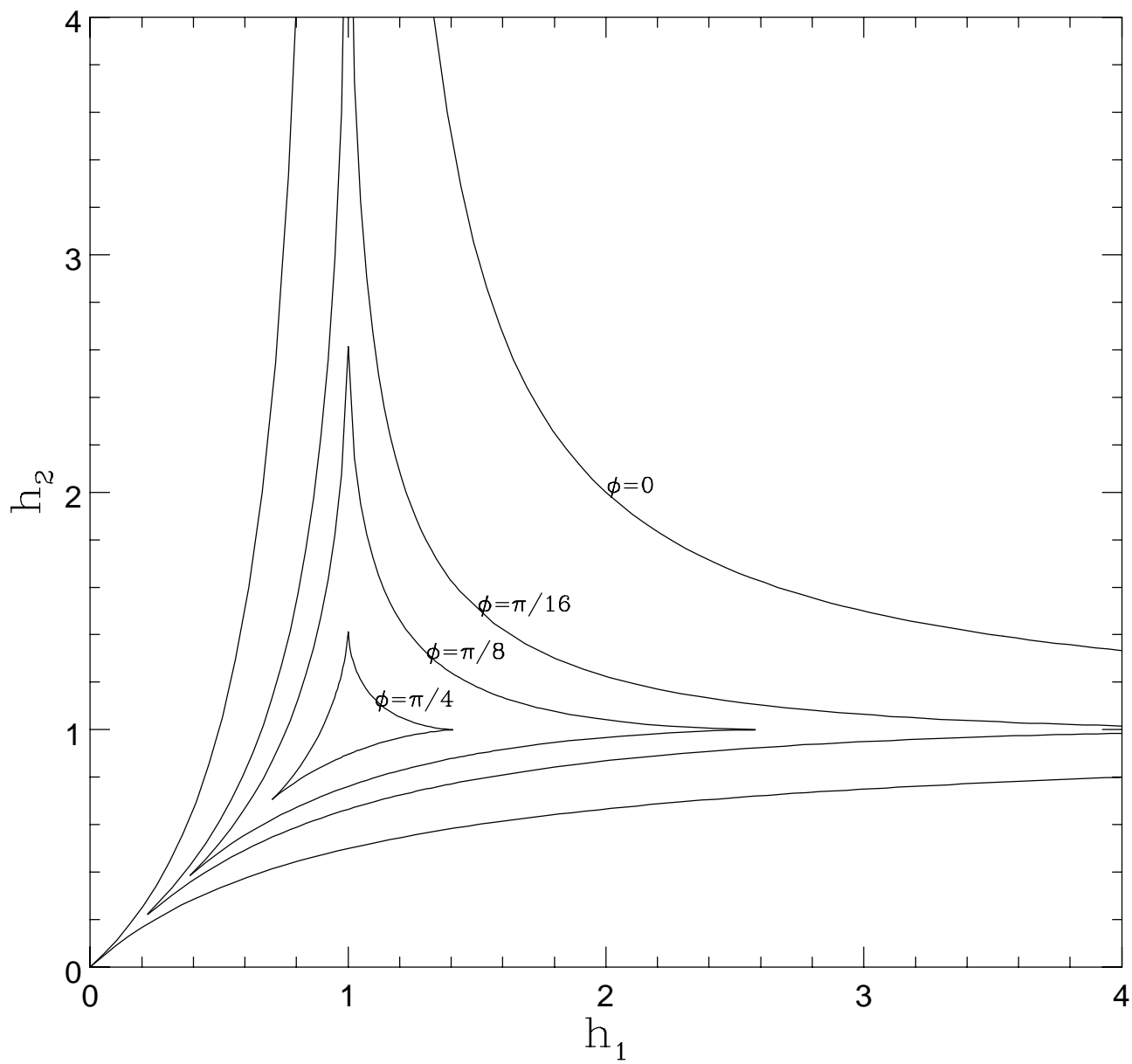


Fig. 6a

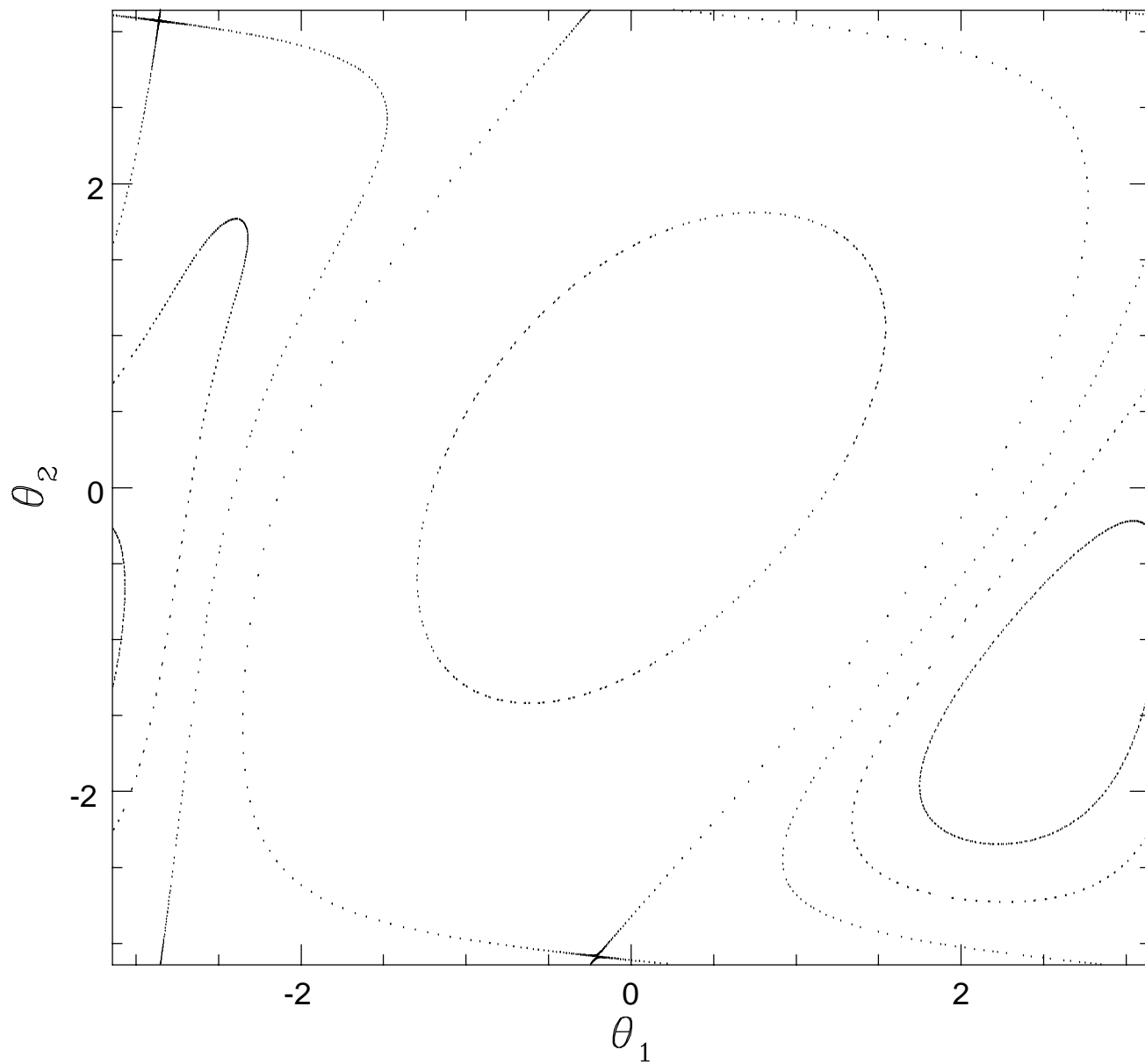


Fig. 6b

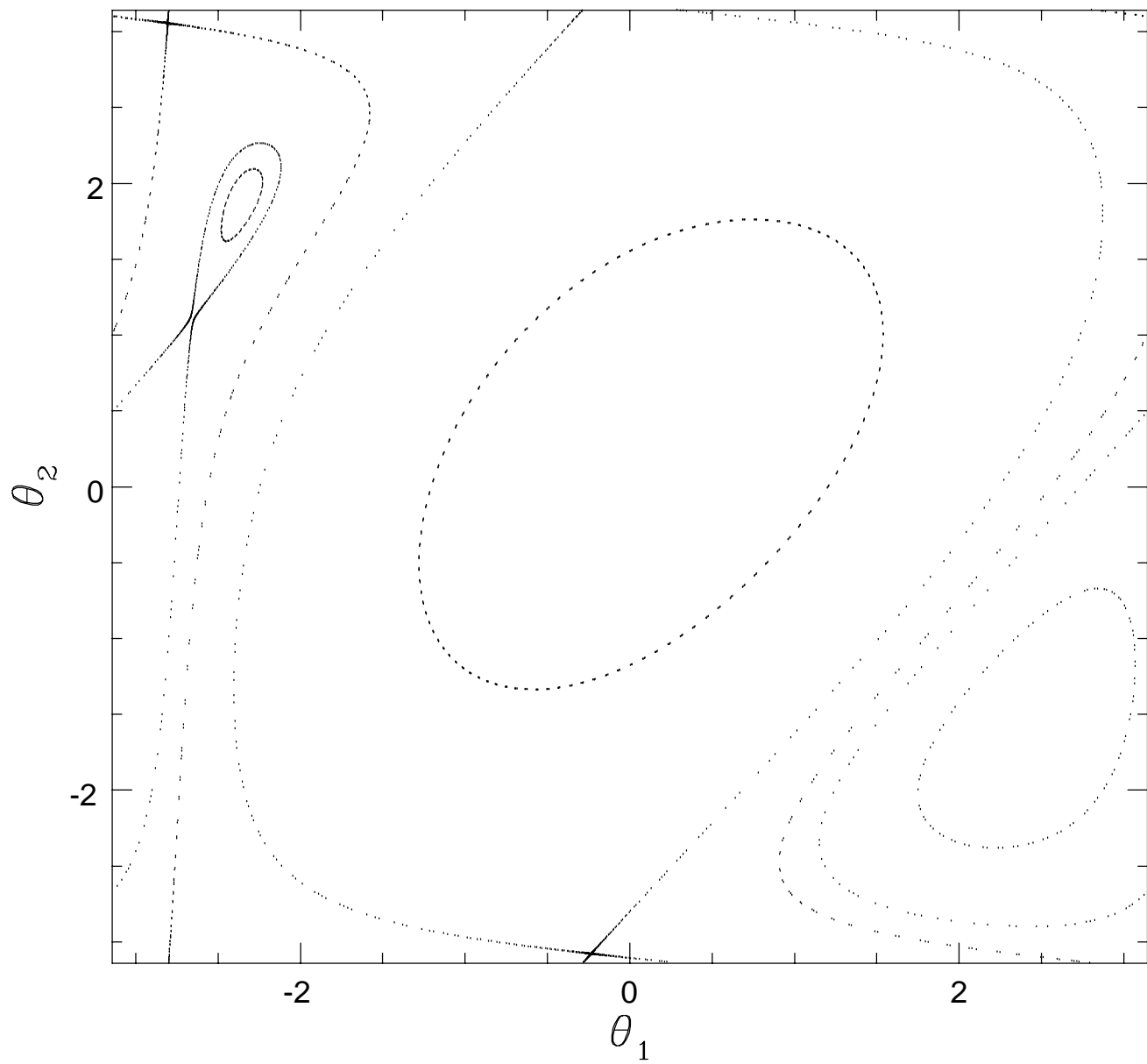


Fig. 7

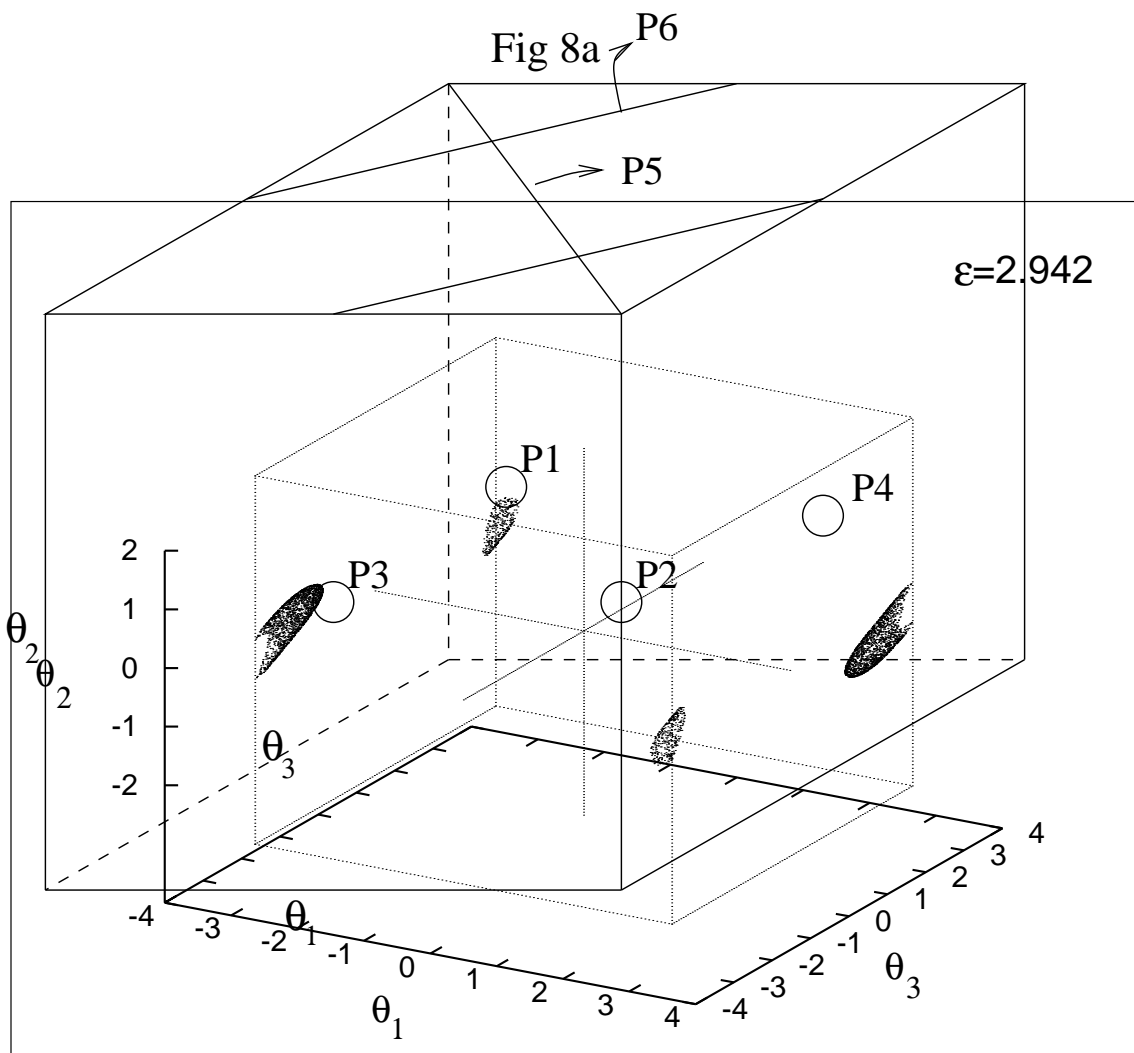
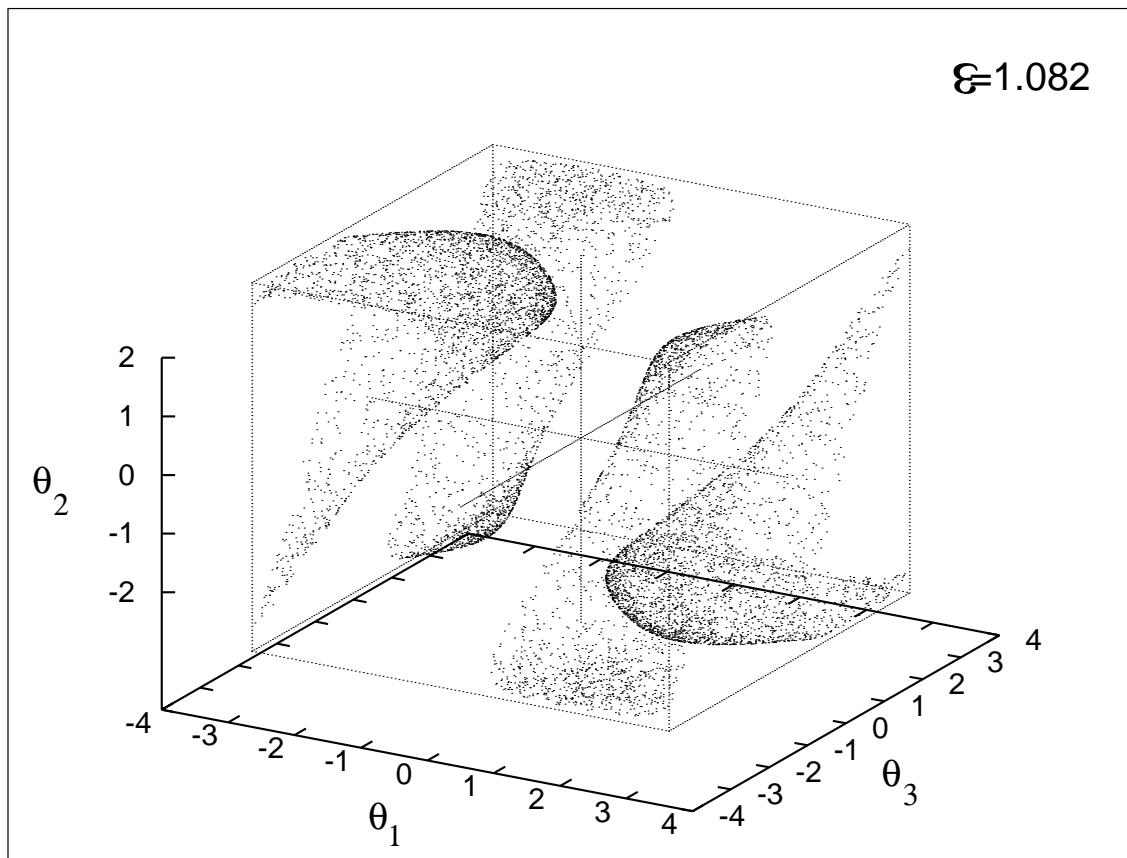


Fig 8b



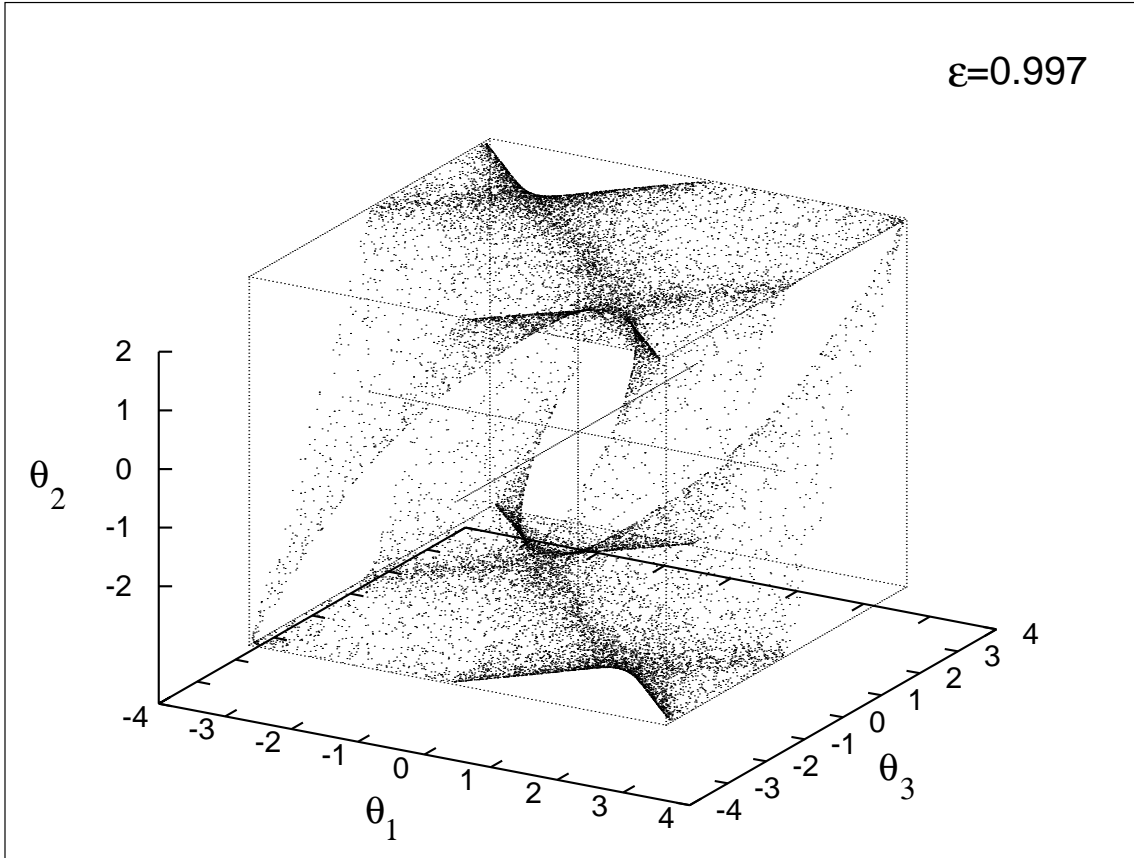


Fig 8c

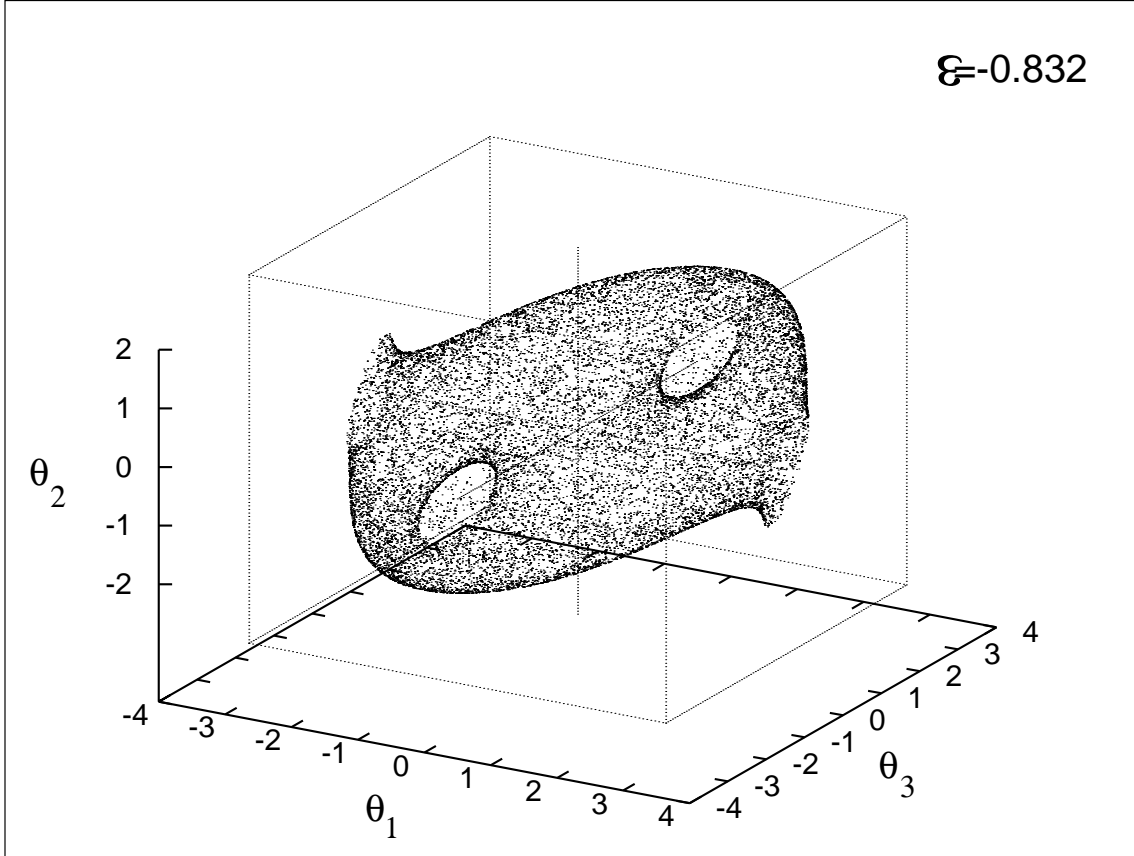


Fig 8d

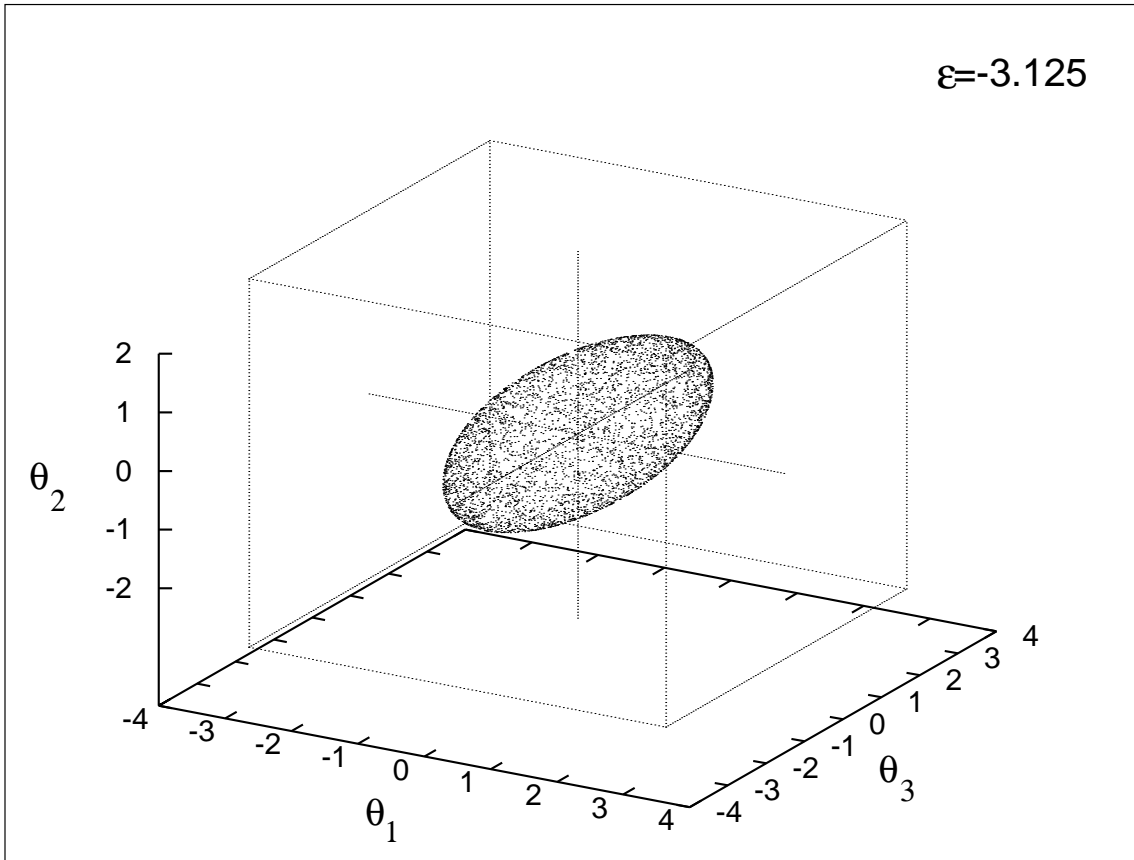


Fig 8e

Fig. 9

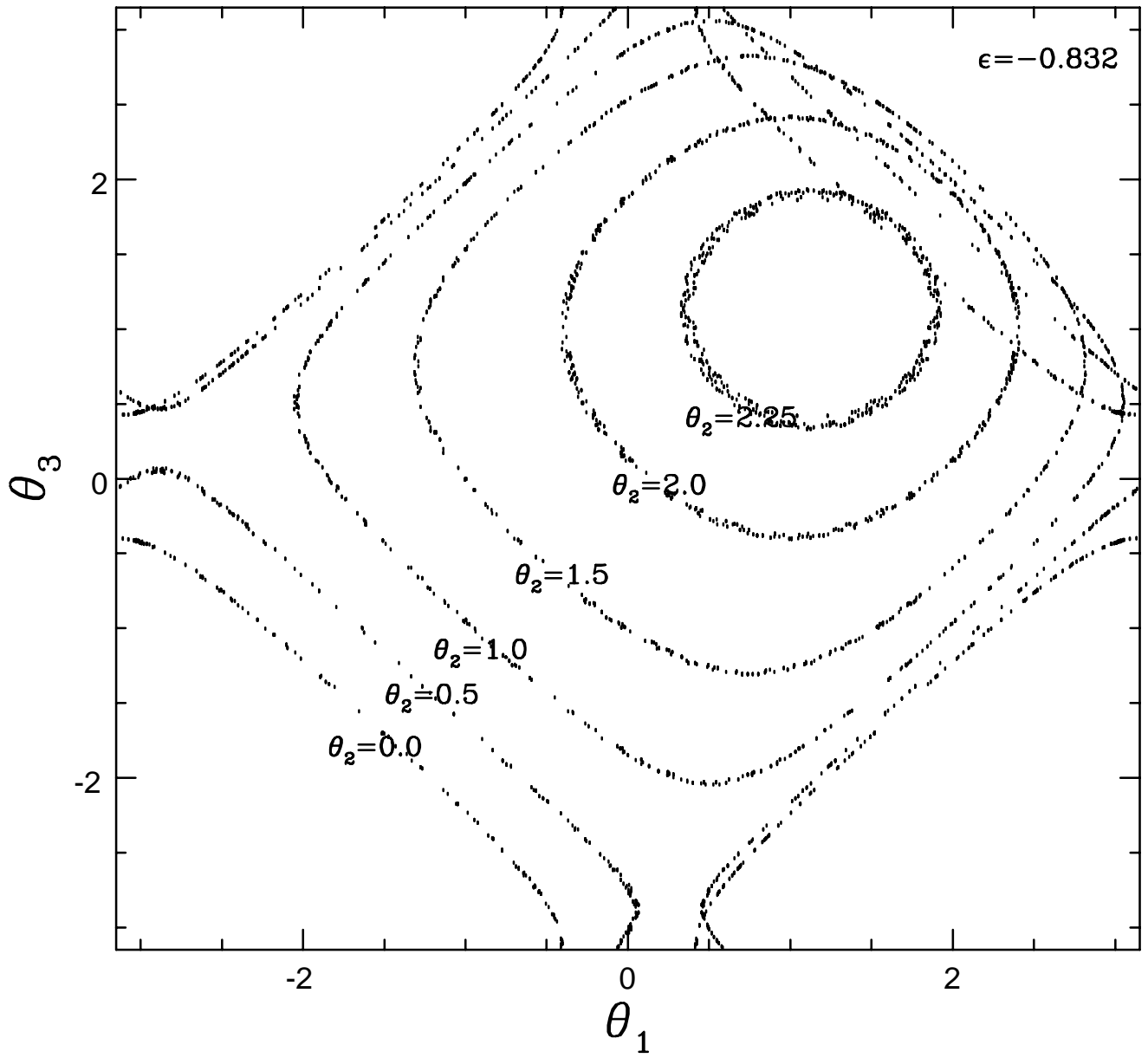


Fig. 10

