

ON THE GENERATING FUNCTION OF POINCARÉ  
PLOTS DEFINING ONE DIMENSIONAL  
PERTURBED HAMILTONIAN SYSTEMS

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**ABSTRACT**

A simple numerical method has been devised for deriving the generating function of an arbitrary, one dimensional Hamiltonian system, represented by its Poincaré plot. In this case, the plot to be numerically processed is an area preserving transformation of a two-dimensional surface onto itself. Although the method in its present form is capable of treating only this case, there are no principal restrictions excluding the analysis of systems with higher dimensionality as well. As an example, the generating function of the motion of a charged particle in a nonsymmetric, toroidal magnetic field is derived and studied numerically.

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INTRODUCTION

In very loose terms, the aim of this paper is to show that the generating function of a Hamiltonian system can be derived by solving a certain boundary value problem. This is done by using a method which is based on the theory of perturbed Hamiltonian systems. The method is applied to the case of a one-dimensional Hamiltonian system with a perturbation which is periodic in one of the coordinates (p,q). The method is also applied to the case of a two-dimensional Hamiltonian system with a perturbation which is periodic in one of the coordinates (p,q).

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**ABSTRACT**

A simple numerical method has been devised, for deriving the generating function of an arbitrary, one dimensional Hamiltonian system represented by its Poincaré plot. In this case, the plot to be numerically processed is an area preserving transformation of a two-dimensional surface onto itself. Although the method in its present form is capable of treating only this case, there are no principal restrictions excluding the analysis of systems with higher dimensionality as well. As an example, the generating function of the motion of alpha particles in a nonsymmetric, toroidal magnetic field is derived and studied numerically.

## INTRODUCTION

In very loose terms, systems of classical-mechanics are those which can be modeled by setting up a well-behaved system of differential equations, which in turn is equivalent to defining a vector field over an even-dimensional phase space with local coordinates  $(p_i, q_i)$ . Here the  $p$ 's and  $q$ 's are canonical momentum and space variables respectively, ( $i \in 1...n$ ), and  $n$  is the number of degrees of freedom of the system.

Although this "definition" is anything but one which satisfies the requirements of precision and generality, it reflects the fact that the notion of a "system of classical-mechanics" unifies a wide variety of physical problems, and allows us to investigate them by using general and standardized methods.

This Hamiltonian analogy has been successfully applied for instance in the field of controlled thermonuclear fusion, and has found widespread application in studying the structure and evolution of the confining magnetic field. (Refs. 1....3.) Formal derivations of this analogy, however, suffer from certain problems, which prevent them to be sufficiently precise and general. (An analysis of the situation and strict demonstration of the equivalence will be the subject of a subsequent paper [4].)

Studies of stellarator vacuum fields with the effects of modeled physical perturbations [5] have shown that it is of practical interest to extend the possibilities of these investigations beyond the existing ones.

Generally speaking, there are two basic problems which have to be solved in order to attain the necessary progress. First of all, the lack of a generally applicable numerical procedure, which would be able to deliver the equivalent Hamiltonian, or the generating function of the associated Poincarè plot (in many respects of equal importance with the Hamiltonian function) of a given magnetic field and specific, realistic perturbations thereof, imposes obvious limitations on the investigations. It results in the necessity of solving the system of equations defining the problem numerically. In many cases this is a time consuming procedure, sometimes beyond practical possibilities, because of the large CPU time needed to complete the study.

On the other hand, there are very interesting problems, which can be investigated only indirectly by restricting oneself to the numerical solution of the mathematical problem. For instance the behaviour of the trajectories in the vicinity of fixed points of the Poincarè plot can be characterised with the trace of the matrix representing the linearised Poincarè plot. The derivation of the numbers involved is very complicated using the method of direct integration, but it is straightforward if the generating function of the Poincarè plot is known in any suitable form.

If one has been given a Poincarè plot of a Hamiltonian system with a single

degree of freedom (which in this case is an area preserving transformation of a two-dimensional surface onto itself) it is possible to construct a numerical procedure which delivers the generating function of this map in the form of a Fourier series. This possibility is the main topic of this paper.

Toward this end a brief summary of the relevant results from the theory of classical mechanical systems will first be given. After this rather short summary, the numerical procedure is presented. As will be clear after this description, the Poincaré plot under study must be numerically described by storing the coordinates of the starting and the corresponding image points of trajectories in the phase space over a set of initial conditions, which covers with a high enough density the entire area of interest. In the case of a system with one degree of freedom this is conveniently achieved by using two-dimensional arrays which contain the canonical momentum and space variables of the corresponding points.

The origin of these arrays is completely arbitrary (it may be devised by solving numerically the system of equations describing the mechanical problem and following the phase trajectories emerging from a suitably chosen set of initial conditions, or can be numerically derived from actual measurements, etc.). In describing the procedure, it is therefore assumed that these matrices have already been given.

The presentation is followed by a numerically analysed problem, borrowed from the transport theory of alpha particles in nonsymmetric confinement geometries. Trajectories of the guiding centres of alpha particles with suitably chosen parameters approximately follow the lines of forces of the confining magnetic field. Taking into account the effects of the finite Larmor radius, this behaviour (which can be described by an integrable Hamiltonian problem) is perturbed due to the drifts of the guiding centres in inhomogeneous fields. By solving the corresponding system of equations, one can easily derive the necessary arrays, following the trajectories of the particles during one transition around the major axis of the torus. Having obtained the arrays, the problem is numerically analysed with respect to the applicability of the method. The reproducibility and the precision attainable is subsequently investigated in detail.

## ANALYTICAL BACKGROUND

As has already been mentioned, the procedure in its present form is only suitable treating an arbitrary system with one degree of freedom. Therefore, in what follows, the description is presented in a form which is restricted to this case. It must be stressed again, that this limitation is rather practical than principal, and the extension to higher dimensionality involves no greater complexity.

There is a strict correspondence between the Poincarè plot of the Hamiltonian system and a specific, area preserving plot generated by the magnetic field defined on a torus. This transformation is generated by the lines of force of the magnetic field as follows: taking a poloidal section of the magnetic field, the map under consideration is defined by bringing into correspondence the start- and endpoints of the lines of forces after one transit around the torus.

Because of the strict analogy of the two transformations, in constructing the numerical procedure it is possible to refer exclusively to the results of classical mechanics. In other words, the procedure devised in this way is a general one, suitable to treat any Hamiltonian problem with one degree of freedom.

Let us assume, that a one dimensional, integrable Hamiltonian system is represented by its Poincarè plot  $\mathbf{A}$ , in a surface lying transverse to the stable periodic, or quasiperiodic orbits. Furthermore, the existence of a coordinate system in the extended phase space is assumed in which one period of motion along the KAM tori is equivalent to a coordinate change of  $2\pi$ .

Because of the fact that the transformation  $\mathbf{A}$  represents an integrable Hamiltonian system, the effect of this transformation is only a shift of the canonical space coordinate of the starting point and the canonical momentum remains constant; that is, the trajectory remains on the same invariant surface. The amount of this shift can naturally depend on the actual stable surface. That is:

$$\mathbf{A} := \quad p_o \rightarrow p = p_o; \quad q_o \rightarrow q = q_o + \Delta q(p) \quad (1)$$

In the numerical procedure this integrable part does not play any specific role (beyond the necessity of taking it into account in the corresponding steps). In what follows, therefore it will not be further specified.

Perturbing this system with a momentum- and space-dependent transformation  $\mathbf{C}$  the perturbed map (the product of these two maps):

CA maps the point with coordinates  $(p_o, q_o)$  onto the point  $(P, Q)$  as follows:

$$\begin{aligned} \text{CA} &:= (p_o, q_o) \rightarrow (P, Q) \\ \text{A} &:= (p_o, q_o) \rightarrow (p, q) \\ \text{C} &:= (p, q) \rightarrow (P, Q) \end{aligned} \quad (2)$$

where  $p$  is the canonical momentum variable and  $q$  is the canonical space coordinate. (In what follows, we shall concentrate ourselves on the transformation C. Therefore capital letters denote transformed quantities in general and the small ones are used for the starting values. This role naturally can be changed in a sequence of transformations.)

The generating function of a given canonical transformation (which will be denoted by using the corresponding letter with a tilde) is a scalar function defined over the Cartesian product of selected coordinates defining the phase space of the system, which has the property, that certain derivatives of it deliver the corresponding values of untransformed and transformed coordinates. The Poincarè transformation — as with any canonical transformation — can be generated by a suitably chosen scalar function, without the necessity of following the trajectories between the initial and transformed states of the system.

This can be readily shown by plausibility arguments, based on the actual, strict mathematical proof.

The Poincarè plot (as any area preserving transformation) has the property:

$$\int p_o dq_o = \int P dQ \quad (3)$$

when one is integrating along a closed line around the same bundles of trajectories in the initial and the transformed states. Because the infinitesimal differences of the form  $p_o dq_o$  and  $P dQ$  can be treated as linear functionals on the tangent vectors to the trajectories, the difference of them is a complete differential of a continuous function  $d(\tilde{C}\tilde{A})$ , where:

$$d(\tilde{C}\tilde{A})(p_o, q_o) = p_o dq_o - P dQ \quad (4)$$

If we rewrite this function  $\tilde{C}\tilde{A}$  using the arguments  $P$  and  $q_o$  — which under certain regularity conditions is always possible — the remaining coordinate values  $p_o$  and  $Q$  are delivered by the partial derivatives of  $\tilde{C}\tilde{A}$  with respect to the arguments. [6]

In these relations, the “time” difference elapsed between the two states is apparently not present, which in other words means that one can determine the corresponding  $\{p_o, q_o\}$  and  $\{P, Q\}$  pairs without following the trajectories of the system once the generating function of the Poincarè plot has been given.

Finally, if the perturbation  $\mathbf{C}$  depends on a parameter,  $\epsilon$ , and when the perturbation is not very much different from the identity transformation, that is  $\mathbf{C} = (\mathbf{1} + \epsilon)\mathbf{C}_0$ , (here  $\mathbf{1}$  is the identity transformation), then the partial derivatives of the transformed variables  $Q$  and  $P$  with respect to  $\epsilon$  obey the Hamilton equation,

$$\left. \frac{dP}{d\epsilon} \right|_{\epsilon=\epsilon_0} = - \frac{\partial \tilde{C} \tilde{A}(p_0, q_0, \epsilon = \epsilon_0)}{\partial q_0} \quad (5)$$

$$\left. \frac{dQ}{d\epsilon} \right|_{\epsilon=\epsilon_0} = \frac{\partial \tilde{C} \tilde{A}(p_0, q_0, \epsilon = \epsilon_0)}{\partial p_0}$$

(Ref. 6). This has the consequence, that once the generating function has been determined, it is possible to study the evolution of the trajectories by a simple rescaling of it by the parameter  $\epsilon$  in an entire vicinity of the parameter value known, ( $\epsilon_0$ ), which — as it will be seen later on — can be advantageously used in the numerical calculations .

There are most diverse possibilities to define a suitable generating function [6], but we have chosen the case treated above, namely the one, which is defined in dependence of the transformed momentum  $P$  and the “old”  $q$  angle variables.

The generating function of a specific perturbation  $\mathbf{C}$  (of the form mentioned before eq. 5.) can be put in a form:

$$\tilde{C}(P, q) = P q + \sum_{k=-\infty}^{\infty} C_k(P) e^{ik q} \quad (6)$$

(where the parameter  $\epsilon$  is understood to be contained in the coefficients,  $C_k(P)$ ) and the following relations hold:

$$Q = q + \sum_{k=-\infty}^{\infty} \frac{\partial C_k}{\partial P} e^{ik q} \quad (7)$$

$$P = p - \sum_{k=-\infty}^{\infty} ik C_k e^{ik q} \quad (8)$$

The examination of eqs 6 to 8., show, that the factor  $Pq$  is actually the generating function of the identity transformation, which means that the transformations  $\mathbf{A}$  and  $\mathbf{CA}$  are the same, if all the Fourier coefficients are zero.



## NUMERICAL PROCEDURE

The Poincaré plot of the system under consideration has to be discretised and stored in a way accessible for the subsequent numerical study.

This immediately leads to the conclusion that the original (untransformed) and transformed-coordinate values can be stored in, suitably sized matrices containing the coordinates of the starting points of the trajectories and the corresponding endpoints after one transition around the major axis, respectively.

With a simple normalisation, the Poincaré plot of a compact set on the plane can be redefined in most cases within the limits

$$0 \leq p \leq 1 \text{ and } 0 \leq q \leq 2\pi \quad (9)$$

therefore it is possible to construct a general procedure which treats numerically only this area.

Within the limits specified, one has to define a set of equally spaced meshpoints. The necessary density depends on the nature of the problem to be solved, but numerical experience has shown, that in a good deal of cases a mesh with a total number of  $\sim 10000$  points is sufficient: that is, one has to store approximately  $100 \times 100$  matrices, in which the coordinates of the initial- and the corresponding transformed points are to be found. The correspondence is established by the row- and column indices.

For the sake of convenience, the "radial" ( $p$ ) and ( $P$ ) variables and the "angular" ( $q$ ) and ( $Q$ ) variables are stored as complex numbers, that is:

$$\text{Re } Z_{(i,j)} = p_i; \quad 1 \leq i \leq 101; \quad \text{Re } Z_{(i,j)}^T = P_i; \quad 1 \leq i \leq 101 \quad (10)$$

and

$$\text{Im } Z_{(i,j)} = q_j; \quad 1 \leq j \leq 101; \quad \text{Im } Z_{(i,j)}^T = Q_j; \quad 1 \leq j \leq 101 \quad (11)$$

$Z$  and  $Z^T$  are the matrices containing the starting points and the corresponding transformed points respectively.

The structure of the generating function (eq. 6.) shows, that one is able to treat the  $P$  and  $q$  dependences separately. Furthermore one has to consider that the generating function chosen depends on the "old" angular variable and the "new" momentum variable. These two characteristics of the problem profoundly affects the numerical algorithm to be followed. Based on these characteristics one has to locate at first the  $P = \text{const}$  lines in the transformed matrix  $Z^T$  at a set of appropriately chosen, constant values, and store them in one-dimensional arrays.

Doing so, one has to Fourier analyse the differences:

$$Q - q|_{P=\text{const}} = \text{Im } Z_{(.,.)}^T - \text{Im } Z_{(.,.)} \quad (12)$$

along the  $P = \text{const}$  lines, where the correspondence is established via the radial and angular indices.

The relation

$$c_k(P) = \frac{1}{2\pi} \int_0^{2\pi} (Q - q)|_{P=\text{const.}} e^{ikq} dq \quad (13)$$

delivers the coefficients sought for.

In choosing an appropriate set of  $P = \text{const.}$  lines one has to consider that the generating function values have to be interpolated among this predefined constant values, and the acceptable modeling requires a certain density of these lines. In general 25 ~ 30 equidistant values are appropriate, but it is only a rough estimate. The density needed can be determined on the basis of numerical study.

This way one arrives at a set of Fourier coefficients depending on the frequency parameter  $k$ , and the  $P = \text{const}$  values. However eqs. (13), (7) and (8) show, that the coefficients determined ( $c_k$ ) are the partial derivatives of the coefficients required ( $C_k$ ).

Furthermore it is to be note, that the subsequent numerical procedure requires the values of the  $C_k(P)$  coefficients and its derivatives not only at the previously chosen, discrete  $P = \text{const.}$  values, but continuously, at any particular  $P$  value, therefore one has to chose an appropriate representation of these coefficients.

After some considerations the choice of using a cubic spline representation turned out to be natural. It has the advantage too being able to determine in the same procedure the necessary integrals and derivatives easily.

Still one circumstance has to be mentioned in this context. As the transformation is stored in a finite set of mesh points, the  $Q - q$  differences determined numerically follow a complicated pattern consisting of finite number jumps, and between them the function is changing slowly (see Fig. 6.a). This fact results in enhanced Fourier coefficients at higher harmonics, introduced by the finite resolution of the procedure, and by the resonance of specific members of the Fourier series. This may lead to substantial deteriorations in the reconstructed Poincarè map. (See Fig. 7.).

After a longer search for a suitable procedure, the polinomial smoothing proved itself to be suitable to tackle the task.(See. Fig. 6.b )

Having got the spline coefficients ( $C_k$ ) in the generating function (eq. 6.), there are two basic possibilities for further numerical calculations.

At first it is possible to determine the corresponding pairs of the coordinates of the starting- and transformed points value using the:

$$p = \frac{\partial \tilde{C}(P, q)}{\partial q} \quad (14)$$

$$Q = \frac{\partial \tilde{C}(P, q)}{\partial P} \quad (15)$$

relations (which correspond to eqs 7 and 8).

This makes it possible to either follow a trajectory with given initial coordinates (field-line tracing) under repeated transformations, or to effectuate the Poincaré transformation of the surface as a whole. Because of the mixed dependence of the generating function on the old angular and the new radial variables, these operations can be performed only after inverting the transformation.

Giving a general method for inverting the transformation results in unnecessary complications, therefore we have chosen a different approach. If the generating function is known, and coordinates of the starting point  $(p, q)$  have been given, one is able to construct an approximation for the corresponding  $P$  radial coordinate using eq. 8, which turns out to be:

$$P_o = p - \frac{\partial \tilde{C}(P, q)}{\partial P} \Big|_{P=p} \quad (16)$$

The error due to this approximation is measured by the deviation,

$$\Delta(P_o) = P_o - \left( p - \frac{\partial \tilde{C}(P, q)}{\partial P} \Big|_{P=P_o} \right) \quad (17)$$

and the corresponding  $p$  and  $P$  pairs are found by searching for the zero of this deviation  $\Delta(P_o)$ .

## NUMERICAL EXAMPLE

The example used to illustrate the applicability of the procedure described here and to test the precision requirements, is one pertaining to the case of the circulating  $\alpha$ -particle in a strongly nonsymmetric stellarator vacuum field.

In what follows, we identify the canonical momentum variable of the corresponding Hamiltonian system with the radial coordinate of the magnetic field and the canonical space variable with the poloidal-angle coordinate on the magnetic surface. Therefore we replace the corresponding symbols of the canonical coordinates by their corresponding and widely used symbols;  $p \rightarrow \psi$  and  $q \rightarrow \theta$ .

Using a coordinate system, in which the lines of force of the magnetic field are straight, the equation of motion of the  $\alpha$  particles can be cast in a form [7]:

$$\frac{d\psi}{d\phi} = -\frac{\rho R}{\psi} \frac{\partial}{\partial \theta} \left[ \frac{(1 - \lambda B)}{B^2} \right]^{1/2} \quad (18)$$

$$\frac{d\theta}{d\phi} = \tau(\psi) + \frac{\rho R}{\psi} \frac{\partial}{\partial \psi} \left[ \frac{(1 - \lambda B)}{B^2} \right]^{1/2} \quad (19)$$

where:  $\rho$  is the gyroradius of the particle,  $R$  is the major radius of the magnetic surface,  $\psi$  is the flux coordinate of the magnetic surface,  $\phi$  is the toroidal coordinate which corresponds with the canonical time variable,  $\tau$  is the rotational transform, and finally  $\lambda$  is the pitch angle variable of the particle. On the magnetic surface the magnitude of the magnetic field ( $B$ ) is supposed to be known in an appropriate form for the subsequent numerical study.

It is easy to see, that in the limiting case of  $\rho = 0$ , the system is an integrable one; that is the Poincaré transformation generated by the trajectories is a simple "twist" map.

Referring to the already mentioned transformations **A** and **C**, the  $\tau(\psi)$  term in eq. 19. represents the "integrable" part of the map, and the factors containing  $\rho$  represent the perturbation **C** in the case of nonzero Larmor radius. The drifts caused by the finiteness of the Larmor radius can substantially deform the trajectories of the corresponding solution.

In practical calculations the factors containing the magnetic field,  $B$ , are written in the form:

$$[1 - f]^{1/2}$$

and:

$$f = \lambda \left[ 1 - \epsilon_0 \cos \theta + \sum_{l=1}^4 \epsilon_l \psi^{l/2} \sin(l\theta - m\phi) \right] \quad (20)$$

here  $\epsilon_l$  and  $\lambda$  are constants determined from the actual magnetic configuration and the characteristics of the particle. [7]. For a given set of these constants, it is possible to construct the two 100 x 100 matrices needed by direct integration, and these matrices serve for the subsequent numerical analysis.

## NUMERICAL TESTS, PRECISION REQUIREMENTS

In assuring the numerical reliability of the method arriving a sufficiently reliable numerics, the first question to be answered is, how many Fourier coefficients are needed for an acceptable description of the system? Naturally the answer depends

on the spectral composition of the perturbation. (eq. 20.) The Fourier coefficients of an analytic function limited from above are monotonically decreasing for large frequencies as the frequency parameter tends to infinity. Because of this fact one is able to determine the length of the Fourier series from

$$|k \cdot C_k| < \Delta \cdot C \cdot n^{-1} \text{ for every } |k| > k_0 \quad (21)$$

where  $n$  is the desired number of repeated Poincarè transformations,  $\Delta$  is a parameter which depends on the required resolution of the plot, and  $C$  is a parameter less than unity which takes into account the "stability" properties of the domain in the phase space to be investigated. (See later.) The parameter  $C$  is necessary because as a second parameter, the length of the Fourier series depends on the properties of the phase space and where the analysis is being done. In a stable region where the invariant tori still exist, the stability of the trajectories is better than in the "stochastic" region, or in the vicinity of hyperbolic points. Experience has shown that the range  $0.5 < C < 0.1$  is in general a satisfactory one. On the basis of the features given, the necessary length of the Fourier series in the cases investigated varied between 6 and 10 members with nonzero frequency parameter.

As has been already mentioned, there is a sensitive property of the procedure, which deserves further clarification. As the function to be Fourier analysed is evaluated in discretised form in a sequence of jump function, the smoothing of the data set to be processed is essential, because the Fourier series of a step function has a very broad frequency spectrum which can introduce unwanted resonances. However, the smoothing can result in unwanted secondary effects with the same characteristics.

If the smoothing is done by using polynomials or splines, one has to impose constraints on the procedure, because the peaks must be reproduced very precisely. This means that one has to use polynomials of fairly high degree, or a large number of interior knots are needed in the case of splines. As a consequence, the fitting curve contains a residual fluctuation which is in resonance with the very important frequency range of  $k = 5 - 10$ . The Fourier decomposition of such a function is very imprecise, and the error in the coefficients derived can amount to several orders of magnitude, even using an adaptive integrator.

The problem has been circumvented by using a numerical procedure which delivers the necessary Fourier coefficients by a minimisation procedure. Namely the sum of the quadratic deviations of the harmonic functions from the function to be expanded into Fourier series in dependence of the Fourier coefficients is sought for. Actually

the minimum of the sum

$$\sum_i (y_{i|x_i} - \sum_{k=-\infty}^{k=\infty} c_k e^{ikx_i})^2 \quad (22)$$

is determined in function of the  $c_k$  coefficient. (The  $y$  above is the function to be expanded into series.)

The precision of this decomposition method is sufficiently high; with analytical test function at least the first nine significant digits of the coefficients are precise. This degree of the precision is inevitable in this context.

Finally the flux conserving property of the Poincarè map is to be rigorously insured. The main parameter in this context is the precision of the local inversion of the map. (eqs 16, 17.). In Figs. 8.a and b. two examples are to be seen, which differ only in the precision of the inversion.

As an exotic example, the case with deliberately distorted flux conservation is shown on Fig. 9. This actually indicates, that the simulation of dissipative systems is also ensured by the method described, which substantially enlarges the field of possible applications.

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Fig. 5.a. The phase space of the system with  $A = 0.15$ , in the vicinity of the stochastic region

Fig. 5.b. The same part of the phase space as simulated numerically.

Fig. 6.a. The  $Q - q|_{P=const}$  function of the system of equations 6 and 7 at the parameter value of  $A = 0.1$ , before smoothing

Fig. 6.b. The effect of smoothing of the curves presented on Fig. 6.a

Fig. 7. Diagrams effects of the enhanced Fourier coefficients without smoothing. The small islands around the two big ones are the islands of the new modes, as they are mentioned in the main text.

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## FIGURE CAPTIONS

Fig. 1. a - The solution of the system of equation 6. and 7.

with  $A = 0.05$ .  $\frac{\rho R}{\psi} = A$ .

Fig. 1. b - The results of the field line tracing with the numerically determined generating function, using the same starting points for the trajectories.

Fig. 2.a. The direct integration of the system at the parameter value:  $A = 0.01$ .

Fig. 2.b. The results of numerical simulation of the same model.

Fig. 3.a. The structure of the phase space of the model at parameter value  $A = 0.05$ .

Fig. 3.b. The numerically simulated phase space of the system using the generating function of Fig. 2.b., but rescaling the coefficients of the Fourier series by a numerical factor equal to five times the original ones. This possibility of rescaling of the generating function of the model contributes to the substantial economy of computer time.

Fig. 4.a. The solution of the system at parameter value  $A = 0.1$ .

Fig. 4.b. The simulation of the trajectories with the generating function of Fig. 2.b, multiplying the coefficients by a factor of 20. The similarity of the phase spaces is acceptable for most studies of practical interest.

Fig. 5.a. The phase space of the system with  $A = 0.15$ , in the vicinity of the stochastic region.

Fig. 5.b. The same part of the phase space as simulated numerically.

Fig. 6.a. The  $Q - q_{|P=const}$  function of the system of equations 6 and 7 at the parameter value of  $A = 0.1$ , before smoothing.

Fig. 6.b. The effect of smoothing of the curves presented on Fig. 6.a.

Fig. 7. Resonance effects of the enhanced Fourier coefficients without smoothing. The small islands around the two big ones are results of the unwanted resonances mentioned in the main text.

Fig. 8. a and b. The effect of the precision of the inversion. (eq. 17.)

In Fig. 8.b. The tolerance of the inversion is 1000 times as large as in Fig. 8.a.

Fig. 9. The effects of the non area preserving character of the generating function.

a and b: the unstable trajectories of the system just outside and inside of the limiting cycle of the resulting classical mechanical system;  
c: the corresponding limiting cycle of this specific system.

Fig. 10. a,b,c. The Poincaré plots of the system with parameter value  $A = 0.08$ .

a - after one transition of the trajectories;

b - after 15 transitions;

c - after 30 transitions.

The formation of the two main chains of islands and the secondary islands may be clearly seen.

## SUMMARY

A numerical method has been described which is capable of deriving the generating function of a Poincaré plot defining a Hamiltonian system with one degree of freedom. There are only very loose conditions to be fulfilled. For instance there has to be found in the mapped region reasonably large intervals in the direction of the canonical impulse coordinate with unbroken KAM surfaces.

The method allows us to follow a trajectory with given initial values of momentum- and space coordinates. The trajectory tracing is approximately ten to fifty times as fast as the direct integration of the corresponding system of differential equation, depending on the actual circumstances.

The possibility of rescaling the generating function by a numerical factor without loss of precision means that the total computer time economy in an extended numerical study of a complicated problem can amount to two orders of magnitude.

It is possible to carry out the Poincaré transformation of the plane of interest at an arbitrarily chosen set of starting points. The time economy in this case is similar to that mentioned above.

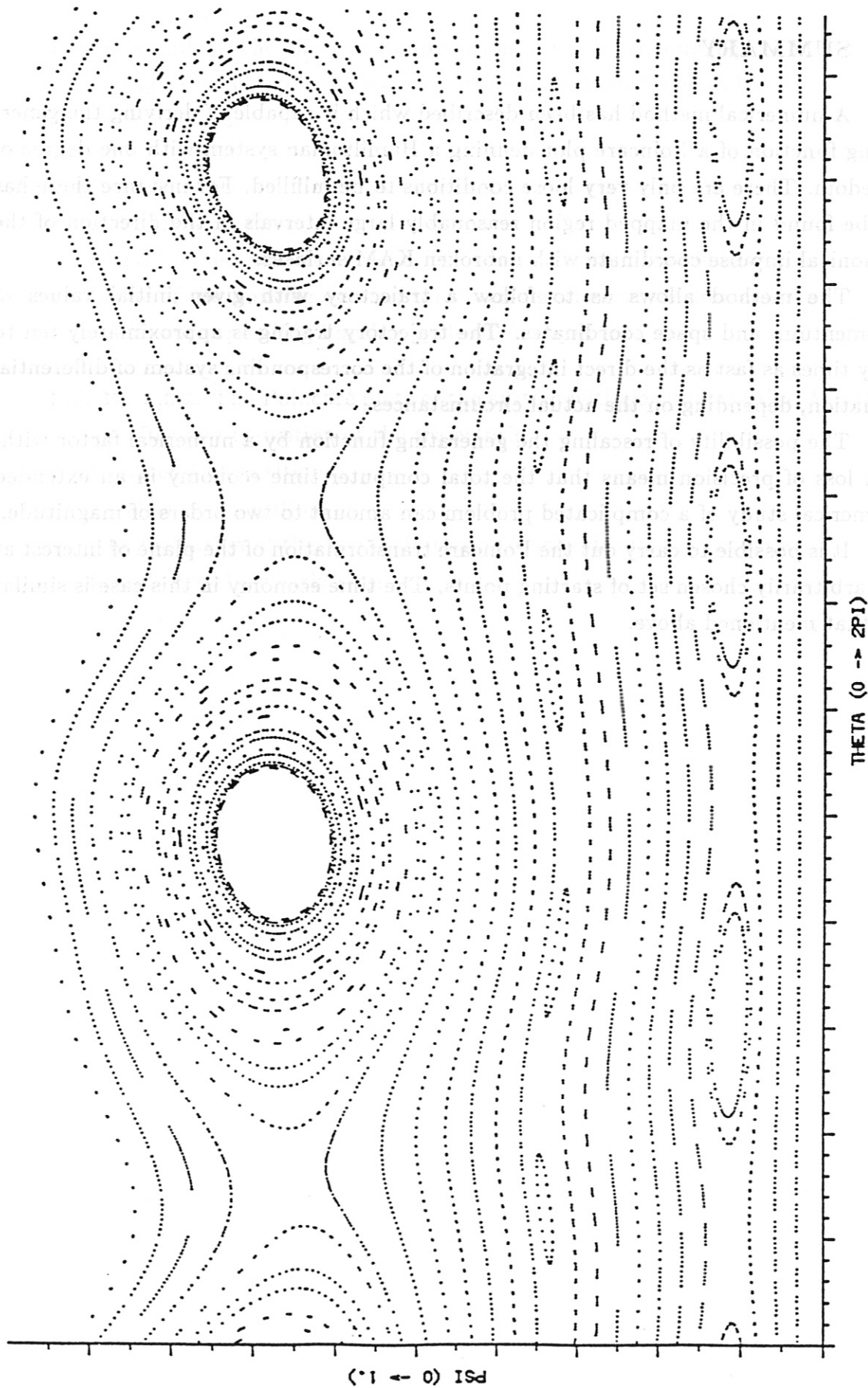
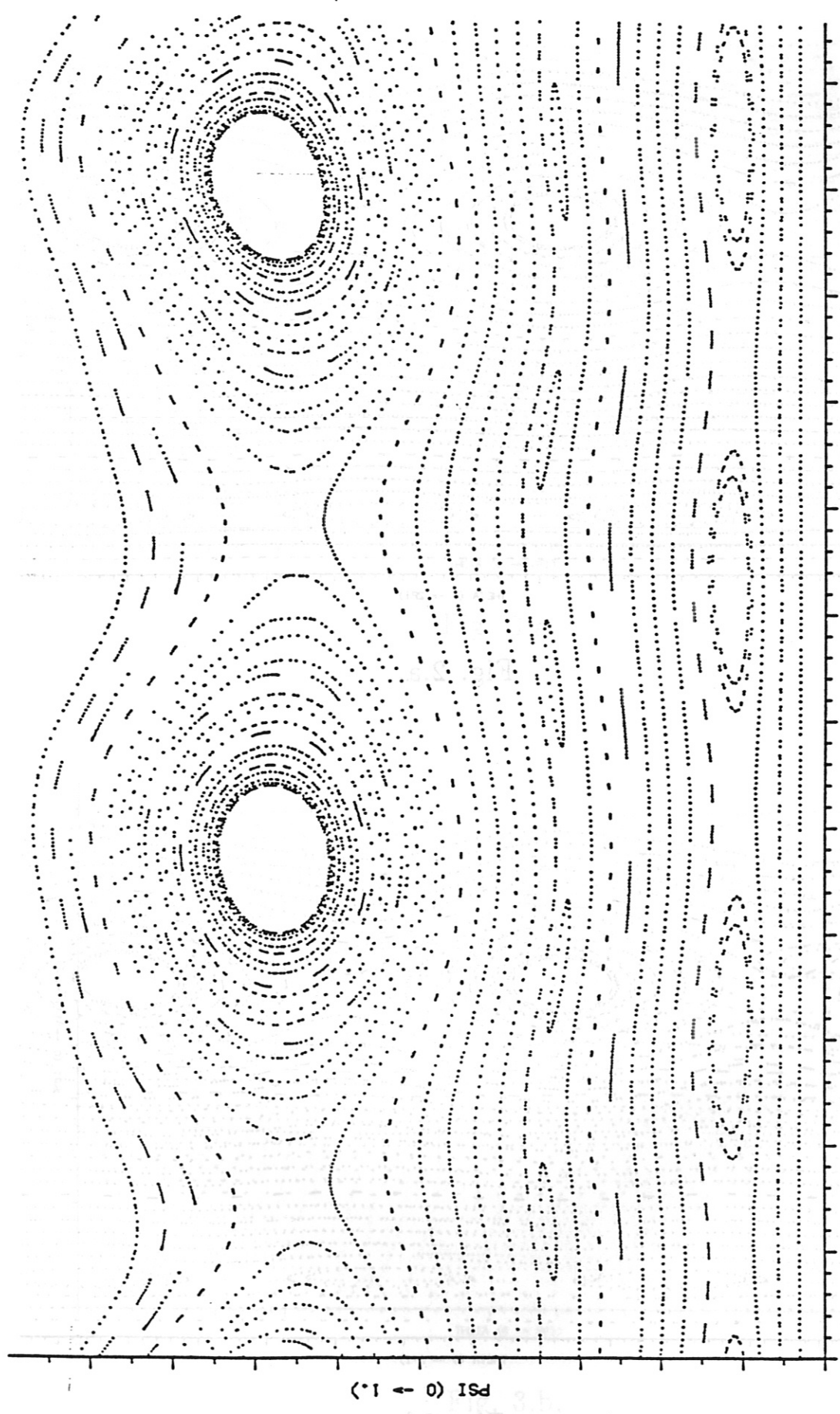


Fig. 1.a.



THETA (0 -> 2PI)

PSI (0 -> 1)

Fig. 1.b.

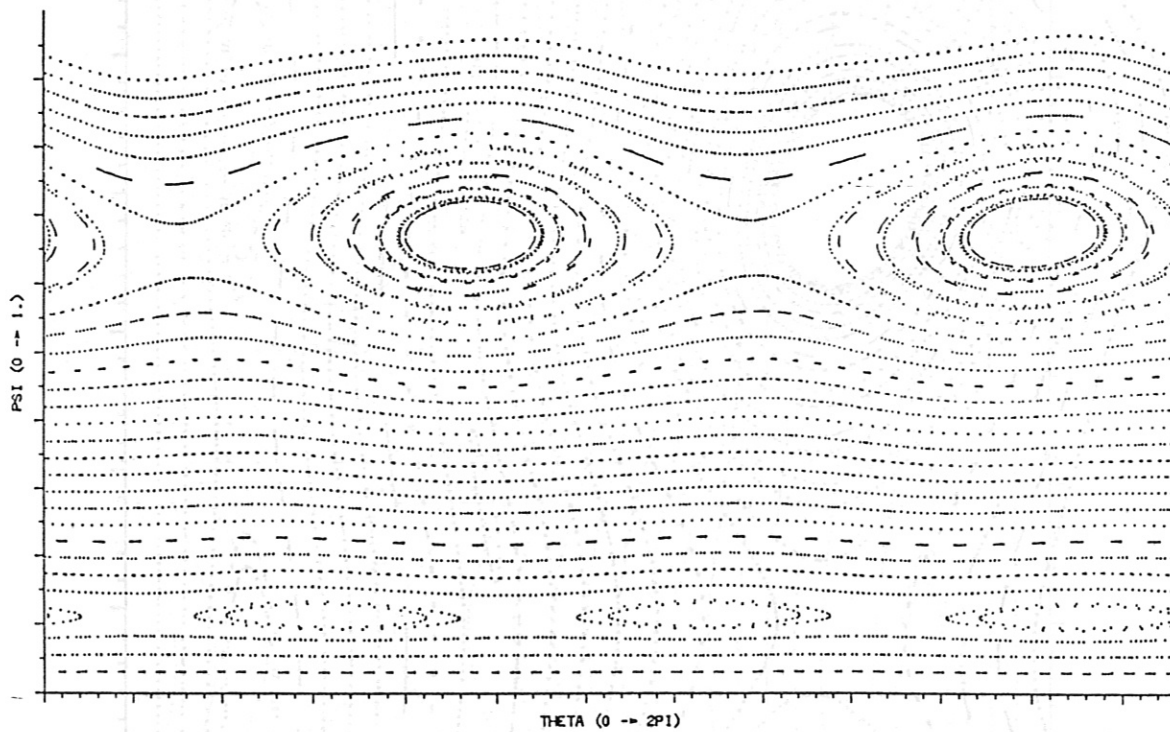


Fig. 2.a.

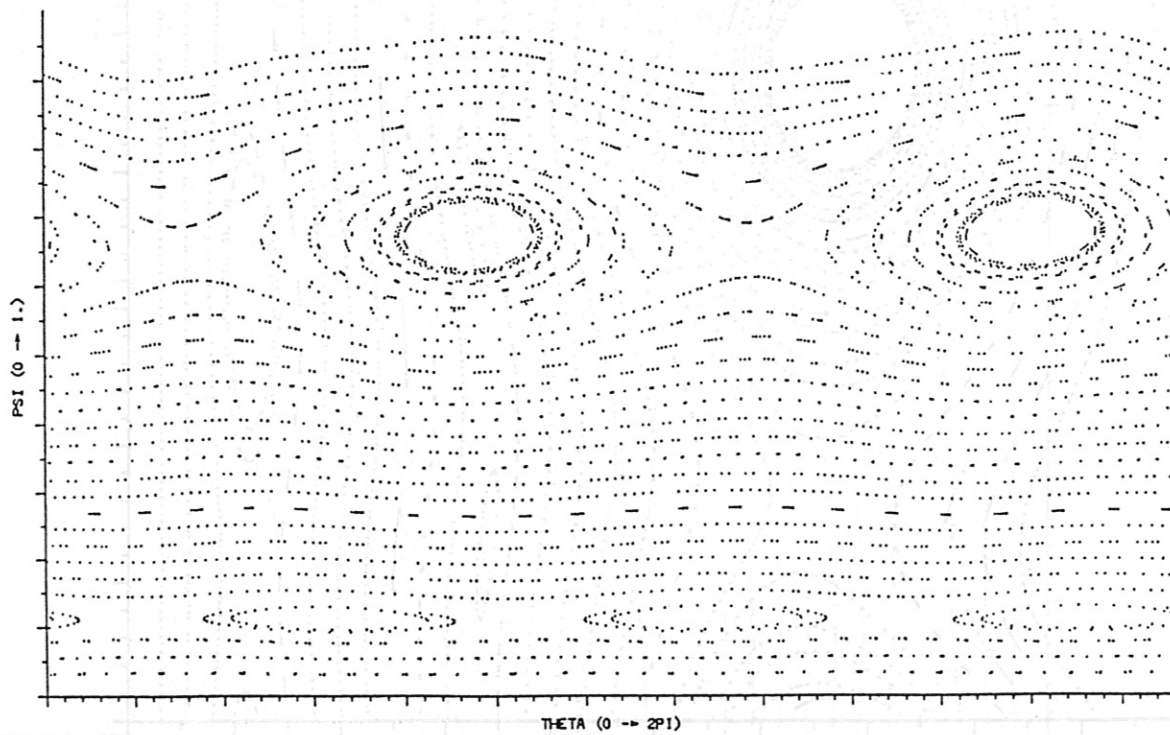


Fig. 2.b

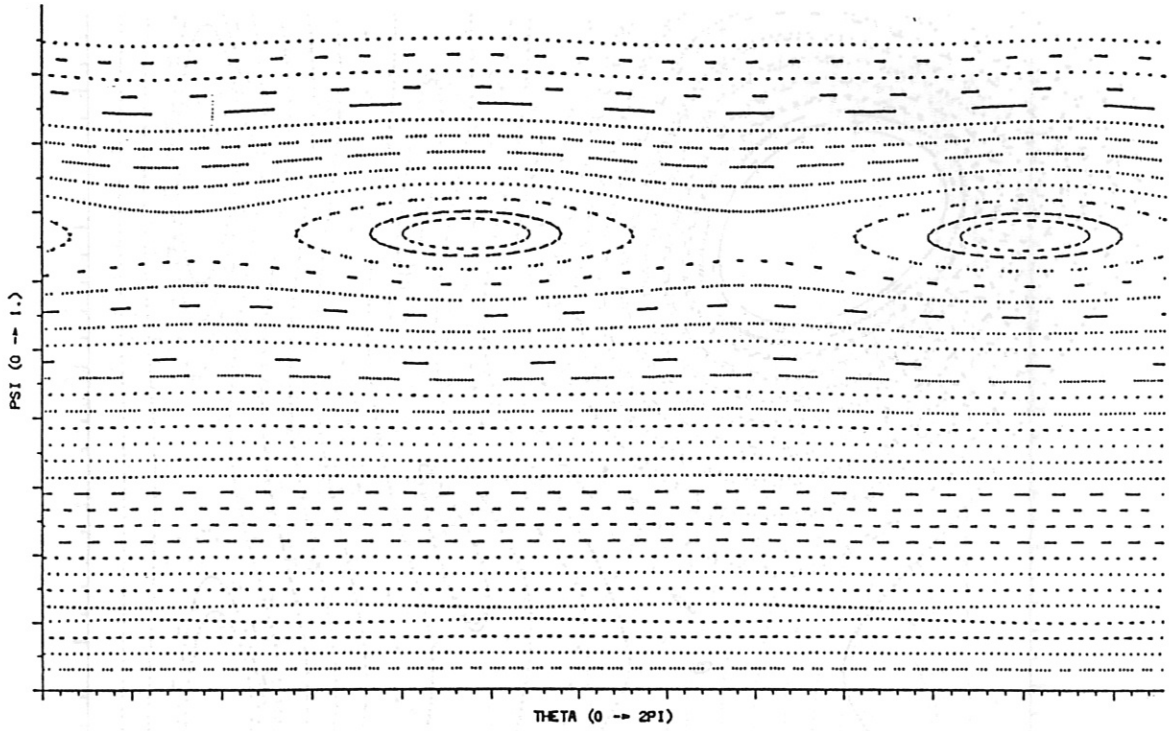


Fig. 3.a.

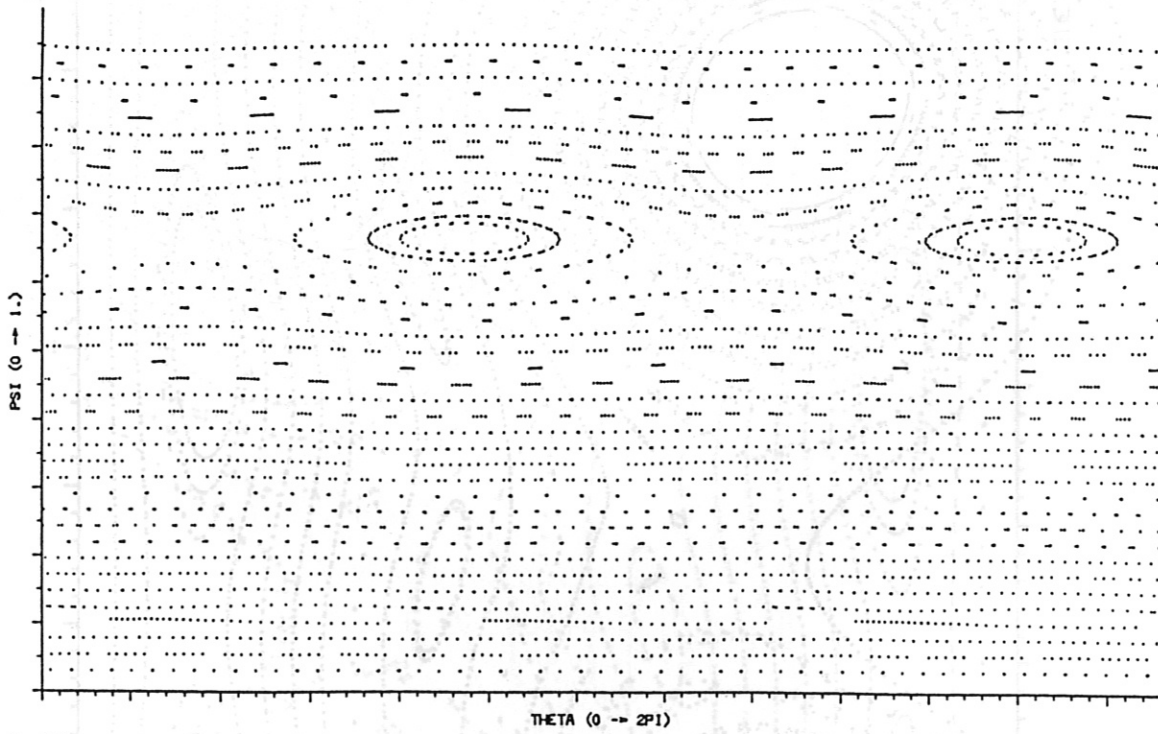


Fig. 3.b.

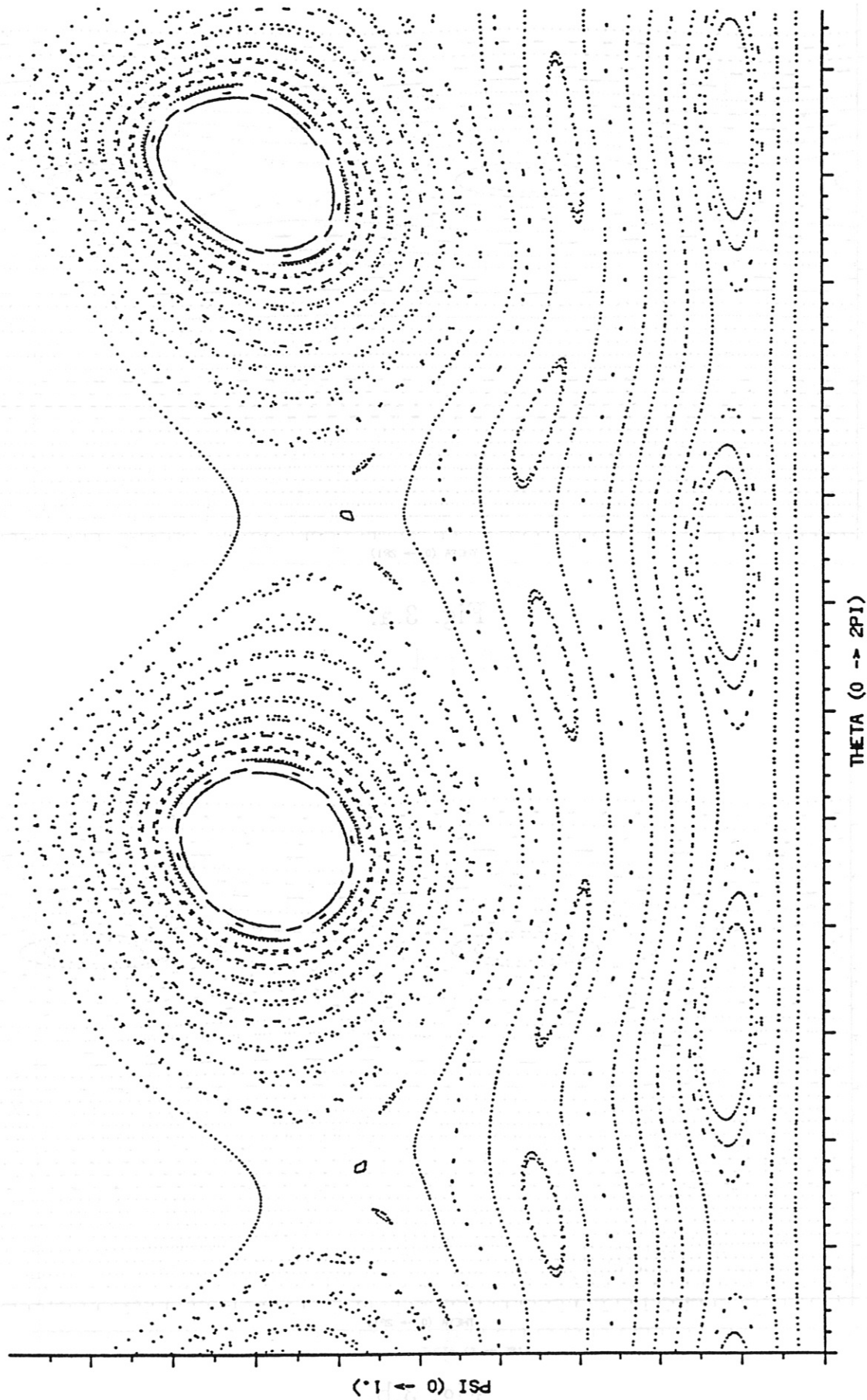


Fig. 4.a.



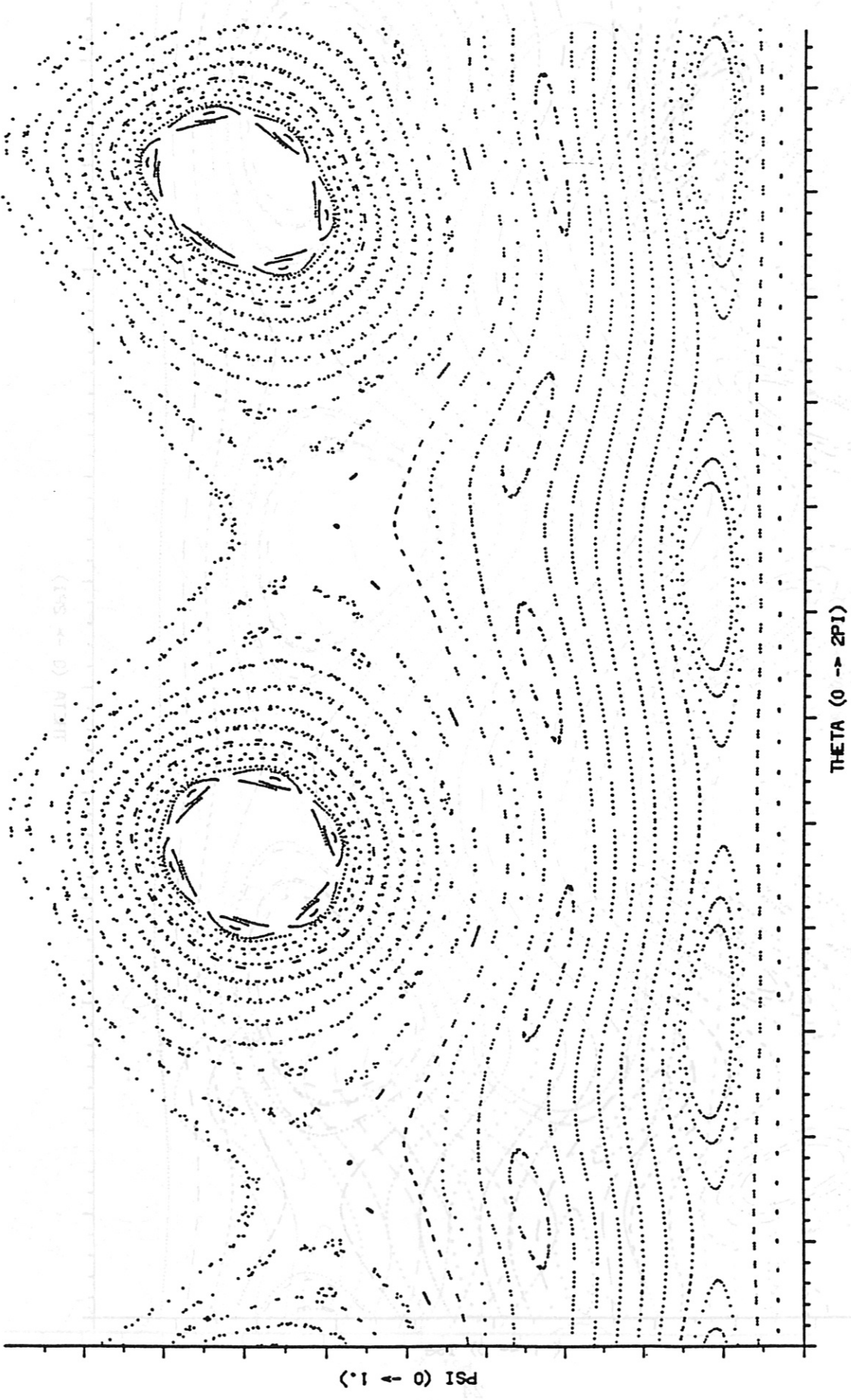
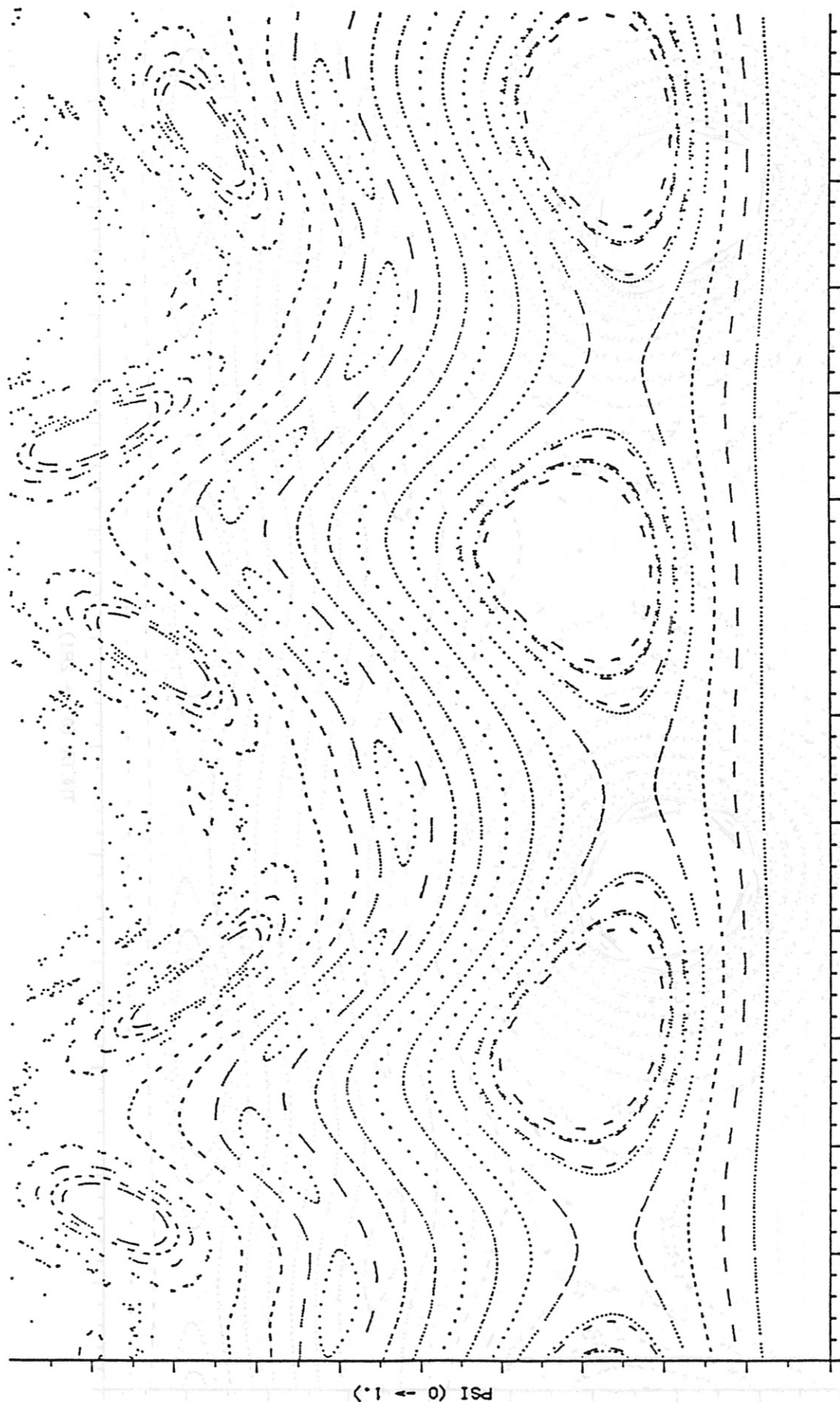


Fig. 4.b.

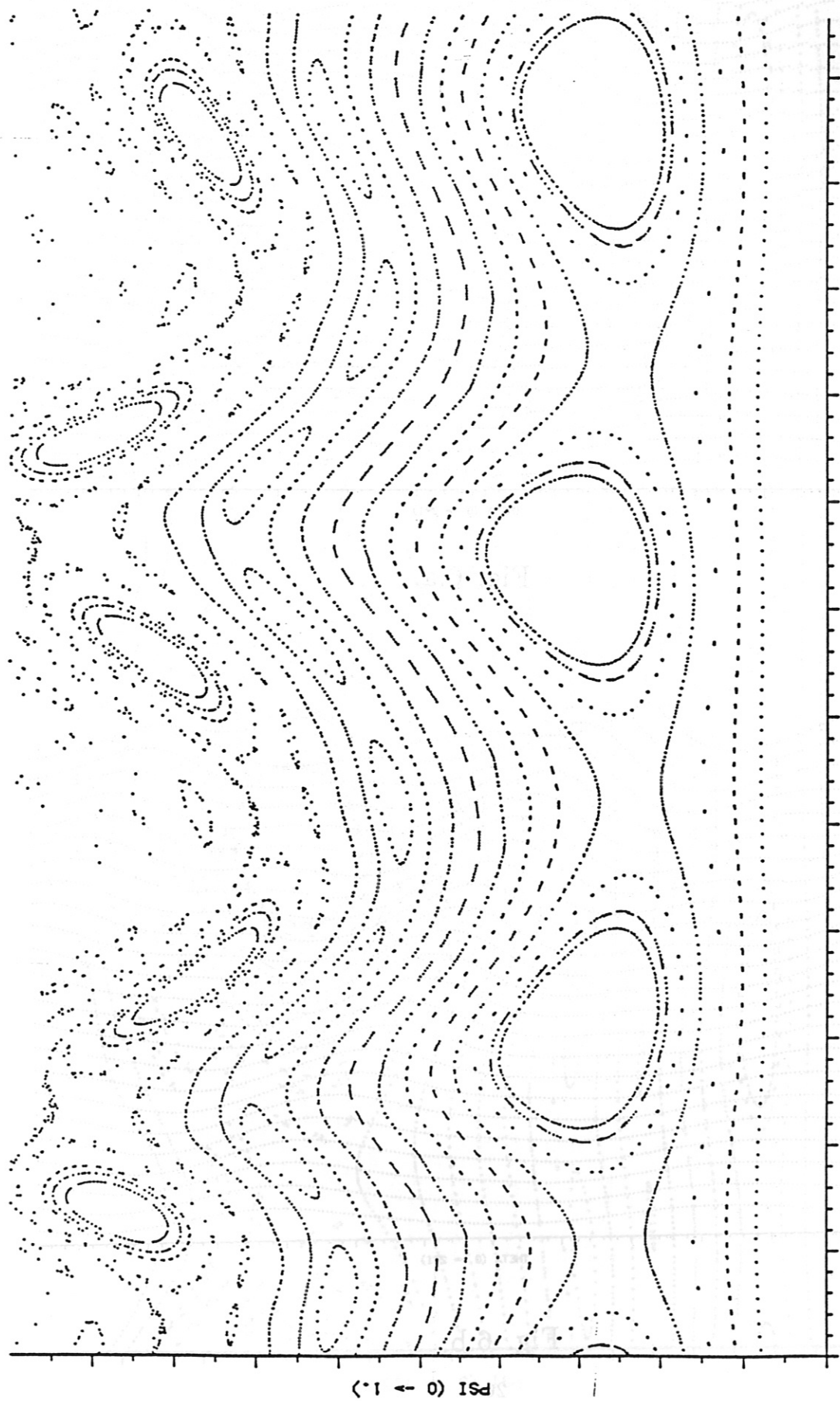
LiF 4P



$\Psi (0 \rightarrow 1)$

$\Theta (0 \rightarrow 2\pi)$

Fig. 5.a.



THETA (0 -> 2PI)

Fig. 5.b.

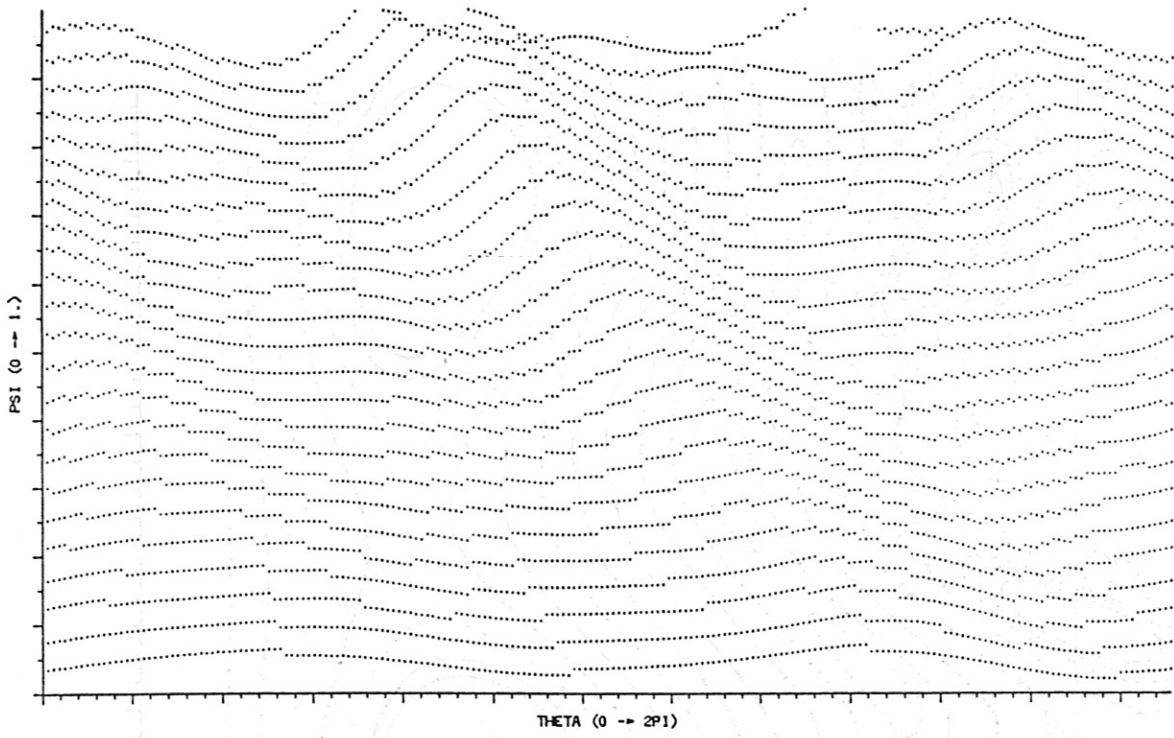


Fig. 6.a.

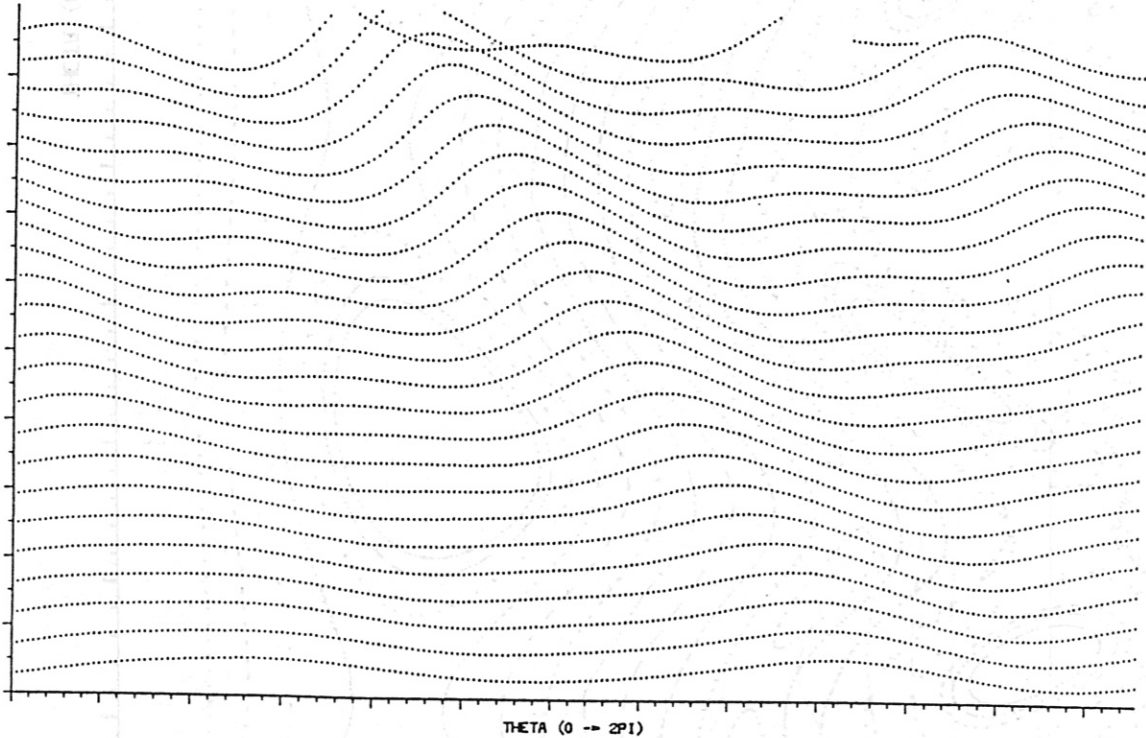


Fig. 6.b.

Fig. 7

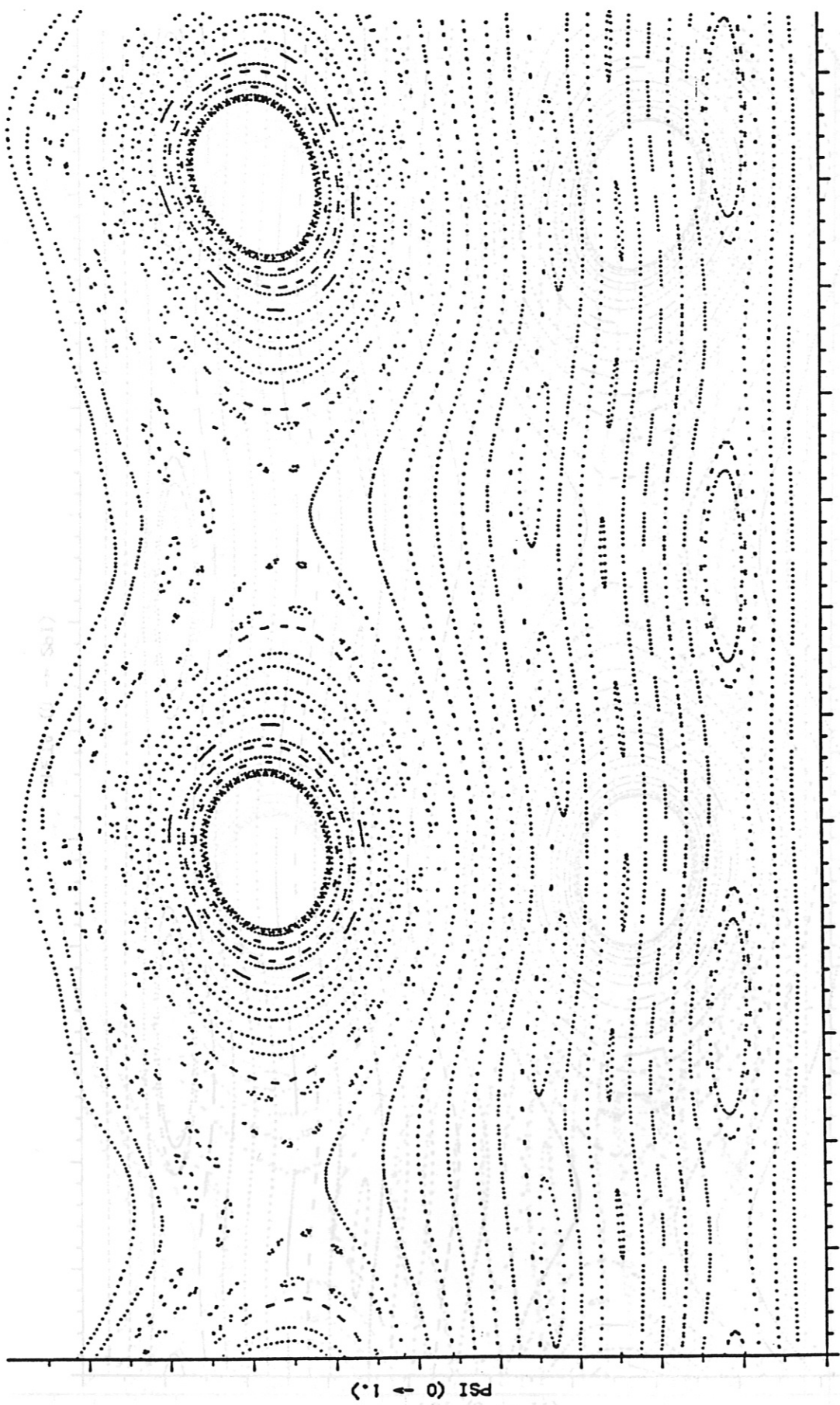


Fig. 7.

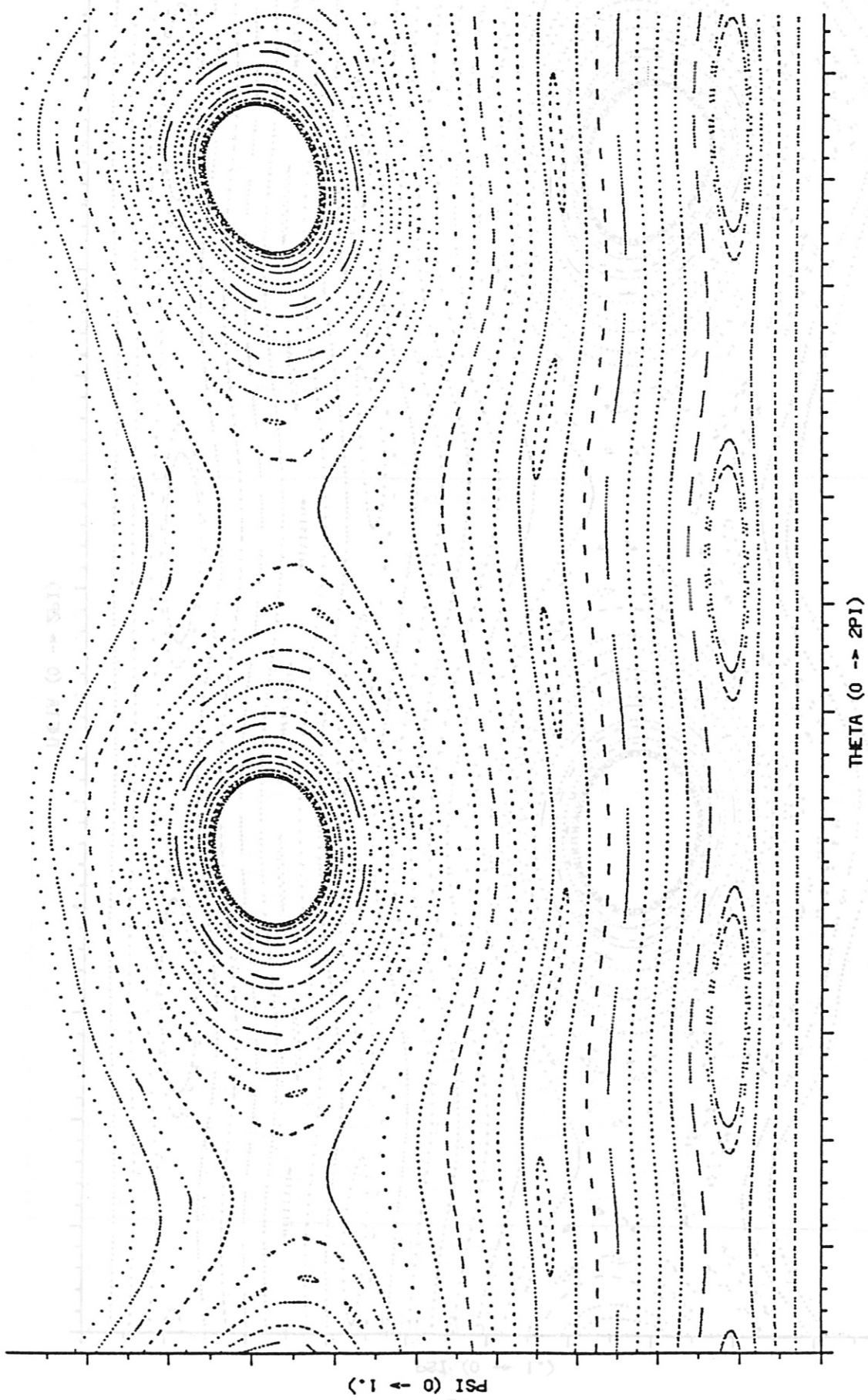


Fig. 8.a

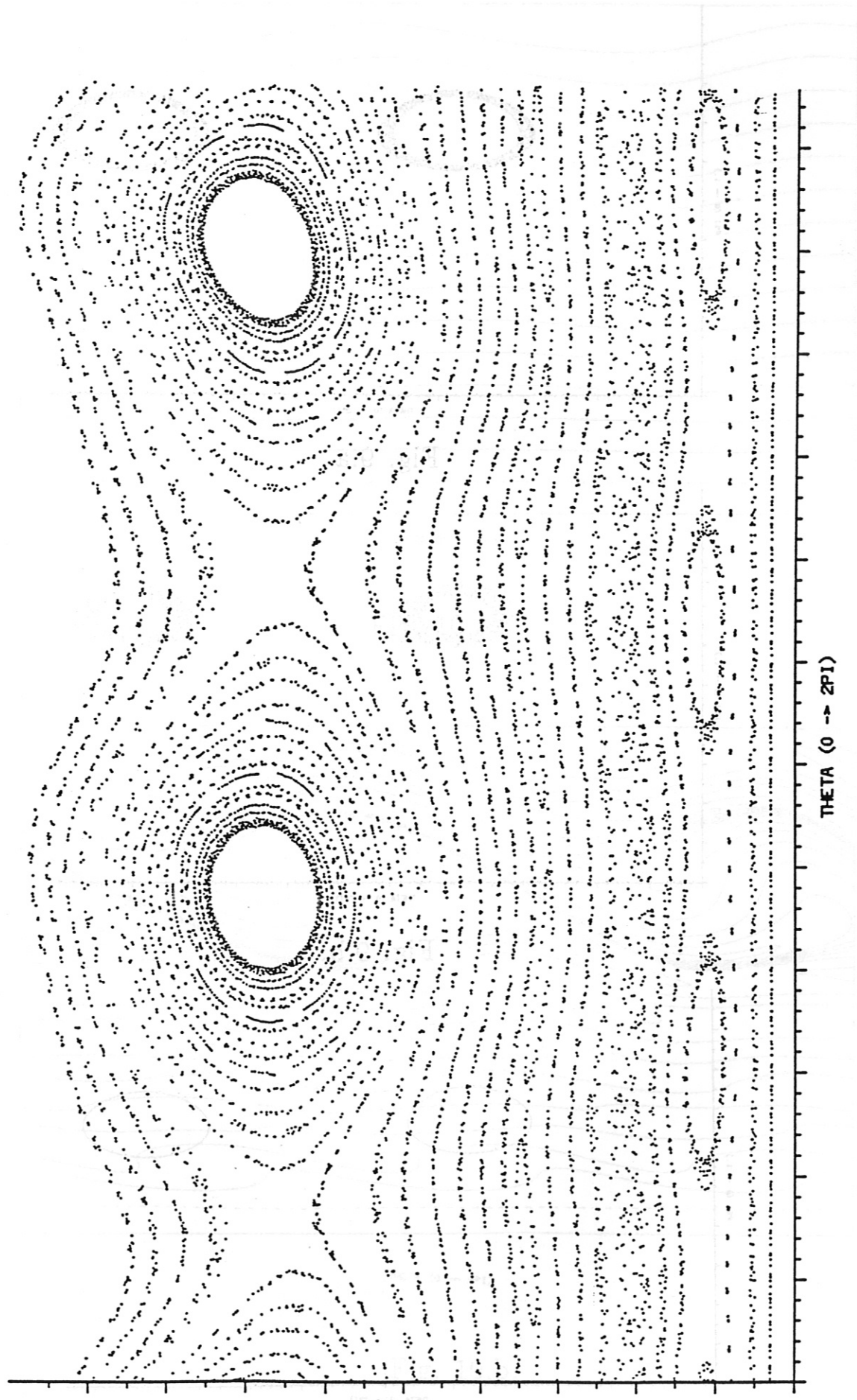


Fig. 8.b.

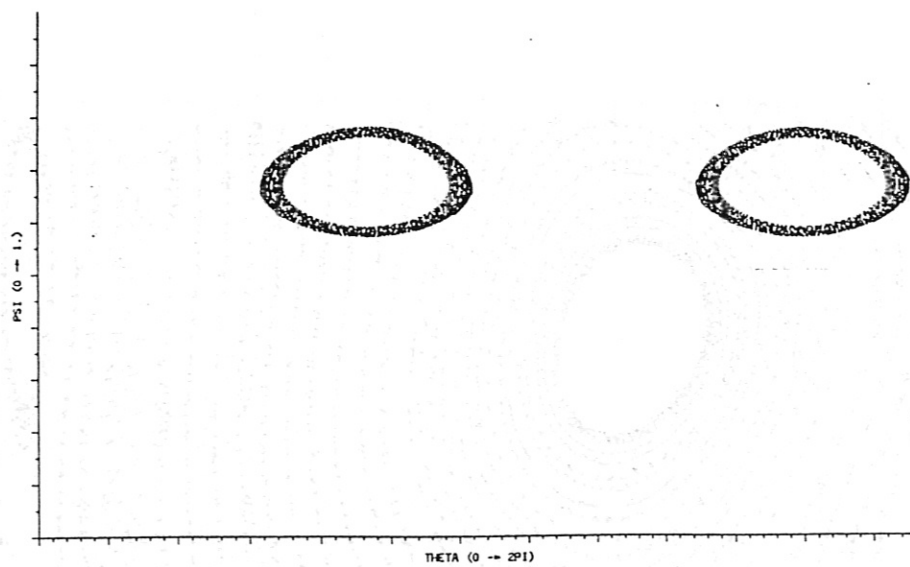


Fig. 9.a



Fig. 9.b.

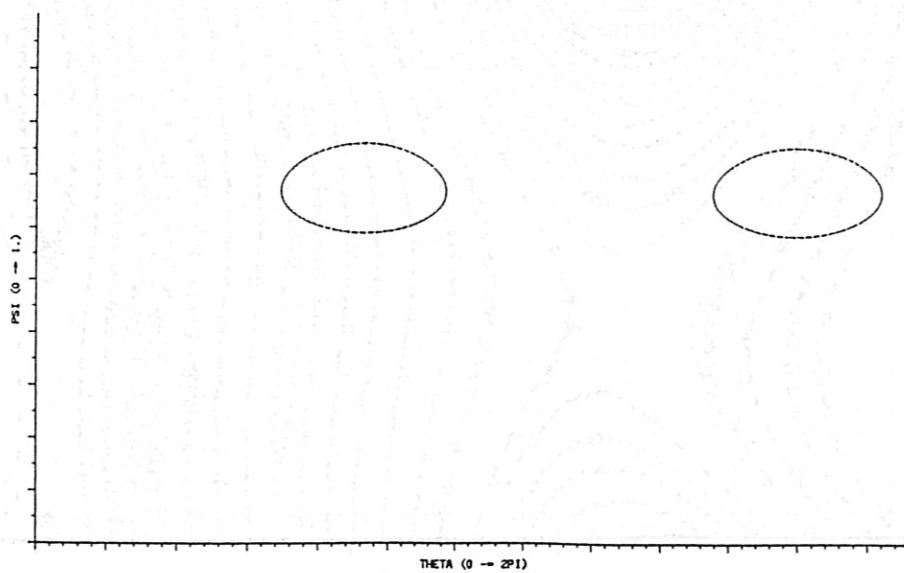


Fig. 9.c.



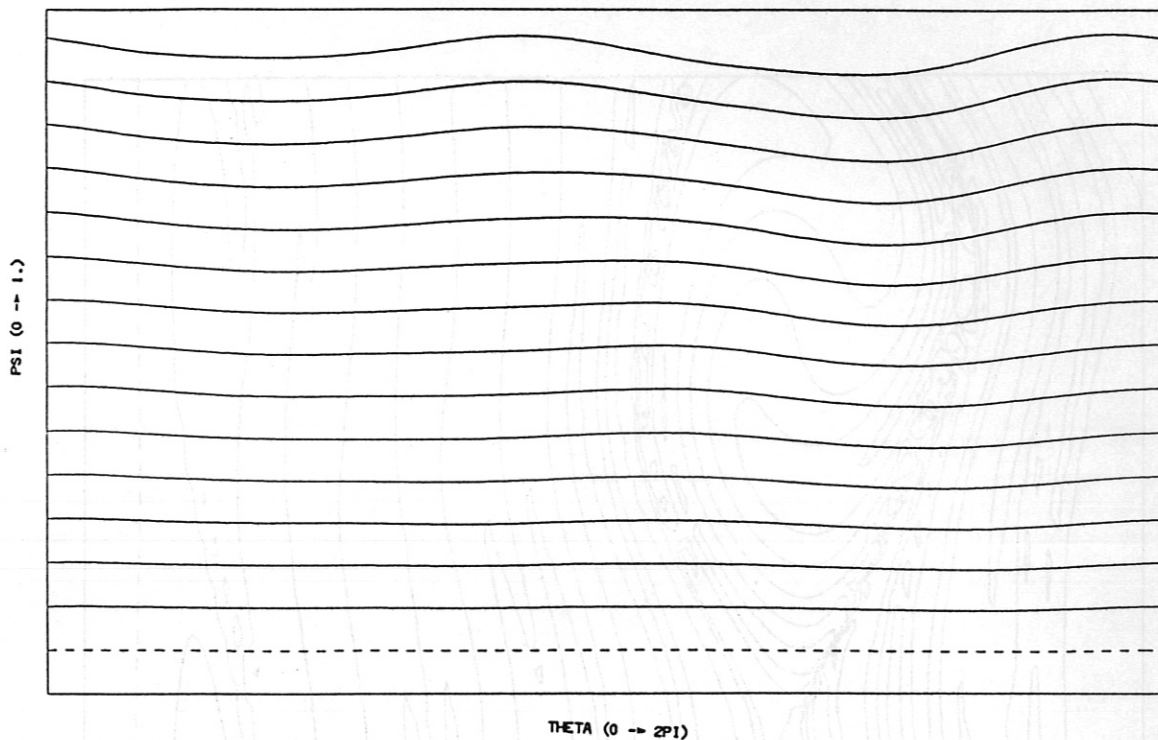


Fig. 10.a.

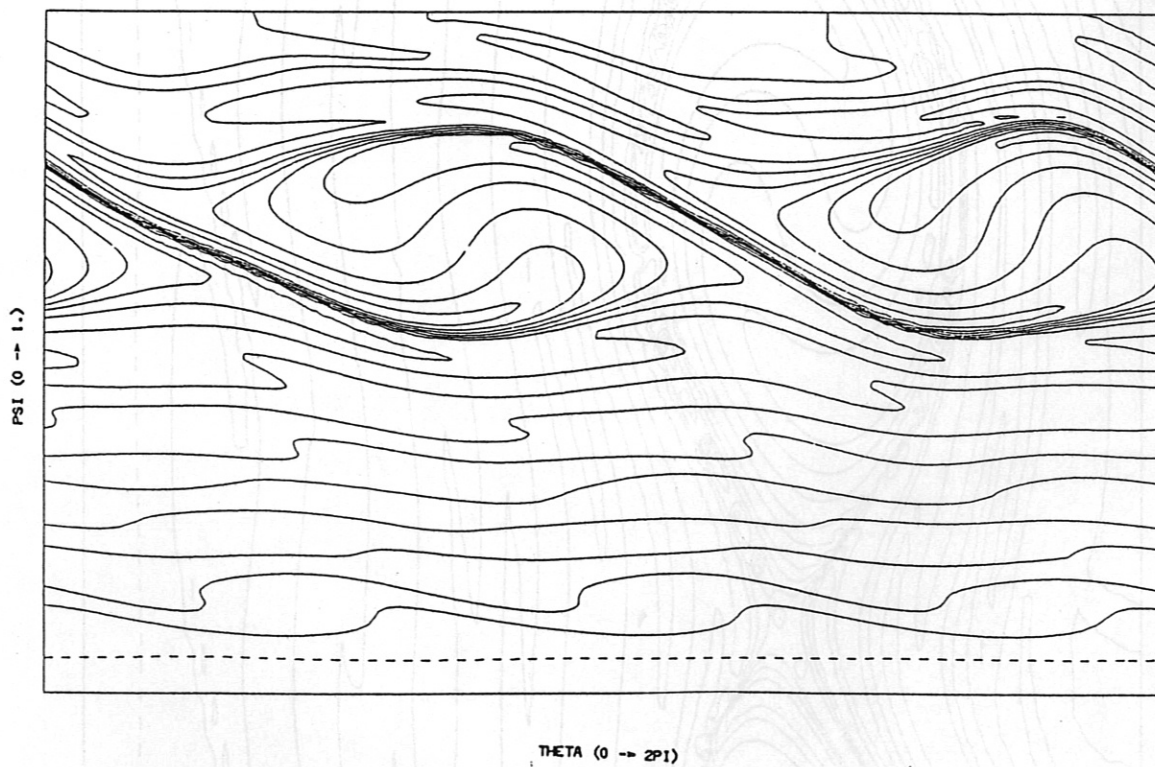


Fig. 10.b.

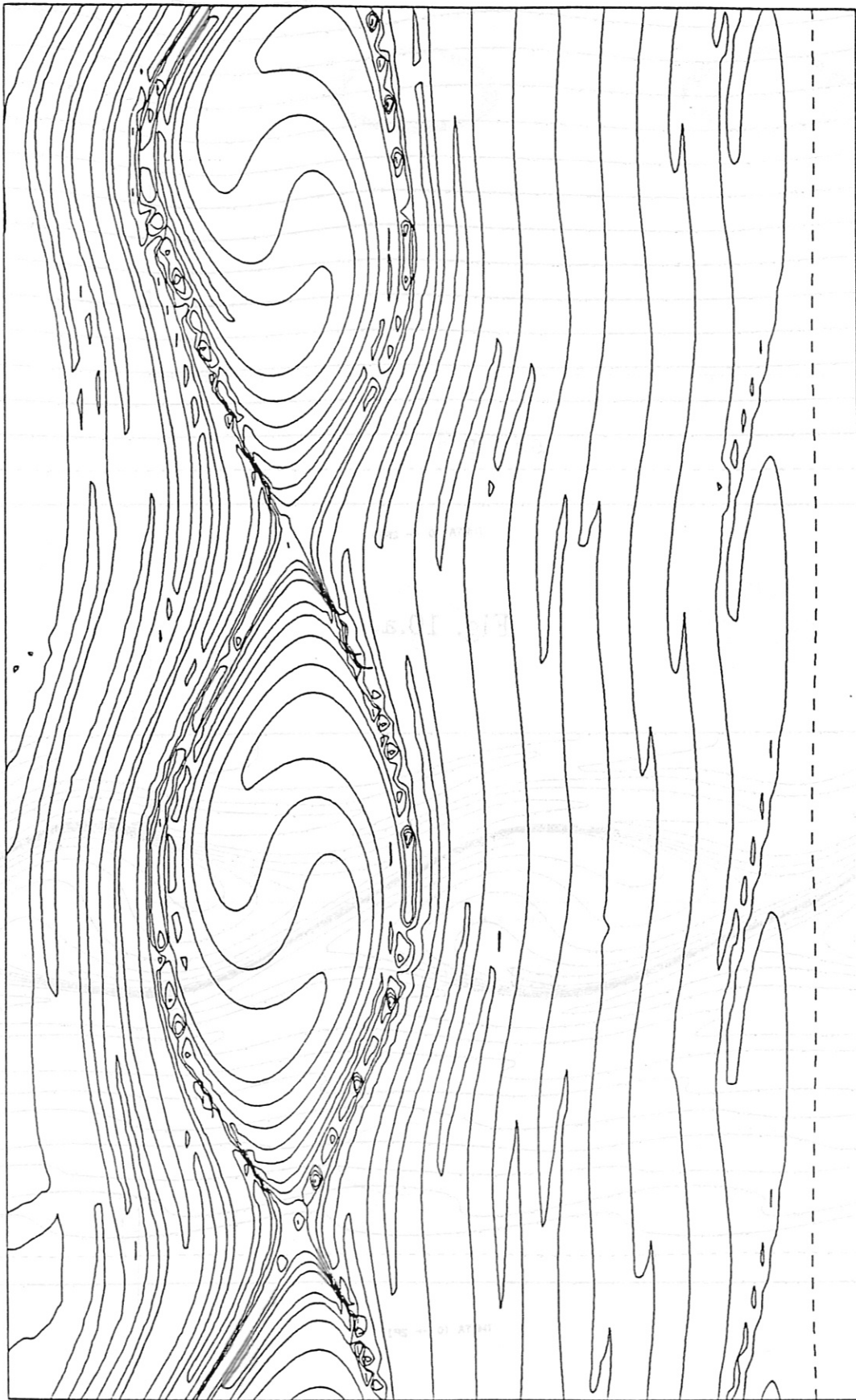


Fig. 10.c.