DOE/ET-53088-277 IFSR #277

Orbit Extension Method for Finding Unstable Orbits

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May 1987

CENTRAL DUPLICATING WORK ORDER FORM

Institute for Fusion Studies: (Acct. #) 26-0921-5050

Fusion Research Center: (Acct. #) _____

Title of Paper: ORBIT EXTENSION METHOD for FINDING UNSTABLE ORBITS

Report #: 277

First Author: Q. CHEN

# of copies needed: 330

# of pages (incl. window and figs.): 27

Single-side window - duplex the rest: ✓

Single side entire manuscript: _____

Collate: ✓ Staple: ✓

Journal name and date submitted: _____

Internal distribution only: _____

Whose mailing list(s)? JDM

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Date sent to CD: 5-14-87 ?

Date picked up from CD: _____

Orbit Extension Method For Finding Unstable Orbits

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April 6, 1987

Abstract The orbit extension method is a technique for building long orbits from shorter ones. Combined with Newton's method, it gives a powerful and efficient tool for finding various orbits of area-preserving twist maps on a cylinder. It is particularly valuable for unstable orbits. We develop this method and use it to find two kinds of orbits: ordered periodic orbits and principal heteroclinic orbits between two resonances. Flux from one resonance to another is obtained as a by-product of the principal heteroclinic orbits.

Keywords area-preserving map, Newton's method, transport, unstable orbits, ordered periodic orbits, heteroclinic orbits.

§1. Introduction

The study of the nature of chaotic behavior and transport in Hamiltonian systems requires the computation of various orbits.[1,2] These orbits are typically unstable; indeed, the stochastic region is characterized by positive Lyapunov exponents, which implies sensitive dependence on initial conditions. It is a delicate procedure to locate highly unstable orbits even for the simplest Hamiltonian systems—area preserving mappings. The easiest method, iteration of the map,[3] is doomed to failure due to the exponential growth of numerical errors. The gradient flow method introduced by Aubry[4] converges well on unstable orbits[1,2] but requires the integration of a large number of coupled differential equations, one for each point on the orbit, and is often too time consuming. The best technique uses Newton's method[5,6] which is superconvergent, and can be arranged so that the time to find an orbit is proportional to its period. However, this method is so sensitive to initial configuration that one often ends up with a different orbit than that desired: in chaotic regions there are many close periodic orbits with the same period. Thus careful choice of initial configuration is necessary for success, and most of the time to find an orbit is often spent searching for good starting points. This slows the method considerably (especially for long orbits) and diminishes its advantage.[1]

In this note we introduce a new technique, orbit extension, for finding appropriate starting points for Newton iteration. It gives both a stable and an economic prescription for finding unstable orbits and resolves the last problem with Newton's method.

Recent investigations[1,2] suggest that the phase space of an area preserving map is decomposed into a countable set of resonances which never overlap. Transport takes place as a result of flux between resonances whose turnstiles overlap. This procedure of analyzing transport processes gives reasonably good agreement with numerical studies[7] and may serve as a starting point for the analysis of the global transport properties.[8] The determination of the flux from one resonance to another requires the calculation of both homoclinic and heteroclinic orbits. In this paper,we apply the orbit extension technique to find two types of orbits, ordered periodic orbits and principal heteroclinic orbits between two resonances.

This paper is organized as follows: in §2, we give a description of the

Newton method, its difficulties and a few relevant methods for determining good initial configurations. An account of the orbit extension method for finding both ordered periodic orbits and principal heteroclinic orbits is presented in §3. The computer program to find ordered periodic orbits will be published elsewhere.[9] Next we apply this method to determine the flux between different resonances and briefly discuss the implications for the study of transport in area-preserving maps. Finally, in the conclusion is a discussion of other applications and possible extensions of the method.

§2 Preliminaries

§2A. Twist Maps

We will consider a twist map acting on a phase space (x,p) given by

$$\begin{aligned} p_{t+1} &= p_t - V'_k(x_t) \\ x_{t+1} &= x_t + p_{t+1} \qquad \mathrm{mod}(1) \end{aligned} \tag{1}$$

or equivalently in Lagrangian form by

$$x_{t+1} - 2x_t + x_{t-1} = - V'_k(x_t) \tag{2}$$

Here V'_k is the derivative of a potential, V_k, which is assumed to be an even, periodic function of x, with period unity.

$$V_k(x+1) = V_k(x) = V_k(-x), \tag{3}$$

The periodicity condition implies that x is an angle variable; we usually assume that x falls in the half open unit interval [0,1). Sometimes, however, it is convenient to consider the lift of x to the real line. The evenness condition implies that the map has a reflection symmetry about x=0, and is not necessary for our method, but convenient for the exposition. Without loss of generality, we also assume that the extremum of V at x=0 is a minimum. For simplicity, we also suppose that this is the only minimum of V_k. Equation (3) then implies that its maximum occurs at $x=1/2$. Finally, the

potential depends on a parameter k, which governs its height, and thus the strength of the nonlinearity.

An orbit is denoted by its configuration $\{x_t\ ,\ t = 0,1,...\}$. Orbits are stationary points of the action

$$W\{x_t\} = \sum_t F(x_t,x_{t+1}) \tag{4}$$

where the generating function is

$$F(x,x') = {}^1/_2(x-x')^2 - V_k(x) \tag{5}$$

If the orbit has period n, we denote it by $\{x_0, x_1, \ldots , x_{n-1}\}$, with additional conditions that $x_n = x_0$, $x_{n+1} = x_1$. Of course, knowledge of the configurations also gives the momenta through (1).

An important class of orbits is the class of ordered orbits. An ordered orbit is topologically equivalent to uniform rotation on a circle, i.e. for any ordered orbit $\{x_t\}$, there exists a monotonic function f (not necessarily smooth) such that $x_t = f^t(x_0)$. Every ordered orbit has a frequency defined as the average rotation per step:

$$\omega = \lim_{t-t'\to\infty} \left[\sum_{i=t'}^{t}(x_{i+1} - x_i)/(t-t')\right] \tag{6}$$

If the orbit is periodic, then $\omega = m/n$ where m is the number of rotations around the circle in n steps. We will denote such orbits by the symbol (m,n). The frequency is also rational if the orbit is homoclinic to a periodic orbit (that is, approaches this orbit asymptotically for $t\to\pm\infty$). When ω is irrational the orbit is quasiperiodic, and can densely cover a circle or a Cantor set, or be homoclinic to the Cantor set.[10]

It has been shown[10,11] that the map (2) has at least two ordered orbits for each ω. These correspond to minimizing and minimax configurations of $W\{x_t\}$. For example, periodic orbits usually come in hyperbolic-elliptic pairs with the hyperbolic orbit being minimizing and the elliptic minimax. Remarkably, minimax orbits are observed to always have a point on the line x=0, while minimizing orbits have none of their points on this line. This is related to the fact that the potential is minimal at x=0, and hence the action tends to be larger for orbits with points near x=0.

A much studied map of this class is the standard map,[3,7,11] with $V_k = -k/(2\pi)^2\cos(2\pi x)$. Another example is the sawtooth map, $V_k = -k(x-1/2)^2/2$ (the force term is discontinuous at x=0 in this case).[12,13]

§2.B Bunching

Our method for finding orbits of twist maps is based on the observation that the configuration points of an orbit tend to cluster into groups as the nonlinearity is increased.[12] An example of this is shown in Fig. (1a) for the (m,n) = (8,21) minimizing orbit of the sawtooth map, and in Fig. (1b) for the standard map. These figures show the configuration points $\{x_t, t=0,1,...20\}$ as k is varied from 0 to 3.5.

At k=0 all orbits are simple rotations. For a minimizing orbit, as $k\to 0^+$ $x_t \to \omega t + 1/2n$. The rotation frequency determines the relationship between the spatial and temporal ordering of the points: upon iteration each point shifts m to the right. The ordering is preserved as k varies since the curves $x_t(k)$ do not cross in Fig. (1).

However, as k increases they do tend to bunch together in groups. For k $\approx$ 0.2 for the sawtooth map, and k$\approx$1.5 for the standard map, some of the points cluster together in pairs, leaving thirteen well separated points or pairs of points. As k increases these clusters successively approach each other in pairs, until near k$\approx$ 3 there are five distinguishable groups, and for k$\approx$10 there are only three. In fact, as $k\to\infty$ all the points approach $x = {}^1/_2$, where the action is minimum. The way in which this bunching occurs is determined by the Farey sequence for the frequency m/n.

A Farey tree is a method for constructing all rationals between a given pair. Begin with a pair of rationals m/n and p/q, which satisfy the relation mq-np = $\pm$1, such rationals are called "neighbors." A "daughter" rational in the interval (m/n,p/q) is obtained by adding numerators and denominators: r/s = (m+p)/(n+q). The parent with the larger denominator, which is closer in frequency to its progeny, will be called the "mother." It is easy to see that r/s is a neighbor to both its parents, m/n and p/q. Two daughters of r/s are obtained by Farey addition to its neighbors: (r+m)/(s+n), and (r+p)/(s+q). Each of these daughters has r/s as mother. Every rational number has two parents, and from each can be obtained two daughters: the tree is binary. All rationals between m/n and p/q appear exactly once on the tree.

The parents of a rational can easily be obtained from its continued fraction expansion:

$$m/n = [a_0,a_1,...a_j] = a_0 + 1/(a_1 + 1/(... + 1/a_j)) , \qquad (7)$$

where the a_i are positive integers With the convention that the final element $a_j > 1$, the continued fraction expansion for the mother is $[a_0,a_1,..., a_{j-1},a_j-1]$ and for the father is $[a_0,a_1,...a_{j-1}]$.

The Farey sequence for a rational is its maternal lineage: thus for 8/21 one obtains the sequence {1/2, 1/3, 2/5, 3/8, 5/13}. In this case the Farey sequence is identical to the sequence of continued fraction convergents; more generally when the $a_i \neq 1$, "intermediates" as well as convergents are included in the Farey sequence. Each convergent in the Farey sequence gives a best approximation to m/n. For example, 3/5 is the nearest rational to 8/21 for any with denominator less than 8.

As is seen in Fig. (1) the bunching of points on an orbit occurs with groups defined by successive levels of the Farey sequence. Furthermore, the order in which groups in the bunch are visited is determined by the Farey rationals. If one identifies the points in a bunch, then the resulting order is that of the mother rational with the appropriate denominator: for $k \approx 3$, the 5 bunches in Fig. 1 are visited as though the orbit had rotation frequency 2/5.

It is observed that the largest, or principal gap between a pair configuration points on a minimizing orbit occurs around x=0 where the generating function has a maximum. Because the points on the orbit are ordered, we know that the iterates of the endpoints of a gap are also gap endpoints. Thus we can follow the iterates of a gap, delineated by its endpoints. For the orbit in Fig. (1), the image of the principal gap is the gap around $x \approx 0.4$, and its preimage is the gap around $x \approx 0.6$. These are both narrower than the principal gap. In fact the size of a gap decreases approximately exponentially with time away from the principal gap; the mean exponent is the Lyapunov exponent of the orbit. This implies that strong bunching is only present when the orbit is strongly unstable, and is the reason that there is no bunching when k is small for the standard map. For the case of the sawtooth map, the local exponentiation rate is spatially constant, and the bunching can be analyzed exactly.[12]

The bunching properties of unstable orbits will be exploited extensively

below.

§2C. Newton's Method

There are two steps to find a periodic orbit with Newton's method: i) choose a trial configuration, and ii) invert the tangent map. For a given trial configuration $\{x_t\}$ the tangent map, or Hessian matrix is denoted

$$H_{i,j} = \delta_{i+1,j} - 2\delta_{i,j} + \delta_{i-1,j} + \delta_{i,j}V''_k(x_j) \tag{8}$$

where δ is the Kronnecker delta. To obtain the correction, $\{\Delta x_t\}$, to $\{x_t\}$ one must solve the linear problem

$$H_{i,j}\,\Delta x_j = R_i \tag{9}$$

where, R_i is the residue vector of the trial configuration:

$$R_i = x_{i+1} - 2x_i + x_{i-1} + V'_k(x_i) \tag{10}$$

Solution of (9) for requires proper consideration of the boundary conditions of the desired orbit. For example, suppose we are interested in an orbit which begins at x_{-1} and reaches x_n after n+1 iterations. In this case the 0^{th} and $(n-1)^{st}$ rows of H must be changed since Δx_{-1} and Δx_n are zero. In contrast, to find a periodic orbit we set $\Delta x_n = \Delta x_0$ and $\Delta x_{-1} = \Delta x_{n-1}$, but allow Δx_0 and Δx_{n-1} to vary. In this case the Hessian becomes a periodic matrix. In Ref. 5 an accurate, stable, and efficient way to solve the linear problem was developed for periodic case. More general boundary conditions can be developed in a similar fashion (see the appendix for a more detailed discussion).

The success of the Newton method depends critically on the choice of initial configuration. Unlike the gradient flow method, for which one is able to find the basin of attraction (in fact, order is preserved by this method[14]), no general results are known about the basin of attraction for the Newton method. This makes the choice of the initial configuration an extremely delicate matter. There are two cases for which a simple choice suffices for ordered orbits: for a stable orbit, uniform rotation gives a sufficiently good

initial guess, and in the opposite limit of extreme instability a sensible choice of initial configuration can be perturbatively obtained to first order in $1/k$.[6]

While these techniques work reasonably well in the two limits, they still suffer from the problem that the Newton iteration must be carried out many times in order to find the correct orbit; this makes the method very time-consuming for long orbits. Furthermore they are applicable only to ordered orbits. Our purpose is to develop a method which will be quicker and more flexible.

§3. Orbit extension method

The orbit extension method is motivated by the fact that often a short orbit already contains a lot of information about a related longer period orbit. This is familiar in the case of quasi-periodic orbits, which can be approximated by periodic orbits with nearby frequencies. The orbit extension method is a technique for systematically exploiting the bunching of points on an unstable orbit.

§3A. Ordered Periodic Orbits

The spatial ordering of points for an (m,n) orbit is defined by their positions in the unit interval. We will denote this ordering by x(j) such that

$$0 \leq x(0) \leq x(1) \leq \ldots \leq x(n-1) < 1 \quad . \tag{11}$$

It is observed that minimizing orbits have all points nonzero, and a minimax orbit has x(0)=0. The principal gap in the orbit is the gap around x=0. For a minimizing orbit, we focus on the endpoints of the principal gap which, since our convention is to put points in the interval [0,1), are x(0) and x(n-1). On the other hand, a minimax orbit has a point in the center of each gap, so we focus on the center point of the principal gap, which is x(0). Choose the origin of time such that $x_0=x(0)$.

There is an easy translation between time ordering and spatial ordering

for an ordered orbit; it is based on the Farey sequence for the orbit frequency. Let p/r and q/ℓ ($p/r < q/\ell$) be the parents of m/n. Suppose $x(j) = x_t$, then its spatial neighbors are given by:

$$x(j-1) = x_{t+\ell} \ , \qquad x(j+1) = x_{t+r} \tag{12}$$

i.e. the right neighbor is obtained upon r iterations, and the left neighbor upon ℓ iterations. With the above formula, we are able to find the endpoints of the largest gap by successive iteration from any point on the orbit. For example, for a minimizing orbit, since x_0 is the right endpoint of the principal gap, x_ℓ is its left endpoint.

The extension method is based on iteration on the levels of the Farey sequence, and is given by the following algorithm:

1) Find the Farey sequence of m/n. Begin at a level which has a sufficiently small period, say ≤ 5. Denote the frequency at this level by p/q.
2) Find an approximate configuration $\{x(j),\ i = 0,1,....q-1\}$ at the lowest level. It is sufficient to choose a simple trial as discussed in §2C, and Newton iterate twice.
3) Proceed to the next Farey level with daughter rotation number p'/q'; denote the denominators of the parents by r' and ℓ'.
4) Obtain the the initial guess for the new configuration at this level. For a minimizing orbit, $\{x'(j)\}$, is obtained from $\{x(j)\}$ first by setting the new endpoints of the principal gap equal to the old. This means that the largest gap in the new trial orbit is approximated by the largest gap in the old one. We then set the second largest gaps equal, and so forth. Since the gaps decrease approximately monotonically away from the largest, this is done by identifying temporal neighbors of the principal gap. Continue to do this until all q' points on the new orbit are assigned:

$$\begin{aligned} x'_t &= x_t \\ x'_{\ell'-t} &= x_{\ell-t} \end{aligned} \qquad t = 0,1,2,\ldots\ [\ell'/2]$$

$$\begin{aligned} x'_{q'-t} &= x_{q-t} \\ x'_{\ell'+t} &= x_{\ell+t} \end{aligned} \qquad t = 1,2,\ldots\ [(q'-\ell')/2] \tag{13}$$

where [ ] indicates integer part. Note there is overlap in the assignments for ℓ' or $q'-\ell'$ even. If this is the case, the best strategy is to use the average of the two assignments. For a minimax orbit, the situation is simpler, since there is only one point to assign per gap:

$$\begin{aligned} x'_t &= x_t & t &= 0,1,2,\ldots [q'/2] \\ x'_{q'-t} &= x_{q-t} & t &= 1,2,\ldots [q'/2] \end{aligned} \qquad (14)$$

5) Apply Newton iteration with periodic boundary conditions to the current configuration.
6) If $q' < n$, remove the primes on the symbols to indicate a transition to the next Farey level, and go to 3).
7) Otherwise, this final configuration is used as the initial guess of the (m,n) orbit. It generally takes only one or two more iterations of the Newton method to obtain the (m,n) orbit to a given precision.

Several levels of orbit extension are shown for the minimizing (13,34) orbit in Fig. 2 The top configuration is that of the 2/5 orbit; the assignment of the points for the next level (3/8) gives the second configuration. Upon Newton iteration the points split apart, resulting in the third configuration. Below that is the result of the next two iterations, giving approximations to the (5,13) and (8,21) orbits. The final configuration shown is indistinguishable from the actual (8,21) orbit, and on the scale of the graph, from the (13,34) orbit as well.

The orbit extension method has the advantage that it only needs the approximating configurations of small period orbits. Newton iteration is applied only once to the intermediate configurations because the general structure of the bunching is only qualitative. It is quite efficient considering that most of the intermediate configurations have very short periods. So the effective time cost of all the intermediate steps is just that for two or three Newton iterations of the (m,n) orbit.

Theoretically, there is no limitation to the period of the orbit one wants to find. Numerically, because of the exponential divergence of the elements of the Hessian matrix with the period of the orbit, very long orbits cannot be found due to computer overflow. We have been able to find periodic orbits up to residue 10^{25} using a double precision (128 bit) algorithm on the ICL 2988

computer (the residue is $^1/_4[2-\mathrm{Tr}\{DT^n\}]$). This is far better than that needed for physically motivated studies because the smallest gap on an orbit scales as the inverse of the residue; so orbits with residue larger than the inverse of the precision are numerically indistinguishable. Similarly, quantities such as the Lyapunov exponent, and the flux also have errors of order the inverse of the residue.

Typically the orbit extension method converges with less than half the computational time than that required for Newton iteration on simple trial configurations of the full orbit. However, the extension method can be slower when the orbit has small residue: the analysis of bunching is based on the existence of a positive Lyapunov exponent, which certainly breaks down for small residue orbits. Thus, the orbit extension is useful when k is larger than the parameter value of the (m,n) orbit for which $R\approx 1$.

§3B. Principal Heteroclinic Orbits

When we study transport, we are primarily interested in quantities such as area and flux.[1,2] The flux out of a resonance is determined by the orbits homoclinic to the resonance. The flux from one resonance to another is determined by the corresponding heteroclinic orbits.

A type (m,n) principal homoclinic orbit is an ordered orbit which approaches a periodic (m,n) orbit in both directions of time. Let h_0 represent a point on such an orbit in the gap (x(0),x(1)) of the (m,n) orbit. Ordering implies that each subsequent point on the homoclinic orbit is in the corresponding gap of the periodic orbit, and furthermore that $h_{jn} \to x(1)$ and $h_{-jn} \to x(0)$ as $j \to \pm\infty$. We call such an orbit right (left)-going and denoted with superscript "±", respectively. The existence of such orbits is proved by Aubry.[10] There are actually two such orbits of each type: they are obtained at minimum and minimax values of the action, and will be denoted by M and S, respectively (see Fig. 4). Choose t=0 such that $S^{\pm}_0 = 0$ and $M^{\pm}_0$ is the leftmost point on the minimizing orbit. Ordering then implies

$$\begin{aligned} M^+_{t-n} < S^+_t < M^+_t \,, \\ M^-_{t+n} < S^-_t < M^-_t \,, \end{aligned} \tag{15}$$

A heteroclinic orbit of type $(m_1,n_1)\to(m_2,n_2)$ approaches an (m_2,n_2) orbit

in the forward time direction and an (m_1,n_1) orbit in the backward time direction. Such orbits clearly do not exist when there is an invariant circle between the two periodic orbits. Birkhoff has shown that non-existence of an invariant circle is sufficient to guarantee the existence of an orbit which goes from some neighborhood of (m_1,n_1) to some neighborhood of (m_2,n_2). Furthermore Mather has proved that heteroclinic orbits do exist in this case.[15] Since all absolutely minimizing configurations are either periodic or quasiperiodic,[10,4] a principal heteroclinic orbit cannot be absolutely minimizing; however, Mather's result implies the existence of locally minimizing and minimax orbits.[15]

There are possibly four types of heteroclinic orbits, depending on whether the orbit leaves (m_1,n_1) from the right or left and on whether it approaches (m_2,n_2) to the right or left. These will be denoted with superscripts $\pm$ as before, i.e. the orbit $(m_1,n_1)^-\rightarrow(m_2,n_2)^+$ leaves (m_1,n_2) on a left-going unstable manifold, and approaches (m_2,n_2) on a right-going stable manifold. At each point on a heteroclinic orbit the unstable manifold of (m_1,n_1) intersects the stable manifold of (m_2,n_2) as shown in Fig. 4 Corresponding to each $(m_1,n_1)\rightarrow(m_2,n_2)$ orbit there is also a $(m_2,n_2)\rightarrow(m_1,n_1)$ orbit; in Fig. 4 these orbits occur at the unlabelled stable-unstable manifold intersections. By Eq. (3) these orbits are equivalent under the symmetry operation; however, they are not symmetric themselves. These heteroclinic orbits characterize the transport from (m_1,n_1) to (m_2,n_2) and vice versa.

A principal heteroclinic orbit is a heteroclinic orbit which is partially ordered in the following sense. Consider for example $(m_1,n_1)^-\rightarrow(m_2,n_2)^+$ and suppose $m_1/n_1 > m_2/n_2$. Let M^{1-} and S^{1-} be the minimizing and minimax $(m_1,n_1)^-$ orbit, etc. Let x_0 be the leftmost point on the heteroclinic orbit: $S^{2+}{}_0 = S^{1-}{}_0 < x_0 < M^{2+}{}_0 , M^{1-}{}_0$. The partial ordering condition is:

$$\begin{aligned} M^{2+}{}_t < x_t < S^{2+}{}_t,\ t > 0 \\ M^{1-}{}_t < x_t < S^{1-}{}_t,\ t < 0 \end{aligned} \qquad (16)$$

Similarly, the ordering conditions can be easily given for the other three types of principal heteroclinic orbits.

The non-existence of invariant circles is not sufficient for the existence of principal heteroclinic orbits. These exist only when the turnstiles of the two resonances overlap.[1,2]

Since a homoclinic orbit lies on the unstable or stable manifolds of the corresponding minimizing periodic orbit, its behavior in the neighborhood of the periodic orbit is governed by the latter's characteristic exponent. Indeed, most points of a homoclinic orbit typically lie very near the corresponding periodic orbit. Furthermore, the ordering condition (16) implies that a heteroclinic orbit is well approximated by the corresponding homoclinic orbits near the periodic points. This suggests the use of segments of homoclinic orbits as the initial guess for the corresponding heteroclinic orbit. This idea corresponds to the method used by Mather in his existence proof.[15]

The method for finding the principal homoclinic orbits is reviewed in Ref. 1. Suppose we want to find the homoclinic orbits for resonance (m,n). We first find the parents (p,r) and (q,ℓ) of m/n ($p/r < q/\ell$). The left-going principal homoclinic orbit is approximated by the (mj+p, nj+r) orbit and the right going one by the (mj+q, nj+ℓ) orbit for j large enough. These periodic orbits can be found by the extension method, as before.

The orbit extension method to find a minimizing $(m_1,n_1)^- \to (m_2,n_2)^+$ orbit consists of the following steps:

1) Find the minimizing $(m_2,n_2)^+$ orbit $\{x^{2+}\}$ and the minimizing $(m_1,n_1)^-$ orbit $\{x^{1-}\}$.
2) Position the time origin of the homoclinic orbits at their leftmost points, take a segment of the $(m_1,n_1)^-$ orbit from some time -T, up to time zero, and a segment of $(m_2,n_2)^+$ orbit from time zero up to T. The initial guess for the $(m_1,n_1)^- \to (m_2,n_2)^+$ heteroclinic orbit consists of the union of these two segments, with the choice of one of the two points at t=0:

$$\{x^{1-}_{-T}, \ldots, x^{1-}_{-1}, \max(x^{1-}_0, x^{2+}_0), x^{2+}_1, \ldots, x^{2+}_T\} \qquad (17)$$

3) Apply the Newton iteration with asymptotically periodic boundary conditions once.
4) Append another segment of the minimizing $(m_1,n_1)^-$ orbit from -2T to -T-1, to the negative time end and the minimizing $(m_2,n_2)^+$ orbit from T+1 to 2T to the positive time end of the resulting orbit.
5) Repeat 3) and 4) until the orbit is sufficiently long to achieved the desired accuracy.

6) This final configuration is used as the initial guess for the $(m_1,n_1)^- \to (m_2,n_2)^+$ orbit; however, usually only one or two Newton iterations are required for convergence at this stage.

A similar prescription can be developed to find the other principal heteroclinic orbits.

We find numerically that the principal heteroclinic orbits are locally minimizing or minimax. These two orbits are labelled as $M^{1\to 2^+}$ and $S^{1\to 2^+}$ respectively in Fig. 4. The difference of the action of these two orbits is the flux which leaves the (m_1,n_1) resonance and moves to the (m_2,n_2) resonance or beyond upon each iteration of the map.[1]

We find that the time used to find a heteroclinic orbit is of the same order as the time used to find a periodic orbit of the same length. In cases where the principal heteroclinic orbits do not exist, the Newton iteration does not convergence.

§4. Flux between resonances

The flux, $\Delta W_{1\to 2}$, between two resonances is obtained by finding the minimax and minimizing principal heteroclinic orbit between these two resonances. Figure 5 shows the typical behavior of this function. Here the first resonance is (1,3), and the second is varied over the rationals on a Farey tree. For example, the lower turnstile of the 1/3 resonance has area $\Delta W_{(1,3)^-} = 1.41(10)^{-3}$, and the area of the overlap region with the $(2,7)^+$ turnstile is $\Delta W_{(1,3)^-\to(2,7)^+} = 1.2(10)^{-3}$. The overlap of the $(1,3)^-$ turnstile with the $(2,7)^-$ turnstile is considerably less $(6.3(10)^{-4})$ because the (2,7) resonance itself intervenes. This is explicitly seen if we plot the resonances in the phase space (Fig. 6). This figure also shows that a one step transition from the (1,3) resonance is limited to the frequency range [1/4,2/5]. This is also seen when an attempt to find the orbit $(1,3)^-\to(1,4)^-$ fails to converge, indicating that this principal heteroclinic doesn't exist for this value of k. Of course, as k increases the transition range grows as more of the turnstiles overlap.

The function $\Delta W_{(1,3)^- \to (m,n)}$ is a devil's staircase: it has discontinuous drops across each rational.

§5. Conclusion

The difficulty of accurate computation of unstable orbits has been a major impediment to the study of transport in Hamiltonian systems. The orbit extension method actually takes advantage of this instability in order to increase the speed of computation. In this paper we applied it to find ordered periodic orbits and the principal heteroclinic orbits between two resonances. We are able to obtain the differences in action required to estimate fluxes at least twice as rapidly as before.

The use of representative shorter orbits to provide information for longer ones is obviously capable of further generalization, for example, to certain disordered orbits, an orbit coding scheme[12] provides a natural relation between orbits of different lengths. It is also desirable to generalize the Newton method to maps other than the Taylor-Chirikov type. Many other area-preserving maps can be put in the standard form (2) by a suitable choice of coordinates, e.g. Henon's quadratic map can be written as $x_{t+1} - 2x_t + x_{t-1} = 2(k - x_t - x_t^2)$, which is of the form (2), except that x is not a periodic variable. Thus the Newton method technique can not be directly applied to this map. It would be interesting if one could develop an efficient and stable method to find unstable orbits of such maps.

Acknowledgements: We thank Dr. Ben Mestel for the use of his Newton iteration program, and for many helpful discussions. The first two authors thank Queen Mary College for its hospitality during the period when this research was carried out. This research was supported by grants from the U.S. Department of Energy and the U.K. Science and Engineering Research Council, and a NATO grant for International Collaboration.

Appendix: Boundary Conditions and Newton's Method

In this appendix we extend the method of Ref. 5 for inversion of the tangent map to general boundary conditions.

Consider first the case of periodic boundary conditions. Define a periodic n×n Hessian matrix by

$$\begin{aligned}\tilde{H}_{0,j} &= \delta_{1,j} - 2\delta_{0,j} + \delta_{n-1,j} + \delta_{0,j}V''_k(x_0)\\ \tilde{H}_{i,j} &= \delta_{i+1,j} - 2\delta_{i,j} + \delta_{i-1,j} + \delta_{i,j}V''_k(x_j) \quad , 0<i<n-1\\ \tilde{H}_{n-1,j} &= \delta_{0,j} - 2\,\delta_{n-1,j} + \delta_{n-2,j} + \delta_{n-1,j}\,V''_k(x_{n-1})\end{aligned} \tag{A1}$$

The periodic Green function is the solution of

$$\sum_{j=0}^{n} \tilde{H}_{i,j}\tilde{g}_{j,k} = \delta_{i,k} \tag{A2}$$

Instead of solving this problem directly, it is more efficient to introduce the Hessian on the infinite domain, defined by (8) for $-\infty< i,j < \infty$. The corresponding Green function is the solution of

$$\sum_{j=-\infty}^{\infty} H_{i,j}g_{j,k} = \delta_{i,k} \tag{A3}$$

The solution of (A3) is a linear combination of the two linearly independent solutions of the homogeneous version of (A3), call them $w^+{}_j$ and $w^-{}_j$:

$$g_{j,k} = A_k w^+{}_j + B_k w^-{}_j \tag{A4}$$

As remarked in Ref. 5, these two solutions can be determined in a stable and efficient manner. The coefficients A_k and B_k must be obtained by the imposition of the boundary conditions, and the jump condition across i=k On the infinite interval this is usually done by requiring that g vanish as $i\to\pm\infty$.

Note, however, that (A2) and (A3) are the same in the range $0<i<n-1$. Thus $g_{j,k}$ will equal $\tilde{g}_{j,k}$ for $0 < j,k < n-1$ if we choose the coefficients A_k, B_k by insisting that

$$g_{-1,k} = g_{n-1,k} \quad , \quad g_{0,k} = g_{n,k} \tag{A5}$$

The point is that the homogeneous solutions, $w^{\pm}$, can be used to compute the periodic Green function. Eq. (A5) is slightly different from Eqs. (16a)-(16c) and (23) in Ref. 5 due to the different choice of interval for the summation indices.

To solve the Newton equation for an orbit with given initial and final points x_{-1} and x_n, we again use the Green function solving (A2), with a slight modification in boundary conditions.

The Hessian matrix $\tilde{H}$ at the endpoints is now given by

$$\begin{aligned} \tilde{H}_{0,j} &= \delta_{1,j} - 2\delta_{0,j} + \delta_{0,j} V''_k(x_0) \\ \tilde{H}_{n-1,j} &= -2\,\delta_{n-1,j} + \delta_{n-2,j} + \delta_{n-1,j}\, V''_k(x_{n-1}) \end{aligned} \qquad \text{(A6)}$$

The Green function solving (A3) will be the same as $\tilde{g}$ if we choose A_k and B_k so that

$$g_{n,k} = 0 \quad , \quad g_{-1,k} = 0 \qquad \text{(A7)}$$

Asymptotic boundary conditions can be treated in exactly the same way as the fixed boundary condition so long as we know the asymptotic behavior.

The linear problems for all three boundary conditions are identical for those points of the orbits far from the boundaries. Thus, if the Newton corrections to the boundary points are small, the periodic method can even be used for the boundary points.

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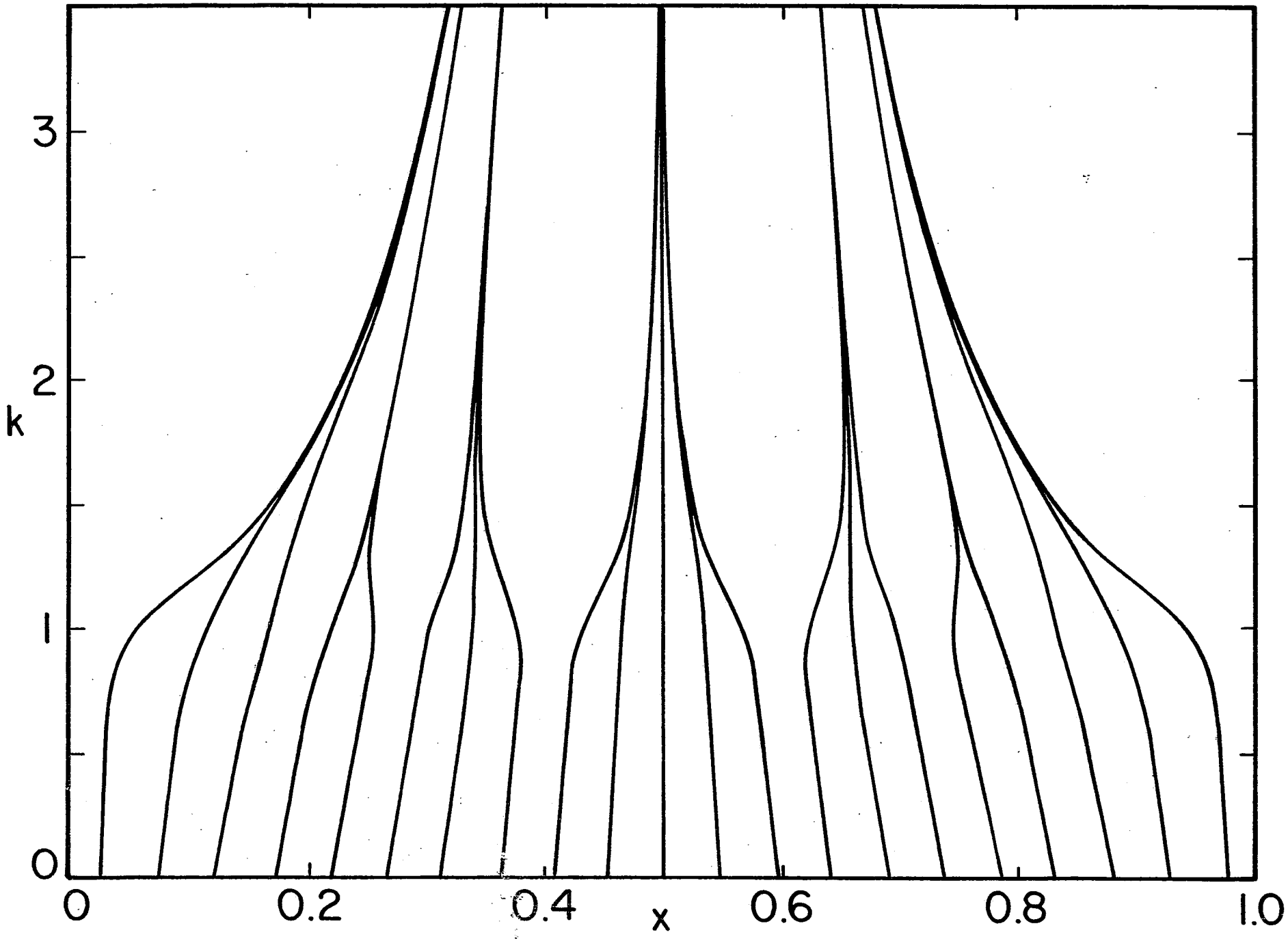
Figure captions

1) Configuration points of the (8,21) minimizing orbit as the parameter k varies. (1a) is for the sawtooth map and (1b) for the standard map. At k=0 the points are equally spaced, but as k increases bunching towards the action minimum occurs.
2) Configurations for four levels approaching the minimizing (13,34) orbit of the standard map at k = 2.0. The uppermost configuration is the exact configuration of (2,5) orbit. Next is the reassignment of the points to give the (3,8) ordering. The third configuration is the result of a single Newton iteration on this trial. The last two are the results of the next two Newton iterations on (5,13) and (8,21) orderings. The final orbit has a residue of order 10^{10}, and higher levels cannot be distinguished on this scale.
3) Phase space plot of the (8,21) minimizing orbit at k=2.0. Note that configuration bunching is equivalent to phase space bunching.
4) Sketch of points on orbits homoclinic to and heteroclinic between minimizing periodic orbits M^1 and M^2.
5) Flux from the (1,3) resonance to other resonances in the standard map for k = 1.4. The other frequencies are generated by Farey tree up to level 4, and the fluxes are obtained from heteroclinic orbits.
6) Phase space plot of the (1,3) resonance and two neighbors [(1,4) and (2,5)] in the phase space of the standard map for k = 1.4. The turnstiles of the (1,3) resonance overlap with these neighbors, but do not extend beyond them.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2
k
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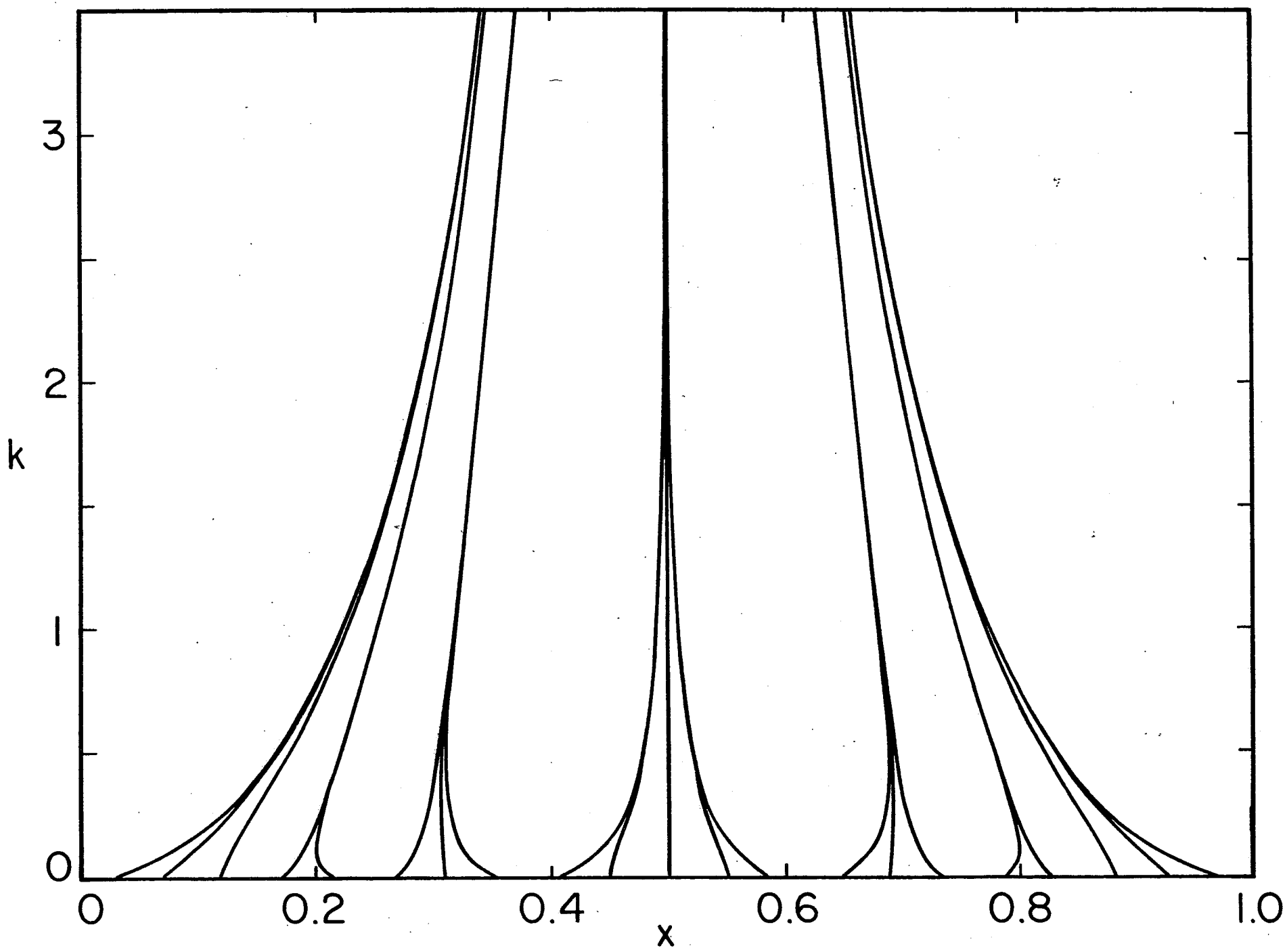
0
0
0.2
0.4
x
0.6
0.8
1.0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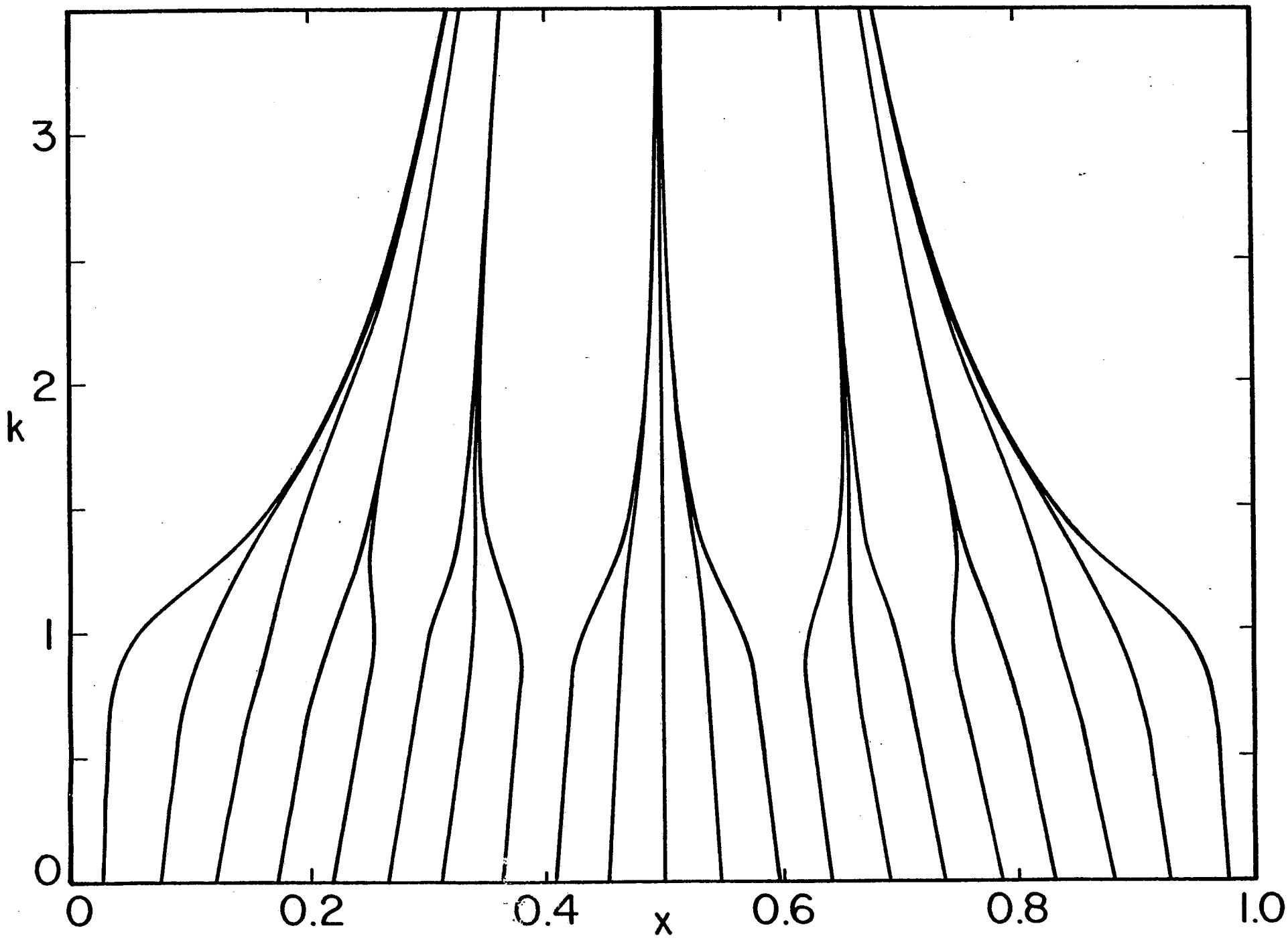
x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k
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x
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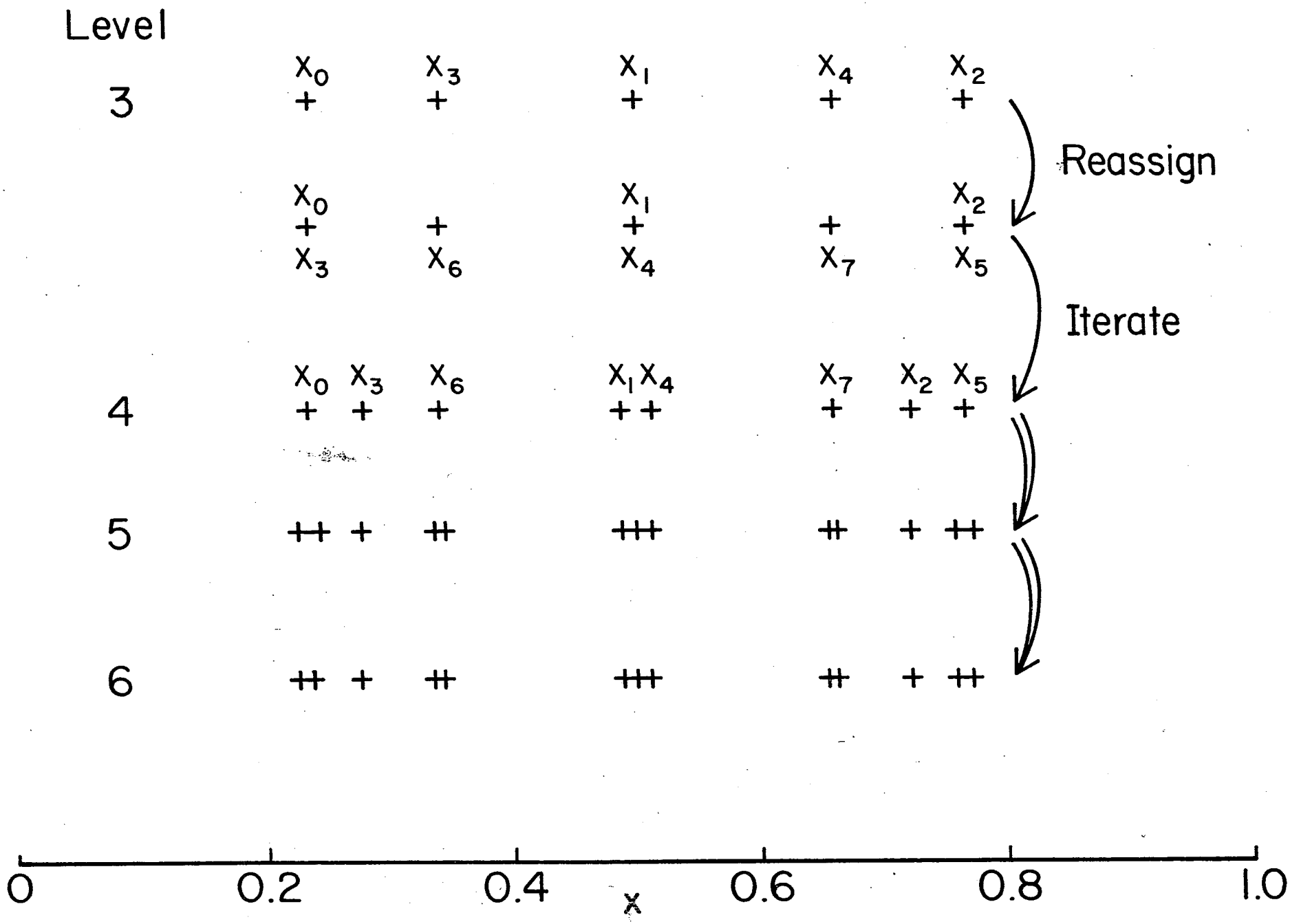
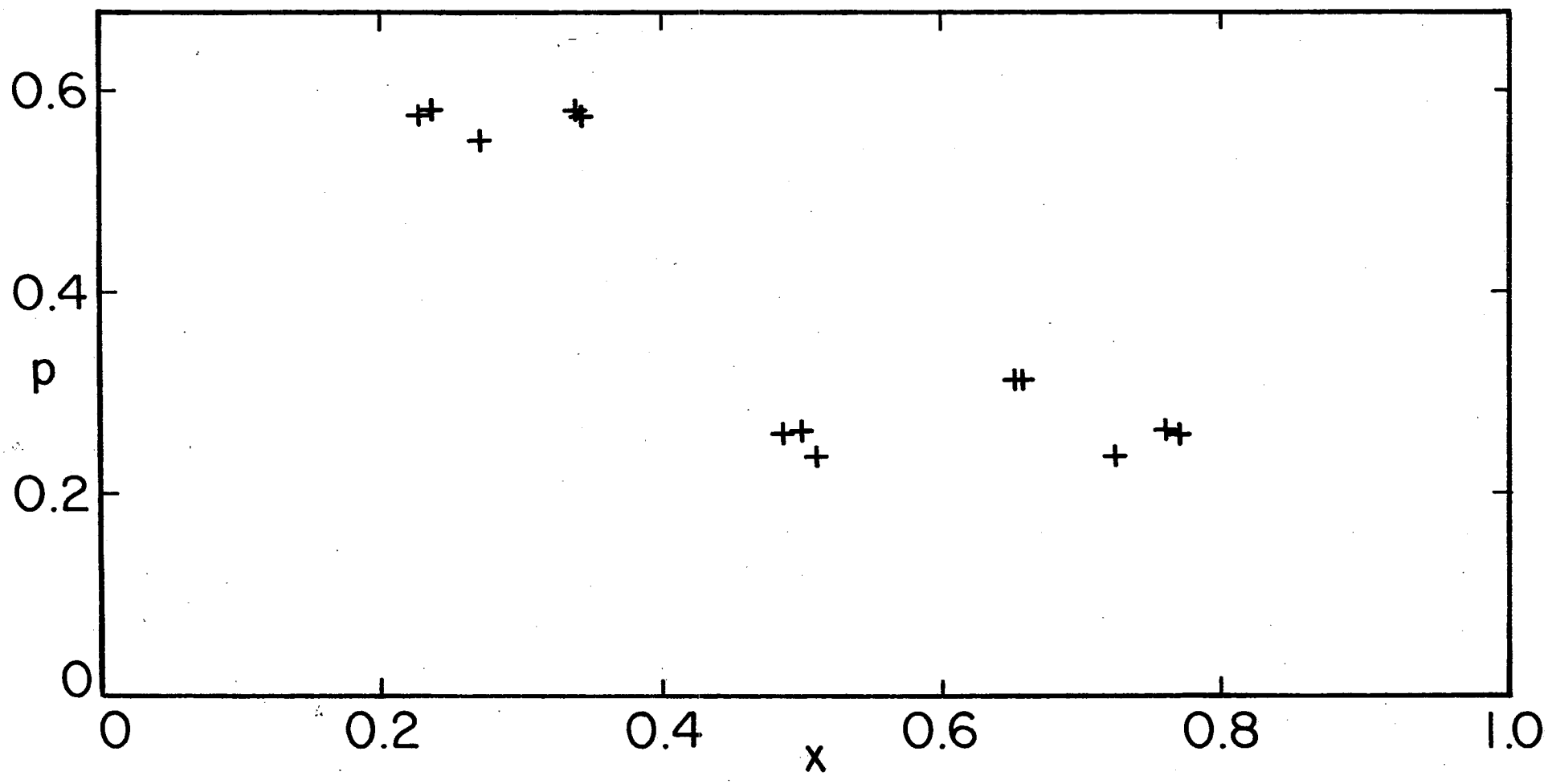
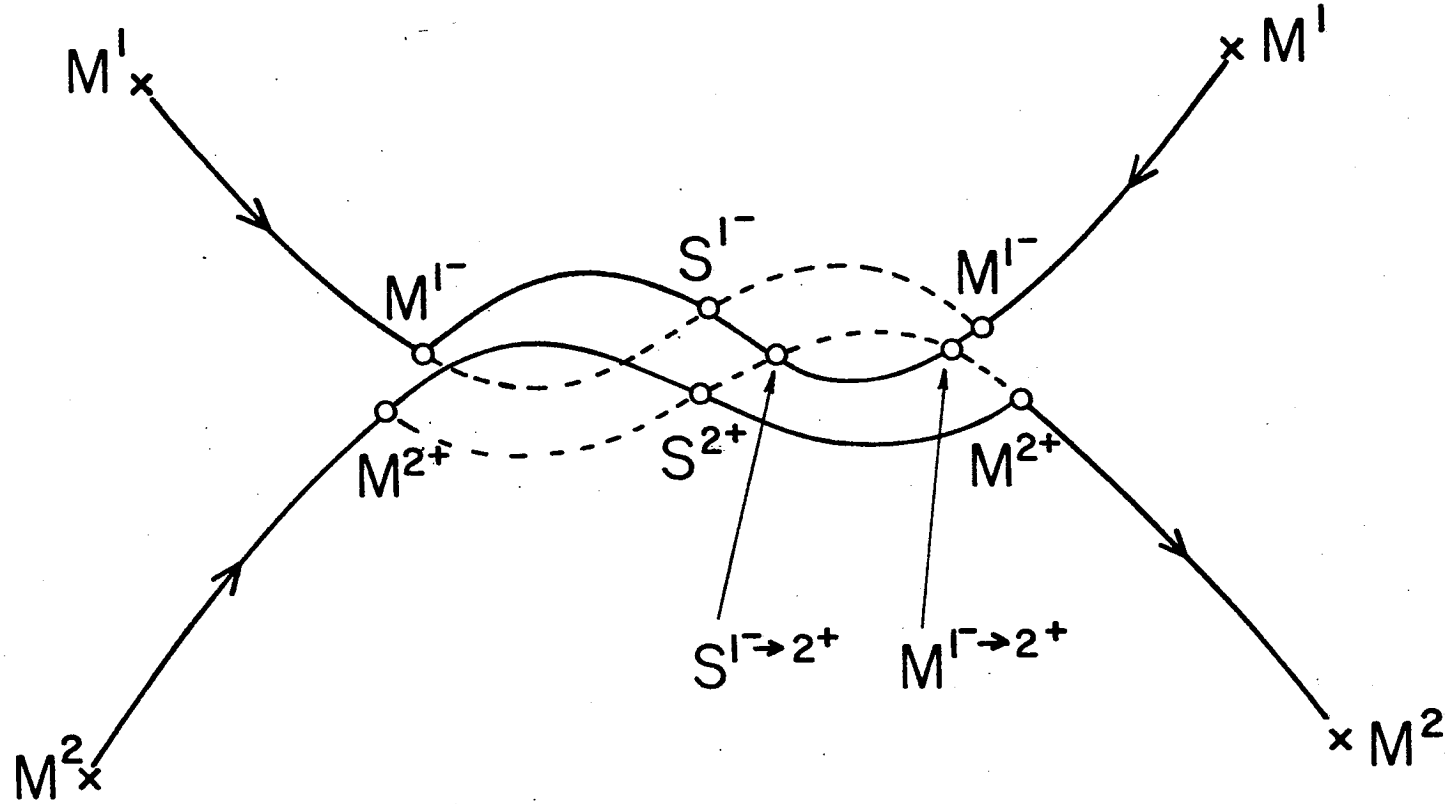
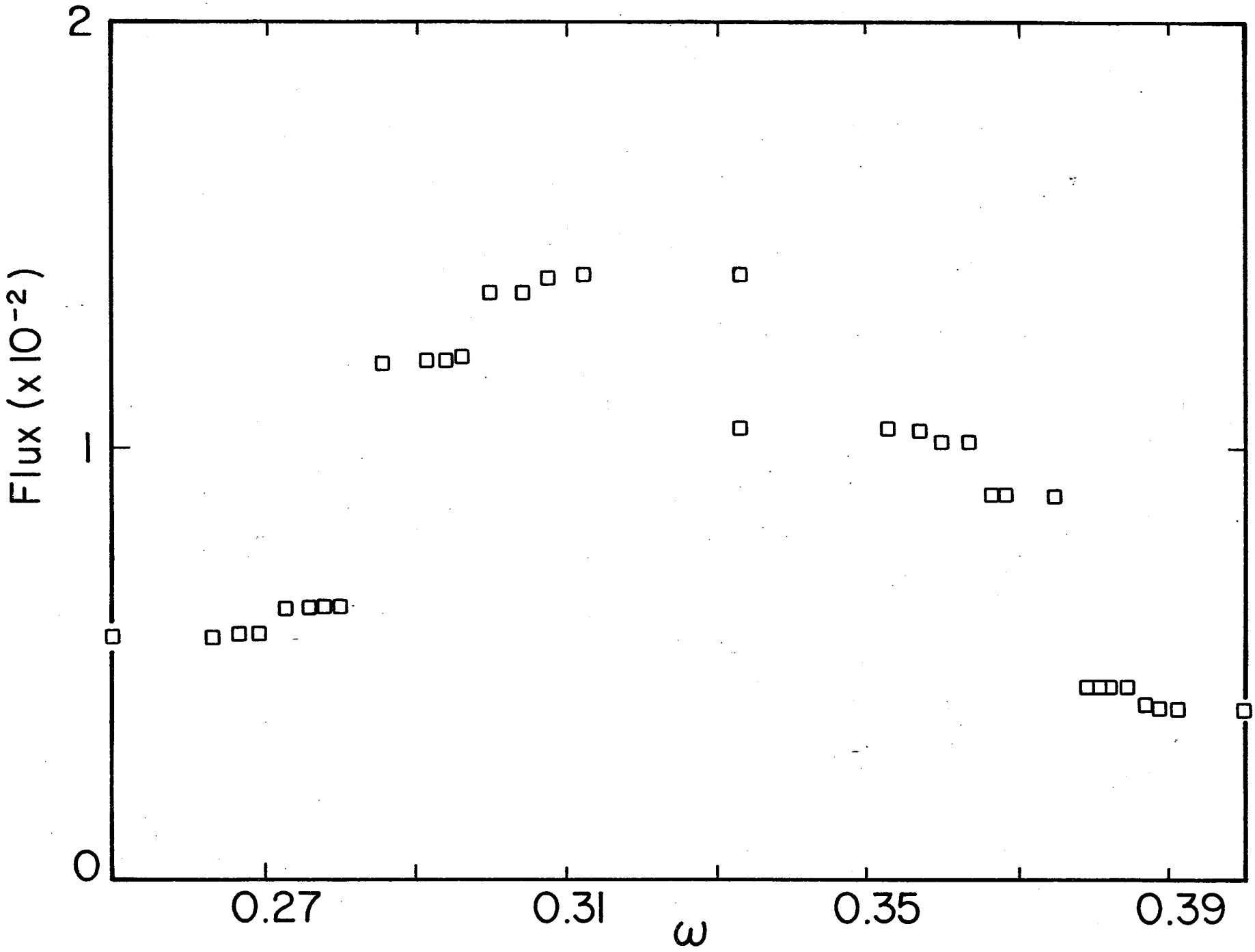
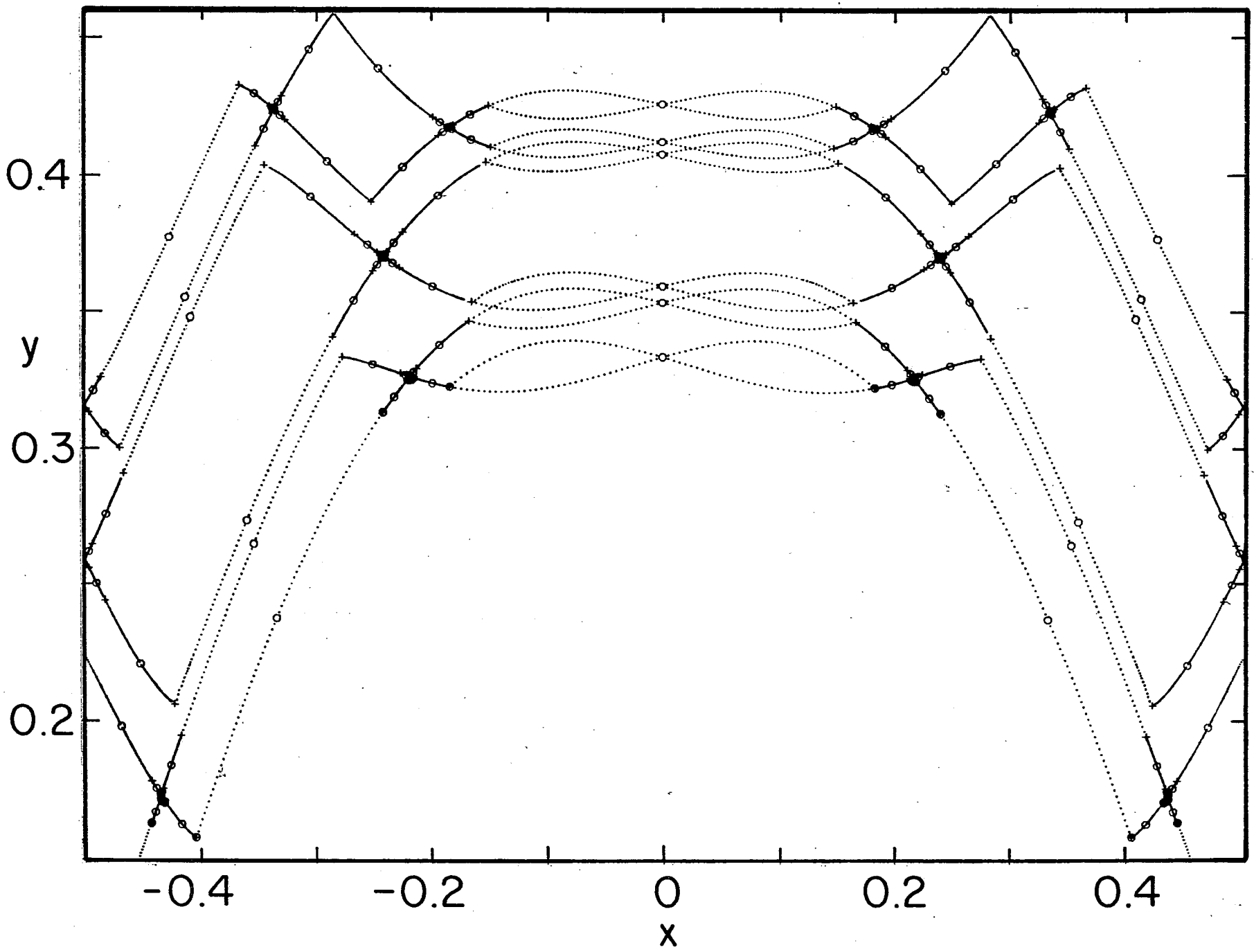
1.0


Level
3
x_0 x_3 x_1 x_4 x_2
Reassign
x_0 x_1 x_2
x_3 x_6 x_4 x_7 x_5
Iterate
4
x_0 x_3 x_6 x_1 x_4 x_7 x_2 x_5
5
6
0
0.2
0.4
0.6
0.8
1.0
x


0.6
0.4
p
0.2
0
0
0.2
0.4
0.6
0.8
1.0
x


M1
M1
M1−
S1−
M1−
M2+
S2+
M2+
S1−→2+
M1−→2+
M2
M2


2
1
0
Flux (x 10⁻²)
0.27
0.31
0.35
0.39
ω


0.4
y
0.3
0.2
-0.4
-0.2
0
0.2
0.4
x