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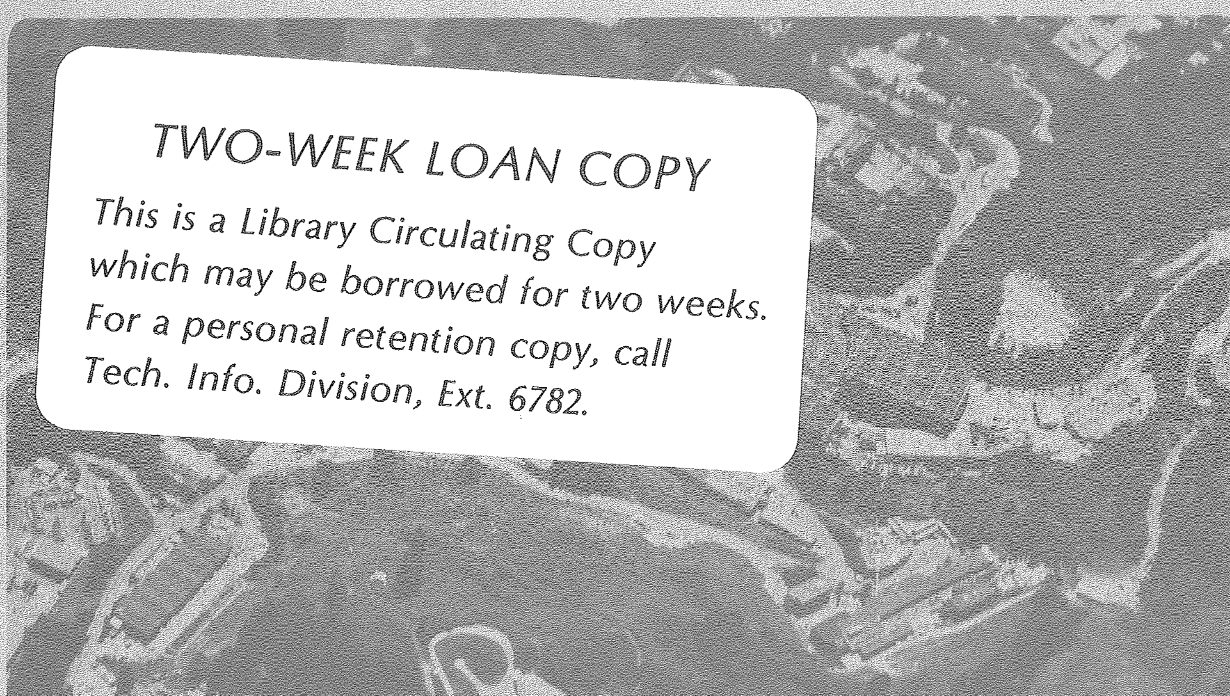

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Strong Coupling Expansions for Nonintegrable Hamiltonian Systems*

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Abstract

We present a method for studying nonintegrable Hamiltonian systems $H(\underset{\sim}{I},\underset{\sim}{\theta}) = H_0(\underset{\sim}{I}) + k\, H_1(\underset{\sim}{I},\underset{\sim}{\theta})$ $(\underset{\sim}{I}, \underset{\sim}{\theta}$ are action-angle variables) in the regime of large k. Our central tool is the conditional probability $P(\underset{\sim}{I},\underset{\sim}{\theta},t|\underset{\sim}{I}_0,\underset{\sim}{\theta}_0,t_0)$ that the system is at $\underset{\sim}{I},\underset{\sim}{\theta}$ at time t given that it resided at $\underset{\sim}{I}_0,\underset{\sim}{\theta}_0$ at t_0. An integral representation is given for this conditional probability. By discretizing the Hamiltonian equations of motion in small time steps, ε, we arrive at a phase volume preserving mapping which replaces the actual flow. When the motion on the energy surface $E = H(\underset{\sim}{I},\underset{\sim}{\theta})$ is bounded we are able to evaluate physical quantities of interest for large k and fixed ε. We also discuss the representation of $P(\underset{\sim}{I},\underset{\sim}{\theta},t|\underset{\sim}{I}_0,\underset{\sim}{\theta}_0,t_0)$ when an external random forcing is added in order to smooth the singular functions associated with the deterministic flow. Explicit calculations of a "diffusion" coefficient are given for a non-integrable system with two degrees of freedom. The limit $\varepsilon \to 0$, which returns us to the actual flow, is subtle and is discussed.

I. Introduction

Extensive study has been made of Hamiltonian dynamical systems which are close to being integrable.[1] The primary means is perturbation theory in the non-integrable piece of the Hamiltonian. Given H in the form

$$H(\underset{\sim}{I},\underset{\sim}{\theta}) = H_0(\underset{\sim}{I}) + k\, H_1(\underset{\sim}{I},\underset{\sim}{\theta}) \tag{1}$$

with $\underset{\sim}{I}=(I_1,\ldots,I_M)$ and $\underset{\sim}{\theta}=(\theta_1,\ldots,\theta_M)$ the canonically conjugate action and angle variables for an M degree of freedom system, one attempts a power series expansion in k of any interesting physical quantity. The KAM theorem is an exposition of the topological structure of phase space orbits based on a superconvergent form of perturbation theory in k.[2] The picture which emerges is one of regular orbits lying on invariant tori with interspersed irregular motion.

When k is large, the physical expectation is that most orbits will become essentially chaotic and that memory of the integrable piece of H, $H_0(\underset{\sim}{I})$, will be hopelessly lost. In this paper we set up a formalism adapted to study systems like (1) when k is large. Our primary tool is an integral representation for the conditional probability $P(\underset{\sim}{z},t|\underset{\sim}{w},t_0)$[2] that at t the system is at the point $\underset{\sim}{z}=(\underset{\sim}{I},\underset{\sim}{\theta})$ of phase space, given that it resided at $\underset{\sim}{w}=(\underset{\sim}{I}_0,\underset{\sim}{\theta}_0)$ at t_0. We give the representation for $P(\underset{\sim}{z},t|\underset{\sim}{w},t_0)$ both for the actual <u>flow in phase space</u> associated with $H(\underset{\sim}{z})$ and for the phase space volume preserving <u>mapping</u> which takes the system across discrete jumps in time.

Chaotic behavior of the deterministic system given by (1) exhibits itself as an apparently random motion of orbits generated by the action of H. This <u>intrinsic stochasticity</u> is the main subject of study in the present paper. It is possible that in addition to this intrinsic chaotic behavior there will be external noise which as <u>extrinsic stochasticity.</u> This will also be considered in the discussion of $P(\underset{\sim}{z},t|\underset{\sim}{w},t_0)$. The role of external fluctuations is to smooth out the δ functions entering $P(\underset{\sim}{z},t|\underset{\sim}{w},t_0)$. These are a manifestation of the determinism in the dynamics. If one wishes to have a smooth transition from k=o (no intrinsic stochasticity) to k large, one can introduce these external fluctuations to keep all operations smooth.[3] If the "size" of the fluctuations is called σ, then for $k \gg \sigma$, all physical quantities should be smooth as $\sigma \to 0$. In the opposite limit, $k \ll \sigma$, intrinsic stochasticity should be unimportant and only the external random driving will be present.

In the next section we derive the representations for $P(\underset{\sim}{z},t|\underset{\sim}{w},t_0)$ and discuss some of its properties. After that we turn to a model Hamiltonian of the form $H_0(\underset{\sim}{I})+k\,H_1(\underset{\sim}{\theta})$ with two degrees of freedom to test our ideas. Our model is treated analytically as well as numerically.

II. Integral Representation of the Conditional Probability

We want to consider the conditional probability $P(\underset{\sim}{z},t\,|\underset{\sim}{w},t_0)$ that the dynamical system governed by the Hamiltonian $H(\underset{\sim}{z})$, with $\underset{\sim}{z}$ or $\underset{\sim}{w}$ a choice of 2M canonical co-ordinates, is in the state $\underset{\sim}{z}$ at time t given it was in $\underset{\sim}{w}$ at time t_0. The M degree of freedom distribution function $f_M(\underset{\sim}{z},t)$ which obeys Liouville's equation

$$\left(\frac{\partial}{\partial t}+L_{\underset{\sim}{z}}\right)f_M(\underset{\sim}{z},t)=0 \tag{2}$$

with

$$L_{\underset{\sim}{z}}=\sum_{\ell=1}^{M}\left(\frac{\partial H}{\partial I_\ell}\frac{\partial}{\partial\theta_\ell}-\frac{\partial H}{\partial\theta_\ell}\frac{\partial}{\partial I_\ell}\right) \tag{3}$$

for $\underset{\sim}{z}=(\underset{\sim}{I},\underset{\sim}{\theta})$, action-angle variables, is connected to $P(\underset{\sim}{z},t\,|\underset{\sim}{w},t_0)$ by [2].

$$f_M(\underset{\sim}{z},t)=\int d\underset{\sim}{w}\;P(\underset{\sim}{z},t\,|\underset{\sim}{w},t_0)\,f_M(\underset{\sim}{w},t_0) \tag{4}$$

So we see that $P(\underset{\sim}{z},t/\underset{\sim}{w},t_0)$ satisfies Liouville's equation

$$\left(\frac{\partial}{\partial t}+L_{\underset{\sim}{z}}\right)P(\underset{\sim}{z},t\,|\underset{\sim}{w},t_0)=0 \tag{5}$$

with the initial condition

$$P(\underset{\sim}{z},t_0/\underset{\sim}{w},t_0)=\delta(\underset{\sim}{z}-\underset{\sim}{w}) \tag{6}$$

The formal solution to (5) is

$$P(\underset{\sim}{z},t\,|\underset{\sim}{w},t_0)=e^{-L_{\underset{\sim}{z}}(t-t_0)}\,P(\underset{\sim}{z},t_0\,|\underset{\sim}{w},t_0) \tag{7}$$

$$=e^{-L_{\underset{\sim}{z}}(t-t_0)}\,\delta(\underset{\sim}{z}-\underset{\sim}{w}) \tag{8}$$

Introduce the solution $\underset{\sim}{Z}(\underset{\sim}{X},t)$ to the Hamilton equations of motion

$$\frac{d}{dt}\underset{\sim}{Z}(\underset{\sim}{x},t) = L_{\underset{\sim}{x}}\,\underset{\sim}{X}\Big|_{\underset{\sim}{X}=\underset{\sim}{Z}(\underset{\sim}{x},t)} , \tag{9}$$

which at $t=0$ satisfies

$$\underset{\sim}{Z}(\underset{\sim}{x},0) = \underset{\sim}{x} . \tag{10}$$

This solution is formally

$$\underset{\sim}{Z}(\underset{\sim}{x},t) = e^{L_{\underset{\sim}{x}}t}\,\underset{\sim}{X} . \tag{11}$$

In terms of this we may write (8) as

$$P(\underset{\sim}{z},t/\underset{\sim}{w},t_0) = \delta(\underset{\sim}{Z}(\underset{\sim}{z},t_0-t)-\underset{\sim}{w}) \tag{12}$$

and noting that $L_{\underset{\sim}{z}}$ is a differential operator

$$P(\underset{\sim}{z},t|\underset{\sim}{w},t_0) = e^{-L_{\underset{\sim}{z}}(t-t_0)}\delta(\underset{\sim}{z}-\underset{\sim}{w}) = e^{+L_{\underset{\sim}{w}}(t-t_0)}\delta(\underset{\sim}{z}-\underset{\sim}{w}) \tag{13}$$

$$= \delta(\underset{\sim}{z}-\underset{\sim}{Z}(\underset{\sim}{w},t-t_0)) . \tag{14}$$

Since $P(\underset{\sim}{z},t|\underset{\sim}{w},t_0)$ is a conditional probability, it must satisfy

$$P(\underset{\sim}{z},t/\underset{\sim}{w},t_0) = \int d\underset{\sim}{y}\; P(\underset{\sim}{z},t|\underset{\sim}{y}\,\tau)\,P(\underset{\sim}{y},\tau|\underset{\sim}{w},t_0). \tag{15}$$

Now we want to use these properties to construct a representation for $P(\underset{\sim}{z},t|\underset{\sim}{w},t_0)$. Break up the interval from t_0 to t into N steps of size ε : $t=t_0+N\varepsilon$. Apply (15) to each of these intervals to find

$$P(\underset{\sim}{z},t|\underset{\sim}{w},t_0) = \int \prod_{n=1}^{N-1} d\underset{\sim}{y}_n \quad P(\underset{\sim}{z},t|\underset{\sim}{y}_{N-1},t_{N-1})P(\underset{\sim}{y}_{N-1},t_{N-1}|\underset{\sim}{y}_{N-2},t_{N-2})$$
$$\times \ldots \times P(\underset{\sim}{y}_2,t_2|\underset{\sim}{y}_1,t_1)\,P(\underset{\sim}{y}_1,t_1|\underset{\sim}{w},t_0) \tag{16}$$

with $t_n = t_0 + n\varepsilon$. We may also write this as

$$P(\underset{\sim}{z},t/\underset{\sim}{w},t_0) = \int \prod_{n=0}^{N} d\underset{\sim}{y}_n \prod_{n=1}^{N} P(\underset{\sim}{y}_n,t_n / \underset{\sim}{y}_{n-1},t_{n-1})$$

$$\times\, \delta(\underset{\sim}{y}_N - \underset{\sim}{z})\, \delta(\underset{\sim}{y}_0 - \underset{\sim}{w}) \qquad (17)$$

We require, then, the elementary conditional probability

$$P(\underset{\sim}{y}_n,t_n / \underset{\sim}{y}_{n-1},t_{n-1}) = \delta(\underset{\sim}{y}_n - \underset{\sim}{Z}(\underset{\sim}{y}_{n-1},\varepsilon)) \qquad (18)$$

noting $t_n - t_{n-1} = \varepsilon$.

To proceed we must discretize the equations of motion (9) and use this result in making the elementary time step of size ε. Let us write

$$\frac{d}{dt} \underset{\sim}{Z}(\underset{\sim}{x},t) = \underset{\sim}{B}(\underset{\sim}{Z}(\underset{\sim}{x},t)) \qquad (19)$$

in place of (9), and for a small time interval of size ε , we replace (19) by

$$\frac{\underset{\sim}{Z}(\underset{\sim}{x},t+\varepsilon) - \underset{\sim}{Z}(\underset{\sim}{x},t)}{\varepsilon} = \underset{\sim}{B}(\underset{\sim}{Z}(\underset{\sim}{x},t)) \qquad (20)$$

For $\underset{\sim}{Z}(\underset{\sim}{y}_{n-1},\varepsilon)$ we have

$$\frac{\underset{\sim}{Z}(\underset{\sim}{y}_{n-1},\varepsilon) - \underset{\sim}{Z}(\underset{\sim}{y}_{n-1},0)}{\varepsilon} = \underset{\sim}{B}(\underset{\sim}{Z}(\underset{\sim}{y}_{n-1},0)) \qquad (21)$$

or

$$\underset{\sim}{Z}(\underset{\sim}{y}_{n-1},\varepsilon) = \underset{\sim}{y}_{n-1} + \varepsilon\, \underset{\sim}{B}(\underset{\sim}{y}_{n-1}) \qquad (22)$$

which yields our final formula for $P(\underset{\sim}{z},t/\underset{\sim}{w},t_0)$

$$P(\underset{\sim}{z},t/\underset{\sim}{w},t_0) = \int \prod_{n=0}^{N} d\underset{\sim}{y}_n\, \delta(\underset{\sim}{y}_N - \underset{\sim}{z})\, \delta(\underset{\sim}{y}_0 - \underset{\sim}{w}) \prod_{n=1}^{N} \delta(\underset{\sim}{y}_n - \underset{\sim}{y}_{n-1} - \varepsilon \underset{\sim}{B}(\underset{\sim}{y}_{n-1})) \qquad (23)$$

By virtue of its construction this representation satisfies

$$\int d\underset{\sim}{z}\; P(\underset{\sim}{z},t/\underset{\sim}{w},t_0) = 1 \quad , \tag{24}$$

as required for a conditional probability.

The passage to the limit $\varepsilon \to 0,\ t-t_0$ fixed, requires $N=(t-t_0)/\varepsilon$ to become infinite. In this limit the representation (23) becomes a functional integral

$$P(\underset{\sim}{z},t/\underset{\sim}{w},t_0) = \frac{\int \left[\prod_\tau d\underset{\sim}{y}(\tau)\right] \delta(\underset{\sim}{y}(t)-\underset{\sim}{z})\, \delta(\underset{\sim}{y}(t_0)-\underset{\sim}{w})\, \delta(\dot{\underset{\sim}{y}}(\tau)-\underset{\sim}{B}(\underset{\sim}{y}(\tau)))}{\int \left[\prod_\tau d\underset{\sim}{y}(\tau)\right] \delta(\underset{\sim}{y}(t_0)-\underset{\sim}{w})\, \delta(\dot{\underset{\sim}{y}}(\tau)-\underset{\sim}{B}(\underset{\sim}{y}(\tau)))} \tag{25}$$

where the denominator is a normalization factor required to maintain (24). Functional integrals for $P(\underset{\sim}{z},t/\underset{\sim}{w},t_0)$ have been discussed by Jouvet and Phythian[4.] and others [5.] Our derivation of (25) yields some insight into the meaning of the functional integral which in any case is defined by our limiting procedure on (23).

Once one has $P(\underset{\sim}{z},t/\underset{\sim}{w},t_0)$ it may be used to answer dynamical questions of physical interest. Suppose we want the time dependence of the phase function $a(\underset{\sim}{z})$. This is given by

$$a(\underset{\sim}{Z}(\underset{\sim}{z},t)) = \int d\underset{\sim}{w}\; P(\underset{\sim}{z},-t/\underset{\sim}{w},0)\, a(\underset{\sim}{w}) = \int d\underset{\sim}{w}\; \delta(\underset{\sim}{Z}(\underset{\sim}{z},t)-\underset{\sim}{w})\, a(\underset{\sim}{w}) \tag{26}$$

or using (23)

$$a(\underset{\sim}{Z}(\underset{\sim}{z},t)) = \int \prod_{n=0}^{N} d\underset{\sim}{x}_n\; \delta(\underset{\sim}{x}_N-\underset{\sim}{z})\, a(\underset{\sim}{x}_0) \prod_{s=1}^{N} \delta(\underset{\sim}{x}_s-\underset{\sim}{x}_{s-1}+\varepsilon\, \underset{\sim}{B}(\underset{\sim}{x}_{s-1})) \tag{27}$$

An approximation to $P(\underset{\sim}{z},t/\underset{\sim}{w},t_0)$ thus yields an approximate value of

$a(\underset{\sim}{Z}(\underset{\sim}{z},t))$. A quantity of physical interest is the direct diffusion tensor[6.] $(a,b=1,\ldots,M)$ defined by

$$\Delta_{ab}(\underset{\sim}{I},t) = \int \frac{d^M\theta}{(2\pi)^M} \frac{\partial H}{\partial \theta_a}(\underset{\sim}{I},\underset{\sim}{\theta}) e^{-Lt} \frac{\partial H}{\partial \theta_b}(\underset{\sim}{I},\underset{\sim}{\theta}) \tag{28}$$

which enters the equation of motion for the angle averaged phase space density $F(\underset{\sim}{I},t) = \int \frac{d^M\theta}{(2\pi)^M} f_M(\underset{\sim}{I},\underset{\sim}{\theta},t)$. In terms of $P(\underset{\sim}{I},\underset{\sim}{\theta},t \,|\, \underset{\sim}{I}',\underset{\sim}{\theta}',t)$ we find

$$\Delta_{ab}(\underset{\sim}{I},t) = \int \frac{d^M\theta\, d^M\theta'\, d^M I'}{(2\pi)^M} \frac{\partial H}{\partial \theta_a}(\underset{\sim}{I},\underset{\sim}{\theta})\, P(\underset{\sim}{I},\underset{\sim}{\theta},t \,|\, \underset{\sim}{I}',\underset{\sim}{\theta}',0) \frac{\partial H}{\partial \theta_b}(\underset{\sim}{I}',\underset{\sim}{\theta}') \tag{29}$$

From (23) or (25) we see that $P(\underset{\sim}{z},t/\underset{\sim}{w},t_0)$ is a product of delta functions. Clearly it is not a very smooth object. When the Hamiltonian gives rise to irregular or chaotic motion, we expect in some physical sense that $P(\underset{\sim}{z},t\,|\,\underset{\sim}{w},t_0)$ is smoother, as it represents diffusion. Rechester and White[3.] have made the suggestion that we "smooth" $P(\underset{\sim}{z},t\,|\,\underset{\sim}{w},t_0)$ by introducing random noise into the equation of motion (19) and dealing only with the conditional probability averaged over this noise. Call the random noise $\underset{\sim}{R}(t)$ and write

$$\frac{d\underset{\sim}{Z}(\underset{\sim}{x},t)}{dt} = \underset{\sim}{B}(\underset{\sim}{Z}(\underset{\sim}{x},t)) + \underset{\sim}{R}(t) \tag{30}$$

In the discretized form we have

$$\underset{\sim}{Z}(\underset{\sim}{y}_{n-1},\varepsilon) = \underset{\sim}{y}_{n-1} + \varepsilon \underset{\sim}{B}(\underset{\sim}{y}_{n-1}) + \varepsilon \underset{\sim}{R}(t_{n-1}) \tag{31}$$

to replace (22).

In (23) we use the integral representation of the delta functions and average over the probability distribution of the noise. Call the resulting conditional probability $\varphi(\underset{\sim}{z},t|\underset{\sim}{w},t_0) \equiv \langle P(\underset{\sim}{z},t|\underset{\sim}{w},t_0)\rangle_{\underset{\sim}{R}}$:

$$\varphi(\underset{\sim}{z},t|\underset{\sim}{w},t_0) = \int \prod_{n=0}^{N} d\underset{\sim}{y}_n\, \delta(\underset{\sim}{y}_N - \underset{\sim}{z})\, \delta(\underset{\sim}{y}_0 - \underset{\sim}{w}) \prod_{m=1}^{N} \int \frac{d\underset{\sim}{u}_m}{2\pi}$$

$$\times \exp i\underset{\sim}{u}_m \cdot [\underset{\sim}{y}_n - \underset{\sim}{y}_{n-1} - \varepsilon \underset{\sim}{B}(\underset{\sim}{y}_{n-1})] \left\langle e^{-i\varepsilon \underset{\sim}{u}_m \cdot \underset{\sim}{R}(t_{n-1})} \right\rangle_{\underset{\sim}{R}} \tag{32}$$

In the average of $\exp[-i\varepsilon \underset{\sim}{u}_m \cdot \underset{\sim}{R}(t_{n-1})]$ we encounter the characteristic function of the $\underset{\sim}{R}$ distribution. This has a cumulant expansion

$$\langle \exp[-i\varepsilon \underset{\sim}{u}_m \cdot \underset{\sim}{R}(t_{n-1})]\rangle_{\underset{\sim}{R}} = \exp \sum_{l=1}^{\infty} (i\varepsilon \underset{\sim}{u}_m)^l \times (l^{th}\ \text{cumulant}) \tag{33}$$

Since the external noise was introduced simply to smooth out the behavior of $P(\underset{\sim}{z},t|\underset{\sim}{w},t_0)$, we are free to choose $\underset{\sim}{R}(t)$ to be gaussian white noise with zero mean $\langle \underset{\sim}{R}\rangle_{\underset{\sim}{R}} = 0$ and co-variance

$$\langle R_a(t) R_b(\tau)\rangle_{\underset{\sim}{R}} = \delta_{ab}\, \sigma_b\, \delta(t-\tau) \qquad a,b = 1,\ldots,M. \tag{34}$$

This leads to

$$\varphi(\underset{\sim}{z},t|\underset{\sim}{w},t_0) = \int \prod_{n=0}^{N} d\underset{\sim}{y}_n\, \delta(\underset{\sim}{y}_N - \underset{\sim}{z})\, \delta(\underset{\sim}{y}_0 - \underset{\sim}{w})$$

$$\times \prod_{m=1}^{N} \frac{d\underset{\sim}{u}_m}{2\pi} \exp i\underset{\sim}{u}_m \cdot (\underset{\sim}{y}_n - \underset{\sim}{y}_{n-1} - \varepsilon \underset{\sim}{B}(\underset{\sim}{y}_{n-1}))\, e^{-\frac{1}{2}\sum_{b=1}^{M} u_{m_b}^2 \sigma_b \varepsilon^2} \tag{35}$$

which has clearly smoothed out the delta functions of the deterministic system over a range in phase space of order $\sqrt{\sigma_b}$ for $b=1,\ldots,M$.

For the calculations we will indicate below on Hamiltonians of the form

$$H(\underset{\sim}{I},\underset{\sim}{\theta}) = H_0(\underset{\sim}{I}) + k H_1(\underset{\sim}{I},\underset{\sim}{\theta}),$$

the external noise will be unimportant in the limit of interest: $k\to\infty$. In this limit the intrinsic stochasticity of the orbits in phase space overwhelms the extrinsic stochasticity given by the external noise $\underset{\sim}{R}$. For studying both the $k\to 0$ and $k\to\infty$ regimes, (35) will prove useful. We do not consider it further here.

III. Strong Coupling Limits for Hamiltonian Dynamics

For our Hamiltonian $H(\underset{\sim}{I},\underset{\sim}{\theta}) = H_0(\underset{\sim}{I}) + k\, H_1(\underset{\sim}{I},\underset{\sim}{\theta})$, we write the equations of motion in the following discretized form

$$\underset{\sim}{I}(n) = \underset{\sim}{I}(n-1) + \varepsilon k\, \underset{\sim}{h}(\underset{\sim}{I}(n), \underset{\sim}{\theta}(n-1)) \tag{36}$$

$$\underset{\sim}{\theta}(n) = \underset{\sim}{\theta}(n-1) + \varepsilon \underset{\sim}{\omega}(\underset{\sim}{I}(n)) + \varepsilon k \frac{\partial H_1}{\partial \underset{\sim}{I}}(\underset{\sim}{I}(n), \underset{\sim}{\theta}(n-1)) \tag{37}$$

where we take N time steps of size ε between t_0 and t and write $\underset{\sim}{I}(t_0+n\varepsilon), \underset{\sim}{\theta}(t_0+n\varepsilon)$ as $\underset{\sim}{I}(n)$, $\underset{\sim}{\theta}(n)$. Also we have introduced the abbreviated notation $\underset{\sim}{\omega}(\underset{\sim}{I}) = \partial H_0/\partial \underset{\sim}{I}$, $\underset{\sim}{h}(\underset{\sim}{I},\underset{\sim}{\theta}) = -\partial H_1(\underset{\sim}{I},\underset{\sim}{\theta})/\partial \underset{\sim}{\theta}$.

This form of discretized motion defines a mapping from $(\underset{\sim}{I}(n-1), \underset{\sim}{\theta}(n-1))$ to $(\underset{\sim}{I}(n), \underset{\sim}{\theta}(n))$ which preserves volume in 2N dimensional phase space.

Our representation for the conditional probability $P(\underset{\sim}{I},\underset{\sim}{\theta},t\,|\,\underset{\sim}{I}_0,\underset{\sim}{\theta}_0,t_0)$ comes from (23) and reads

$$\begin{aligned} P(\underset{\sim}{I},\underset{\sim}{\theta},t\,|\,\underset{\sim}{I}_0,\underset{\sim}{\theta}_0,t_0) = &\int \prod_{n=0}^{N} d\underset{\sim}{J}(n)\, d\underset{\sim}{\chi}(n)\; \delta^M(\underset{\sim}{J}(0)-\underset{\sim}{I}_0)\; \delta^M(\underset{\sim}{J}(N)-\underset{\sim}{I}) \\ &\times \delta^M(\underset{\sim}{\chi}(0)-\underset{\sim}{\theta}_0)\; \delta^M(\underset{\sim}{\chi}(N)-\underset{\sim}{\theta}) \Big\{ \prod_{s=1}^{N} \delta^M\big[\underset{\sim}{J}(s) - \underset{\sim}{J}(s-1) - \varepsilon k\, \underset{\sim}{h}(\underset{\sim}{J}(s), \underset{\sim}{\chi}(s-1))\big] \\ &\times \delta^M\Big[\underset{\sim}{\chi}(s) - \underset{\sim}{\chi}(s-1) - \varepsilon\, \underset{\sim}{\omega}(\underset{\sim}{J}(s)) - \varepsilon k \frac{\partial H_1}{\partial \underset{\sim}{J}}(\underset{\sim}{J}(s), \underset{\sim}{\chi}(s-1))\Big] \Big\} \end{aligned} \tag{38}$$

The idea is to now represent each of the δ functions in (38) by <u>fourier series</u>. For the evolution of the angle variables this is quite natural since they are defined to lie in the interval $0 \le \theta_a(s) \le 1$, $s = 0, \ldots, N$. For actions to remain in a finite interval, we must require that the energy surface $E = H(\underset{\sim}{I},\underset{\sim}{\theta})$, on which the orbits lie, be bounded. We restrict our attention to this case. Then if the highest power of

$I_a, a=1, \ldots, M$, occuring in $H(\underset{\sim}{I}, \underset{\sim}{\theta})$ is $(I_a)^P$, the values of I_a lie more or less in the range $0 \le |I_a| \le (E)^{1/p}$. Of course, the actual values of I_a are more complicated, but what is essential is that each I_a lies in a finite domain for fixed E. With this in mind we write (38) as

$$P(\underset{\sim}{I}, \underset{\sim}{\theta}, t \,|\, \underset{\sim}{I}_0, \underset{\sim}{\theta}_0, t_0) = \int \prod_{n=0}^{N} d\underset{\sim}{J}(n)\, d\underset{\sim}{\chi}(n)\, \delta^M(\underset{\sim}{J}(0) - \underset{\sim}{I}_0)\, \delta^M(\underset{\sim}{J}(N) - \underset{\sim}{I})$$

$$\times \delta^M(\underset{\sim}{\chi}(0) - \underset{\sim}{\theta}_0)\, \delta^M(\underset{\sim}{\chi}(N) - \underset{\sim}{\theta}) \prod_{s=1}^{N} \Bigg\{ \Bigg(\sum_{\underset{\sim}{l}_s = -\infty}^{\infty} \exp 2\pi i\, \underset{\sim}{l}_s \cdot \Big[\underset{\sim}{\chi}(s) - \underset{\sim}{\chi}(s-1)$$

$$- \varepsilon\, \underset{\sim}{\omega}(\underset{\sim}{J}(s)) - \varepsilon k \frac{\partial H_1}{\partial \underset{\sim}{J}} (\underset{\sim}{J}(s), \underset{\sim}{\chi}(s-1)) \Big] \Bigg)$$

$$\times \prod_{a=1}^{M} \frac{1}{L_{as}} \sum_{m_{as}=-\infty}^{\infty} \exp \frac{i 2\pi}{L_{as}} m_{as} \Big[J_a(s) - J_a(s-1) - \varepsilon k\, h_a(\underset{\sim}{J}(s), \underset{\sim}{\chi}(s-1)) \Big] \Bigg\} \tag{39}$$

where $\underset{\sim}{l}_s$ is an M vector of integers and L_{as} is the length of the interval covered by $I_a(t_s)$ on the energy surface.

To evaluate $P(\underset{\sim}{I}, \underset{\sim}{\theta}, t \,|\, \underset{\sim}{I}_0, \underset{\sim}{\theta}_0, t_0)$ for large k we proceed by choosing those values of l_{as} and m_{as} which result in the smallest number of factors of oscillating integrands of form exp[i k (functions of $\underset{\sim}{J}(s)$ and $\underset{\sim}{\chi}(s)$]. The smallest number of such factors will always be zero from the choice $l_{as}, m_{as} = 0$ for all a and s. Then we can arrange to have one factor exp i k ( ) by judicious choice of the $\underset{\sim}{l}_s$ and $\underset{\sim}{m}_s$; then, two; etc. Each oscillating integral over the $\underset{\sim}{I}(s)$ and $\underset{\sim}{\chi}(s)$ will contribute powers of $k^{-\frac{1}{2}}$ to the expansion for large k. This is readily seen by use of a stationary phase approximation on such integrals. Although the convergence of such a large k expansion is likely to be problematic, a useful asymptotic series will result. For purposes of illustration of these general statements we will now restrict ourselves to Hamiltonians of the form

$$H(\underset{\sim}{I}, \underset{\sim}{\theta}) = H_0(\underset{\sim}{I}) + k H_1(\underset{\sim}{\theta}) \tag{40}$$

For this choice all the $\underset{\sim}{I}(n)$ integrations can be performed leaving us with

$$P(\underset{\sim}{I}, \underset{\sim}{\theta}, t \,|\, \underset{\sim}{I}_0, \underset{\sim}{\theta}_0, t_0) = \int_0^1 \prod_{n=0}^{N} d\underset{\sim}{\chi}(n)\, \delta^M(\underset{\sim}{\chi}(0) - \underset{\sim}{\theta}_0)\, \delta^M(\underset{\sim}{\chi}(N) - \underset{\sim}{\theta})$$

$$\times\, \delta^M(\underset{\sim}{I} - \underset{\sim}{I}_0 - k\varepsilon \underset{\sim}{S}(N-1)) \prod_{s=1}^{N} \sum_{\underset{\sim}{l}_s = -\infty}^{\infty} \exp 2\pi i\, \underset{\sim}{l}_s \cdot \left[\underset{\sim}{\chi}(s) - \underset{\sim}{\chi}(s-1) - \varepsilon \underset{\sim}{\omega}(\underset{\sim}{I}_0 + \varepsilon k \underset{\sim}{S}(s-1))\right] \tag{41}$$

where

$$\underset{\sim}{S}(n) \equiv \sum_{r=0}^{n} \underset{\sim}{h}(\underset{\sim}{\theta}(r)) \tag{42}$$

A quantity of some physical interest in chaotic systems is the value of $(\underset{\sim}{I}(N) - \underset{\sim}{I}_0)^2$ after a large number of steps N. The mean value

$$D(\underset{\sim}{I}_0, k) = \lim_{N\to\infty} \frac{1}{2N} \int P(\underset{\sim}{I}, \underset{\sim}{\theta}, t \,|\, \underset{\sim}{I}_0, \underset{\sim}{\theta}_0, t_0)\, d\underset{\sim}{\theta}\, d\underset{\sim}{\theta}_0\, d\underset{\sim}{I}\, (\underset{\sim}{I} - \underset{\sim}{I}_0)^2 \tag{43}$$

$$= \lim_{N\to\infty} \frac{1}{2N} \int_0^1 \prod_{n=0}^{N} d\underset{\sim}{\chi}(n)\, \varepsilon^2 k^2 \left(\underset{\sim}{S}(N-1)\right)^2$$
$$\times \prod_{s=1}^{N} \sum_{\underset{\sim}{l}_s=-\infty}^{\infty} \exp 2\pi i \underset{\sim}{l}_s \cdot \left[\underset{\sim}{\chi}(s) - \underset{\sim}{\chi}(s-1) - \varepsilon \underset{\sim}{\omega}\left(\underset{\sim}{I}_0 + \varepsilon k \underset{\sim}{S}(s-1)\right)\right], \tag{44}$$

represents a diffusion coefficient telling how far the system will wander in $\underset{\sim}{I}$ space from its initial value $\underset{\sim}{I}_0$ after a long time $t = N\varepsilon + t_0$. $D(\underset{\sim}{I}_0)$ is clearly related to the trace of the direct diffusion tensor, Eq. (29), given at present by

$$\Delta_{ab}(\underset{\sim}{I}, N) = \int_0^1 \prod_{n=0}^{N} d\underset{\sim}{\chi}(n)\; k^2 h_a\left(\underset{\sim}{\chi}(0)\right) h_b\left(\underset{\sim}{\chi}(N)\right)$$
$$\times \prod_{s=1}^{N} \sum_{\underset{\sim}{l}_s=-\infty}^{\infty} \exp 2\pi i \underset{\sim}{l}_n \cdot \left[\underset{\sim}{\chi}(s) - \underset{\sim}{\chi}(s-1) - \varepsilon \underset{\sim}{\omega}\left(\underset{\sim}{I} + \varepsilon k\left(\underset{\sim}{S}(s-1) - \underset{\sim}{S}(N-1)\right)\right)\right]. \tag{45}$$

Turning from these general remarks we choose a specific Hamiltonian with two degrees of freedom. We required the unperturbed or integrable part of H to be at most quadratic in $\underset{\sim}{I} = (I_1, I_2)$ and to have two resonances which can overlap inside the energy surface[7]. By canonical transformation such an H can always be cast in the form

$$H(I_1, I_2, \theta_1, \theta_2) = \sum_{a,b=1}^{2} \left(I_a m_{ab} I_b\right) + \frac{k}{2\pi}\left[\cos 2\pi\theta_1 + \rho \cos 2\pi\theta_2\right] \tag{46}$$

with m_{ab} some numerical 2x2 matrix. If m_{ab} has positive eigenvalues, the energy surface contains bounded $\underset{\sim}{I}$. The choice we have made to study is

$$H(\underset{\sim}{I}, \underset{\sim}{\theta}) = \frac{I_1^2 + I_2^2 + I_1 I_2}{2} + \frac{k}{2\pi}\left[\cos 2\pi\theta_1 + \rho \cos 2\pi\theta_2\right] \tag{47}$$

The discretized equations of motion read

$$I_1(n) = I_1(n-1) + \varepsilon k \sin 2\pi\theta_1(n-1) \tag{48}$$

$$I_2(n) = I_2(n-1) + \varepsilon k\rho \sin 2\pi\theta_2(n-1) \tag{49}$$

$$\theta_1(n) = \theta_1(n-1) + \varepsilon\left(I_1(n) + \tfrac{1}{2}I_2(n)\right) \tag{50}$$

and

$$\theta_2(n) = \theta_2(n-1) + \varepsilon\left(I_2(n) + \tfrac{1}{2}I_1(n)\right) \tag{51}$$

Choosing $H_0(\underset{\sim}{I})$ quadratic in $\underset{\sim}{I}$ was clearly to make $\underset{\sim}{\omega}(\underset{\sim}{I})$ linear. Choosing $\rho \neq 0$ is to make $H(\underset{\sim}{I},\underset{\sim}{\theta})$ nonintegrable. This choice of discretization makes the mapping $(\underset{\sim}{I}(n-1), \underset{\sim}{\theta}(n-1)) \rightarrow (\underset{\sim}{I}(n), \underset{\sim}{\theta}(n))$ volume preserving in phase space for any ε. Notice that this mapping becomes the Chirikov standard mapping[7]. when $\rho = 0$.

We have investigated the orbits of the system defined by (48) - (51) by the surface of section method. We present in Figures 1 - 6, the I_1, θ_1 plane for $\theta_2 = 0$ for various choices of ρ for a large k. Note that $\rho = 0$ (Figure 1) is integrable.

Note an essential difference between the mapping (48) - (51) and the flow. When $\rho = 0$, the flow is integrable. When $\rho = 0$, the mapping is not. The usual parameter of the standard mapping is $2\pi\varepsilon^2 k$ in the notation used here. In doing the numerical integrations presented in Figures 1-6 we took $k = 110 \times 2\pi$, and the value of ε used in Figure 1 was 3.6×10^{-4}. This gives a standard mapping parameter of 4.6×10^{-4} which is so small as not to destroy the regularity of motion in I_1, θ_1, seen in the plot.

Now we use (44) to evaluate $D(\underset{\sim}{I}_0, k)$ for our mapping. The ingredients we need for the calculation are

$$\underset{\sim}{\omega}(I_1, I_2) = \left(I_1 + I_2/2,\ I_2 + I_1/2\right) \tag{52}$$

and

$$\underset{\sim}{S}(n) = \sum_{r=0}^{n} \left(\sin 2\pi\theta_1(r),\ \rho \sin 2\pi\theta_2(r)\right) \tag{53}$$

The leading contributions to $D(\underset{\sim}{I}_0, k)$ are $(K = 2\pi\varepsilon^2 k)$

$$D(\underset{\sim}{I}_0, k) \xrightarrow[\varepsilon,\rho \text{ fixed}]{K \text{ large}} \frac{\varepsilon^2 k^2}{2} \left\{ \frac{1+\rho^2}{2} - \left[J_2(K) J_0(K\rho/2) + \rho^2 J_2(K\rho) J_0(K/2) \right] \right.$$

$$+ J_0^2(K\rho/2)\left[J_2^2(K) - J_1^2(K) + J_3^2(K)\right]$$

$$+ \rho^2 J_0^2(K/2)\left[J_2^2(K\rho) - J_1^2(K\rho) + J_3^2(K\rho)\right]$$

$$\left. + \cdots \right\} \qquad (54)$$

where $J_l(z)$ is the ordinary Bessel function of order l. For ρ=o the results of Reference 3 are recovered including a correction, the $J_2^{\,2}(K)$ term, pointed out by R. Cohen. The standard mapping parameter for ρ=o is $K = 2\pi\varepsilon^2 k$ as it should be.

The initial condition enters only in terms not proportional to N and thus are absent in the limit, Equation (43), defining $D(\underset{\sim}{I}_0, k)$. This is actually a nice result for one would hope that diffusion in a chaotic system would be independent of one's starting point in phase space.

In Figures 7 and 8 we compare numerical calculations for $D(\underset{\sim}{I}_0, k)$ with ρ=1.0 and $\varepsilon = 0.5$ and 0.1 respectively with the asymptotic form of (54)

$$D(\underset{\sim}{I}_0, k) \sim \frac{\varepsilon^2 k^2}{2}\left\{1 - \frac{4\sqrt{2}}{\pi K}\cos\left(K - \frac{5\pi}{4}\right)\cos\left(K/2 - \pi/4\right) + \mathcal{O}(1/K^3)\right\} \qquad (55)$$

To return to the $\varepsilon = 0$ limit which gives us the original Hamiltonian flow is somewhat subtle. We take up that subject next.

IV. The $\varepsilon \to 0$ Limit

To this point we have focused our attention on the behavior of phase space volume preserving mappings such as Equations (36) and (37) which are derived from discretizing Hamiltonian flows. Our concentration has been on the limit where k, the "size" of the non-integrable part of the original Hamiltonian, becomes large while the time step ε remains fixed. To return to the actual flow we must investigate the $\varepsilon \to 0$ limit of our methods.

It is clear from the representation of the conditional probability $P(\underset{\sim}{z}, t | \underset{\sim}{w}, t_0)$ as a product of delta functions or from the form of our expression Equation (54) or (55) for the diffusion coefficient in our model problem that one may not take the $\varepsilon \to 0$ limit directly on the large k asymptotic expansion. The issue we are encountering here is familiar from strong coupling expansions in quantum field theory[8.] and statistical physics[9.].

To pose the problem in the context of our model Hamiltonian we note that in the $\varepsilon \to 0$ limit one is interested in

$$\tilde{D}(\underset{\sim}{I}_0, k) \equiv \frac{\left\langle \left(\underset{\sim}{I}(t = t_0 + N\varepsilon) - \underset{\sim}{I}_0\right)^2 \right\rangle_{\theta_0}}{2N\varepsilon} \tag{56}$$

in the limit $\varepsilon \to 0$, $t - t_0 = N\varepsilon$ large. Now the dimensions of k are $(\text{time})^{-2}$ and the dimensionsions of $\underset{\sim}{I}$ are $(\text{time})^{-1}$ while the dimensions of $\tilde{D}$ are $(\text{time})^{-3}$. $\tilde{D}(\underset{\sim}{I}_0, k)$ must take the form $(K = 2\pi k \varepsilon^2)$

$$\tilde{D}(\underset{\sim}{I}_0, k) = k^{3/2} \Psi(K, \varepsilon \underset{\sim}{I}_0) \tag{57}$$

indeed our expression for Ψ can be read off from (54) to be (defining $\eta = 1/K$)

$$\Psi(1/\eta, \varepsilon \underset{\sim}{I}_0) = \frac{1}{2} \eta^{-\frac{1}{2}} \left\{ \frac{1}{2}(1+\rho^2) - \left[J_0\left(\frac{\rho}{2\eta}\right) J_2(1/\eta) + \rho^2 J_2(\rho/\eta) J_0(1/\eta) \right] + \dots \right\} \tag{58}$$

We know the function ψ for $\eta \to \infty$ and we wish to evaluate it for $\eta \to 0$. Assuming this function has a finite limit we learn that

$$\tilde{D}(k, \underset{\sim}{I}_0) = k^{3/2}\, \chi\left(k/\underset{\sim}{I}_0^2\right) \tag{59}$$

for the flow. Our expectation from the form of (54) is that for the particular problem at hand χ will be a function of the dimensionless quantity ρ alone and $\underset{\sim}{I}_0$ will be absent.

Various methods are available for making the extrapolation from $\eta \sim \infty$ to $\eta \sim 0$.[8,9,10] We have not yet undertaken this project for our model Hamiltonian. What is needed are many more terms of the series we have begun in (54); this work will be reported in a subsequent publication.

V. Conclusions

We have presented in this paper a method for evaluating physical properties of non-integrable Hamiltonian dynamics with $H(\mathbf{I},\boldsymbol{\theta}) = H_0(\mathbf{I}) + k\,H_1(\mathbf{I},\boldsymbol{\theta})$ when the parameter k is large. Our procedure requires the calculation of the conditional probability $P(\mathbf{I},\boldsymbol{\theta},t\,|\,\mathbf{I}_0,\boldsymbol{\theta}_0,t_0)$ that the system is in $\mathbf{I},\boldsymbol{\theta}$ at t given it was in $\mathbf{I}_0,\boldsymbol{\theta}_0$ at t_0. To determine $P(\mathbf{I},\boldsymbol{\theta},t\,|\,\mathbf{I}_0,\boldsymbol{\theta}_0,t_0)$ for large k we put our system on a time "lattice" of spcing ϵ between discrete time steps. This transforms the actual flow which occurs for $\epsilon = 0$ into the volume preserving mapping, Equations (39) and (37). For k large, ϵ fixed we were able to give a procedure for evaluating $P(\mathbf{I},\boldsymbol{\theta},t\,|\,\mathbf{I}_0,\boldsymbol{\theta}_0,t_0)$. The return to the actual flow at $\epsilon = 0$ is subtle, and we have not yet explored the various existing approaches to that problem.

The $\epsilon \neq 0$ limit of the Hamiltonian flow is of some interest in itself from a theoretical point of view. Numerical solutions of the Hamilton equations of motion on digital computers are, of course, done with $\epsilon \neq 0$. There is thus a body of numerical "experiment" against which to compare the large k, fixed ϵ limits discussed here. More physically one often encounters situations in which the flow can be approximated by "free" or unperturbed motion with occasional bumping of adiabatic invariants by resonance crossing. The motion of a charged particle in an electrostatic field of eikonal form is a case of some interest in plasma physics[11]. The "free" motion is that of the oscillation center over which one can average to arrive at a mapping to be studied by the methods given here.

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Figure Captions

Figure 1. Surface of Section Plot for orbits generated by our Hamiltonian, Equation (47). We show the I_1, θ_1 plane for $\theta_2 = 0$. The initial conditions are $I_1(0) = 3.0, I_2(0) = 1.0, \theta_1(0) = 0.743, \theta_2(0) = 0.0$. The parameters k, and ρ were $\frac{k}{2\pi} = 110.0$, $\rho = 0.0$.

Figure 2. Same as Figure 1, except $\rho = 0.05$

Figure 3. Same as Figure 1, except $\rho = 0.25$

Figure 4. Same as Figure 1, except $\rho = 0.51$

Figure 5. Same as Figure 1, except $\rho = 0.75$

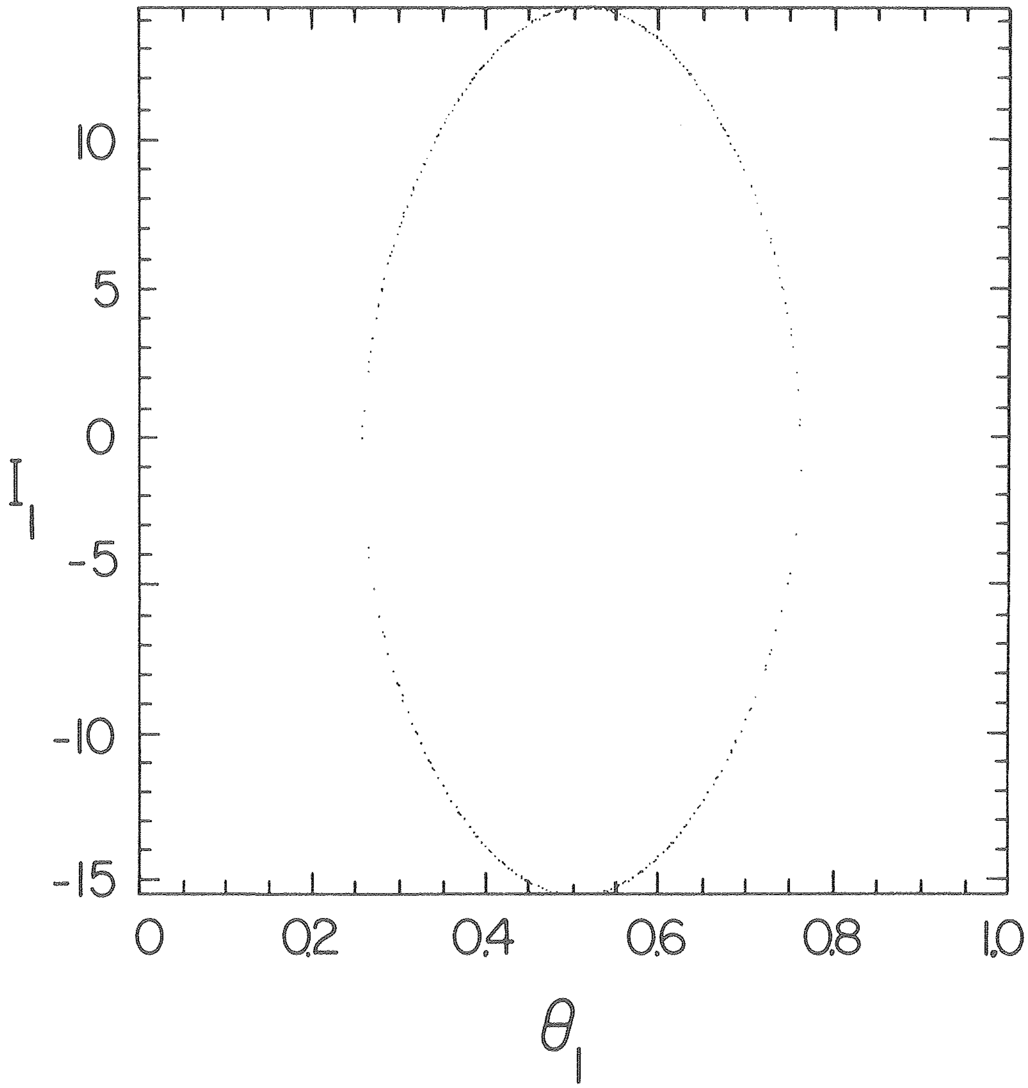
Figure 6. Same as Figure 1, except $\rho = 1.0$

Figure 7. The analytic asymptotic form, Equation (55), for

$$D(k, \underset{\sim}{I}_0) = \lim_{N\to\infty} \frac{1}{2N} \left\langle (\underset{\sim}{I}(N) - \underset{\sim}{I}_0)^2 \right\rangle_{\underset{\sim}{\theta}_0}$$

compared to numerical results (labeled by the N's) from the discretized equations of motion, Equations (48) - (51). In this graph D/k^2 is shown for $10 \le k \le 50, \rho = 1.0, \varepsilon = 0.5$. The range of $K = 2\pi\varepsilon^2 k$ is $15.7 \le K \le 78.5$. The integration over initial angles $\underset{\sim}{\theta}_0 = (\theta_{1_0}, \theta_{2_0})$ was performed with a 96 point Gaussian quadrature. The deviation of the numerical points from the asymptotic formula is less than 4% and is consistent with the numerical error arising from the use of only 96 initial θ_{1_0}'s and 96 initial θ_{2_0}'s.

Figure 8. The same as Figure 7 with $\varepsilon = 0.1$, $50 \le k \le 90$. The range of $K = 2\pi\varepsilon^2 k$ here is $3.14 \le K \le 5.65$.



XBL 8012-2490

Fig. 1

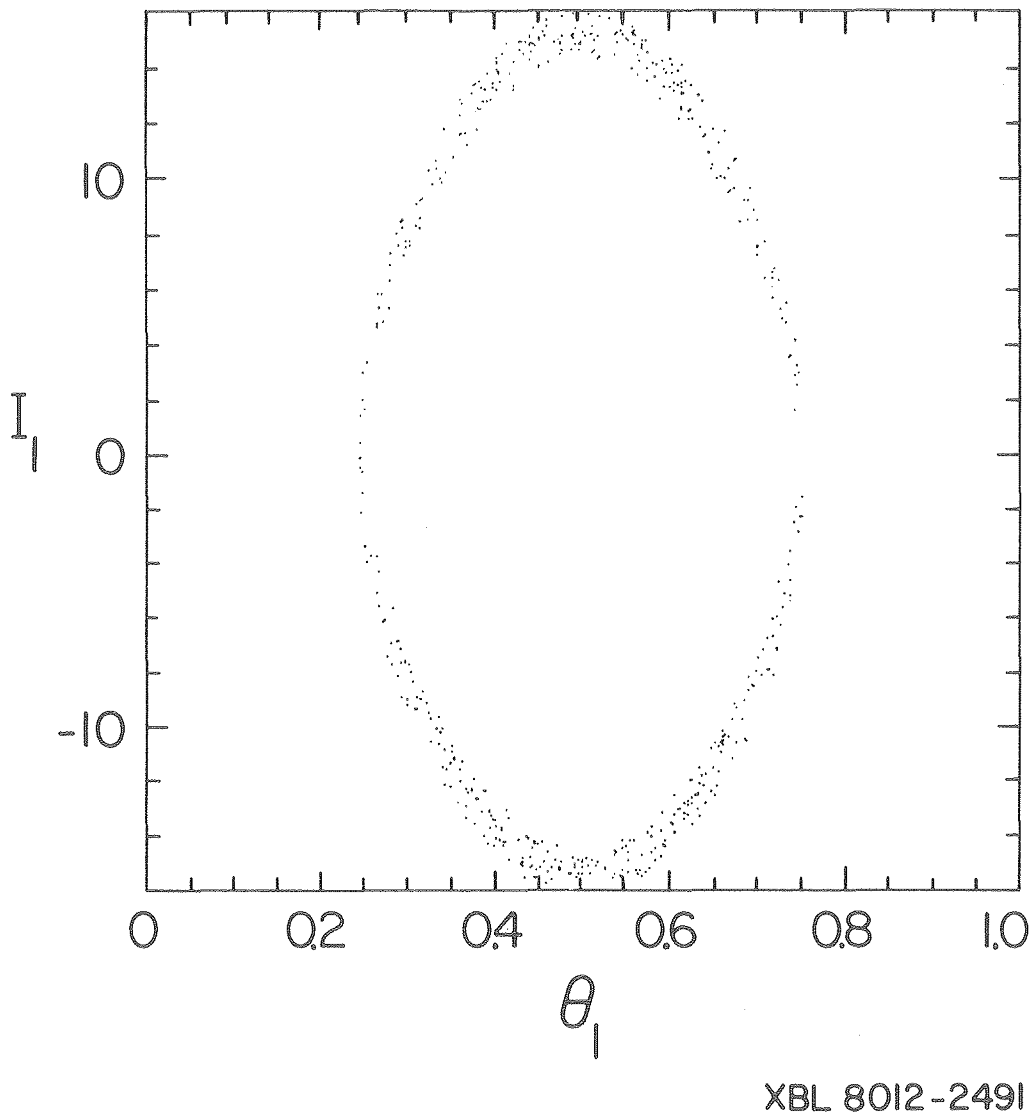
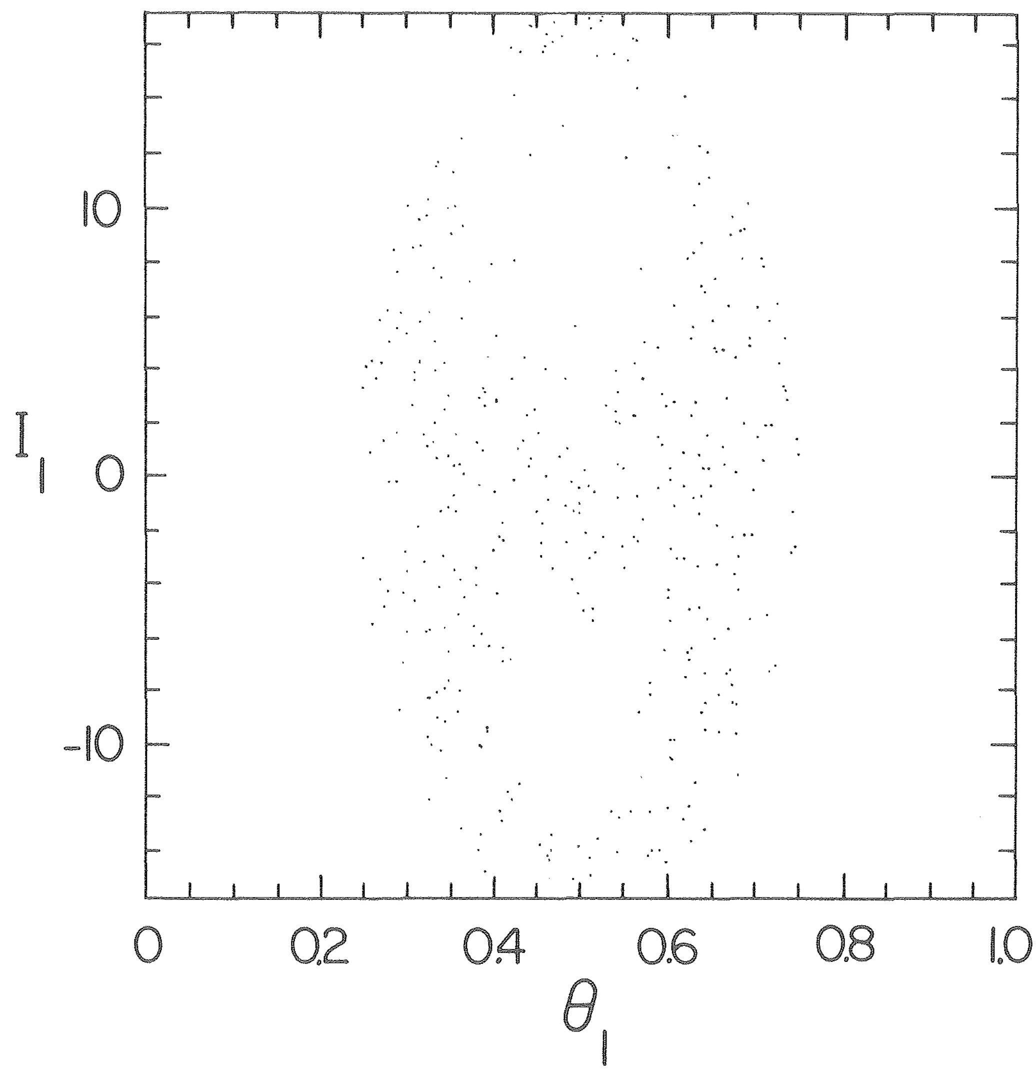
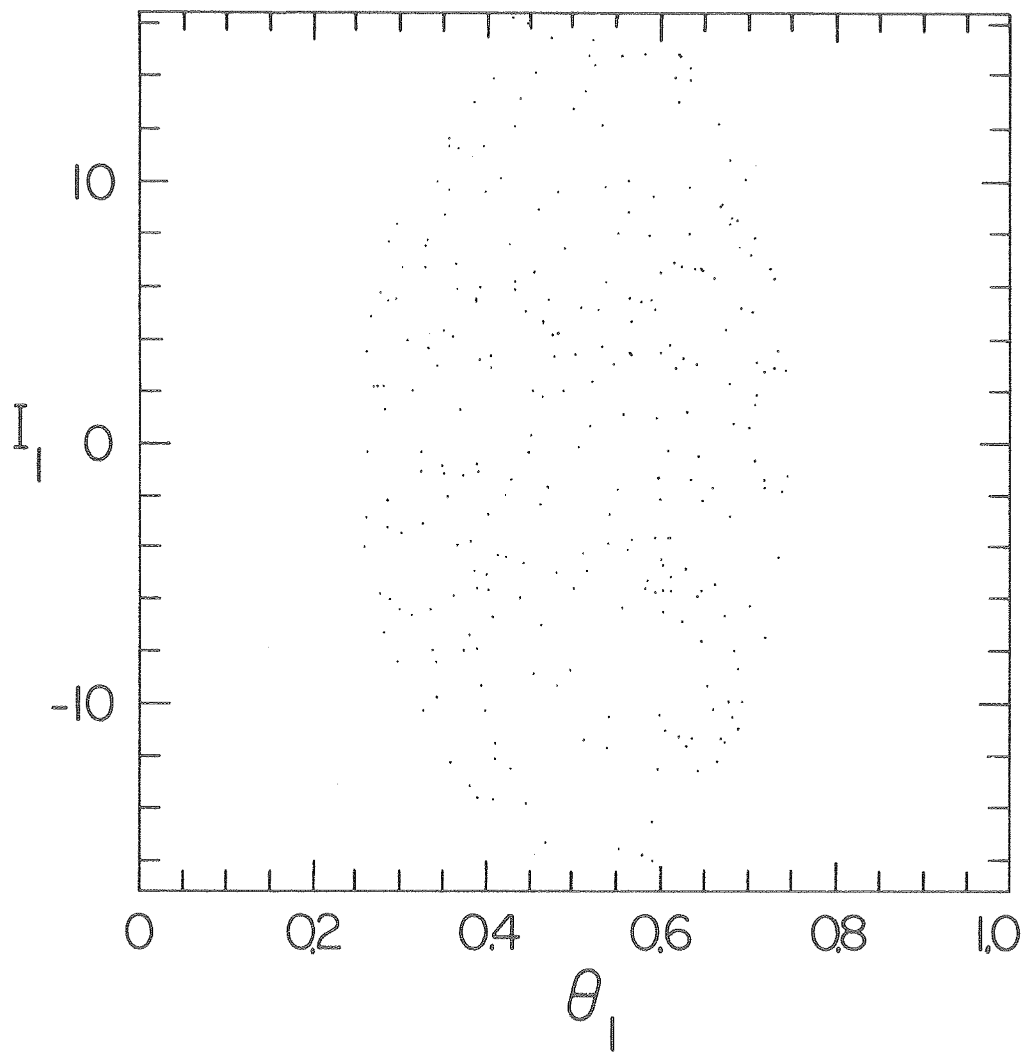


Fig. 2



XBL 8012-2492

Fig. 3



XBL 8012-2493

Fig. 4

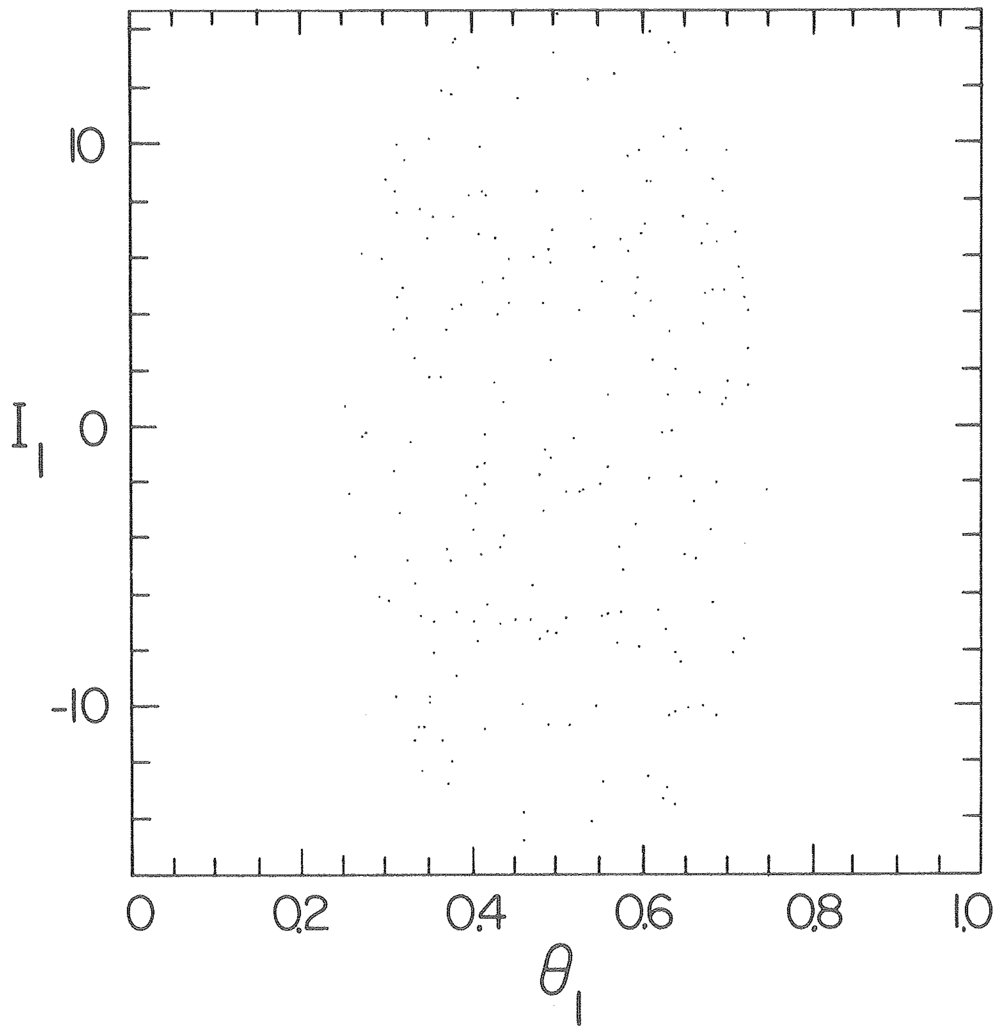


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Fig. 5

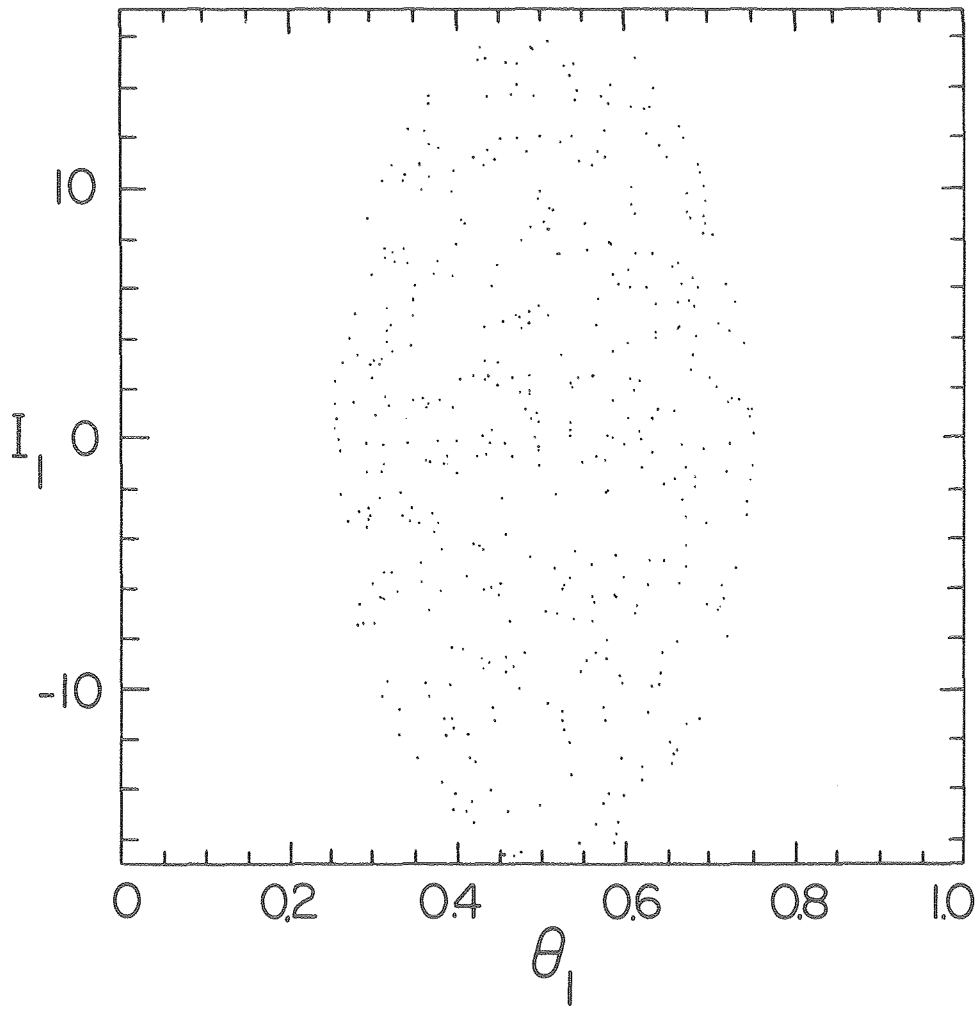

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Fig. 6

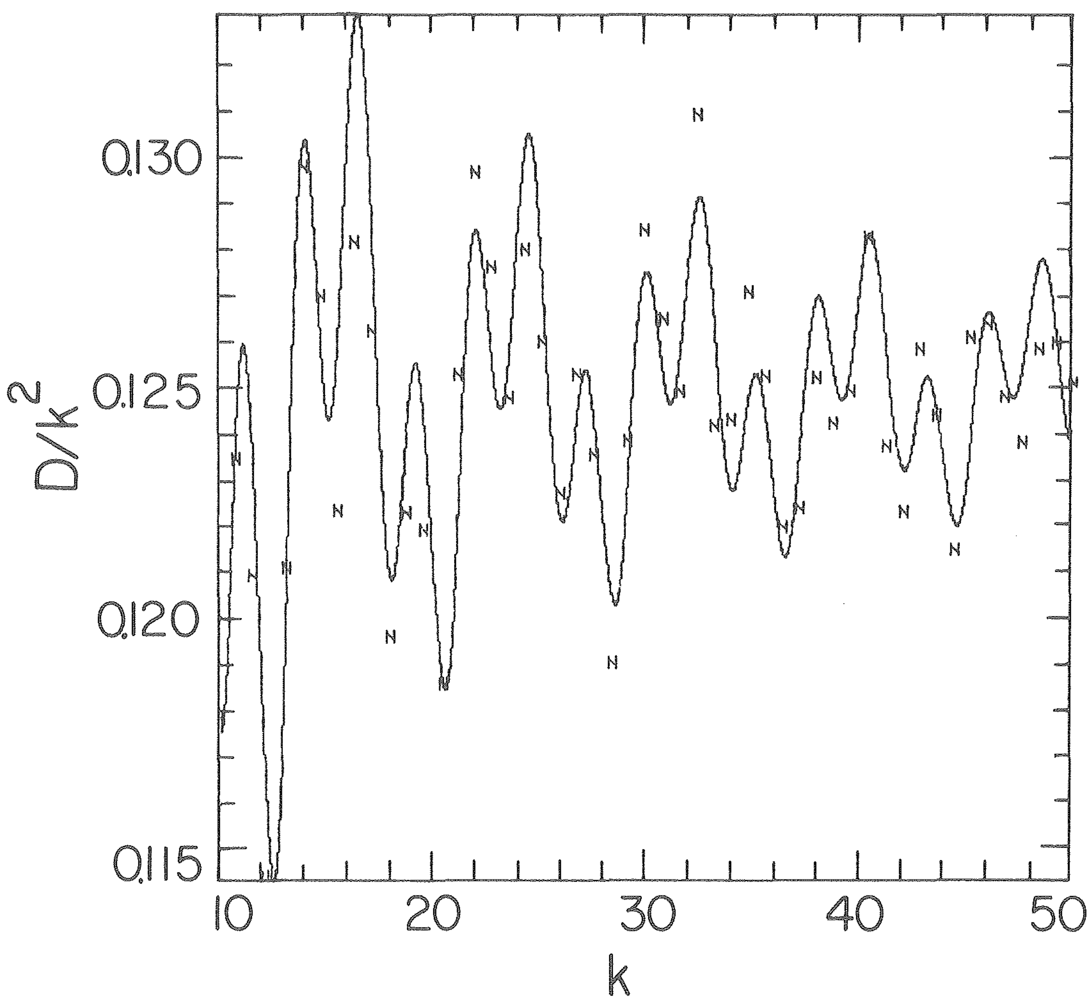

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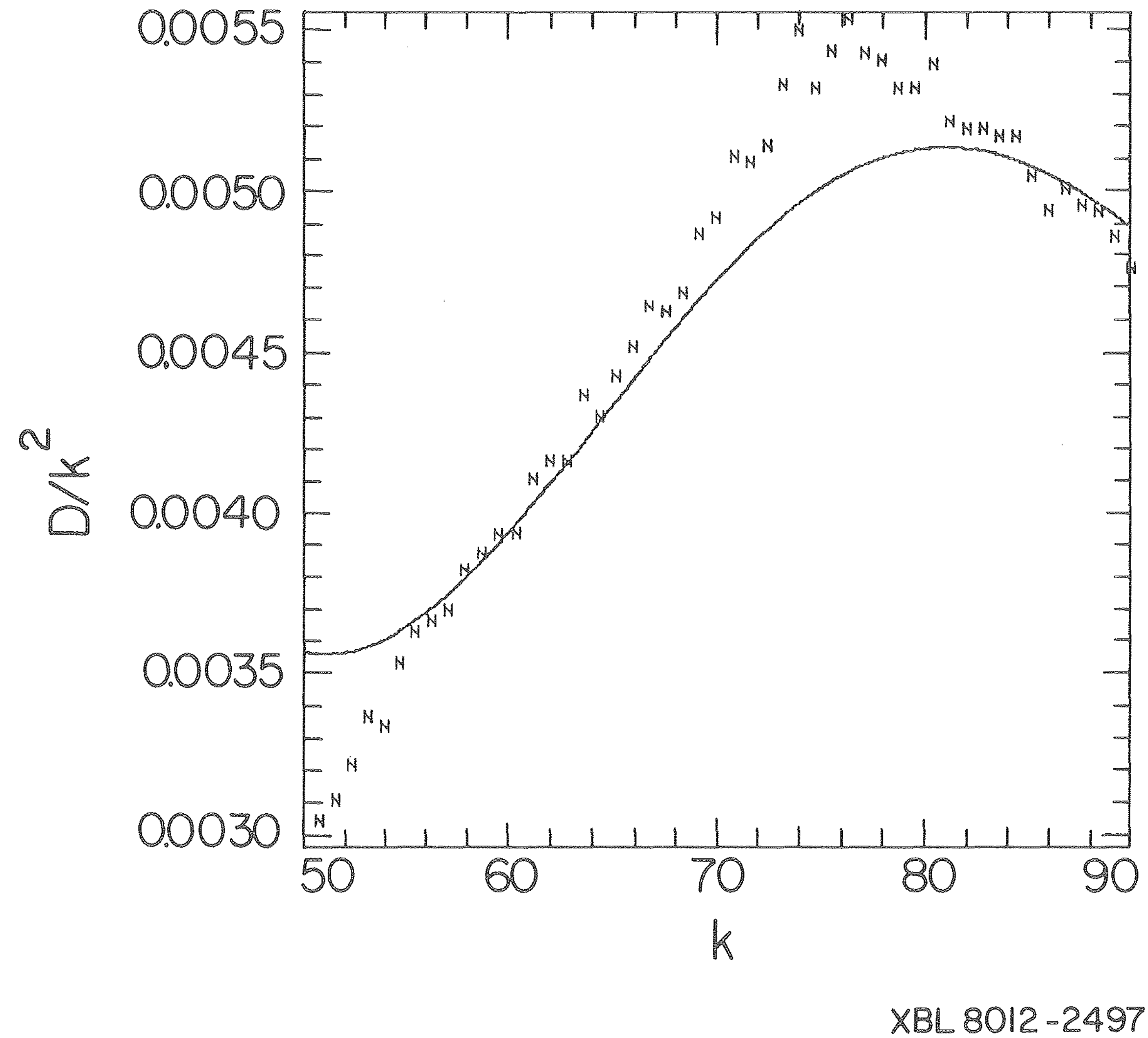
Fig. 7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0.0050
0.0045
0.0040
0.0035
0.0030
D/k^2
50
60
70
80
90
k
XBL 8012-2497

Fig. 8