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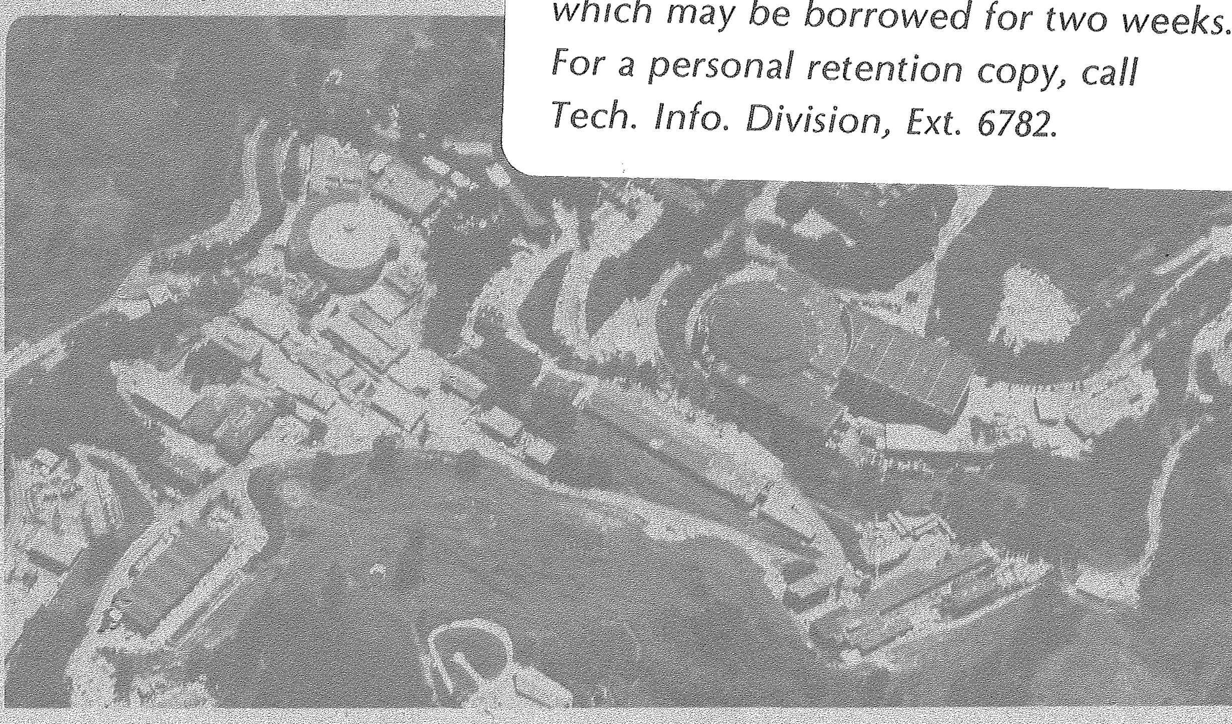

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Diffusion in Very Chaotic Hamiltonian Systems*

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Abstract

We study nonintegrable Hamiltonian dynamics: $H(\underline{I},\underline{\theta}) = H_0(\underline{I}) + kH_1(\underline{I},\underline{\theta})$, for large k;that is,far from integrability. An integral representation is given for the conditional probability $P(\underline{I},\underline{\theta},t|\underline{I}_0,\underline{\theta}_0,t_0)$ that the system is at $\underline{I},\underline{\theta}$ at t, given it was at $\underline{I}_0,\underline{\theta}_0$ at t_0. By discretizing time into steps of size ε ,we show how to evatuate physical observables for large k, fixed ε . An explicit calculation of a diffusion coefficient in a two degree of freedom problem is reported. Passage to ε = 0, the original Hamiltonian flow, is discussed.

In this note we study Hamiltonian systems which are very far from integrable. For action ($\underset{\sim}{I}$), angle ($\underset{\sim}{\theta}$) canonical co-ordinates we are interested in Hamiltonians of the form

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

when k is large. The small k behavior of the motion generated by (1) has been extensively studied in perturbation theory. We are interested here in the opposite limit where one encounters complicated, irregular motion.[1]

Our central tool is the conditional probability $P(\underset{\sim}{z},t|\underset{\sim}{w},t_0)$ that the system is at $\underset{\sim}{z} = (\underset{\sim}{I},\underset{\sim}{\theta})$ at t given it resided at $\underset{\sim}{w} = (\underset{\sim}{I}_0,\underset{\sim}{\theta}_0)$ at t_0. The motion arising from (1) is, of course, deterministic, but we expect the irregular behavior at large k to be describable by probabilistic ideas such as diffusion. The use of the conditional probability to discuss this <u>intrinsic stochasticity</u> is quite appropriate.

The conditional probability satisfies Liouville's equation[2]

$$\left(\frac{\partial}{\partial t} + \sum_j \left[\frac{\partial H}{\partial I_j}\frac{\partial}{\partial \theta_j} - \frac{\partial H}{\partial \theta_j}\frac{\partial}{\partial I_j}\right]\right) P(\underset{\sim}{z},t|\underset{\sim}{w},t_0) = 0 \tag{2}$$

with the initial condition

$$P(\underset{\sim}{z},t_0|\underset{\sim}{w},t_0) = \delta(\underset{\sim}{z}-\underset{\sim}{w}). \tag{3}$$

The general solution to this is given in terms of the solution to Hamilton's equations of motion, $\underset{\sim}{X}(\underset{\sim}{w},t)$, which at t=0 satisfies $\underset{\sim}{X}(\underset{\sim}{w},0) = \underset{\sim}{w}$. We have

$$P(\underset{\sim}{z},t|\underset{\sim}{w},t_0) = \delta(\underset{\sim}{z} - \underset{\sim}{X}(\underset{\sim}{w},t-t_0)). \tag{4}$$

If we split the interval t_0 to t into N segments of length ε, $t - t_0 = N\varepsilon$, we may repeatedly use the property of a conditional probability

$$P(\underset{\sim}{z},t|\underset{\sim}{w},t_0) = \int d\underset{\sim}{z}'\, P(\underset{\sim}{z},t|\underset{\sim}{z}',t')\, P(\underset{\sim}{z}',t'|\underset{\sim}{w},t_0) \tag{5}$$

to write

$$P(\underset{\sim}{z},t|\underset{\sim}{w},t_0) = \int \prod_{\ell=0}^{N} d\underset{\sim}{x}(\ell)\,\delta(\underset{\sim}{x}(0)-\underset{\sim}{w})\,\delta(\underset{\sim}{x}(N)-\underset{\sim}{z}) \times \tag{6}$$

$$\times \prod_{s=1}^{N} P(\underset{\sim}{x}(s), t_s = t_0 + s\varepsilon \,|\, \underset{\sim}{x}(s-1), t_{s-1} = t_0 + (s-1)\varepsilon).$$

We require,then, the elementary conditional probability

$$P(\underset{\sim}{x}(s), t_s \,|\, \underset{\sim}{x}(s-1), t_{s-1}) = \delta(\underset{\sim}{x}(s) - \underset{\sim}{X}(\underset{\sim}{x}(s-1),\varepsilon)). \tag{7}$$

Now we must discretize the equations of motion

$$\frac{d\underset{\sim}{X}}{dt}(\underset{\sim}{w},t) = \underset{\sim}{B}(\underset{\sim}{X}(\underset{\sim}{w},t)), \tag{8}$$

which we do in the form

$$\frac{1}{\varepsilon}\left[\underset{\sim}{X}(\underset{\sim}{w},t_s) - \underset{\sim}{X}(\underset{\sim}{w},t_{s-1})\right] = \underset{\sim}{B}(\underset{\sim}{X}(\underset{\sim}{w},t_{s-1})) \tag{9}$$

leading to

$$P(\underset{\sim}{z},t|\underset{\sim}{w},t_0) = \int \prod_{\ell=0}^{N} d\underset{\sim}{x}(\ell)\,\delta(\underset{\sim}{x}(0)-\underset{\sim}{w})\,\delta(\underset{\sim}{x}(N)-\underset{\sim}{z}) \times$$

$$\times \prod_{s=1}^{N} \delta(\underset{\sim}{x}(s) - \underset{\sim}{x}(s-1) - \varepsilon\,\underset{\sim}{B}(\underset{\sim}{x}(s-1))). \tag{10}$$

In the case of Hamiltonian dynamics coming from(1), we take for the discretized equations of motion the phase space volume preserving mapping

$$\underset{\sim}{I}(n) = \underset{\sim}{I}(n-1) + \varepsilon k\,\underset{\sim}{h}(\underset{\sim}{I}(n),\underset{\sim}{\theta}(n-1)), \tag{11}$$

$$\underset{\sim}{\theta}(n) = \underset{\sim}{\theta}(n-1) + \varepsilon\,\underset{\sim}{\omega}(\underset{\sim}{I}(n)) + \varepsilon k\,\underset{\sim}{h}'(\underset{\sim}{I}(n),\underset{\sim}{\theta}(n-1)), \tag{12}$$

where $\underset{\sim}{I}(t_n)$, $\underset{\sim}{\theta}(t_n)$ are written as $\underset{\sim}{I}(n)$ and $\underset{\sim}{\theta}(n)$, $\underset{\sim}{\omega} = \partial H_0/\partial\underset{\sim}{I}$, $\underset{\sim}{h} = -\partial H_1/\partial\underset{\sim}{\theta}$, $h' = \partial H_1/\partial\underset{\sim}{I}$. The conditional probability $P(\underset{\sim}{I},\underset{\sim}{\theta},t|\underset{\sim}{I}_0,\underset{\sim}{\theta}_0,t_0)$ follows directly from (10). In the limit $\varepsilon\to 0$,we return to the actual Hamiltonian flow, and (10) becomes

$$P(\underset{\sim}{I},\underset{\sim}{\theta},t|\underset{\sim}{I}_0,\underset{\sim}{\theta}_0,t_0) =$$

$$\int \prod_{\tau} d\underset{\sim}{J}(\tau)\, d\underset{\sim}{\chi}(\tau)\, \delta(\underset{\sim}{J}(t_0)-\underset{\sim}{I}_0)\, \delta(\underset{\sim}{J}(t)-\underset{\sim}{I})\, \delta(\underset{\sim}{\chi}(t_0)-\underset{\sim}{\theta}_0)\, \delta(\underset{\sim}{\chi}(t)-\underset{\sim}{\theta})$$

$$\times\, \delta\left(\dot{\underset{\sim}{J}}(\tau) - k\, \underset{\sim}{h}(\underset{\sim}{J}(\tau), \underset{\sim}{\chi}(\tau))\right) \delta\left(\dot{\underset{\sim}{\chi}}(\tau) - \underset{\sim}{\omega}(\underset{\sim}{J}(\tau)) - k\, \underset{\sim}{h}'(\underset{\sim}{J}(\tau), \underset{\sim}{\chi}(\tau))\right), \tag{13}$$

up to an overall normalization factor. This functional integral representation has been given earlier.[3]

Our goal is to utilize (10) to study physical properties of our Hamiltonian dynamics at fixed ε for large k, and then we use this information to extrapolate back to $\varepsilon = 0$. We proceed by representing each $\delta(\underset{\sim}{\chi}(s) - \underset{\sim}{\chi}(s-1) - \varepsilon \underset{\sim}{B}(\underset{\sim}{\chi}(s-1)))$ in (10) by a <u>fourier series</u>. For the delta functions representing evolution in the angle variables, this is quite natural since each $\underset{\sim}{\theta}(t_s) = (\theta_1(t_s), \theta_2(t_s), \cdots)$ lies in $0 \le \theta_a(t_s) \le 1$. For the actions to remain in a finite interval, we require that the energy surface $H(\underset{\sim}{I}, \underset{\sim}{\theta})$ = constant--on which the orbits lie, be bounded. Then if any I_a appears in H with maximum power p, the values of $I_a(t_s)$ lie more or less in the range $0 \le |I_a(t_s)| \le |E|^{1/p}$. Thus, on the energy shell, each $I_a(t_s)$ takes values in some finite interval. Denoting the length of this interval by L_{as}, we write (13) as

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

$$\times\, \delta(\underset{\sim}{J}(N) - \underset{\sim}{I})\, \delta(\underset{\sim}{\chi}(N) - \underset{\sim}{\theta}) \prod_{s=1}^{N} \Big\{ \sum_{\underset{\sim}{\ell}_s=-\infty}^{+\infty} \exp 2\pi i\, \underset{\sim}{\ell}_s \cdot [\underset{\sim}{\chi}(s) - \underset{\sim}{\chi}(s-1) -$$

$$- \varepsilon \underset{\sim}{\omega}(\underset{\sim}{J}(s)) - \varepsilon k\, \underset{\sim}{h}'(\underset{\sim}{J}(s), \underset{\sim}{\chi}(s-1))] \times \prod_a \frac{1}{L_{as}} \sum_{m_{as}=-\infty}^{+\infty} \exp \frac{2\pi i}{L_{as}} m_{as}$$

$$[J_a(s) - J_a(s-1) - \varepsilon k\, h_a(\underset{\sim}{J}(s), \underset{\sim}{\chi}(s-1))] \Big\}, \tag{14}$$

where $\underset{\sim}{\ell}_s$ is a vector of integers.

To evaluate $P(\underset{\sim}{I}, \underset{\sim}{\theta}, t \mid \underset{\sim}{I}_0, \underset{\sim}{\theta}_0, t_0)$ for <u>large</u> k, <u>fixed</u> ε, we choose that combination of ℓ_{as} and m_{as} values which result in the smallest number of oscillating integrands of the form exp ik(functions of $\underset{\sim}{J}(s)$ and $\underset{\sim}{\chi}(s)$). This smallest number will be zero, resulting from the choice $\ell_{as} = m_{as} = 0$. Then we can arrange to have the next smallest number of oscillating integrands by judicious choice of ℓ_s and m_s. If this number is n_1, then corrections to the leading term will be (oscillating function of k)/ $k^{n_1/2}$ which we derive from the stationary phase approximation. After that we go on to $n_2 > n_1$ oscillating integrands, then $n_3 > n_2$, etc., so deriving an asymptotic series for $P(z,t|w,t_0)$.

We illustrate these general remarks by the Hamiltonian with two degrees of freedom

$$H(I,\theta) = \frac{I_1^2 + I_2^2 + I_1 I_2}{2} + \frac{k}{2\pi}\Big[\cos 2\pi\theta_1 + \rho\cos 2\pi\theta_2\Big] , \tag{15}$$

which has a bounded energy surface and for small k always has overlapping resonances[4.] in the physical region. By the surface of section method[1.] we have numerically concluded that for $\rho \neq 0$, the motion generated by (15) is non-integrable. In Figure 1 we show the I_1, θ_1 plane at $\theta_2 = 0$ for $\rho = 1.0, k/2\pi = 110$.

Using the technique outlined above we evaluated the diffusion coefficient defined by ($t = t_0 + N\varepsilon$)

$$D(I_0,k) \equiv \lim_{N\to\infty} \frac{1}{2N} \left\langle (I(N) - I_0)^2 \right\rangle_{\theta_0} \tag{16}$$

$$= \lim_{N\to\infty} \frac{1}{2N} \int dI\, d\theta\, d\theta_0\, P(I,\theta,t|I_0,\theta_0,t_0)\,(I - I_0)^2 \tag{17}$$

$$= \lim_{N\to\infty} \frac{1}{2N} \int_0^1 \prod_{\ell=0}^{N} d^2\chi(\ell)\; \varepsilon^2 k^2 \left(\sum_{r=0}^{N-1} h(\theta(r))\right)^2 \times \prod_{s=1}^{N} \sum_{\ell_s=-\infty}^{+\infty} \exp 2\pi i\, \ell_s\cdot\Big[\chi(s)-\chi(s-1)-\varepsilon\,\omega\Big(I_0+\varepsilon k\sum_{r=0}^{s-1} h(\theta(r))\Big)\Big]. \tag{18}$$

The leading terms in D are ($\varkappa = 2\pi\varepsilon^2 k$)

$$D(I_0,k) \underset{\substack{k\ \text{large}\\ \varepsilon,\rho\ \text{fixed}}}{\sim} \frac{\varepsilon^2 k^2}{2}\Big\{\frac{1+\rho^2}{2} - \Big[J_2(\varkappa)\,J_0(\varkappa\rho/2) + \rho^2 J_2(\varkappa\rho)\,J_0(\varkappa/2)\Big] +$$

$$+ J_0\left(\frac{\varkappa\rho}{2}\right)^2 \left[J_2(\varkappa)^2 + J_3(\varkappa)^2 - J_1(\varkappa)^2 \right] + \tag{19}$$

$$+ \rho^2 J_0(\varkappa/2)^2 \left[J_2(\varkappa\rho)^2 + J_3(\varkappa\rho)^2 - J_1(\varkappa\rho)^2 \right] + \cdots \Big\},$$

where $J_\ell(z)$ is the ordinary Bessel function. For $\rho = 0$ the discretized volume preserving mapping arising from the Hamiltonian (15) is the Chirikov standard mapping[4.] with parameter $\varkappa$. Indeed, for $\rho = 0$, (19) reduces to the results of Rechester and White[5.] including a correction, the $J_2(\varkappa)^2$ term, pointed out by R. Cohen[6.]. It is important to note that our derivation of $D(\underset{\sim}{I}_0,k)$ contains no assumed randomness added to the Hamiltonian equations of motion. A non-zero diffusion coefficient arises from the intrinsic stochasticity of the motion. (External random forcing can be incorporated into our representation for $P(\underset{\sim}{z},t \mid \underset{\sim}{w},t_0)$ in a straightforward fashion. This will be discussed by us in the near future.[7.]) In Figure 2 we compare the asymptotic form (19) for $\rho = 1.0$ to a direct numerical evaluation of $D(\underset{\sim}{I}_0,k)$ from its definition (16).

Returning to the original flow, namely $\varepsilon = 0$, is accomplished by the following observations. When $\varepsilon \to 0$, we require the diffusion coefficient $\hat{D}(\underset{\sim}{I}_0,k)$ given by

$$\hat{D}(\underset{\sim}{I}_0,k) \equiv \lim_{N\varepsilon\to\infty} \frac{\left\langle (\underset{\sim}{I}(N\varepsilon) - \underset{\sim}{I}_0)^2 \right\rangle_{\underset{\sim}{\theta}_0}}{2N\varepsilon}. \tag{20}$$

From (19) we see this has the form

$$\hat{D}(\underset{\sim}{I}_0,k) = k^{3/2}\,\mathcal{D}(y,\rho), \tag{21}$$

with $y = \varkappa^{-1}$ and $\mathcal{D}$ a dimensionless function. We have evaluated $\mathcal{D}(y,\rho)$ as a series in y near $y = 0$, and require its value at $y = \infty$. The standard techniques for making such an extrapolation[8.] need knowledge of a large number of terms in the series we have begun in (19). The result of determining these terms and carrying out the desired extrapolation will yield $D = k^{3/2}\hat{\mathcal{D}}(\rho)$,

$\tilde{\mathcal{D}}$ dimensionless. This work will be reported in another paper. We note here only the change in k dependence from the diffusion of actions in the mapping.

Our general technique has provided us with a tool for learning the behavior of physical quantities in the limit where the Hamiltonian,Equation (1), is very non-integrable. Most interesting among these physical quantities are those, like our diffusion coefficient, which characterize the intrinsic stochasticity of the chaotic orbits of the system. These are not amenable to calculation by perturbation theory in k; they must vanish in every order since diffusion or intrinsic stochasticity is not a small k phenomenon. Passage to the original flow from our discretized phase space volume preserving mapping requires some labor and may be subtle; still our results find direct application to mappings known to accurately approximate a physical flow. Finally by use of these methods one may hope to learn much about more complicated intrinsically stochastic motions,such a fluid turbulence at large Reynolds' number with no artificial external forcing or externally imposed random boundary or initial conditions.

References

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Figure Captions

Figure 1 Surface of section plot for an orbit generated by our Hamiltonian, Equation (15). We show the I_1, θ_1 plane for $\theta_2 = 0$. The initial conditions were $I_1(0) = 3.0$, $I_2(0) = 1.0$, $\theta_1(0) = 0.743$, and $\theta_2(0) = 0.0$. The parameters k and ρ were $k/2\pi = 110$ and $\rho = 1.0$.

Figure 2 D/k^2 from the asymptotic form of (19) compared to the numerical evaluation (points labeled by N) for $10 \leq k \leq 50$, $\rho = 1.0$, $\varepsilon = 0.5$. In this plot $\kappa = 2\pi\varepsilon^2 k$ has the range $15.7 \leq \kappa \leq 78.5$. The deviation of the numerical results from the analytic form is less than 4% and is consistent with the relatively small number of initial values of θ_0 - 96 in each angle.

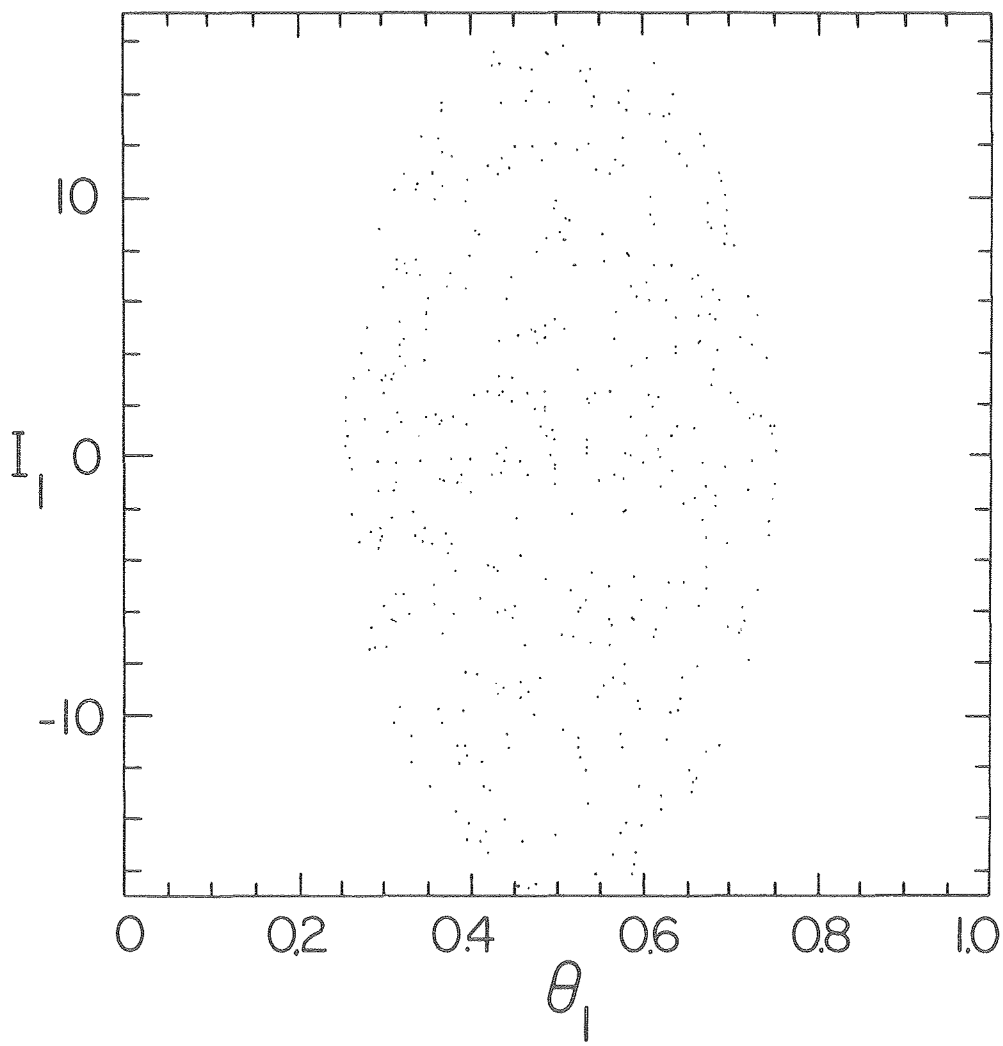

Fig. 1

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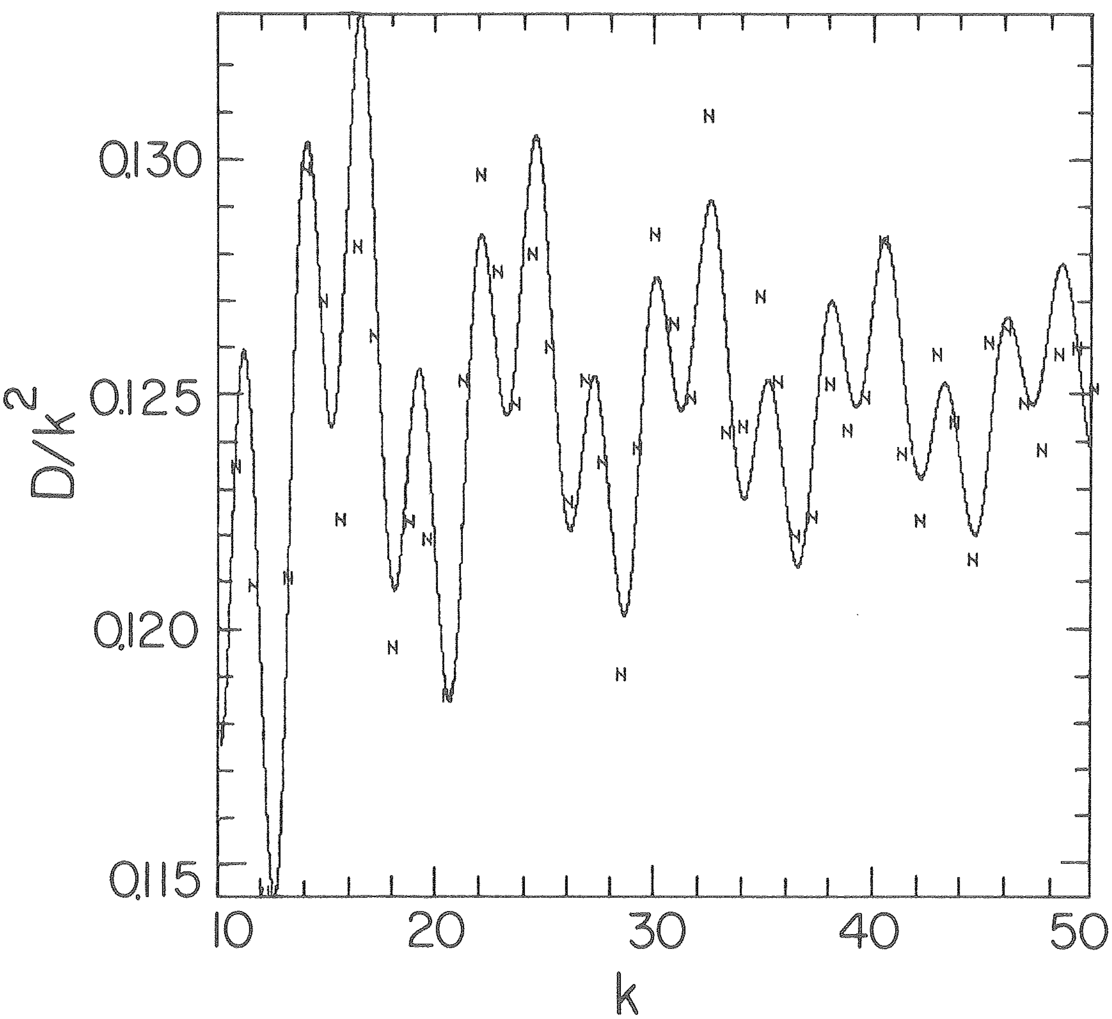

Fig. 2

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