CHAOS AND QUANTUM DYNAMICS OF SIMPLE MODELS

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Abstract

We discuss the manifestations of classical chaotic behaviour in quantum mechanics. We show that, typically, quantum mechanics introduces strong limitations to chaotic motion. In particular we discuss the problem of excitation and ionization of an hydrogen atom under a monochromatic, linearly polarized, electric field and predict new results which can be tested in laboratory experiments.

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Chaos in classical Hamiltonian systems is today a widely studied subject. It is connected with the appearance of strong local instability of orbits, which leads to a rapid loss of memory and calls for statistical description [1]. Motion in the chaotic regime exhibits truly stochastic features and is unpredictable in a well defined sense. For this reason, chaos is often referred to as "self-generated stochasticity", in order to stress that unpredictability, and other stochastic features, are not due to the introduction of external random disturbances into the system.

In particular, self-generated stochasticity is a very common occurrence in Hamiltonian systems subject to time-periodic perturbations; indeed, in macroscopic systems of this type, chaos is directly responsible for easily observable, and often undesirable effects.

In this paper we will be concerned with the problem, whether any such effect survive in Quantum Mechanics also. This is a very important question, as we shall now explain.

Atoms and molecules in external electromagnetic fields are often described by time-periodic Hamiltonians, and, upon investigating the classical mechanics of these models, one often realizes that, for sufficiently high fields, a transition to chaos occurs. Then, an unlimited diffusion in phase space takes place, eventually leading to ionization of atoms or to dissociation of molecules; this classical mechanism of ionization/dissociation is also a very efficient one.

On the other hand, quantum mechanics is the appropriate description for microphysical systems such as atoms or molecules. Therefore, the question about persistence of chaotic or at least diffusive effects in quantum dynamics is a crucial one, whose answer affects the actual phenomenology of atoms and molecules in external electromagnetic fields.

An integrable Hamiltonian system subject to an external periodic perturbation is described by an Hamiltonian

$$H(\mathbf{I}, \boldsymbol{\varphi}, t) = H_0(\mathbf{I}) + \epsilon\, V(\mathbf{I}, \boldsymbol{\varphi}, t) \qquad (1)$$

where $V(\mathbf{I}, \boldsymbol{\varphi}, t)$ is periodic in $\boldsymbol{\varphi}$ and t with periods 2π and T respectively, and $\mathbf{I}$, $\boldsymbol{\varphi}$ are action-angle variables for the unperturbed system described by the Hamiltonian H_0.

As specific examples, we will consider the "δ-kicked rotator"[2]:

$$H(I, \varphi, t) = I^2/2 + \epsilon \cos\varphi \sum_n \delta\,(t-nT) \qquad (2)$$

and the one-dimensional model for a hydrogen atom in a monochromatic electric field[3]:

$$H(I, \varphi, t) = -1/2I^2 + \epsilon\, x(I,\varphi) \cos \omega t; \qquad \omega = 2\pi/T;\ x > 0. \tag{3}$$

Here, $x(I, \varphi)$ is the x coordinate of the electron, expressed as a function of action-angle variables of the unperturbed atom.

Model (3) has a direct physical relevance, in that it can be used to study the effect of a microwave field on a hydrogen atom initially prepared in an "extended" state. The use of the one-dimensional approximation (3) proves theoretically and experimentally justified for such initial states [3].

Instead, model (2) has no such immediate physical meaning. Nevertheless, it is a particularly convenient one in order to analyze the transition to chaos; indeed, by studying this model, an insight on the effect of quantization on dynamical chaos was gotten, which proved very useful for model (3) also.

Both classical systems (2) and (3) exhibit a transition to chaos when the coupling parameter ϵ exceeds some "stochasticity threshold", that can be estimated by means of Chirikov's resonance overlapping criterion[4] .

For model (2), this transition occurs for

$$\epsilon T > 1 \tag{4}$$

Above this threshold, motion is more conveniently described in statistical terms. Specifically, considering an ensemble of trajectories leaving with a fixed value I_0 of the action and with randomly distributed phases φ, one finds that the distribution function $f(I, t)$ in action space is well approximated by the solution of the Fokker- Planck equation:

$$\partial f(I, t)/\partial t = 1/2\ D\ \partial^2 f(I,t)/\partial I^2$$

with $D \approx \epsilon^2/2T$ and with the initial condition $f(I,0) = \delta(I-I_0)$.

In particular, the rotator kinetic energy increases linearly with time, according to the law $\overline{\Delta I^2} \approx Dt$.

For model (3), trajectories leaving from initial states with $I=n_0$ undergo a stochastic transition for[5]

$$\epsilon_0 > \epsilon_s = 1/(50\omega_0^{1/3}); \quad \epsilon_0 = \epsilon n_0^4 ; \quad \omega_0 = \omega n_0^3 . \qquad (5)$$

The motion in the stochastic regime can again be described by a Fokker-Planck equation:

$$\partial f/\partial t = 1/2\ \partial/\partial I\ (D(I)\partial f/\partial I\ ) \ . \qquad (6)$$

Here the diffusion coefficient D(I) depends on the action I:
$D(I) \approx \pi^{-1}\epsilon^2 I^3 \omega^{-4/3}$. A quite remarkable feature of the diffusion ruled by eq.(6) is that the moment $\langle I\rangle = \int I f(I, t)dI$ grows to infinity -i.e., the atom ionizes - in a finite time $t_1 \approx 2\omega^{4/3}/(\epsilon^2 n_0)$.

Let's now quantize models (2) and (3). In both cases we get Schroedinger equations of type

$$i\ \partial\psi/\partial t = H_0\ \Psi + \epsilon\ V(t)\Psi \qquad (7)$$

with V(t) an operator depending periodically on time.

A particularly convenient way to study equations of this type is introducing the Floquet operator $S = U(0,T)$ where U(s,s+t) is the unitary operator which gives the evolution of states ψ over the time t according to $\psi(t+s) = U(s,s+t)\psi(s)$. Indeed, in order to analyze the long-time behaviour of the solutions of eq.(7), it is sufficient to study the iterates S^n of this Floquet operator[6].

A first qualitative classification of various types of behaviour that solutions of (7) can show is provided by the nature of the quasi-energy spectrum, which is by definition the spectrum of the self-adjoint operator G such that $S = \exp(iG)$. As a matter of fact, in both models (2) and (3) the unperturbed Hamiltonian H_0 possesses a discrete spectral component, and one is interested in the time evolution of states initially coinciding with some unperturbed eigenstate. Then, it can be shown[6] that a continuous quasi-energy spectrum would enforce an indefinite spreading of such wave packets over the unperturbed spectrum. Instead, a pure point quasi-energy spectrum would be associated with a recurrent behaviour of the wave packets.

In the rotator case (model (2)) it was found that the nature of the quasi-energy spectrum depends in a sensitive way on the value of the period T. If T is a rational multiple of 4π, then the spectrum of the Floquet operator S possesses an (absolutely) continuous component,

which causes the spread of the wave packet over the unperturbed eigenstates $\langle n^2 \rangle$ (which in this case is proportional to the kinetic energy of the rotator) to increase with time according to an asymptotic t^2 law. This phenomenon is known as quantum resonance and cannot be understood in classical terms; its appearance in model (2) is due to the particular nature of the unperturbed spectrum of this model[7].

When $T/4\pi$ is irrational, numerical experiments provide evidence that, in most cases, the quasi-energy spectrum is pure point. Far from spreading indefinitely, the wave packet remains localized in momentum space. Thus, even in the semiclassical regime ($\epsilon >> 1, T << 1$) and for such parameter values that the classical rotator is chaotic ($\epsilon T >> 1$) the quantum rotator does not reproduce the classical diffusive increase of $\langle n^2 \rangle$, except for a more or less extended, but anyway finite, time scale t_B, after which $\langle n^2 \rangle$ enters a seemingly steady-state oscillatory regime.

However, even though localization seems to be a fairly typical occurrence for irrational $T/4\pi$, we were able to prove[8] that a dense set of irrational $T/4\pi$ values exists, yielding a continuous quasi-energy spectrum. It is not yet clear whether this continuous nonresonant spectrum has any physical relevance, nor it is clear whether it is possible to observe it also in different models where the unperturbed spectrum is pure point.

On account of numerical and theoretical analysis, these values of the period look somewhat exceptional. Therefore, despite the intriguing character of the spectral problem, our basic question about the persistence of chaos in quantum mechanics must be answered in the negative for model (2). The typical picture for the quantum rotator in the classically chaotic regime is the following: wave packets initially concentrated on a single unperturbed eigenstate start spreading in momentum space, but after a certain "*break-time*" t_B, quantum interference effects become dominant, which prevent further spreading. Then, the average number of unperturbed eigenstates significantly excited by the wave packet evolution, setttles to a stationary value, which is called localization length and provides also a measure for the number of unperturbed eigenstates significantly excited by one single quasi-energy eigenstate.

In the semiclassical region a simple estimate can be given for both the localization length and the break time. We now sketch this estimation since the idea behind it is basic also to our present understanding of the quantum model (3).

Before the time t_B, the spread Δn of the wave packet over the unperturbed levels (quantized actions $I = n$) will grow in time, following to some extent the law $\Delta n = \Delta n(t)$ that is predicted by the Fokker Planck equation that rules classical diffusion. However, this diffusive growth will stop, because the discrete character of the quasi-energy spectrum will eventually become manifest; the time t_B necessary for this can be assumed to be $t_B \approx \alpha N$, with α a constant and N the number of q.e. eigenstates significantly excited by the single initial unperturbed eigenstate. In fact, $2\pi/N$ is just the average spacing of q.e. eigenvalues significantly contributing in the wave packet evolution. Then we can reasonably assume that N also measures the number of unpertubed eigenstates spanned by a single q.e. eigenstate, i.e., $N \sim l$ (the localization length). On the other hand, the latter coincides in order of magnitude with $\Delta n(t_B)$; thus we get an equation for t_B:

$$\alpha \Delta n(t_B) \approx t_B$$

In the rotator case, classical diffusion obeys $(\Delta n(t))^2 \approx Dt$, whence it follows that $t_B \approx \alpha^2 D$. Numerical experiments support very well this estimate, provided that the value $\alpha \approx 1$ is chosen.

Now we come to the hydrogen atom model (3). Here the question about the nature of the quasi-energy spectrum is clearer; indeed, it is known that the q.e. spectrum is absolutely continuous[10]. This means that, unlike the classical atom, the quantum atom will eventually ionize, no matter how small ϵ. The corresponding ionization mechanism, however, at least for small ϵ has nothing to do with the classical chaotic phenomenon, and involves very long time scales. From the mathematical point of view, this entails that identifying the nature of the q.e. spectrum is not enough for answering the question of the existence of "quantum chaos". Indeed, this question calls for the analysis of time evolution of wave packets over the time scale in which quantum and classical evolution may be expected to agree to some extent.

In the present case, the short time behaviour of the atom is dominated by resonances (in the sense of scattering theory). In other words, the q.e. spectrum is absolutely continuous, but there are poles of the resolvent operator lying very close to the real axis[10]. For practical purposes, it can still be assumed that the q.e. spectrum has a pure point component, in which each level has a small width.

Therefore, we can expect that the same mechanism which leads to quantum localization of the classical dynamical chaos in the rotator case will be working here, too. There is an essential difference, however; indeed, if it is possible to choose such parameter values that the quantum $\Delta n(t)$ follows the classical diffusion for a time larger than the classical chaotic ionization time, then we may expect "diffusive" ionization also in the quantum case. Conditions for this delocalization phenomenon can be easily derived; in fact, the break time can be estimated by the same procedure outlined above for the rotator case - the difference being that here the appropriate Fokker-Planck equation (6) must be used. In this way we find that delocalization will occur for[9]

$$\epsilon_0 \geq \epsilon_s \quad , \qquad \epsilon_0 \geq \epsilon_q = \omega_0^{7/6}/\sqrt{(6n_0)} \tag{8}$$

A remarkable fact is that in order to obtain the estimate (8) for the *delocalization border*, the parameter α was taken ≈ 1 just like in the rotator case. The good agreement of (8) with numerical results implies that, however particular, the rotator model still retains features that have some generality in problems about quantization of chaotic systems.

Like in the rotator case, the model (3) was the object of extensive numerical investigations, which fully confirm the main result of the above discussion[9]. Namely, three distinct quantum regimes can be observed according to the particular choice of ϵ_0, ω_0 and of the initial state n_0 . If ϵ_0 lies below both the classical stochasticity border ϵ_s and the delocalization border ϵ_q , then both the classical and the quantum model will exhibit localization in action space; this is the case of fig. 1, where $\omega_0 = 1.5$, $n_0 = 100$, $\epsilon_0 = .01$ and where the quantum and classical distributions over unperturbed actions are shown after 120 periods of the external field.

If ϵ_0 lies in between the thresholds ϵ_s and ϵ_q , we observe classical chaotic motion and quantum localization; here the classical atom would ionize diffusively, but the quantum one does not. (Fig. 2: $n_0 = 100$, $\omega_0 = 1.5$, $\epsilon_0 = .03$, distributions after 480 periods). In Fig. 3 we show the comparison of classical and quantum probability of excitation above $n = 1.5\, n_0$, as functions of time. Quantum localization of classical chaos is here quite evident.

Finally, if ϵ_0 exceeds both thresholds, we observe a qualitative agreement between classical and quantum results (Fig. 4, $n_0 = 100$, $\omega_0 = 1.5$, $\epsilon_0 = .15$). Here a quantum ionization mechanism is at work, that

cannot be understood in terms of standard perturbation theory. Indeed, this mechanism is effective at much lower frequencies than those ($\omega_0 > n_0/2$)-predicted by the pertubative theory of the photoelectric effect.

To summarize, for the model (3) of a 1-dimensional hydrogen atom in a microwave field it is possible to observe a memory of the classical chaotic motion, surviving in the quantum domain, which manifests in a diffusive mechanism of ionization of the atom.

On these grounds, we can predict a photoionization effect occuring at much lower frequencies than usually expected, that should be observable in actually feasible laboratory experiments.

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FIGURES CAPTION.

Fig.1 Classical(-)and quantum(-) distribution function $\bar{\Gamma}_n$ averaged over 40 values of $\tau=\omega t/(2\pi)$ within the interval $80<\tau<120$. Here $\omega_0=1.5$, $\epsilon_0=.01$, $n_0=100$. For these parameters value, both classical and quantum packets are localized. Notice the small quantum tunneling through the classical Kolmogorov invariant curves.

Fig.2 Same as Fig. 1 but with $\epsilon_0=.03$. The classical (-) and quantum (-)distribution functions are averaged over 40 values of τ within the interval $440<\tau<480$. In this case $\epsilon_s < \epsilon_0 < \epsilon_q$, and the quantum packet is localized as expected (besides a small resonant plateau).On the contrary, the classical packet is strongly diffusing as it is also shown in fig. 3.

Fig.3 Classical(1) and quantum(2) total probability $W_{n>1.5n_0}$ above level $n=1.5n_0$ for the case of fig.2. The classical ionization probability is order of magnitudes higher than the quantum one(fig.3a). The comparison of the two ionization probabilities for short times is shown in fig. 3b.

Fig.4 Same as fig.1 but with $\epsilon_0=.15$. Here, the classical (-) and quantum (-) distribution functions are averaged over 40 values of τ within the interval $0<\tau<40$. In this case $\epsilon_0>\epsilon_q$ and both classical and quantum motion obey a diffusion law given by Fokker-Planck equation. The dotted line gives the solution of the Fokker Planck equation.

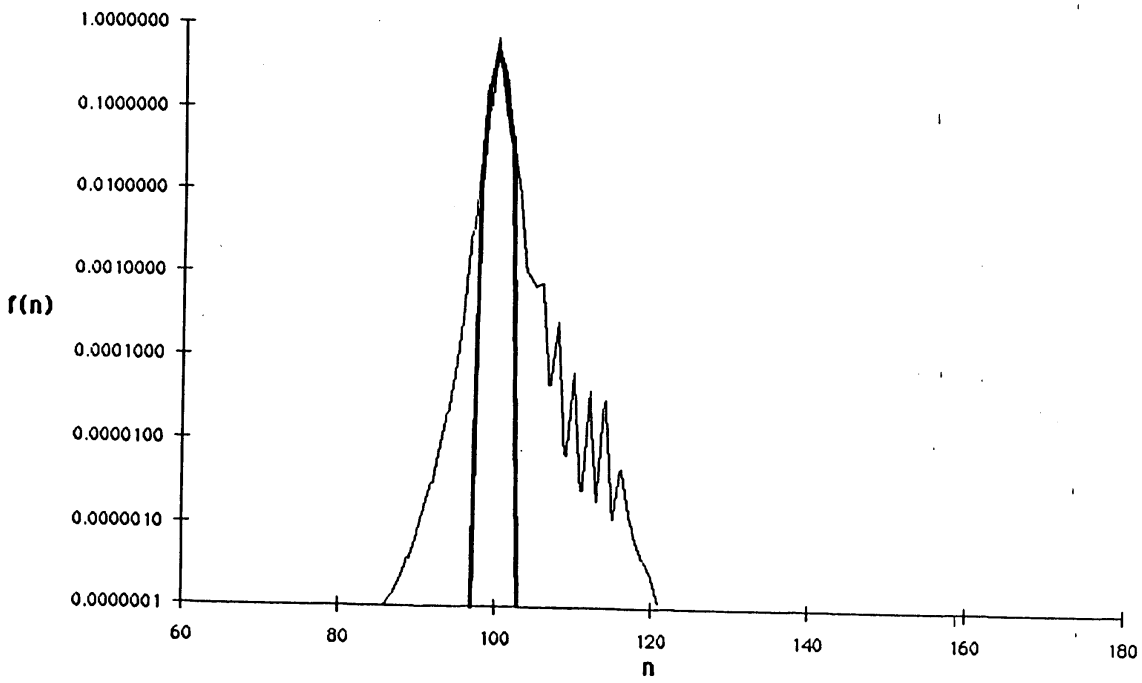
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FIG. 1

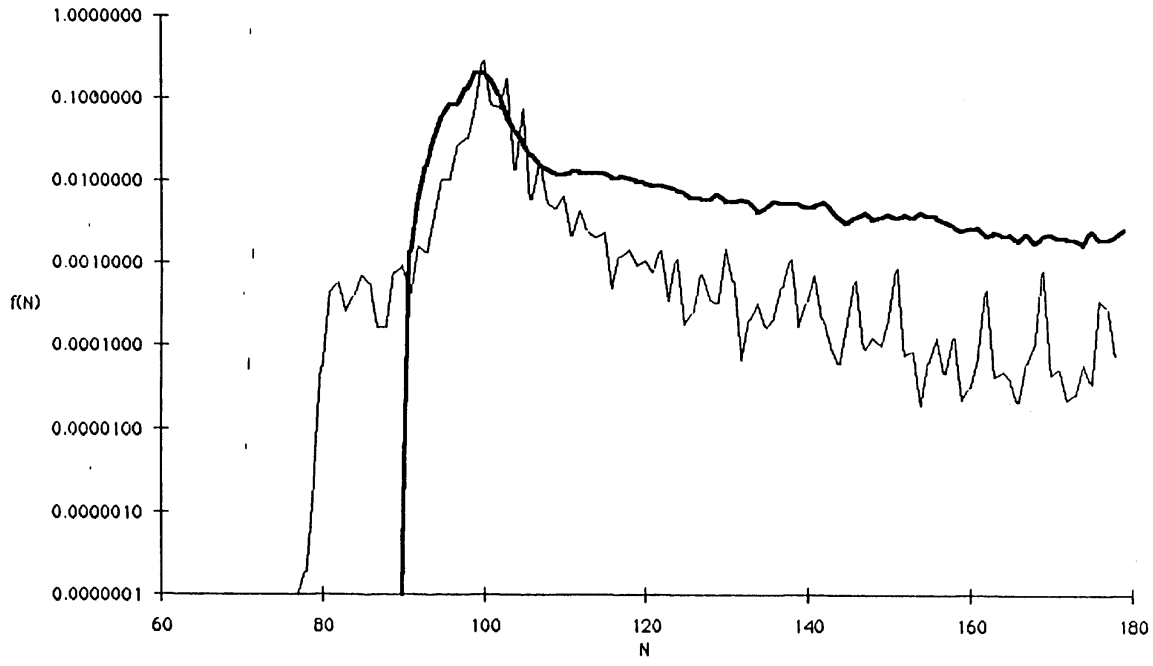
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FIG 2

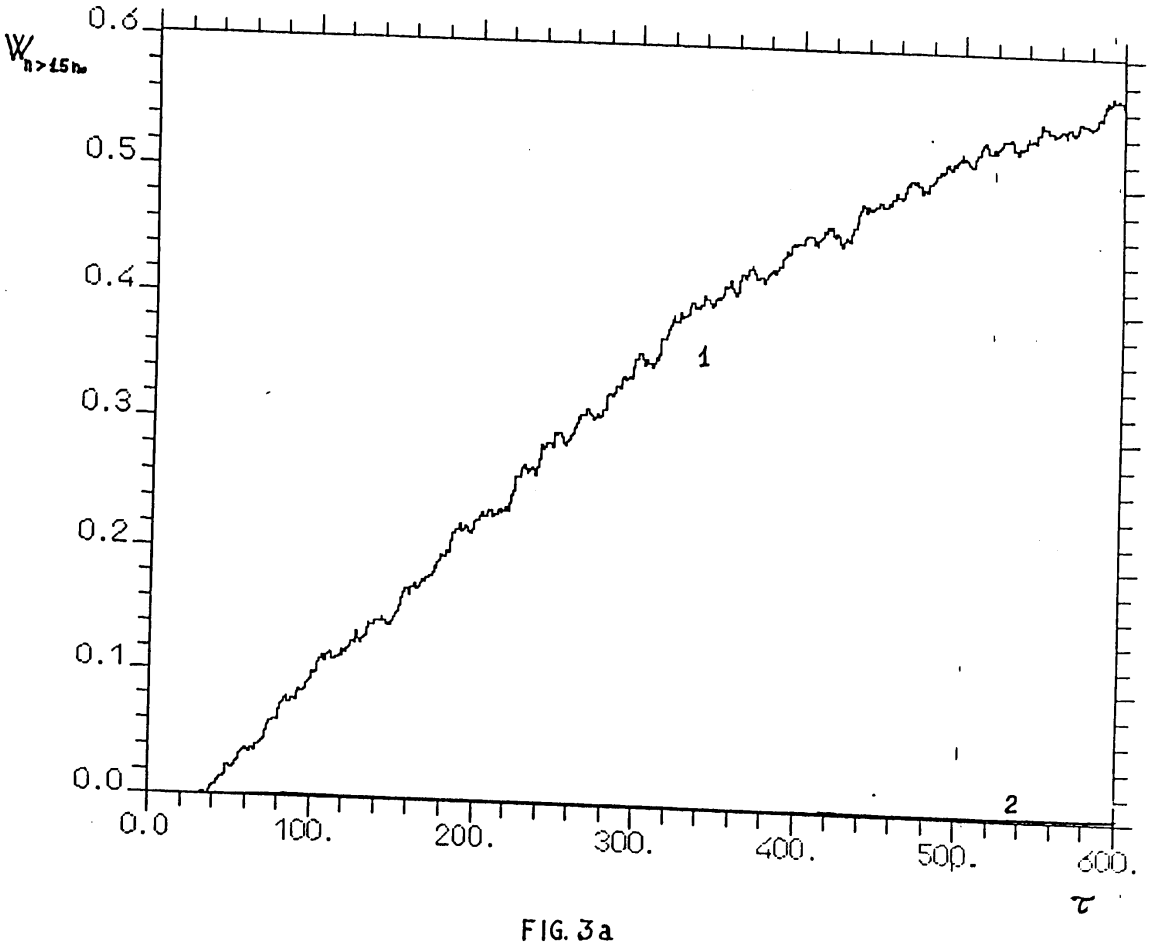

FIG. 3a

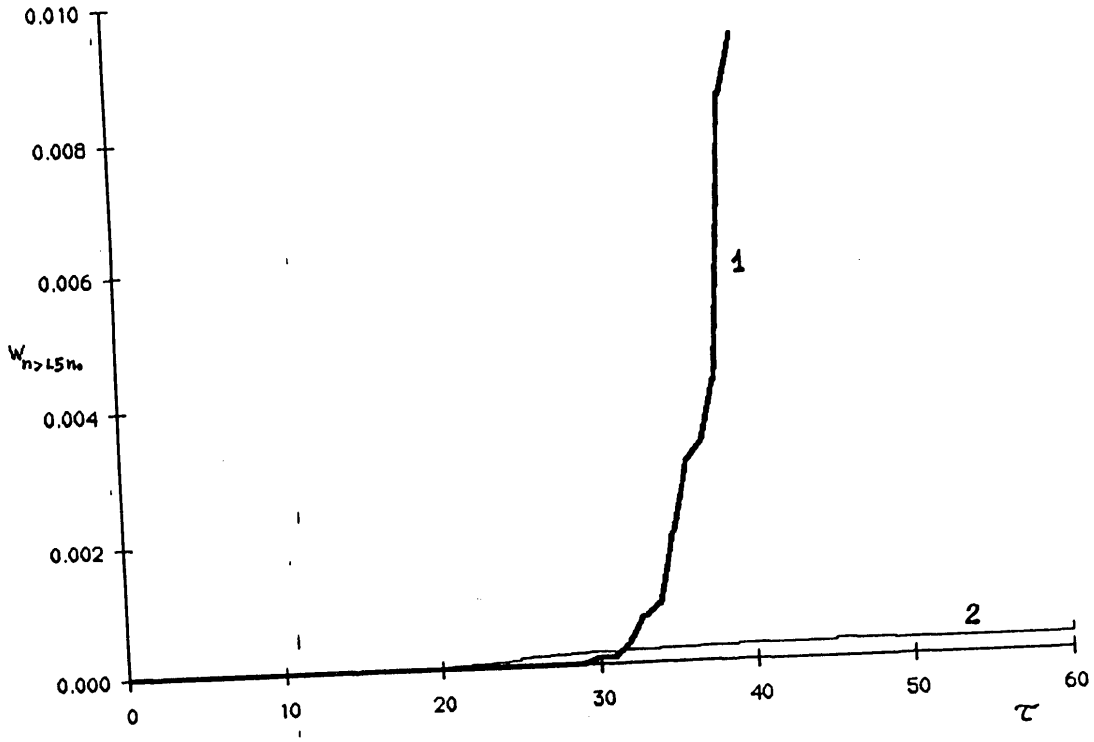

FIG. 3b

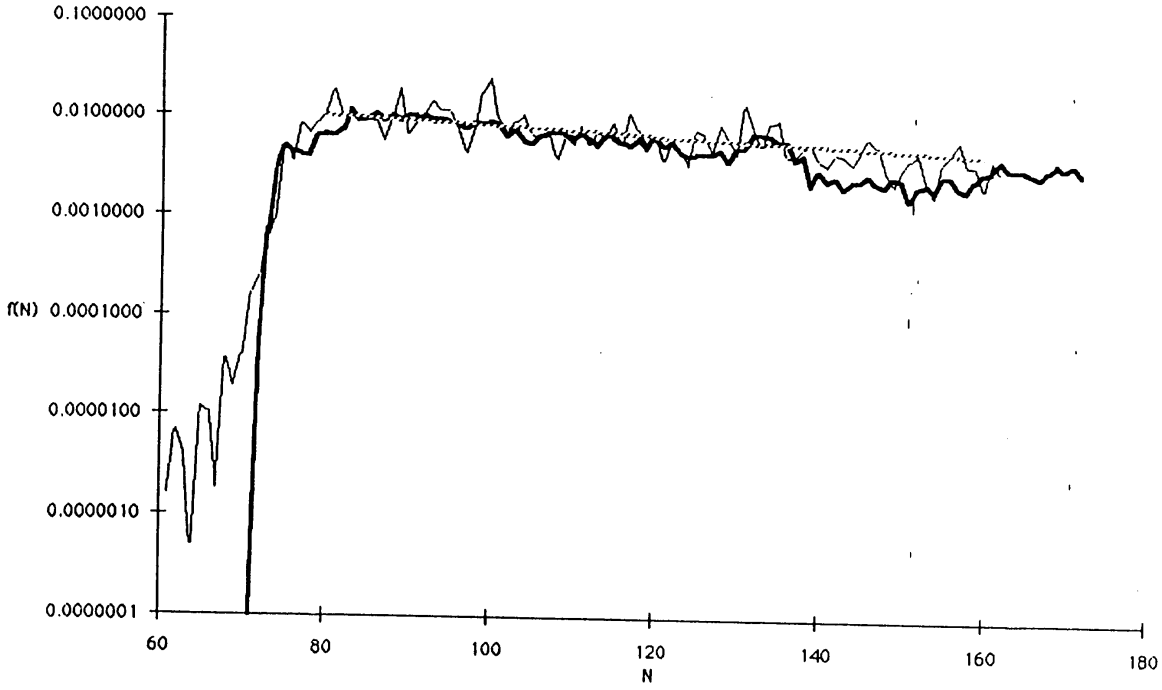
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FIG 4