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CHAOS IN CLASSICAL NONLINEAR FIELDS

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Summary

Chaos in Classical Nonlinear Fields

We studied chaotic behavior in a high-dimensional periodic lattice version of the classical Hamiltonian phi-four field theory. Both single and double well potentials were considered. We examined the existence of a global stochasticity threshold that varied with energy and initial conditions. The model was discretized using an algorithm due to Hirota that guarantees stability and energy conservation. Chaotic behavior was diagnosed using the Lyapunov exponent, with additional information from space-time profiles, Fourier power spectra, and phase space plots. We found long time scales which made it difficult to distinguish between asymptotically chaotic and integrable behavior.

1. Background and Motivation

The importance of understanding infinite (or high) dimensional nonlinear systems is clear: we are surrounded by fluids, plasmas, solids and other continuous (or very high dimensional) systems whose behavior is critical to us. In some cases, when dissipation is present, the long-time behavior of such systems may be adequately described by low dimensional models. But for Hamiltonian systems with no asymptotic description on attractors possible, and where regular and chaotic regions can be strongly intermixed, we usually must seek understanding and intuition in a different way.

Another reason for the importance of high dimensional Hamiltonian systems is their relevance to basic questions in statistical mechanics, including the nature of the approach to equilibrium and the equipartition of energy. Recent equipartition studies[1] in large Hamiltonian systems containing no *a priori* natural time scale, suggest that very long times are necessary for some modes to reach equilibrium.

In the present work we studied a non-integrable classical Hamiltonian field theory, the ϕ^4 model (which will be described below). This arises physically as a useful simple model in condensed matter systems (e.g., polyacetylene, ferroelectrics) and elementary particle physics. But its basic significance, for our purposes, is as an example of a nearly-integrable, high-dimensional, nonlinear Hamiltonian system.

Our working hypothesis was that chaotic behavior is to be expected in a non-integrable system for some values of the parameters and types of initial conditions. We expect that at sufficiently high energy (or energy density) global stochasticity will occur in both the single- and double-well potentials, with the two cases being rather similar in the high energy regime. Since only the double well allows solitary wave (and near-breather) solutions, we expected the low energy behavior of the two models to be rather different.

Previous numerical studies[2] have found conflicting results, some finding no chaos or chaotic behavior which appears as the energy (or energy density) increases and then disappears at higher energies. How the partial differential equation is discretized, what initial conditions are considered, choice of lattice parameters, and especially the length of integration times are expected to be crucial to the results.

2. The ϕ^4 Model

The Lagrangian and Hamiltonian densities of the (one space dimensional) ϕ^4 field theory are:

$$\mathcal{L} = \frac{1}{2}\left(\frac{\partial\phi}{\partial t}\right)^2 - \frac{1}{2}\left(\frac{\partial\phi}{\partial x}\right)^2 + V(\phi)$$
$$\mathcal{H} = \frac{1}{2}p^2 + \frac{1}{2}\left(\frac{\partial\phi}{\partial x}\right)^2 + V(\phi)$$

where

$$p = \frac{\partial\phi}{\partial t}, \qquad V(\phi) = \frac{1}{2}\mu\phi^2 + \frac{1}{4}\lambda\phi^4$$

The equation of motion for this potential is

$$\frac{\partial^2\phi}{\partial t^2} - \frac{\partial^2\phi}{\partial x^2} + \mu\phi + \lambda\phi^3 = 0$$

This model can be regarded as a truncation of the exactly-integrable sine-Gordon ($\mu < 0$) and sinh-Gordon ($\mu > 0$) equations. With $\mu < 0$, $V(\phi)$ is a double-well potential (leading to spontaneous symmetry breaking in the corresponding quantum field theory); the classical theory then allows solitary wave solutions.

It is possible to remove the ϕ^2 and ϕ^4 coefficients in $V(\phi)$ by scaling x, t, and ϕ :

$$x \to |\mu|^{-1/2}x$$
$$t \to |\mu|^{-1/2}t$$
$$\phi \to \left(\frac{|\mu|}{\lambda}\right)^{1/2}\phi$$

Thus the equation of motion can always be written in the form

$$\phi_{tt} - \phi_{xx} \pm \phi + \phi^3 = 0 \qquad \left(\phi_t \equiv \frac{\partial\phi}{\partial t}\text{, etc.}\right) \tag{1}$$

In this form we see that the only parameters which can be varied are the total energy and sign of the quadratic term in the potential (corresponding to the single and double well cases). For the lattice version of the model there are additional parameters, the number of lattice points and length of the lattice.

The ϕ^4 model has two known conserved quantities:

$$E = \int \mathcal{H}(x,t)dx \qquad P = -\int \phi_x \phi_t dx$$

The absence of an infinite number of conserved quantities[3] is also supported by studies of ϕ^4 solitary wave scattering which show that the initial kink and antikink shapes need not survive the collision.[4]

3. Progress

This work began as a Master's thesis of D. Bradley-Hutchison,[5] supervised by one of us (HKS). He used a 300 site spatial lattice (with periodic boundary conditions), a lowest order finite difference approximation to the equation of motion, and initial conditions consisting of a sharply peaked static gaussian at the center of the lattice. A simple diagnostic was used to measure the separation of neighboring trajectories in phase space:

$$[D(t)]^2 \equiv \frac{1}{L}\int_0^L dx \left\{ \left[\phi(t) - \bar{\phi}(t)\right]^2 + \left[\phi_t(t) - \bar{\phi}_t(t)\right]^2 \right\}$$

where ϕ and $\bar{\phi}$ are initially infinitesimally close trajectories . For an integrable system we expect $D(t) \sim t$ for large t, while for a chaotic system we expect $\ln D(t) \sim t$ asymptotically.

Bradley-Hutchison studied the separation distance, $D(t)$, as the total energy was varied over the range $43 < E < 1865$. He found that $D(t)$ grows linearly for "low" energies and "short" times, corresponding to typical integrable behavior, and that $\ln D(t)$ grows linearly for "high" energies, corresponding to chaotic behavior. For "moderate" energies, there can be a sudden onset of chaotic behavior after "long" times. In the strongly chaotic cases, "saturation" is generally observed; i.e., $\ln D(t)$ reaches a maximum value at some t value and remains constant thereafter (see Fig. 1).[6]

These preliminary results were interesting enough to warrant a more detailed and sophisticated study. There are two primary components in the calculation: the discretization algorithms for the partial differential equation, eq.[1], and the selection of diagnostics for the spatial-temporal behavior. Ideally we would like to discretize in such a way that any known conserved quantities for the continuous system are preserved, and also in such a way that stability is guaranteed as the spatial and time step sizes are varied in the integration algorithms.

We chose a discretization scheme due to Hirota[7] that guarantees stability and conservation of energy. The discretized Hamiltonian density is

$$\mathcal{H} = \frac{1}{2}\rho^2 + \frac{1}{2}(\Delta_{2x}\phi)^2 + V(\phi).$$

The corresponding first order equations of motion are

$$\begin{aligned} \Delta_t\phi &= \Pi_t\rho \\ \Delta_t\rho &= \Delta_{2x}^2\Pi_t\phi - \Delta_\phi V(\phi)\Big|_t \end{aligned}$$

where the central difference operator, Δ, and averaging operator, Π, are defined as

$$\begin{aligned} \Delta_x f(x) &\equiv \frac{1}{\epsilon}[f(x+\frac{\epsilon}{2}) - f(x-\frac{\epsilon}{2})] \\ \Pi_x f(x) &\equiv \frac{1}{2}[f(x+\frac{\epsilon}{2}) + f(x-\frac{\epsilon}{2})] \end{aligned}$$

with

$$\Delta_{2x} f(x) = \Delta_x\Pi_x f(x)\,, \quad \text{etc.}$$

Combining the first order equations, we obtain

$$\Delta_t^2\phi = \Delta_{2x}^2\Pi_t^2\phi - \Pi_t\Delta_\phi V(\phi)\Big|_t$$

The implicit nature of the Hirota integration algorithm means that in general we must solve a set of coupled nonlinear equations. When the equations are linear, the resulting equations can be solved using techniques for inverting a tridiagonal matrix (modified for the periodic boundary conditions that we are imposing). With the nonlinear terms included in the evolution equations, we use an explicit scheme as an approximation to the nonlinear term and then iterate the inversion until the field becomes self-consistent.

In our work we used a simple measure of chaotic behavior, the maximum Lyapunov exponent, to search for the onset of global stochasticity. This exponent is a function of the linearized equations of motion which are in turn dependent on the full equations of motion. On a discrete lattice, the equations for the field become a set of N coupled oscillators governed by the equations of motion of the form

$$\frac{d\vec{\phi}}{dt} = \vec{F}(\vec{\phi})$$

where $\vec{\phi}$ is a $2N$ dimensional vector, N components are the field and the other N are its time derivative. We linearize the equations of motion about our initial trajectory by introducing the variable $\vec{\Theta}$:

$$\vec{\Theta}(\vec{\phi}_0, t) \equiv \lim_{|\delta\vec{\phi}| \to 0} \frac{\vec{\phi}(\vec{\phi}_0 + \delta\vec{\phi}, t) - \vec{\phi}(\vec{\phi}_0, t)}{|\delta\vec{\phi}|}$$

where $\vec{\phi}_0$ indicates the initial values for the variables. These new variables evolve in time according to the the linear equations

$$\frac{d\Theta_i}{dt} = \sum_j \left. \frac{\partial F_i}{\partial \phi_j} \right|_{\vec{\phi}(\vec{\phi}_0, t)} \Theta_j$$

These time evolution equations for Θ_i are a set of $2N$ coupled ordinary differential equations and were integrated using a fourth order Runge-Kutta algorithm. Finally, the maximum Lyapunov exponent is given by

$$\lambda(\vec{\phi}_0) = \lim_{t \to \infty} \frac{1}{t} \ln \frac{||\vec{\Theta}(\vec{\phi}_0, t)||}{||\vec{\Theta}(\vec{\phi}_0, 0)||}$$

If there is sensitivity to initial conditions, nearby trajectories diverge exponentially and the Lyapunov exponent is positive. For integrable systems the divergence of nearby trajectories is linear and the finite time Lyapunov exponent decreases toward zero as t^{-1}. $D(t)$ and the Lyapunov exponent measure essentially the same property of the system; however the Lyapunov exponent procedure is preferable in that it takes the limit of the initial separation going to zero.

Figures 2-4 show some of our results. In these calculations (performed on the UNH VAX 8820 and the San Diego SDSC CRAY X-MP) we imposed periodic boundary conditions on discrete lattices with 128 or 256 points. Energy was conserved to 6 or 7 digits at each time step. The initial conditions examined to date include static gaussians of varying amplitude centered on the lattice and pure sinusoidal modes.

As a general summary of these runs, we note (for initial static gaussians): (a) there is little dependence of the Lyapunov exponent on the number of lattice points (for N above 100); (b) for energies up to 80 in both the single and double well, we see the Lyapunov exponent decreasing as t^{-1}, indicating non-chaotic behavior; (c) at $E \approx 300$ the Lyapunov exponent approaches a positive constant value, indicating chaos; here the double well has a larger exponent than the single well; (d) for all energies between $E = 300$ and $E = 2600$ the asymptotic t behavior is not yet clear, since the data shows regions of flatness as well as sharp decreases; (e) for high energies (2600 and 17356) the system again has a decreasing Lyapunov exponent. Thus, from our search in energy space with static gaussian initial conditions, it appears that there might be an onset and later disappearance of global stochasticity. The study of this question became the focus of our work at the end of the grant period.

Code development for all the additional useful diagnostics: space-time profiles, power spectra, and phase space plots has also been completed.

In examining the Lyapunov exponents over very long times, we became aware of the sensitivity of our results to the details of the discretization procedure. For this reason it became difficult to be certain if the Lyapunov exponent differed significantly from zero and thus whether the system was chaotic or not. We are currently devising more sophisticated statistical tests to be applied to our Lyapunov exponent data in order to distinguish between zero and non-zero values.

4. Communications and Publications

This grant has resulted in the publication *A Numerical Study of Chaos in the One-Dimensional ϕ^4 Model*, Douglas A. Bradley-Hutchison and Harvey K. Shepard, *Physica Scripta* **40**, 731 (1989), and the presentation of a poster at Dynamics Days Conference, Houston, Texas in January 1989.

5. Partcipating Professionals

Those professionals involved in this work were Harvey Shepard (Professor of Physics), Dawn Meredith (Assistant Professor of Physics), Rob Braswell, and Douglas Bradley-Hutchison (Physics graduate students).

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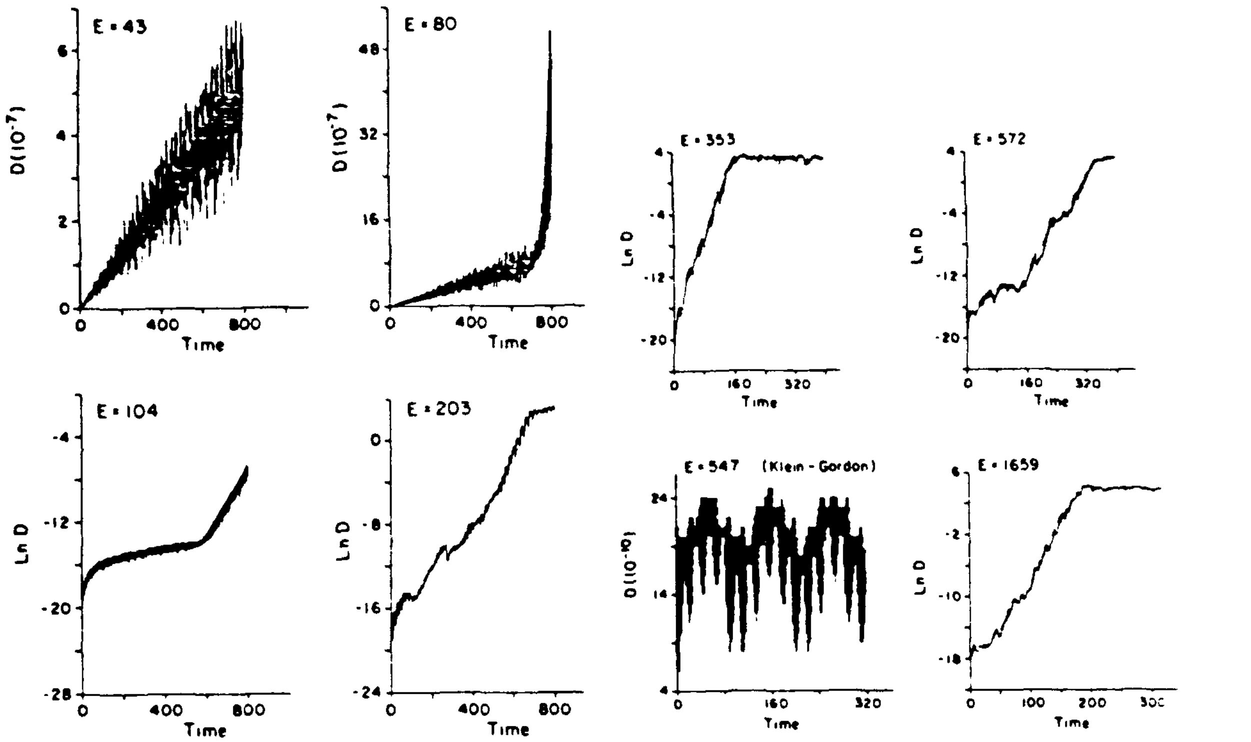
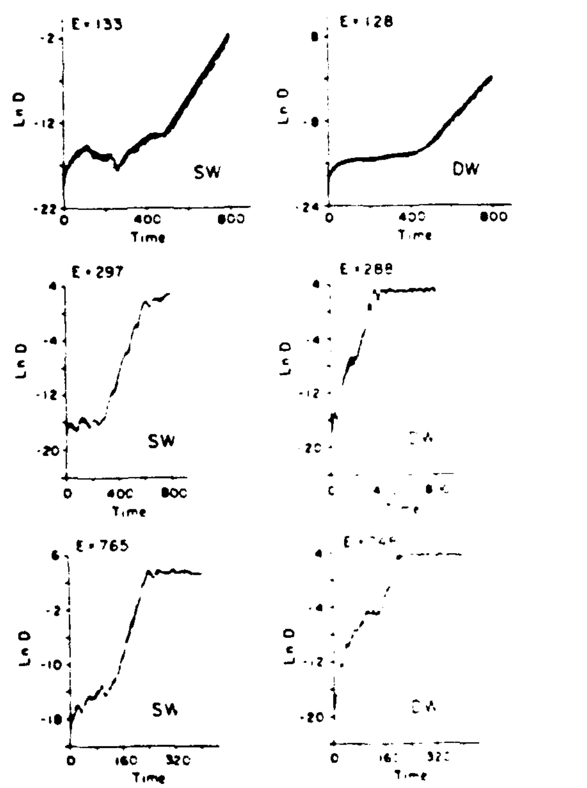
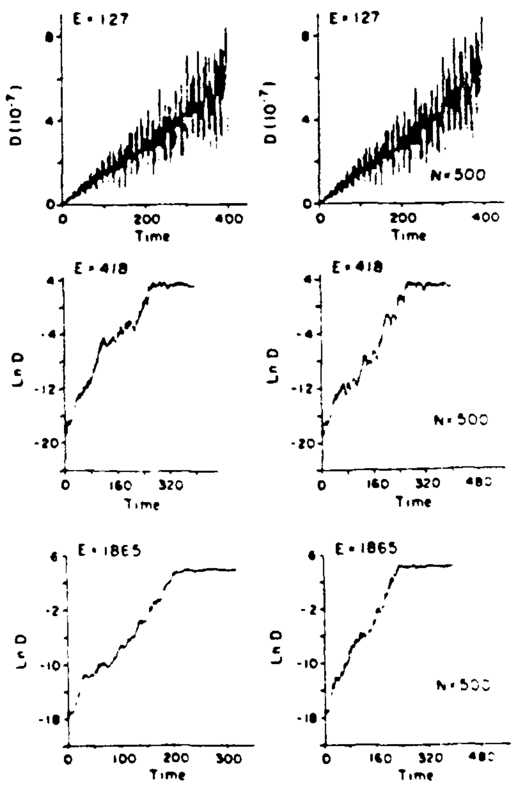


$D(t)$ vs. time for different energy values in the single well potential (b) $D(t)$ vs. time for different energy values. Except for the Klein–Gordon case (see text), the potential is single well

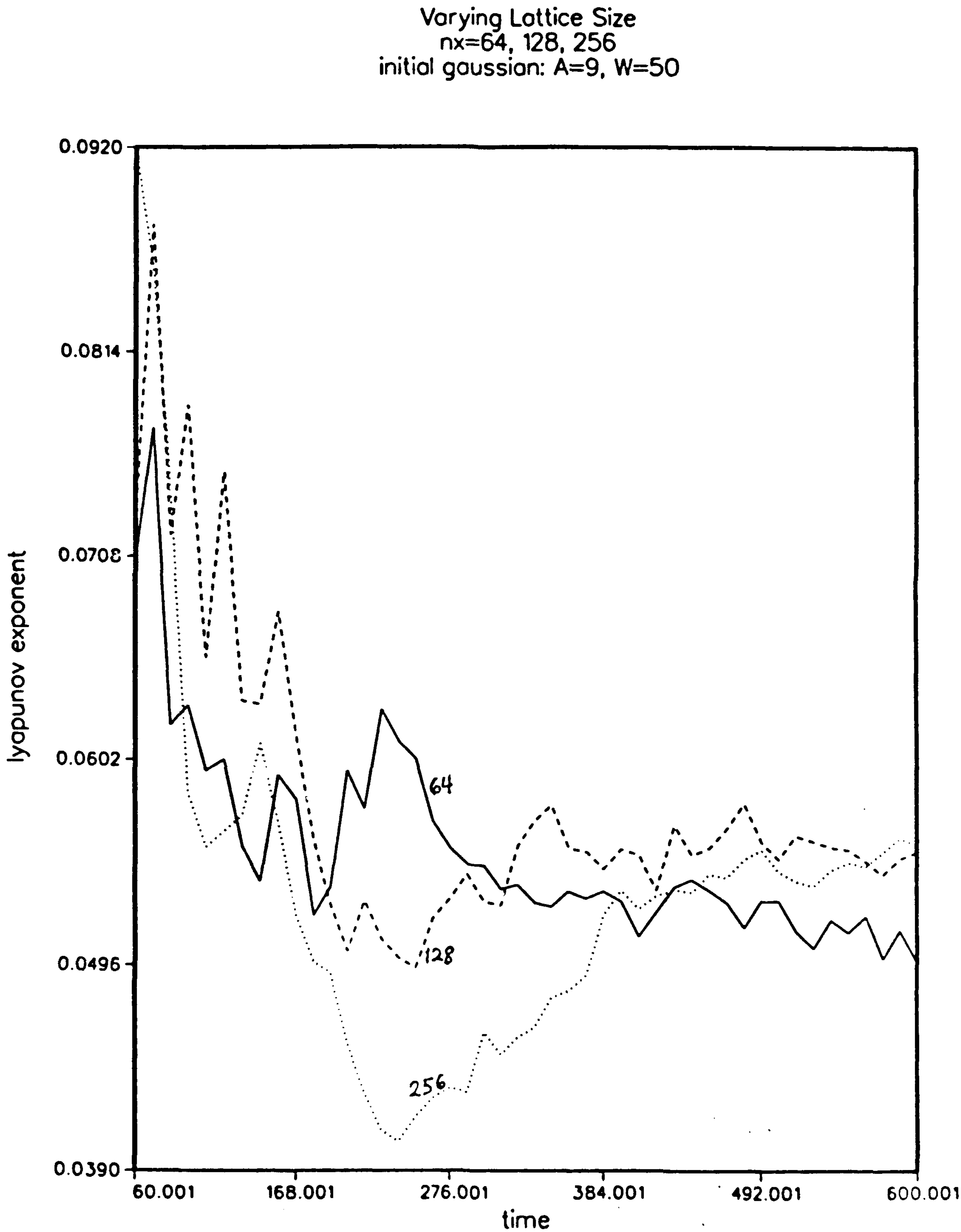


Comparison of $D(t)$ vs. time for the single well (SW) and double well (DW) potential at several energy values



Comparison of $D(t)$ vs. time for two different lattice sizes, N = 300 and N = 500, at several values of the energy

Fig. 1



Varying Lattice Size
nx=64, 128, 256
initial gaussian: A=9, W=50
0.0920
0.0814
0.0708
0.0602
0.0496
0.0390
lyapunov exponent
64
128
256
60.001
168.001
276.001
384.001
492.001
600.001
time

Fig 2

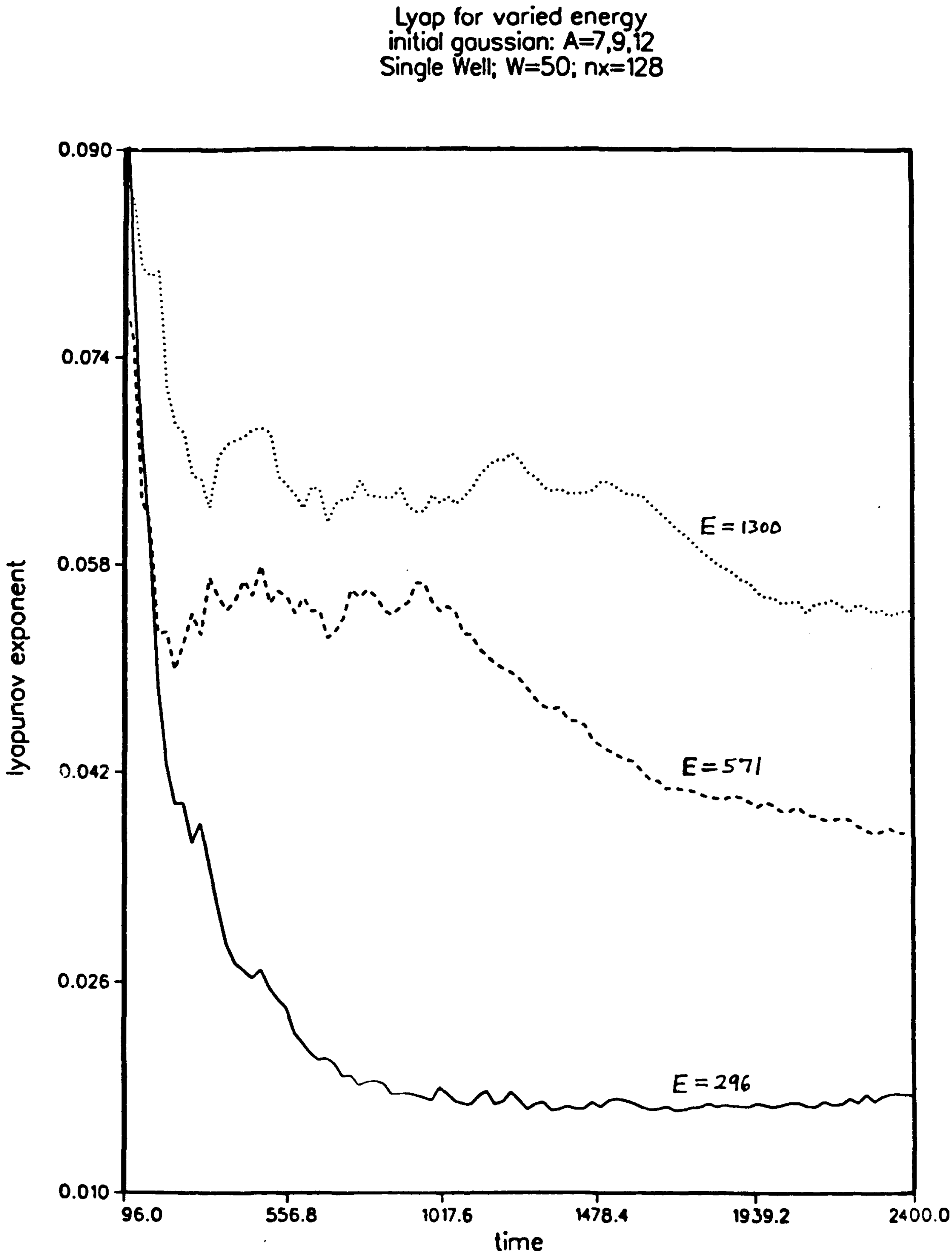

Lyap for varied energy
initial gaussian: A=7,9,12
Single Well; W=50; nx=128
lyapunov exponent
0.090
0.074
0.058
0.042
0.026
0.010
96.0
556.8
1017.6
1478.4
1939.2
2400.0
time
E = 1300
E = 571
E = 296

Figure 3.

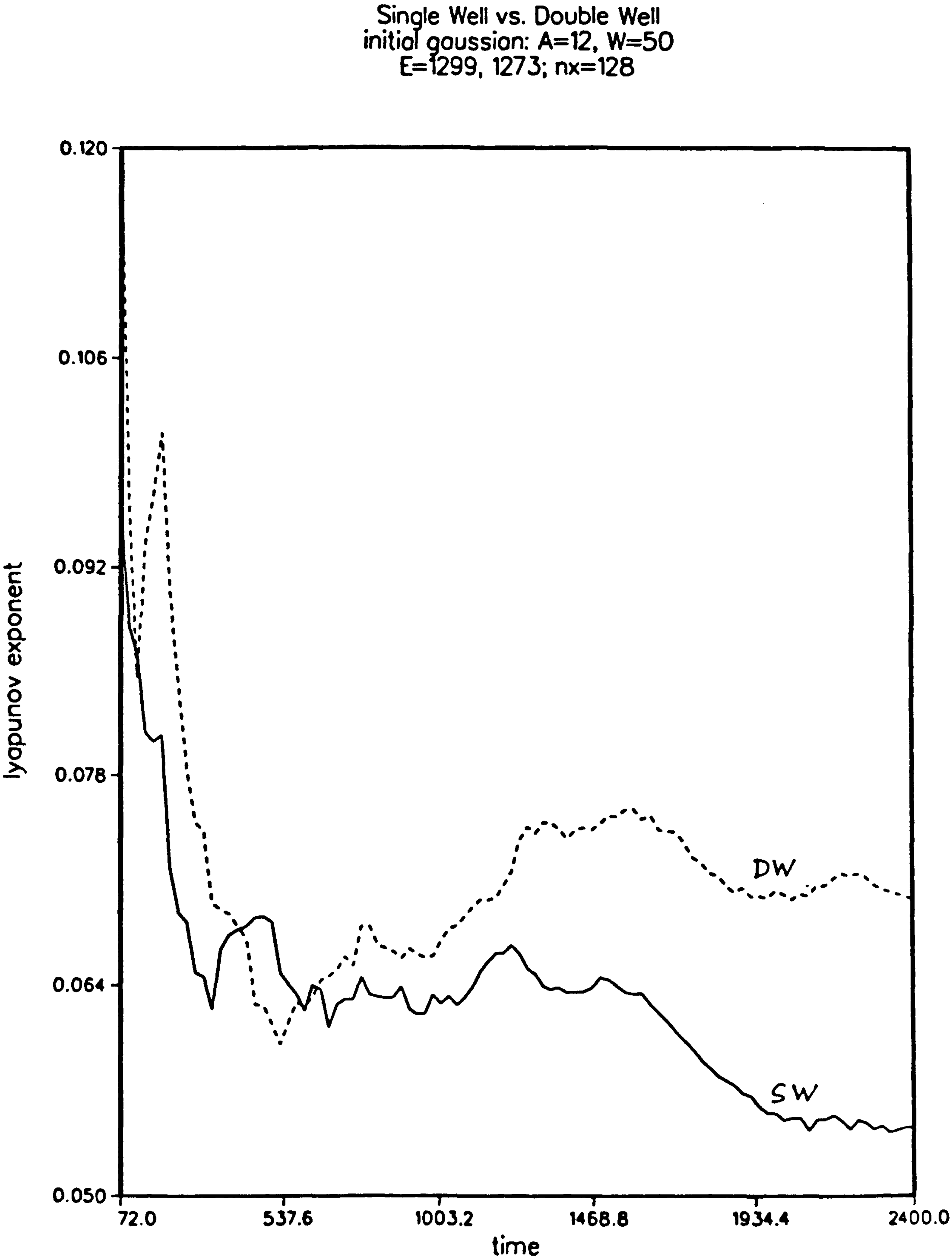

Single Well vs. Double Well
initial gaussian: A=12, W=50
E=1299, 1273; nx=128
0.120
0.106
0.092
0.078
0.064
0.050
lyapunov exponent
72.0
537.6
1003.2
1468.8
1934.4
2400.0
time
DW
SW

Figure 4.