and in its immediate vicinity, Fig. 1, and fit the asymptotic behavior $L(y) \sim y^{\tau}$ for large y. The results do *not* coincide in the periodic regime, Fig. 2, but they could have been made to agree if we had chosen noise amplitudes differing by factors of κ, instead of factors of 100. This more restricted scaling follows from considerations of the type enunciated above.

These results appear to us to be both exciting and highly provocative. A theoretical picture of the transition to turbulence is just beginning to emerge; the analogy to critical phenomena should lead to new and important insights into the nature and characteristics of this transition.

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Scaling Theory for Noisy Period-Doubling Transitions to Chaos

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The effect of noise on systems which undergo period-doubling transitions to chaos is studied. With the aid of nonequilibrium field-theoretic techniques, a correlation-function expression for the Lyapunov parameter (which describes the sensitivity of the system to initial conditions) is derived and shown to satisfy a *scaling theory*. Since these transitions have previously been shown to exhibit *universal behavior*, this theory predicts *universal effects* for the noise. These predictions are in good agreement with numerical experiments.

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During the past few years, the onset of chaotic behavior, after a sequence of period-doubling transitions, has been extensively studied. Feigenbaum[1] has observed that these transition sequences exhibit "universal" features akin to those of phase transitions; Collet and Eckmann[2] have noted that these universal features are shared by differential equations and multidimensional maps in which chaos is preceded by a sequence of period doublings; and Libchaber and Maurer[3] have observed this phenomenon in a convective cell with small aspect ratio. Recently, Huberman and Rudnick[4] have related one of the pretransitional parameters identified by Feigenbaum with the growth of disorder (i.e., the Lyapunov parameter) in the chaotic regime, and Huberman and Crutchfield[5] have examined numerically the effect of external noise on the onset of chaos. Nevertheless, many connections between period-doubling chaotic transitional phenomena and the critical phenomena at second-order phase transitions remain unclear.

The purpose of this Letter is the following: (1) to present a scaling theory (in which "noise" and "stress" play the role of external field and temperature) for systems that become chaotic

via the period-doubling mechanism, and (2) to compare the dependence on noise and stress of the Lyapunov exponent predicted by this theory with numerical experiments performed by Huberman and collaborators.[6] Our results, found by field-theoretic methods designed for nonequilibrium systems, clarify some connections between phase transitions and the onset of chaos. These methods identify the Lyapunov exponent with the "long-time" limit of the nonequilibrium response function introduced by Martin, Siggia, and Rose.[7]

The Lyapunov exponent, λ, describes how solutions that were initially close to one another evolve after a long time (or many steps). Its sign and magnitude provide a measure of the "sensitivity of the system to initial conditions"; a large negative value implies great insensitivity to initial differences, a vanishing value implies that initial differences neither grow nor decay, and a large positive value implies rapid separation and great sensitivity.

Our principal quantitative result is that, at corresponding stress points between successive period doubling transitions, as a function of the noise amplitude, σ, of the noise and the magnitude of the difference between the stress, r, and the stress, r_∞, at which the onset to chaos occurs without noise, the Lyapunov parameter satisfies

$$\lambda(r_\infty - r;\sigma) = (r_\infty - r)^t \Phi((r_\infty - r)^{-t}\sigma^u); \tag{1}$$

with

$$t = (\ln 2)/\ln\delta = 0.4498\ldots \tag{2a}$$

and

$$u = (\ln 2)/\ln\beta \approx 0.34\ldots. \tag{2b}$$

The quantity, $\delta = 4.669\ldots$, is Feigenbaum's universal scaling parameter for functions $f(x)$ with quadratic maxima and β is a scaling parameter, associated with the noise, whose value we have calculated in a second-order approximation to be $\beta \approx 7.7\ldots$.

Let us consider the one-dimensional difference equation

$$x_{m+1} = f_r(x_m) + \xi_m. \tag{3}$$

The dynamical variable x_m ranges over the interval $[-1, 1]$, the function $f_r(x)$ has its maximum value, $f_r(0) = 1$, at $x = 0$, and ξ_m is a Gaussian random variable with $\langle \xi_m \rangle = 0$ and $\langle \xi_m \xi_{m'} \rangle = \sigma^2 \delta_{mm'}$. We analyze this stochastic difference equation, using a discrete version of the path-integral formulation[8] developed for stochastic nonlinear Langevin equations. The average of the functional $F[\{x\}]$ over sequences $\{x\}$ which obey Eq. (3) is given by

$$\langle F[\{x\}]\rangle = Z^{-1}\langle \pi_m \int dy_m\, \delta(y_m - x_m) F[\{y\}]\rangle = Z^{-1}\int [\mathfrak{D}y][\mathfrak{D}s] F[\{y\}]\langle \exp\{i\sum_m s_m[y_{m+1} - f_r(y_m) - \xi_m]\}\rangle$$
$$= Z^{-1}\int [\mathfrak{D}x][\mathfrak{D}s] F[\{y\}] \exp\Omega_r(x, s, \sigma)$$

with

$$\Omega_r(x, s, \sigma) \equiv \sum_m \{is_m[x_{m+1} - f_r(x_m)] - \tfrac{1}{2}\sigma^2 s_m^2\}. \tag{4}$$

Specifically, the correlation function is given by

$$\langle x_m x_{m'}\rangle = Z^{-1}\int [\mathfrak{D}x][\mathfrak{D}s] x_m x_{m'} \exp\Omega_r(x, s, \sigma). \tag{5}$$

We also introduce the Martin-Siggia-Rose response function, $R(r, \sigma; m - m') \equiv i\langle x_m s_{m'}\rangle$,

$$R(r, \sigma; m - m') = Z^{-1}\int [\mathfrak{D}x][\mathfrak{D}s] i x_m s_{m'} \exp\Omega_r(x, s, \sigma) \tag{6}$$

which depends on both x and s, the variable "conjugate" to x, to define the Lyapunov parameter in the presence of noise. Let $X_N(y)$ be the expectation value of x_N in the ensemble with the initial condition $x_0 = y$. We then have for large N

$$\exp(\lambda N) \equiv \lim_{N\to\infty,\,\epsilon\to 0} [X_N(y+\epsilon) - X_N(y)]/\epsilon = Z^{-1}\epsilon^{-1}\int [\mathfrak{D}x][\mathfrak{D}s] x_N \exp\Omega_r(x, s, \sigma)\{\exp[i\epsilon s_0 f_r'(x_0)] - 1\}$$
$$\approx i f_r'(y)\langle x_N s_0\rangle = f_r'(y) R(r, \sigma; N). \tag{7}$$

As observed originally by Feigenbaum, it is sometimes preferable to study the iterated equation which, for weak noise, takes the form

$$x_{m+1} = f_r(x_m; n) + \xi_m' g_r(x_m; n)$$

in terms of the 2^n-th iterate of f_r

$$f_r(x;n) = \underbrace{f_r \circ f_r \circ f_r \circ \cdots \circ f_r}_{2^n \text{ terms}}(x). \tag{8}$$

We call this iterative process "coarse-graining." If $f_r(x) = f_r(x;0)$ has a period-2 limit cycle, then $f_r(x;1)$ has a pair of isolated fixed points; similarly, a four-cycle becomes a pair of two-cycles, etc. As a result of coarse graining, the function $g_r(x;n)$ appears, which, along with $f_r(x;n)$, is assumed to approach a fixed point through the coarse graining and rescaling transformations. Approximate expressions for the scaling variables are obtained by explicitly integrating over every other x_m variable in the functional integral.

With these ideas in mind, let us introduce $\langle\ \rangle_n$ to describe expectations computed at the nth coarse-graining level, i.e.,

$$R(r,\sigma;N;n) \equiv i\langle x_N s_0\rangle_n = Z^{-1}\int[\mathfrak{D}x][\mathfrak{D}s]\, i x_N s_0 \exp\Omega_r(x,s,\sigma;n)$$

with

$$\Omega_r(x,s,\sigma;n) \equiv \sum_m \{ i s_m [x_{m+1} - f_r(x_m;n)] - \tfrac{1}{2}\sigma^2 s_m{}^2 g_r{}^2(x;n)\}. \tag{9}$$

We can also express the Lyapunov parameter in terms of the coarse-grained response function,

$$\exp(\lambda N) = f_r'(y;n) R(r,\sigma;N;n). \tag{10}$$

Note that the quantity $f_r'(y;n)$ is the "stability parameter" for a 2^n-cycle with given r.

To find the desired recursion relations for $f_r(x)$ and $g_r(x)$ we first integrate over every even s_m in the "partition function"

$$Z \equiv N\int[\mathfrak{D}x][\mathfrak{D}s]\exp\Omega_r(x,s,\sigma;n) = N\int_{\text{odd}}[\mathfrak{D}x][\mathfrak{D}s]\exp\bar{\Omega}_r(x,s,\sigma;n)$$

with

$$\bar{\Omega}_r(x,s,\sigma;n) \equiv \sum_{\text{odd } m}\{ i s_m [x_{m+1} - f_r(x_m;n)] - \tfrac{1}{2}\sigma^2 s_m{}^2 g_r{}^2(x_m;n)\} - \tfrac{1}{2}\sigma^{-2}\sum_{\text{even } m}\{ g_r{}^{-2}(x_m;n)[x_{m+1} - f_r(x_m;n)]^2\}. \tag{11}$$

We next calculate the x_m integrals for odd values of m in the saddle-point approximation, obtaining

$$Z = N\int_{\text{even}}[\mathfrak{D}x]\int_{\text{odd}}[\mathfrak{D}s]\exp\Omega_r'(x,s,\sigma;n)$$

with

$$\Omega_r'(x,s,\sigma;n) \equiv \sum_{\text{odd } m}\{ i s_m [x_{m+1} - f_r(f_r(x_{m-1};n);n)] - \tfrac{1}{2}\sigma^2 s_m{}^2 [g_r{}^2(f_r(x_{m-1};n);n) + f_r'{}^2(f_r(x_{m-1};n);n) g_r{}^2(x_{m-1};n)]. \tag{12}$$

Equation (12) leads to the coarse-graining recursion relations,

$$f_r(x;n+1) = f_r(f_r(x;n);n), \quad g_r{}^2(x;n+1) = f_r'{}^2(f_r(x;n);n) g_r{}^2(x;n) + g_r{}^2(f_r(x;n);n). \tag{13}$$

Rescaling Eq. (13) by

$$x_m' = -\alpha^{-1} x_{2m} \text{ and } s_m' = -\alpha s_{2m+1},$$

using Feigenbaum's result,

$$f_{r_{n+1}}(x;n+1) = -\alpha^{-1} f_{r_n}(-\alpha x;n),$$

and assuming the existence of a fixed point for

$$g_{r_{n+1}}(x;n+1) = \beta\alpha^{-1} g_{r_n}(\alpha x;n)$$

(where β is a multiplicative renormalization constant for the noise amplitude, and r_n and r_{n+1} are, respectively, points with corresponding stability for the 2^n- and 2^{n+1}-cycle), we find

$$\Omega_{r_{n+1}}(x, s, \sigma; n+1) = \Omega_{r_n}(x', s', \beta\sigma; n). \tag{14}$$

This leads to a scaling form for the response function

$$R(r_n, \sigma; N; n) = Z^{-1} \int [\mathfrak{D}x][\mathfrak{D}s]\, i x_N s_0 \exp\Omega_{r_n}(x, s, \sigma; n)$$
$$= Z^{-1} \int [\mathfrak{D}x'][\mathfrak{D}s']\, i x_{N/2}' s_0' \exp\Omega_{r_{n-1}}(x', s', \beta\sigma; n-1) = R(r_{n-1}, \beta\sigma; \tfrac{1}{2}N; n-1). \tag{15}$$

The factor $\frac{1}{2}$ multiplies N since coarse graining doubles the length of the unit iteration step.

We have searched for the approximate fixed points of Eq. (13) by using linear and quadratic approximations for $g_r(x)$. The linear approximation leads to an expression for $\beta^2 = \alpha^2 + \delta^2$, entirely in terms of Feigenbaum's universal constants. In the quadratic approximation we obtain the value[9] $\beta \approx 7.7$. For large enough n, Eqs. (10) and (15) imply that $\lambda(r_n; \sigma) = 2\lambda(r_{n+1}; \beta^{-1}\sigma)$ which, upon iteration, yields

$$\lambda(r_n; \sigma) = 2^m \lambda(r_{n+m}; \beta^{-m}\sigma). \tag{16}$$

Let us first examine the behavior of λ as a function of σ at r_∞. From Eq. (16), we see that

$$\lambda(r_\infty; \sigma) = 2^m \lambda(r_\infty; \beta^{-m}\sigma);$$

whence, assuming that $\lambda(r_\infty; \sigma)$ is proportional to σ^u, we find

$$u = (\ln 2)/\ln\beta \approx 0.34\ldots. \tag{2b'}$$

Since $r_k - r_\infty$ is proportional to δ^{-k}, we can rewrite Eq. (16) as

$$\lambda(r_\infty - r_n; \sigma) = 2^m \lambda(\delta^{-m}(r_\infty - r_n); \beta^{-m}\sigma). \tag{17}$$

Introducing $t = (\ln 2)/\ln\delta = 0.4498\ldots$, and fixing the first argument on the right-hand side of Eq. (17) at some small constant value, we are led to

$$\lambda(r_\infty - r_n; \sigma) = (r_\infty - r_n)^t \Phi((r_\infty - r_n)^{-t}\sigma^u), \tag{1'}$$

and the zero-noise scaling relation,

$$\lambda(r_\infty - r_n; 0) \sim (r_\infty - r_n)^t. \tag{18}$$

Equation (18) gives the same scaling exponent for the Lyapunov parameter below threshold that Huberman and Rudnick previously obtained for this parameter beyond threshold in the chaotic regime. Our relation, which complements theirs, holds only when the Lyapunov exponent is calculated for corresponding values of the stability parameter, i.e., it describes the curve connecting the points in each 2^n-cycle which have equal stability parameters. With this understanding, we see that the same power law describes the Lyapunov exponent above and below threshold.

From Eq. (1), we can calculate how, as the external noise is varied, the point r_c, at which the Lyapunov parameter changes sign, is shifted. Since $(r_\infty - r_c)^{-t}\sigma^u$ must be constant for $\sigma \neq 0$, we see that γ, defined by $(r_\infty - r_c) \sim \sigma^\gamma$, satisfies

$$\gamma = u/t \approx 0.75\ldots. \tag{19}$$

In careful numerical experiments, Huberman and collaborators[6] have found

$$u = 0.37 \pm 0.02 \text{ and } \gamma = 0.82 \pm 0.02$$

which agree satisfactorily with our simple approximate values, 0.34 and 0.75.

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μ, the ratio of the intensity of successive subharmonics in the power spectrum studied by M. Feigenbaum [Phys. Lett. 74A, 375 (1979)], who found $\mu \simeq 4\alpha[2(1+\alpha^{-2})]^{1/2}$. The current best values of β and μ are, respectively, 6.618 and 6.557. That β and the "noise-free" parameter μ are related can be made plausible by requiring the ratio of the intensities of the noise-induced power spectra for chaotic transitions at r_n and r_{n+1} to coincide with the ratio of the spectral peaks at corresponding values of the control parameter, and performing a field-theoretic calculation which identifies the former ratio with the ratio of noise levels causing the transition.

Ion Beam Crystallography at the Si(100) Surface

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The geometric structures of the clean 2×1 reconstructed and the hydrogen-stabilized $(1\times1)2H$ Si(100) surface have been studied by means of ion channeling and blocking. The latter surface appears to be contracted by 0.08 ± 0.03 Å and has a surface Debye temperature of ~230 K. For the 2×1 surface it is shown that only the surface dimer models by Appelbaum and Hamann and by Chadi agree well with the backscattering data. The silicon atoms in the very surface are displaced more than 0.45 Å in the surface dimer direction, but those in deeper layers are displaced less than ~0.2 Å.

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A large number of investigations, both theoretical and experimental, have been dedicated to the problem of determining the structure of the clean Si(100) surface. These efforts have yielded structural models for this surface, but have not yet yielded a solution to the problem.[1] The models proposed can be divided into two main categories. First there are models that explain the observed low-energy electron-diffraction (LEED) patterns by assuming missing rows in the surface, leading to an increase in the surface unit cell. All other models attribute the reconstruction to displacements of surface atoms from bulk lattice positions. Recently subsurface displacements have been included in both types of models. The simplest surface-vacancy model has missing rows giving rise to a 2×1 LEED pattern. A more complicated model, proposed by Poppendieck, Gnoc, and Webb,[2] combines missing rows in the two outer layers of the crystal with displacements in the three outer layers. The LEED pattern belonging to this model is $c(4\times2)$, observed in several LEED experiments and with He diffraction.[3] The dimer model is an example of the second category. Surface atoms, having two dangling bonds, form a dimer to lower their energy. In the simplest case, only surface atoms are involved.[4] The conjugated-chain model[5] also features a pairing of rows in the outer crystal layer. Appelbaum and Hamann[6] showed that the energy can be lowered further by displacing subsurface atoms from their bulk positions when a symmetric dimer is formed between Si surface atoms. Chadi calculated that tilting the surface dimer is energetically even more favorable.[7] LEED studies show reasonable agreement with models from both classes, even when these models differ drastically. He diffraction results have confirmed the existence of the $c(4\times2)$ structure, along with $p(2\times2)$ and possibly $c(2\times2)$ regions.[3] Chadi presented arguments in favor of 2×2 reconstructions against a pure 2×1 reconstruction.[8] The 2×2 reconstructions are obtained by a rearrangement of the asymmetric surface dimers, still including subsurface distortions. Photoemission experiments, in which the dispersion of the intrinsic surface state was determined, gave evidence for an asymmetric-dimer model.[9]

Medium-energy ion scattering with the combined effects of channeling and blocking has been shown to be extremely sensitive to surface structural parameters such as atomic displacements and thermal vibrations.[10] It is a quantitative technique and the experimental results are, in general, easily interpreted. We have used this technique to determine the structure of the Si(100)-$(1\times1)2H$ surface,[11] to establish some essential structural parameters of the Si(100)-(2×1) reconstructed surface, and to investigate

