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Numerically Induced Chaos in the Nonlinear Schrödinger Equation

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The cubic nonlinear Schrödinger equation and some of its discretizations, one of which is integrable, are studied. Apart from the integrable version the discretizations produce chaotic solutions for intermediate levels of mesh (mode) refinement. Chaos disappears when the discretization is fine enough and convergence to a quasiperiodic solution is obtained. Details are given for finite-difference calculations, although similar results are also obtained by Fourier spectral methods. Results regarding a forced nonlinear Schrödinger equation are briefly described.

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The cubic nonlinear Schrödinger (NLS) equation,

$$iu_t+u_{xx}+Q|u|^2u=0, \tag{1}$$

where Q=const, $i^2=-1$, plays a ubiquitous role in physics. It arises as an asymptotic limit of a slowly varying dispersive wave envelope in a nonlinear medium and as such has significant applications; e.g., nonlinear optics, water waves, plasma physics, etc. Moreover, it has the distinction of being completely integrable via the inverse scattering transform (IST). As such we are ensured that the NLS equation does not possess chaotic behavior for the standard initial-value problem (see Ref. 1 for a review of IST and a discussion of physical applications). Recently there has also been significant interest in particular forced versions of the NLS equation and approximate solutions via low-mode truncations.[2] There are numerous popular discretizations of the NLS equation which provide a vehicle for numerical solutions. Some of these discretizations are physically important in their own right, with applications to nonlinear dimers, self-trapping phenomena, biological systems, etc.[3-5]

The NLS equation and some of its discretizations are excellent models to study the phenomenon of numerically induced chaos. Some advantages are the following: The equation is relatively simple, has known exact solutions (see Refs. 1 and 6), and the discretizations are straightforward. The discretizations we shall consider here are of finite-difference type, although at the end we remark upon another discretization—via Fourier spectral decompositions. We will consider the schemes (assuming periodic boundary conditions, given by $u_{j+N}=u_j$ in the finite-difference case),

$$iu_j+(u_{j+1}+u_{j-1}-2u_j)/h^2+Q|u_j|^2u_j^{(k)}=0, \quad k=1,2, \tag{2}$$

where (a) $u_j^{(1)}=u_j$ and (b) $u_j^{(2)}=(u_{j+1}+u_{j-1})/2$. Both schemes are of second-order accuracy and Hamiltonian. In case (2a) there are two constants of the motion, the L^2 norm, $I=\sum_{j=0}^{N-1}|u_j|^2$, and the Hamiltonian

$$H=-i\sum_{j=0}^{N-1}(|u_{j+1}-u_j|^2/h^2-\tfrac{1}{2}Q|u_j|^4). \tag{3}$$

Hence, when $N=2$ the system is integrable. In fact, this system has been used as a model for a nonlinear dimer.[3] The Poisson brackets are the standard ones.

The Hamiltonian structure of scheme (2b) is given (for $h=1$) by the Hamiltonian[7]

$$H=-i\sum_{j=0}^{N-1}[u_j^*(u_{j-1}+u_{j+1})=4Q^{-1}\ln(1+\tfrac{1}{2}Qu_ju_j^*)], \tag{4}$$

together with the nonstandard Poisson brackets $\{q_m,p_n\}=(1+\frac{1}{2}Qq_np_n)\delta_{m,n}$ and $\{q_m,q_n\}=0=\{p_m,p_n\}$. This system has been demonstrated to be solvable by IST and there is an infinite number of conserved quantities.[8] General solutions can be obtained on the infinite line (see Refs. 1 and 8) as well as on the periodic interval.[9] In fact, there are further partial-difference analogs to case (2b) which also have special properties and can be used as effective numerical schemes.[10] However, in this note we shall concentrate on integration of the schemes (2) for long periods of time and shall see that for intermediate levels of discretizations, the schemes are markedly different.

It is well known (see Ref. 11) that the NLS equation allows steady wavelike solutions that are unstable under small perturbations (the so-called Benjamin-Feir instability[12]). This means that if (1) is solved with the initial values $u(x,0)=a[1+\epsilon\cos(\mu_n x)]$, $|\epsilon| \ll 1$, as the initial condition, where $\mu_n=2\pi n/L$, a,ϵ are constants, and L is the period, then all wave numbers n for which

$$0<\mu_n^2<2Q|a|^2 \tag{5}$$

will grow exponentially according to linear analysis. These instabilities will then display the phenomenon known as recurrence which has been observed both experimentally and numerically.[13] Here we use this initial condition to solve (2) with $Q=4$, $L=2\sqrt{2}\pi$, $a=0.5$, and $\epsilon=0.1$. These choices imply that the second mode $n=2$ is just on the edge of the instability region given by (5). The time integration is performed by the Runge-Kutta-Merson routine in the NAG (Numerical Algorithms Group) software library and sufficiently high accuracy is specified in all our computations to ensure that the results reported here are not consequences of the time integration.

Recall that both schemes are integrable for $N=2$ and in this case both methods have quasiperiodic solutions, with scheme (2a) displaying qualitative behavior resembling the behavior of the corresponding continuous solution of (1) (see Ref. 14). Surprisingly enough, if N is increased it does not lead to a better approximation of the NLS solution in the case of scheme (2a). In fact, if N is increased through $N=4$ and higher values, the integrability of scheme (2a) is lost and the solution displays a weak form of chaos, typified by a broadband Fourier spectrum of the time evolution. Figure 1(a) shows the modulus of the solution at $x=0$ for $N=32$ up to a time $T=256$. The broadband Fourier spectrum is evident from Fig. 1(b). For larger values of N the chaos gradually disappears until no trace is left at $N=50$. A steady convergence to the analytical solution is observed if N is further increased.

The solutions obtained from the integrable scheme (2b) are in marked contrast with the previous results. The solution is always quasiperiodic with steady convergence observed for increasing values of N. The solution obtained with $N=32$ is shown in Fig. 2. It is clearly quasiperiodic and has nothing in common with the solution of the nonintegrable scheme, shown In Fig. 1 for the same value of N.

When the NLS equation is perturbed its integrability is lost, in general. For instance, Bishop *et al.*[2] study the following perturbed problem (apart from an elementary transformation):

$$-iu_t+u_{xx}+|u|^2u=i\epsilon[\alpha u+\Gamma\exp(-it)]\,, \tag{6}$$

where α,Γ are real constants, $\epsilon=1$, and the initial condi-

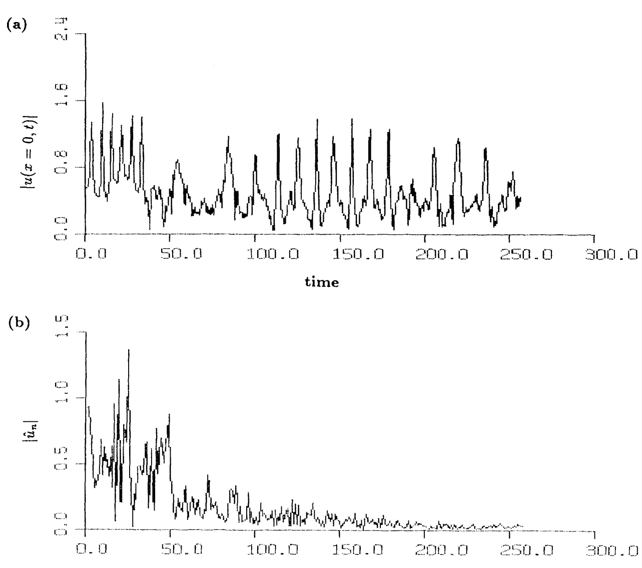

FIG. 1. The NLS equation; standard differences, $N=32$. (a) The time evolution of the modulus of the solution. (b) The Fourier spectrum of the time evolution of the modulus.

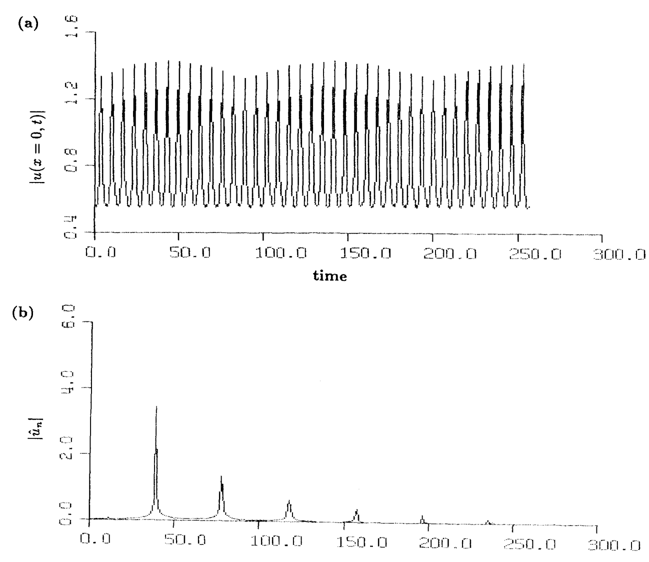

FIG. 2. The NLS equation; the integrable difference scheme, $N=32$. (a) and (b) as before.

tion is given by $u(x,0)=c+b\cos(\mu x)$ with $\mu=2\pi/L$, $L=12\sqrt{0.26}$, and c and b complex constants. Fixing $\alpha=0.155$, the equation is destabilized by increasing the magnitude of the driver, Γ. Chaos is found for $\Gamma=0.275$, using $c=-0.4641+0.6103i$, $b=0.3883-0.5206i$, and this was confirmed by our own numerical experiments. We are interested in qualitative differences between solutions of the perturbed NLS equation using the finite-difference methods (2a) and (2b). Solutions are compared as the value of ϵ is increased, with the values of the remaining parameters fixed.

For $\epsilon=0$, the solutions from both methods, for all N tried, show quasiperiodic behavior, illustrating that only certain regions of the phase space of scheme (2a) contain chaotic solutions. For small positive values of ϵ, the damping dominates and the solutions from both methods quickly settle down to a rest state. However, as the value of ϵ increases into the chaotic region, the solutions from the two methods again differ markedly. The modulus of the solution at $x=0$ up to a time $T=256$, using $\epsilon=1$ and $N=8$ for the two schemes (2a) and (2b), are shown in Figs. 3(a) and 4(a). Although both solutions display irregular behavior, the qualitative features of the solutions are quite different. This is supported by the Fourier spectra of the two solutions, shown in Figs. 3(b) and 4(b). The solution obtained from the integrable method, (2b), is dominated by a few low frequencies, superimposed on a continuous background. This is in contrast with the solution of the nonintegrable method, (2a), where the Fourier spectrum is more evenly spread over the whole domain.

Our numerical results illustrate the marked differences in the solutions of two finite-difference methods, which are identical except for the small change in the discretization of the nonlinear term. Both are second-order accurate and the usual comparisons based on convergence estimates predict similar results for the two methods. The fact that this is not the case in practice stems from the crucial difference between the two methods—that of integrability. Indeed, our numerical experiments confirm that chaos is present even in the exponentially convergent Fourier spectral method.[15] The situation for the Fourier methods is similar to the one described above. For $N=2$ the methods are integrable and reasonable qualitative agreement with the analytical solution is obtained.[14] This qualitative agreement is lost when N is increased and the solution becomes chaotic as well. The exponential convergence only comes into play if N is increased even further; considerably beyond the number of modes one would expect intuitively. The situation is analogous to the time-step restrictions imposed on numerical methods to prevent numerical instabilities; the nonintegrable scheme (2a) being analogous to conditionally stable methods (N needs to be large enough) and the integrable scheme (2b) analogous to the unconditionally stable schemes.

It should be stressed that the examples discussed in this Letter are relatively simple. The spatial structure of the initial condition consists of two Fourier modes and only a relatively small number of spatial Fourier modes are significant throughout the computations. The situation becomes more complicated when initial conditions involving more modes are used. In this case even the full spectral method, despite its exponential convergence, has

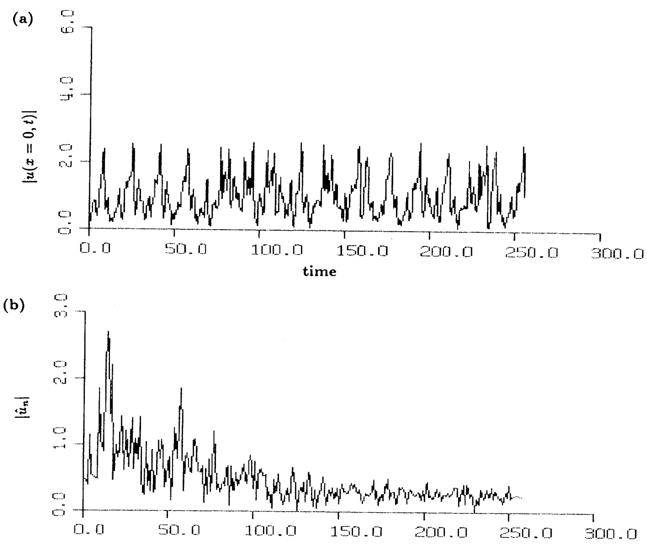

FIG. 3. The driven NLS equation; standard differences. (a) and (b) as before.

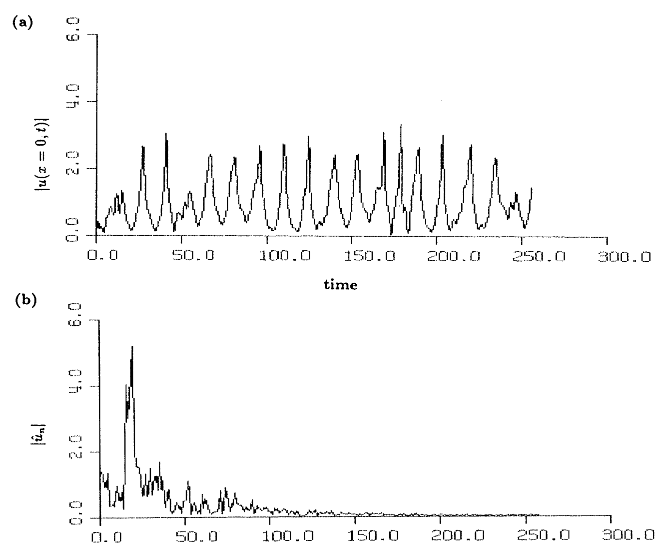

FIG. 4. The driven NLS equation; the integrable difference scheme. (a) and (b) as before.

difficulty approximating the analytical solution, requiring more than 64 modes in some cases.[15] Against this background it is not surprising that numerically induced chaos has also been observed in a much more complicated situation—Rayleigh-Bénard convection[16] (see also Ref. 17), where it is no longer known *a priori* whether the solution is indeed chaotic for given parameter values or not. Since our results show that chaos may disappear for values of N much higher than what one would normally consider to be sufficient for adequate resolution of the spatial structure, computational considerations for realistic problems in higher dimensions may preclude refining the spatial resolution to the relatively high degree necessary to remove numerically induced chaos.

We shall refer to the numerical instability observed here as numerical homoclinic instability (NHI). The NLS equation has its own homoclinic structure, ascertainable both numerically and analytically,[15] which is perturbed by the numerical schemes. Unlike the integrable scheme, standard discretizations apparently allow frequent homoclinic transversals at intermediate levels of mesh refinement. Analytical studies of this process are in progress. In fact, NHI can even be induced by roundoff error (same initial conditions, $Q=2$; see Ref. 15).

NHI is similar to the chaos observed by Bishop *et al.*[2] They find good qualitative description of the analytical situation by means of a two-mode Fourier truncation that is known to be integrable for the nearby unperturbed problem. It is unclear whether the inclusion of an intermediate number of modes, as in our calculations, will still give a reasonable qualitative description of the analytical situation.

Admittedly, integrability is a special property. Numerically viable integrable discretizations may not always be available and many problems are not even close to integrable ones. The danger of confusing numerically induced chaos with physical chaos in these cases emphasizes the importance of current attempts at estimating the Fourier dimension of inertial manifolds (see, for example, Ref. 18). Knowledge of the finite dimensionality of an attractor is of considerable value and estimates of the dimension might provide information regarding the resolution required for eliminating spurious numerical effects and the ability of the numerical scheme to capture the intrinsically important properties of the nonlinear evolution equation at intermediate levels of discretization.

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