PHYSICAL REVIEW E VOLUME 58, NUMBER 1 JULY 1998

Creation and annihilation of intrinsic localized excitations

K. Ø. Rasmussen, A. R. Bishop, and Niels Grønbech-Jensen
Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545
(Received 6 March 1998)

Creation and annihilation of intrinsic localized excitations in a nonintegrable discrete one-dimensional nonlinear Schrödinger system is studied numerically. We demonstrate that the distribution $p(x)$ of the amplitudes x of the created excitations has the form $p(x)=x^{\alpha}\exp(\beta x^{\gamma})$. The log-normal form $\gamma=2$ has previously been found in non-Hamiltonian continuous systems. [S1063-651X(98)50107-9]

PACS number(s): 03.40.Kf, 63.20.Pw

An important and longstanding problem in nonlinear science is the existence and dynamics of intrinsic localized excitations, that have broad physical significance in plasmas, fluids, optics, biomolecular systems [1], etc. It is also expected that intrinsic localized excitations play an important role in the dynamics of anharmonic crystals [2]. Rigorous examples of self-localized states are provided by solitons in completely integrable systems and are well understood by now [3,4]. The dynamics of these examples is simple in that the localized excitations (solitons) do not interact within the nonlinear spectral space defined by the inverse scattering transform. Also, the soliton spectra are separated from spectra arising from other excitations (e.g., radiation). As a consequence, soliton creation and annihilation is at most a recurrence process in integrable systems. In realistic physical models, complete integrability is almost always absent, due to physical properties such as discreteness, dimensionality, disorder, and fluctuations [5–7]. Consequently, the creation and annihilation process of localized excitations becomes much more complicated physically and less understood mathematically.

It is becoming apparent that discrete intrinsic localized excitations do not require integrability for either existence or stability [8,9]. This physically important observation has recently been established rigorously via, e.g., an application of the implicit functions theorem [10–12]. A multitude of aspects of the dynamics of intrinsic localized excitations has been explored using approximate analytical methods [13–15] and well-founded numerical techniques [16]. Also, full dynamical simulations have illustrated the dynamical behavior of such excitations [17,18]. However, the main area of research on intrinsic localized excitations has considered the behavior of single discrete localized excitations and only a few works have been concerned with their interaction [19,20], and even less research has been devoted to the creation and possible annihilation of discrete localized excitations. Addressing such issues is an important step towards understanding the role played by intrinsic localized states in nonergodic and nonequilibrium properties in real physical contexts.

Previous studies of creation and annihilation of solitonlike states have been conducted mainly in continuous systems such as the Kuramoto-Sivashinski equation [21,22], complex Ginzburg-Landau equation [23], and the damped and driven nonlinear Schrödinger equation [24–26]. These equations are necessarily nonintegrable, and they are also dissipative and, therefore, non-Hamiltonian. Initializing the systems in either a uniform state or a uniformly distributed random state leads to localized excitations forming and annihilating in a nonperiodic sequence. Analytical explanations of these observed phenomena in numerical simulations have been promoted in various forms of a ''soliton-lattice'' model [23,21], which build on the superposition of randomly positioned exact soliton excitations. Such models appear to work well when solitons are available and when they are allowed to move freely in the system. An interesting common feature of these continuum systems is that the distribution of certain characteristics (such as amplitude [24], width, or mutual separation [23]), of the localized excitations in all cases studied, has a near-log-normal form.

In the present work, we perform a detailed numerical study of creation and annihilation of localized excitations in a discrete nonintegrable nonlinear Schrödinger (DNLS) system. In contrast to the studies noted above, the DNLS system is a discrete *Hamiltonian* system. The existence and stability and several other aspects of intrinsic localized excitations have been clarified using inverse scattering transform [27], Melnikov analysis [15], and the concept of ''anti-integrability'' [17]. The importance of the DNLS system, as one of the most widely studied discrete nonlinear systems, stems not only from its applicability in diverse physical situations but also from its simple, yet rich, mathematical structure. It is worth mentioning that the dynamics of the DNLS system exhibits a richness that the system in its integrable version does not, either in the discrete version (Ablowitz-Ladik discretization [3]) or in its continuum limit.

We study the one-dimensional DNLS equation

$$i\dot{\psi}_n+(\psi_{n+1}+\psi_{n-1})+2\nu|\psi_n|^2\psi_n=0, \tag{1}$$

where the overdot denotes the time derivative, n is a site index, and ν is a tunable coefficient to the nonlinear term. Using the standard Poisson brackets

$$\{\psi_n,\psi_n^*\}=i\delta_{nm}, \tag{2}$$

$$\{\psi_n,\psi_m\}=\{\psi_n^*,\psi_m^*\}=0, \tag{3}$$

Eq. (1) becomes the equation of motion,

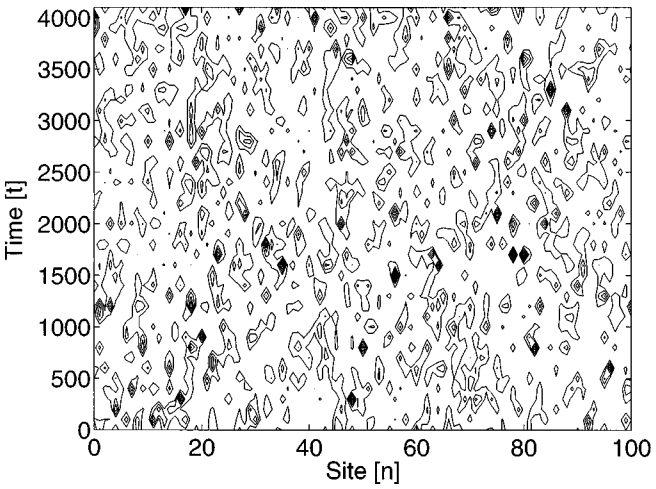

FIG. 1. Spatiotemporal contour image ($|\psi_n|$) of a small part (101 sites) of the periodic chain. Parameters are $\mathcal{N}=2000$, $\nu=10$, and the system size is 2.5×10^5 sites.

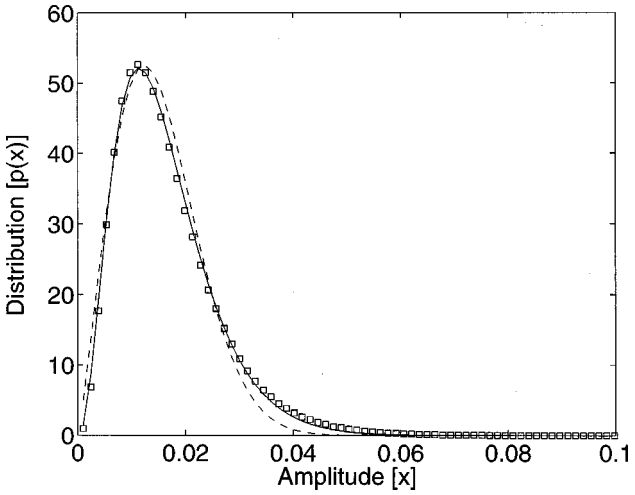

FIG. 2. Distribution of amplitudes of intrinsic localized excitations. Squares indicate numerically obtained data, the solid line indicates least-squares fit to p_1 Eq. (7), and the dashed line indicates least-squares fit to p_2 Eq. (8). System parameters are the same as in Fig. 1.

$$\dot{\psi}_n=\{\mathcal{H},\psi_n\}, \tag{4}$$

where $\mathcal{H}$ is the Hamiltonian given by

$$\mathcal{H}=-\sum_n\ (\psi_n\psi_{n+1}^*+\psi_n^*\psi_{n+1})-\nu\sum_n\ |\psi_n|^4. \tag{5}$$

In addition to the conserved energy $\mathcal{H}$, the quantity

$$\mathcal{N}=\sum_n\ |\psi_n|^2 \tag{6}$$

is also conserved under the dynamics of Eq. (1) and serves as the norm of the system. The quantities $\mathcal{H}$ and $\mathcal{N}$ were frequently monitored during the numerical simulation to ensure appropriate accuracy of the numerical fourth-order Runge-Kutta scheme that we used to simulate the system. The system (1) possesses, as exact solutions, a class of exact intrinsic localized states that however, cannot be found analytically; their existence and stability can be analytically proven in various ways [10,15,17] and they can be found numerically to a high degree of accuracy [15,17].

A numerical experiment of Eq. (1) was performed on a lattice consisting of 2.5×10^5 sites. As initial states every site is assigned a random real value uniformly distributed in the interval $[-v,v]$, where v is chosen to give a total $\mathcal{N}=2000$. Finally, the nonlinear coefficient was chosen to be $\nu=10$. The large system size is chosen in order to obtain reliable statistics while still being able to control the conserved quantities $\mathcal{H}$ and $\mathcal{N}$.

Figure 1 shows the spatial-temporal contour image of a small part of the system as it evolves. Clearly, some coherent structures emerge, indicating a dynamical creation and annihilation process. The mechanism behind this creation and annihilation process is the modulation instability [28] which allows creation of localized structures. In the present case it is an extremely complex process, since the random initial conditions, in a sense, contains all possible modulational frequencies. This, combined with the persistent noisy background caused by the discreteness and nonintegrability of the systems, causes the annihilation process. It is evident that there is very little direct interaction between the various localized excitations, contrary to what has been observed in similar cases for continuous equations [23,24,21]. The reason for this is that the emerging excitations are localized within only a couple of sites and, therefore, the probability that any two excitations are close is low. Also, the individual excitations are very unlikely to move because narrow excitations are more strongly pinned by the lattice discreteness [29,30]. Therefore, all interaction arises almost entirely from the small amplitude background excitations. Since the localized structures are created and annihilated in a seemingly stochastic manner (although it is worth noting that the positions of the structures show some regularity in the way the creation of high amplitude excitations is confined to certain regions of the lattice), the appropriate way to characterize the system is in terms of the distributions of suitable characteristic features. Figure 2 shows the distribution of the amplitude of the localized excitations that are created after a long time (see below). The squares in Fig. 2 show the numerically obtained distribution of the excitation amplitudes, x, while the solid line is the distribution function

$$p_1(x)=p_{1n}x^{\alpha_1}\exp(-\beta_1 x), \tag{7}$$

and the dashed line is the distribution function

$$p_2(x)=p_{2n}x^{\alpha_2}\exp(-\beta_2 x^2), \tag{8}$$

where α_i and β_i are fitting parameters, $p_{1n}=\beta_1^{(\alpha_1+1)}/\Gamma[(\alpha_1+1)]$, and $p_{2n}=2\beta_2^{(\alpha_2+1)/2}/\Gamma[(\alpha_2+1)/2]$; the two latter are normalization constants. The fits are shown for $\alpha_1=2.3$, $\beta_1=208.7$, and $\alpha_2=1.2$, $\beta_2=3810.0$. Both sets of parameters are found from a least-squares fit to the numerical data. It is clear from Fig. 2 that the fit of p_1 is excellent, while the distribution p_2 fails to fit the slowly decreasing tail. To ensure that the distribution is stationary, we fit p_1 to the numerically found distribution in

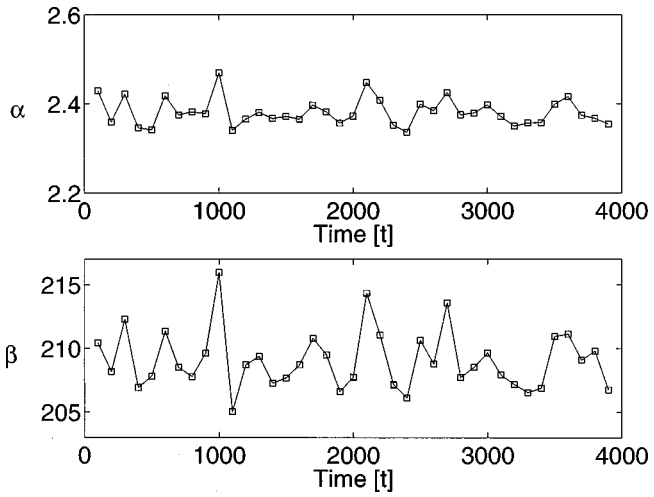

FIG. 3. Evolution of the fitting parameters α_1 and β_1 defined in Eq. (7). Systems parameters are the same as in Fig. 1.

time intervals of length 100 time units and show the resulting α_1 and β_1 versus time t in Fig. 3. From Fig. 3 we clearly observe that the distribution is indeed stationary since there is no time dependence of the fitting parameters except for small fluctuations. The quality of the fit is the same over the entire time interval. In order to test the results further we have performed other similar simulations of the system, varying $\mathcal{N}$ between $\mathcal{N}=2000$ and $\mathcal{N}=10\,000$, and the same overall behavior was found, namely, that the distribution p_1 is able to fit the numerical data well with the same value of α, but with β changing proportionally to $\mathcal{N}$. A few longer simulations ($t\sim 100\,000$) on smaller systems (~ 1000 sites) were done to ensure that the distribution is not changing on an extremely slow time scale, and this was found not to be the case.

As is well known [28] spatially uniform initial conditions with small modulations will, due to the modulational instability, cause certain modes to dominate the initial dynamics of the system. However, the three-wave mixing of the nonlinear term produces all frequency components in the long-time dynamics and a behavior similar to what is reported here may occur.

Since the initial condition is real, the phase of ψ_n is initially zero or π. The distribution of the phase was observed to change smoothly into a completely uniform distribution between 0 and 2π. The uniform distribution is reached after a relatively short time ($t\sim 300$).

Another interesting question is what the effect of integrability on the observed behavior is. The DNLS system is ''close'' to being integrable in the sense that it becomes integrable in the continuum limit. One way to remove this feature is to change Eq. (1) to

$$i\dot{\psi}_n+(\psi_{n+1}+\psi_{n-1})+2\nu|\psi_n|^{2\sigma}\psi_n=0, \tag{9}$$

where σ is a parameter different from $\sigma=1$. The system (9) is itself an interesting system and is well studied [31–33]. Performing similar simulations in this system, we found for $\sigma=2$ no change in the distribution, as compared to the system where $\sigma=1$.

Considering x as a stochastic variable governed by a stochastic differential equation, it is possible [34], via a Fokker-Planck equation, to determine the appropriate equation yielding the distribution p_1,

$$\dot{x}=ax-bx^2+\epsilon(t)x, \tag{10}$$

where

$$\langle\epsilon(t)\rangle=0 \quad \text{and} \quad \langle\epsilon(t)\epsilon(t')\rangle=D\delta(t-t'). \tag{11}$$

The relation between the parameters α_1, β_1 and a, b, and D is

$$\alpha=2a/D-1$$

and

$$\beta=2b/D. \tag{12}$$

The apparent way to explain the appearance of a multiplicative stochastic term $\epsilon(t)$ in Eq. (10) is to ascribe it to the spatial diffusion and fluctuating background created by the moving small amplitude excitations (radiation and low amplitude local excitations). There is, however, no *a priori* reason why the noise should be white; indeed, the remaining very small but systematic deviation from log-normal distribution in the tail region (see Fig. 2) may indicate some color. From the numerics we know that α is intrinsic to the system in that it is unchanged when the parameters of the system are changed, indicating that the a and the noise variance D are intrinsic to the system. So, starting from a random state, the system generates a stochastic background with a specific strength. Furthermore, we know that b is proportional to $\mathcal{N}$, indicating that the term bx^2 arises from the nonlinearity of the system.

The nonlinear stochastic differential equation (9) can also describe a bimolecular chemical reaction [34]. In this connection it is interesting to observe that a similar trimolecular reaction would lead to Eq. (9) with the term bx^2 replaced with bx^3, which in turn leads to the distribution p_2. As we have seen p_2 approximates the numerical data much worse than p_1. It is difficult to interpret this fact in detail in our context, but it suggests that the distribution is a result of the coexisting interaction of intrinsic localized excitations and radiation via the nonlinear term in Eq. (1).

In conclusion, we have numerically studied creation and annihilation of intrinsic localized excitations in a nonintegrable Hamiltonian system, starting from a random initial condition. The observed continuous creation and annihilation process results in a characteristic near-log-normal distribution of the amplitudes of the localized states. We further observed that the phenomena can be described by a nonlinear stochastic differential equation with multiplicative white noise. In contrast to other studies, the system studied in the present paper is Hamiltonian, without any external perturbations. The system is, however, nonintegrable and consequently possesses a finite number conserved quantities. An integrable system would have exhibited recurring behavior under the applied conditions. The prevalence of near-log-normal distributions in nonlinear, nonintegrable systems is important for characterizing mesoscale complexity, and evidently is worthy of further study and analysis.

This work was performed under the auspices of the DOE.

[1] See, e.g., Physica D **68** (1) (1993), special issue on future directions of nonlinear dynamics in physical and biological systems, edited by P. L. Christiansen, J. C. Eilbeck, and R. D. Parmentier.
[2] A. J. Sievers and J. B. Page, in *Dynamical Properties of Solids VII: Phonon Physics—The Cutting Edge*, edited by G. K. Horton and A. A. Maradudin (Elsevier, Amsterdam, 1995), p. 137.
[3] M. J. Ablowitz and P. A. Clarkson, *Solitons, Nonlinear Evolution Equations and Inverse Scattering* (Cambridge University Press, New York, 1991).
[4] L. D. Faddeev and L. A. Takhtajan, *Hamiltonian Methods in the Theory of Solitons* (Springer-Verlag, Berlin, 1987).
[5] A. B. Aceves *et al.*, Phys. Rev. Lett. **75**, 73 (1995).
[6] S. A. Gredeskul and Yu. Kivshar, Phys. Rep. **216**, 1 (1992).
[7] *Fluctuation Phenomena: Disorder and Nonlinearity*, edited by A. R. Bishop, S. Jiménez, and L. Vázquez (World Scientific, Singapore, 1995).
[8] S. Aubry, Physica D **103**, 201 (1997).
[9] S. Flach and C. R. Willis, Phys. Rep. **295**, 182 (1998).
[10] R. S. MacKay and S. Aubry, Nonlinearity **7**, 1623 (1994).
[11] P. C. Bressloff, Phys. Rev. Lett. **75**, 962 (1995).
[12] D. Bambusi, Nonlinearity **9**, 433 (1996).
[13] A. J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988).
[14] S. Takeno, J. Phys. Soc. Jpn. **61**, 2821 (1992).
[15] D. Hennig, N. G. Sun, H. Gabriel, and G. P. Tironis, Phys. Rev. E **52**, 255 (1995); D. Hennig, K. Ø. Rasmussen, H. Gabriel, and A. Bülow, *ibid.* **54**, 5788 (1996).
[16] J. L. Marín and S. Aubry, Nonlinearity **9**, 1501 (1996).
[17] M. Johansson and S. Aubry, Nonlinearity **10**, 1151 (1997).
[18] J. B. Page, Phys. Rev. B **41**, 7835 (1990).
[19] T. Dauxois and M. Peyrard, Phys. Rev. Lett. **70**, 3935 (1993).
[20] David Cai, A. R. Bishop, and Niels Grønbech-Jensen, Phys. Rev. E **56**, 7246 (1997).
[21] S. Toh, J. Phys. Soc. Jpn. **67**, 949 (1987).
[22] C. C. Chow and T. Hwa, Physica D **84**, 494 (1995).
[23] S. Kishiba, S. Toh, and T. Kawahara, Physica D **54**, 43 (1991).
[24] H. Konno and P. S. Lomdahl, Phys. Lett. A **193**, 35 (1994).
[25] K. Nozaki and N. Bekki, Phys. Lett. A **102**, 383 (1984).
[26] K. Nozaki and N. Bekki, Physica D **21**, 381 (1986).
[27] D. Cai, A. R. Bishop, and N. Grønbech-Jensen, Phys. Rev. Lett. **72**, 591 (1994).
[28] Yu. S. Kivshar and M. Peyrard, Phys. Rev. A **46**, 3198 (1992).
[29] K. W. Sandusky, J. B. Page, and K. E. Schmidt, Phys. Rev. B **46**, 6161 (1992).
[30] Yu. S. Kivshar and D. K. Campbell, Phys. Rev. E **48**, 3077 (1993).
[31] E. W. Laedke, K. H. Spatscheck, and S. K. Turitsyn, Phys. Rev. Lett. **73**, 1055 (1994); E. W. Laedke, O. Kluth, and K. H. Spatscheck, Phys. Rev. E **54**, 4299 (1996).
[32] B. Malomed and M. I. Weinstein, Phys. Lett. A **220**, 91 (1996).
[33] P. L. Christiansen *et al.*, Phys. Rev. B **56**, 14 407 (1997).
[34] C. W. Gardiner, *Handbook of Stochastic Methods* (Springer-Verlag, Berlin, 1997).