

Wave energy self-trapping by self-focusing in large molecular structures: A damped stochastic discrete nonlinear Schrödinger equation model

Brenton LeMesurier*, Barron Whitehead

Department of Mathematics, College of Charleston, Charleston, SC 29424, USA

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Abstract

Wave self-focusing in molecular systems subject to thermal effects, such as thin molecular films and long biomolecules, can be modeled by stochastic versions of the discrete self-trapping equation of Eilbeck et al. [J.C. Eilbeck, P.S. Lomdahl, A.C. Scott, The discrete self-trapping equation, *Physica D* 16 (1985) 318–338], which gives as a continuum limit approximation the stochastic nonlinear Schrödinger equation (SNLS): NLS plus a noise term in the form of a random, time dependent potential.

Previous studies directed at such SNLS approximations have indicated that the self-focusing of wave energy to highly localized states can be inhibited by phase noise (modeling thermal effects) and can be restored by phase damping (modeling heat radiation).

Here, the discrete models are studied directly, with some discussion of the validity and limitations of continuum approximations. Also, as has been noted by Bang et al. [O. Bang, P.L. Christiansen, F. If, K.Ø. Rasmussen, Yu.B. Gaididei, Temperature effects in a nonlinear model of monolayer Scheibe aggregates, *Phys. Rev. E* 49 (1994) 4627–4636], omission of damping produces highly unphysical results.

Numerical results are presented here for the first time for discrete models that include the highly nonlinear damping term, and a new numerical method is introduced for this purpose.

The results in general confirm previous conjectures and observations that noise can inhibit energy self-trapping (the discrete counterpart of NLS self-focusing blow-up), while damping can reverse this and restore self-trapping. Damping is also shown to strongly stabilize the self-trapped states of the discrete models. It appears that the previously noted inhibition of nonlinear wave phenomena by noise is an artifact of models that includes the effects of heat input, but not of heat loss.

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1. Introduction

Combinations of mildly nonlinear wave motion in molecular structures with localized excitation modes can lead to intense localization or *self-trapping* of wave energy onto one or a few molecular subgroups. The relevant mathematical modeling started with Davydov's soliton theory of *exciton waves* in protein molecules interacting with localized *phonons*, localized vibrations at CO bonds, where a continuum limit gave the integrable one dimensional focusing cubic nonlinear Schrödinger (NLS) equation [9,11,10]. The discrete self-trapping phenomenon was discovered and named by Scott [24]

along with Eilbeck and Lomdahl [16,17], who extended Davydov's work to vibrations in other molecular systems such as crystalline acetanilide and smaller molecules such as benzene; see also [19,2]. Approximations that eliminate the fastest internal vibration modes again lead to systems that are discrete counterparts of the 1D focusing cubic NLS, or coupled systems of such.

Two dimensional molecular structures such as Scheibe aggregates [4] lead to similar mathematical models related to the 2D focusing cubic NLS [21,3]. In the 2D discrete NLS, a version of discrete self-trapping is also seen, in the sense of the formation of standing trapped narrow spikes, as has been shown by Christiansen et al. [7,6].

Bang et al. [1] added stochastic terms to modeling effects such as random spatial variations in the medium (*fixed pattern*

* Corresponding author.

E-mail address: lemesurierb@cofc.edu (B. LeMesurier).

noise: time independent) and thermal agitation (*space–time noise*). Nonlinear optics has also produced continuum or semi-discrete examples including intense CW lasers and multi-cored optical fibers with random imperfections in the medium or in the strength of the coupling between signals in the different cores or different propagation modes.

However, excitation of vibrational modes by noise without balancing losses can lead to an unphysical degree of spatial disorder or *thermal runaway*, impeding wave propagation in contradiction to experimental observations [1]. Even worse, the obvious continuum limits give stochastic NLS (SNLS) equations which seem to be well-posed only when the noise has adequate spatial correlation [12], which is not necessarily consistent with the length scales in the molecular systems. In other words, noise can destroy the spatial smoothness needed to justify a continuum limit.

More realistic modeling thus requires a mechanism for loss of phonon energy, such as linear damping of those phonon vibrations, in order to allow the attainment of thermal equilibrium. This leads to the damped stochastic discrete nonlinear Schrödinger equation (DSNLS)

$$i \frac{d\psi_n}{dt} + \sum_m J_{nm} \psi_m + |\psi_n|^{2\sigma} \psi_n + \gamma \psi_n \dot{W}_n - \lambda \psi_n \frac{d}{dt} (|\psi_n(t)|^{2\sigma}) = 0, \quad (1)$$

with $\sigma = 1$ giving the cubic case typical in physical applications, as derived and studied in [8]. Here the $W_n(t; \omega)$ are noise processes with ω labeling realizations, the dot denoting formal time derivatives; the physical meanings of other variables and parameters are explained in the next section.

Spatially discrete models such as this are the main object of this paper, but possible continuum limits will also be discussed, mostly in Section 6: the most obvious is the damped stochastic nonlinear Schrödinger equation (DSNLS)

$$i \frac{\partial \psi}{\partial t} + \Delta \psi + |\psi|^{2\sigma} \psi + \gamma \psi \dot{w} - \lambda \psi \frac{\partial (|\psi|^{2\sigma})}{\partial t} = 0, \quad (2)$$

also introduced in [8].

The next section surveys the background for this study: physical origins, mathematical modeling, and some basic properties, and then Section 3 summarizes previous numerical results and establishes conjectures to be studied here. Section 4 describes the numerical methods used, and Section 5 presents the main numerical results, using the surrogate case of a one dimensional structure with quintic nonlinearity $\sigma = 2$. The continuum approximation is discussed in Section 6, with some suggestions as to how to overcome problems with previous approaches, followed by conclusions and a discussion of directions for further work in Section 7.

2. Mathematical modeling

We review here the mathematical modeling of a two dimensional example from chemistry and biochemistry, following [4,22,3,1,8]. This is a model of *Scheibe aggregates*, a class of highly ordered thin films of molecules coupled by

dipole interactions predominantly within a plane: an essentially two dimensional wave medium. However much of the modeling is also relevant to a variety of other molecular systems such as the essentially one dimensional protein models discussed above; see [10,24,16,17] and references therein.

2.1. Scheibe aggregates: Highly ordered thin molecular films

Scheibe aggregates are highly regular arrangements of molecules in thin films, sometimes a single molecule thick, or with only weak interaction between neighboring layers of molecules. These structures have important biological roles such as in photo-chemical reactions, and one laboratory example is provided by the cyanine dye Scheibe aggregates first studied by Bücher, Kuhn, Möbius et al. [4,22]. They establish an arrangement of the molecules in a single layer “brick-wall” lattice, with the dominant dipole interactions being those with six nearest neighboring molecules, arranged in a hexagonal array of approximately dihedral D_2 symmetry (half-turns and reflection in two perpendicular axes).

The molecules also have internal excitation states, which are coupled to the excitons and are also subject to thermal effects: random external forces due to collisions with molecules from outside the thin film.

2.2. An exciton–phonon system with phase noise and damping

Such thin films can be modeled as an exciton–phonon system with noise and damping acting on the internal modes as described by Bang et al. in [1], which adds damping to the purely quantum mechanical modeling of Bartnick and Tuszyński [3]:

$$i\hbar \frac{d\psi_n}{dt} + \sum_{m \neq n} J_{nm} \psi_m + \chi u_n \psi_n = 0 \quad (3)$$

$$M \frac{d^2 u_n}{dt^2} + M\lambda \frac{du_n}{dt} + M\Omega_0^2 u_n - \chi |\psi_n|^2 = \gamma \dot{B}_n \quad (4)$$

where

$\psi_n(t)$ is the exciton wave at molecule (node) n ,

$u_n(t)$ is the elastic degree of freedom of the molecule n ,

J_{nm} is the dipole–dipole interaction energy,

χ is the exciton–phonon coupling constant,

$\gamma \dot{B}_n$ is a random external force acting on molecule n , \dot{B}_n the formal time derivatives of independent Wiener processes at each n ,

γ is the strength of the random external forces,

λ is the damping coefficient,

M is the molecular mass, and

Ω_0 is the Einstein frequency of each oscillator.

These equations conserve the exciton energy $\mathcal{N} = \sum_n |\psi_n|^2$ under the Stratonovic interpretation of the stochastic term as discussed below, at least on a fully infinite lattice or with suitable boundary conditions.

The form of Eqs. (3) and (4) also covers a wide range of other applications such as the one dimensional case of protein molecule models mentioned above: the indices will often be

taken below to simply enumerate a collection of *nodes*, with details such as spatial relationships between nodes encoded in the coupling terms J_{nm} .

For further mathematical flexibility, the coupling term will henceforth be written as a general power law $\chi|\Psi_n|^{2\sigma}$, though all physical models we know of have the cubic nonlinearity $\sigma = 1$. The underlying spatial dimension will be denoted by D , so $D = 2$ in the model above.

Without noise and damping, the system in (3) and (4) is Hamiltonian, giving a second conserved quantity

$$\mathcal{H} = - \sum_{n,m \neq n} J_{nm} \Psi_n \bar{\Psi}_m - \frac{2\chi}{1+\sigma} \sum_n u_n |\Psi_n|^{2\sigma} + \frac{M}{2} \sum_n (\dot{u}_n^2 + \Omega_0^2 u_n^2).$$

2.3. Eliminating the phonon terms u_n

The phonon terms u_n can be eliminated using the variation of parameters formula which gives an integral expression for u_n in terms of Ψ_n [8]. To eliminate the resulting time integral and initial data transients, one must restrict to times $\lambda t \gg 1$ and make the slowly varying envelope approximation: that the exciton energy $|\Psi_n(t)|^2$ is slowly varying relative to the phonon frequency Ω_0 . Thus, the presence of damping ($\lambda > 0$) is essential.

The reduced system is

$$0 = i\hbar \frac{d\Psi_n}{dt} + \sum_{m \neq n} J_{nm} \Psi_m + V |\Psi_n|^{2\sigma} \Psi_n + \frac{\gamma\chi}{M\hbar\Omega} \Psi_n \dot{W}_n - \frac{\lambda V}{\Omega_0^2} \frac{d}{dt} [|\Psi_n(t)|^{2\sigma}] \Psi_n, \quad (5)$$

where $V = \chi^2/M\Omega_0^2$, $\Omega^2 = \Omega_0^2 - (\lambda/2)^2$, and

$$\dot{W}_n = \lambda \int_0^t e^{-\lambda s/2} \sin(\Omega s) \dot{B}_n(t-s) ds. \quad (6)$$

Note that the new noise processes \dot{W}_n are temporally correlated.

2.4. Rephrasing as a damped stochastic discrete nonlinear Schrödinger equation

If the coupling J_{nm} is homogeneous, in that the quantities

$$J_{nn} := - \sum_{m \neq n} J_{nm}$$

have a common value J_0 , then the Ψ_n have a common average phase evolution $e^{tJ_0/\hbar}$. This can be removed by adding J_{nn} to each coupling sum, and with some rescalings including $\gamma\chi/(M\hbar^2\Omega) \rightarrow \gamma$, $\lambda/(\hbar\Omega_0^2) \rightarrow \lambda$, one gets the damped stochastic discrete nonlinear Schrödinger equation (1).

Even if the J_{nm} are not all equal, one can use their average value \bar{J} as the phase shift, and absorb the differences $J_{nn} - \bar{J}$ into the noise coefficients as fixed pattern noise.

The exciton energy $\mathcal{N} = \sum_n |\Psi_n|^2$ is still conserved, and without noise or damping the system still has a conserved

Hamiltonian,

$$\mathcal{H} = - \sum_{n,m} J_{nm} \Psi_n \bar{\Psi}_m - \frac{1}{1+\sigma} \sum_n |\Psi_n|^{2(1+\sigma)}.$$

Simple examples are uniform nearest neighbor interaction on a line (1D) or square lattice (2D) of spacing l with all the non-zero J_{nm} having the same value, J/l^2 . The coupling term is then J times the standard three point second derivative (1D) or five point discrete Laplacian (2D), and the equation is a discretization of the damped stochastic nonlinear Schrödinger equation (2), with

$$\dot{W}_n = \int_0^t e^{-\lambda\Omega_0^2 s/2} \sin(\Omega s) \dot{B}_n(t-s) ds. \quad (7)$$

As Ω_0 (like the unrescaled λ in Eq. (6)) comes from the fast time scale that has been otherwise eliminated, the correlation time of this new noise term is typically very short. Thus we use the approximation that the new noise term is still temporally uncorrelated.

Also, the Hamiltonian for the case of no noise or damping is the natural discretization using simple forward difference quotients for the gradient terms of the Hamiltonian for NLS,

$$\mathcal{H} = \int \|\nabla \psi\|^2 - \frac{1}{1+\sigma} |\psi|^{2(1+\sigma)} d\mathbf{x}.$$

It can be useful in places to think of the ODE systems in relation to the familiar NLS equation, but a more careful consideration of continuum limit approximations is needed, as discussed in Section 6.

2.5. Removing the extra time derivative term, and Stratonovic differential form

For some purposes, the time derivative should be eliminated from the damping term. Also, the rigorous mathematical formulation must be in terms of stochastic integrals and differentials, and in order to conserve the exciton energy \mathcal{N} , products involving stochastic terms must be interpreted in the Stratonovic sense. (Loosely, the Stratonovic integral is defined as the limit of mid-point rule (or trapezoid rule) approximations, whereas the Itô integral is the limit of left-hand end point Riemann sums: see [23] for details.) Solving for $d\Psi_n/dt$, substituting into the other time derivative leads to the stochastic differential form

$$d\Psi_n = i \left[\sum_m J_{nm} \Psi_m + |\Psi_n|^{2\sigma} \Psi_n + 2\lambda\sigma \Psi_n |\Psi_n|^{2(\sigma-1)} \text{Im} \left(\bar{\Psi}_n \sum_m J_{nm} \Psi_m \right) \right] dt + i\gamma \Psi_n \circ dW_n \quad (8)$$

with $\circ d$ denoting the Stratonovic differential.

2.5.1. Why not convert to the Itô integral form?

Any system of stochastic ODE's in terms of the Stratonovic integral can be replaced by an equivalent system which gives

the same solution under the Itô interpretation, by replacing the above Stratonovic differential by the corresponding Itô differential plus a correction term [23], and the Itô form is far more amenable to analysis such as existence and uniqueness proofs. In the current case, this gives

$$d\Psi_n = [\text{as before}] + i\gamma \Psi_n dW_n - \frac{\lambda^2}{2} \Psi_n. \quad (9)$$

However, this form is undesirable for current purposes, particularly numerical simulations. The new term adds rapid exponential decay, destroying the manifestly conservative form. This reflects the fact that the Itô differential term itself generates rapid exponential growth of individual realizations, related to the fact that the ensemble average of Itô solutions satisfies the underlying noise-free equation, and so conserves the exciton energy \mathcal{N} .

This would prevent the use of time discretizations that inherently conserve exciton energy \mathcal{N} ; such conservative discretizations are used here for the Stratonovic form.

Also, the Itô form has no continuum limit with spatially uncorrelated noise. This might reflect the conjectured lack of existence of solutions to such continuum limits, even when the limit formally exists for the Stratonovic form.

3. Heuristics, conjectures and prior numerical results on SNLS blow-up and SDNLS self-trapping

Though our primary subject is the discrete model above with both damping and stochastic terms, far less is known for this model than for the continuum limit PDE approximation, so it is convenient to start with the better understood PDE, SNLS, and then seek heuristic arguments and conjectures on how these results might translate to the discrete model, to guide numerical experiments.

3.1. Wave self-focusing and blow-up in SNLS

In the continuum model of 2D cubic or 1D quintic NLS, self-focusing can lead to the formation of single point singularities, sometimes called *blow-up*. The proof of this for the NLS is based on a variance argument, which has been extended to various cases of stochastic NLS by Gaididei and Christiansen [20] and DeBussche and Di Menza [15], and in more developed form by Fannjiang [18] and de Bouard and DeBussche [13]. All require noise that is sufficiently correlated in space and uncorrelated in time: the former condition is arguably analogous to our situation of a discrete system, but the latter is not exactly true with our model. The relevant results, for critical nonlinearity $\sigma D = 2$, can be summarized as follows.

For data of sufficiently rapid decay at infinity, the pulse width can be measured by its spatial variance

$$V(t) = \int |\psi|^2 \|\mathbf{x}\|^2 d\mathbf{x}.$$

The ensemble average $\langle V \rangle$ is related to the ensemble average $\langle \mathcal{H} \rangle$ of the Hamiltonian by

$$\frac{d^2 \langle V \rangle}{dt^2} = 8 \langle \mathcal{H} \rangle, \quad (10)$$

and in turn noise modifies conservation of the Hamiltonian to

$$\frac{d \langle \mathcal{H} \rangle}{dt} = R := \frac{1}{2} \int \Phi(\mathbf{p}) \|\mathbf{p}\|^2 d\mathbf{p}, \quad (11)$$

where $\Phi(\mathbf{p})$ is the power spectral density of the noise distribution.

For spatially uncorrelated noise, $\Phi(\mathbf{p})$ is a positive constant, so $R = \infty$: the formulas break down, but strongly suggest that SNLS has no solutions, at least in Sobolev space H^1 .

Without noise, $R = 0$, $\langle V \rangle = V$ evolves quadratically, and $\mathcal{H} < 0$ is a sufficient condition for finite time singularity formation, as otherwise, V would become negative. Noise changes the evolution to the cubic

$$\langle V \rangle = \langle V \rangle(0) + bt + 4 \langle \mathcal{H} \rangle(0)t^2 + 2R/3t^3. \quad (12)$$

Clearly for $\mathcal{H}(0) < 0$, weak enough noise still leads to a prediction of negative $\langle V \rangle$ by some positive time t_0 , so with positive probability, solutions must cease to exist before that time. However, for noise having $R > -27 \langle V \rangle(0)/(320 \langle \mathcal{H} \rangle(0))$, the variance stays positive, so that this argument no longer guarantees blow-up. This raises the possibility that sufficiently strong noise restores global existence. For noise of correlation length scale l ,

$$R = O\left(\frac{1}{l^{2+D}}\right) \quad (13)$$

which suggests that both increasing the noise strength and decreasing its correlation length increase the possibility that the noise can prevent blow-up in SNLS that would occur in the noiseless NLS with the same initial data.

These indications should not be overinterpreted: blow-up can occur with positive variance, and indeed simulations without noise typically show blow-up occurring while the variance is still clearly positive. Also, it is shown in [13] for the supercritical case $\sigma D > 2$ under mild technical conditions that blow-up occurs with positive probability for any initial data and level of noise, though that leaves open the intuitive possibility that for initial data not giving blow-up in the noise-free case, adding noise might produce only a low probability of blow-up.

Such formulas have not yet been extended to account for damping, but as seen below, there are hints of damping contributing an additional negative term in $d\mathcal{H}/dt$, in some sense favoring blow-up.

3.2. Exciton energy self-trapping in the discrete system

With no noise or damping, numerical simulations of discrete counterparts of the NLS equation show phenomena analogous to blow-up, which has been named *discrete self-trapping*. That is, solutions can have the exciton energy concentrate until a substantial fraction of the total is at a single node (molecule), and then stay trapped in a solution that seems to oscillate around a stable steady state. This was first described by Davydov [10] in models of protein molecules, and further analyzed and simulated by Eilbeck, Lomdahl and Scott [24,16,17].

No analogues of the above formulas and results are known for discrete NLS equations, even without noise, but for a

heuristic comparison, note that a discrete SNLS with spatially uncorrelated noise on a grid of spacing l effectively has noise correlation length scale l so that Eqs. (12) and (13) hint that both increasing the noise strength and refining the mesh spacing in a discretization of SNLS could favor inhibition of self-trapping.

For the discrete systems with noise, no formulas are known for the evolution of ensemble averages considered above. The closest analogue to the results for SNLS is that from Eq. (1) the Hamiltonian evolution for individual realizations satisfies

$$\frac{d\mathcal{H}}{dt} = \sum_n \left\{ \dot{W}_n \frac{d}{dt} (|\psi_n|^2) - \lambda \left[\frac{d}{dt} (|\psi_n|^{2\sigma}) \right]^2 \right\}. \quad (14)$$

This no longer makes it clear that noise causes the previously noted linear increase in $\langle \mathcal{H} \rangle$, or corresponding growth in beam spatial variance or inhibition of wave collapse, but all these phenomena are still seen in numerical studies of discrete systems with spatially uncorrelated noise, such as in Section 5. This is to be expected, since those discrete systems are effectively discretizations of SNLS with noise of spatial correlation on a length scale comparable to the mesh spacing of the discretization.

3.3. Prior numerical results

The full 2D stochastic NLS equation with spatially uncorrelated noise has been simulated by Bang et al. [1], and the 1D quintic case of the stochastic NLS equation by DeBussche and Di Menza [14,15]. In each case it is observed that spatially uncorrelated noise can prevent blow-up.

In [1] it is concluded that this noise effect is too strong to match physical experiments: noise levels so low as to correspond to temperatures of a few kelvins are needed to reproduce behavior seen in experiments at far higher temperatures. The likely cause is “thermal runaway” due to the absence of a mechanism for “heat loss”, such as the damping term used here.

In [15] a large number of simulations of SNLS on a fixed spatial grid all have the maximum amplitude reach at least three times its initial value at some time, and this is interpreted as showing that spatially correlated noise (as is effectively imposed by a fixed spatial discretization) can only delay blow-up in critical SNLS with initially negative Hamiltonian, but cannot prevent blow-up. However Fig. 15 of that paper shows a case where a finer fixed spatial grid shows inhibition of blow-up, with the maximum amplitude never reaching twice its initial value and then decaying at later times: similar to Fig. 5.

The spatial structure seen in Fig. 4 suggests another possible interpretation of the growth of the maximum amplitude observed in [15]: that noise causes many brief, narrow spikes, and over long enough time almost inevitably at least one of these will have three or more times the initial maximum amplitude, but these noise induced spikes are typically far narrower than a developing self-focusing blow-up, and thus are transient, not continuing on to blow-up. Indeed, in our simulations, such spikes are typically only one or a few nodes wide, narrower than the spatial discretization can accurately

resolve in a solution of the SNLS, so that they are phenomena only of the discrete system, not of the PDE.

A more reliable criterion for numerical detection of NLS blow-up is that some substantial fraction of the exciton energy is concentrated in a very small part of the spatial domain. In terms of discrete NLS, self-trapping is indicated by a substantial fraction of the exciton energy occurring at a single node. In the simulations below, self-trapping is manifested by a majority of all exciton energy reaching and then staying at a single node, with this trapping persisting for considerably longer than the rise time of the self-trapping.

As to damping effects, Eq. (14) indicates that damping has the opposite effect to noise, causing reduction of \mathcal{H} . Combined with the expectation that (10) still holds approximately for discretizations of SNLS, this suggests the possible return of self-trapping.

Christiansen et al. [8] have done the only simulations known to us of the model with damping in Eq. (2). They do this with further approximation by a single stochastic ODE, first imposing radially symmetry and then using the method of collective coordinates. Such modeling has led to some analytical results on self-focusing in the NLS equation, but with the stochastic terms, it still requires study primarily by simulation.

They start with simulations without damping, corroborating the above described observations about inhibition of blow-up by sufficiently strong noise, leading instead to dispersion of initially concentrated wave energy. With damping added, they observe that the effect of noise can be reversed, leading to blow-up where with noise alone it would not occur, as suggested by Eq. (14). Again there appears to be a threshold damping level for this to occur with given initial data and noise level.

With this survey done, we are ready to consider new numerical methods and results of simulations based on Eq. (1).

4. Numerical method: A variant of the iterative trapezoid method of Chang and Xu

With noise but no damping, and with homogeneous coupling and periodic boundary conditions, a Fourier split-step method could be used, as was done by Bang et al. [1] for SNLS.

Instead, an implicit time discretization based on fixed point iterative solution of the trapezoid rule is used, similar to one described and analyzed by Chang and Xu [5]. It has several virtues:

- it satisfies the needed Stratonovic interpretation (no need for the Itô correction term),
- it conserves the exciton energy \mathcal{N} , and
- with no noise or damping, it conserves the Hamiltonian \mathcal{H} .

The main disadvantage is the need for iterative solution (so that conservation is no longer exact, but still highly accurate). Fortunately, most solutions of interest here develop spatial features at the single node spacing level, due to either self-trapping or the spatially uncorrelated noise, producing maximal spatial frequencies that generate the need to resolve the “worst-case” time scales indicated by the leading order term: we must

expect to need $\delta t = O(1/J)$. This step size ensures that even the simplest iterative methods will converge; Newton-style iterations and the updating of the linearization of the nonlinear terms are not needed.

4.1. A modified trapezoid method for conservation of \mathcal{N} and sometimes \mathcal{H}

Writing ψ_n^j for the approximations of $\Psi_n(t^j)$, $\delta t = t^{j+1} - t^j$, and $\delta W_n^j/\delta t$ for the approximation of \dot{W}_n , constant on $t^j \leq t \leq t^{j+1}$, the scheme used for the quintic case is

$$\begin{aligned} & i \frac{\psi_n^{j+1} - \psi_n^j}{\delta t} + \sum_m J_{nm} \frac{\psi_m^j + \psi_m^{j+1}}{2} \\ & + \left[\frac{|\psi_n^j|^4 + |\psi_n^j|^2 |\psi_n^{j+1}|^2 + |\psi_n^{j+1}|^4}{3} \right. \\ & \left. + \gamma \frac{\delta W_n^j}{\delta t} + \lambda \text{Im} \left(\overline{\psi_n^j} \sum_m J_{nm} \psi_m^j + \overline{\psi_n^{j+1}} \sum_m J_{nm} \psi_m^{j+1} \right) \right] \\ & \times \frac{\psi_n^j + \psi_n^{j+1}}{2} = 0. \end{aligned} \quad (15)$$

The quintic nonlinearity needs this special form to conserve the Hamiltonian in the absence of noise and damping; for the cubic case, the familiar trapezoid form $(|\psi_n^j|^2 + |\psi_n^{j+1}|^2)/2$ suffices.

For the case studied so far of totally uncorrelated noise, the noise components δW_n^j are independent with normal distribution of mean zero, standard deviation $\sqrt{\delta t}$. Thus $\delta W_n^j/\delta t$ has standard deviation $1/\sqrt{\delta t}$, a hint at the time step restrictions needed to resolve noise effects accurately.

4.2. Linearly implicit iterative approximation of the trapezoid method, conserving \mathcal{N}

The coupled nonlinear equations given by the trapezoid method can be solved by a *linearly implicit* fixed point iteration, in which certain occurrences of the unknown ψ_n^{j+1} are replaced by the approximation from the latest iteration, producing simultaneous linear equations for the new iterate.

Writing $\psi_n^{j+1,k}$ for the k th iterate, the initial approximation used for the new time step is $\psi_n^{j+1,0} = \psi_n^j$, and the components $\psi_n^{j+1,k}$ of each subsequent iterate are found by solving

$$\begin{aligned} & i \frac{\psi_n^{j+1,k} - \psi_n^j}{\delta t} + \sum_m J_{nm} \frac{\psi_m^j + \psi_m^{j+1,k}}{2} \\ & + \left[\frac{|\psi_n^j|^4 + |\psi_n^j|^2 |\psi_n^{j+1,k-1}|^2 + |\psi_n^{j+1,k-1}|^4}{3} + \gamma \frac{\delta W_n^j}{\delta t} \right. \\ & \left. + \lambda \text{Im} \left(\overline{\psi_n^j} \sum_m J_{nm} \psi_m^j + \overline{\psi_n^{j+1,k-1}} \sum_m J_{nm} \psi_m^{j+1,k-1} \right) \right] \\ & \times \frac{\psi_n^j + \psi_n^{j+1,k}}{2} = 0. \end{aligned} \quad (16)$$

Note the use of the new unknown iterate in the final factor of the nonlinear term rather than the previous iterate as would

normally be done to get a linear iterative scheme: this change is what guarantees exact conservation of the exciton energy at each iteration while still giving linear equations.

Experiment and heuristic error analysis show that only three iterations are needed in this scheme; when convergence to the exact solution of the implicit trapezoid scheme is too slow for three steps to suffice, this indicates that implicit trapezoid solution is itself insufficiently accurate, so that time step reduction is needed rather than more iterations.

The iterative approximation no longer conserves the Hamiltonian \mathcal{H} exactly, but with these three iterations the error in \mathcal{H} is already far less than the overall second order accuracy suggests. This is presumably because this error comes only from the difference between the third iterate and the exact solution of the implicit trapezoid scheme, which is third order: $O(\delta t^3)$.

4.3. Time step size choice and accuracy checking

As already noted above, we expect to need time steps no larger than $O(J^{-1})$. However, even more is probably needed. The local truncation error (per unit time) of the trapezoid method is $\|u_{ttt}\delta t^2/12\|$ and considering just the coupling term $du_n/dt = iJ\Delta u_n + \dots$ (with Δ the second difference operator), $d^3u_n/dt^3 = -iJ^3\Delta^3u_n + \dots$. Thus we must expect $\|u_{ttt}\|$ of magnitude up to $\|\Delta\|^3\|u\|J^3$ and relative errors of up to $(4J)^3\delta t^2/12 = 16J^3\delta t^2/3$, so that for error tolerance ϵ we expect to need $\delta t \lesssim \sqrt{3\epsilon/J^3}/4$, which is $O(J^{-3/2})$ rather than $O(J^{-1})$.

For a modest error tolerance $\epsilon = 10^{-2}$ and $J = 100$ as used below, this suggests $\delta t \lesssim \sqrt{\epsilon/J^3} = 10^{-4}$.

Accuracy is tested in practice by repeated halving of step size. In order to do this while maintaining a consistent noise realization, noise is generated on a time scale δ_{noise} finer than is expected to be needed, and then the time steps tried are of the form $2^p\delta_{\text{noise}}$. Due to the above estimate, our computations use $\delta_{\text{noise}} = 10^{-5}$, with the values of δt needed ranging from 10^{-5} to 8×10^{-5} .

5. Numerical results

For computational efficiency, simulations of the damped stochastic discrete NLS equation (1) have been done with a single computational space dimension, using two different approaches to this reduction of dimension.

The main studies are done for the one dimensional quintic case $D = 1$, $\sigma = 2$, with this somewhat unnatural nonlinearity power used for the sake of remaining in the critical case for collapse in NLS. Homogeneous nearest neighbor coupling is used. Nearest neighbor coupling makes sense in the physical models, since dipole interactions are very short range. It also makes little sense to use higher order spatial discretizations of stochastic NLS equations, because the noise eliminates the higher order smoothness needed to make such discretizations more accurate. This case, without damping, was also studied by DeBussche and Di Menza [14,15], as discussed in Section 3.2.

The second reduction used is imposing radial symmetry on the two dimension cubic NLS ($D = 2$, $\sigma = 1$), and then again

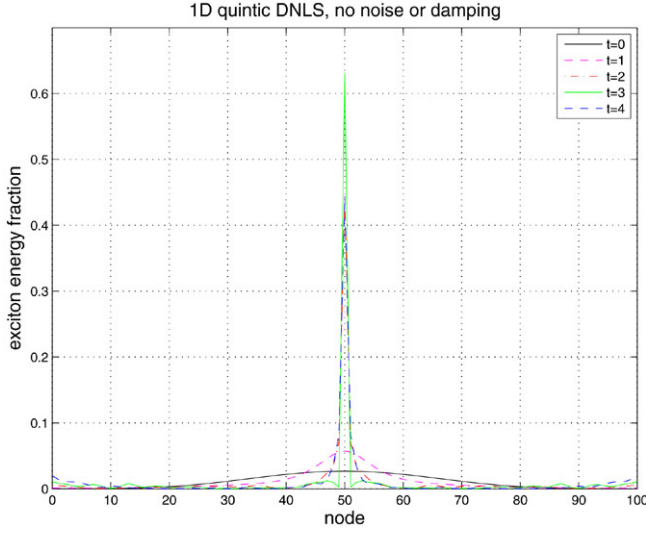


Fig. 1. Exciton energy distribution for 1D quintic, no noise or damping.

using standard three point discretization of spatial derivatives. This allows comparison to the results of Bang, Christiansen et al. [1,8] also discussed above.

5.1. 1D lattice with quintic nonlinearity and homogeneous nearest neighbor coupling

The solutions in this section all have $J = 100$, $N + 1 = 101$ nodes, and initial data $\Psi_n(0) = \psi_0(x_n) = (1 - \cos 2\pi x_n)/2$, $x_n = n/N$, $0 \leq n \leq N$. These are chosen to give Hamiltonian \mathcal{H} just slightly negative, corresponding to the sufficient condition for blow-up in NLS, and indeed they lead to discrete self-trapping when noise and damping are absent.

Noise when present has strength $\gamma = 0.5$, and the default damping strength is $\lambda = 0.01$, with these choices explained below. Also, results for a single “standard noise realization” are presented in many graphs, with corroboration by data from multiple realizations where appropriate.

5.1.1. Self-focusing and exciton energy self-trapping without noise or damping

The time evolution of Eq. (1) in the 1D quintic case without any noise or damping is illustrated in Figs. 1 and 2, which show the distribution of the fraction of exciton energy at each node, $|\Psi_n(t)|^2/\mathcal{N}$, for various times t . The first figure shows all nodes, at two times before self-trapping occurs at $t = t^* \approx 1.3$ and three times afterwards. The second graph shows the details of nodes near the self-trapping locus, showing the trapping of a majority of all energy at a single node.

Note that by the time that the exciton energy fraction at any node exceeds about one half, energy is largely concentrated on at most a couple of nodes, so that the solution is no longer accurate as a discrete approximation of NLS. Likewise, in all subsequent solutions data past the time when the exciton energy at any node first exceeds one half are only relevant to the spatially discrete model.

The evolution of the degree of exciton energy self-trapping is shown in Fig. 3, as measured by the maximum fraction of

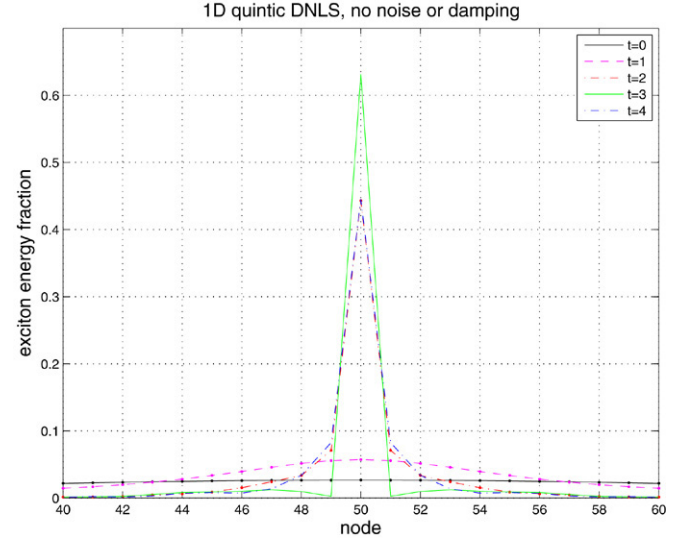


Fig. 2. As in Fig. 1 but restricted to nodes near the self-trapping locus, showing exciton energy persistently concentrated largely at a single node.

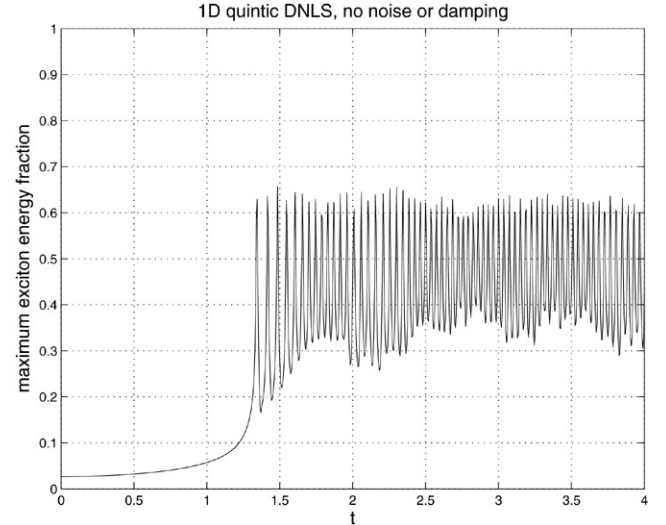


Fig. 3. Evolution of the maximum exciton energy fraction, for 1D quintic, no noise or damping.

exciton energy at any one node, as a function of time. Once energy self-trapping has occurred, it is seen to persist, but with significant oscillations. The oscillations fit with the idea of the solution entering a neighborhood of an orbitally stable stationary state that is a center: the existence of such localized stable center stationary states has been proven in the minimal case of $N = 2$ by Eilbeck et al. [17].

Note that this oscillatory behavior is purely a property of the discrete system, as it only sets in after the maximum single node energy becomes too high for the numerical solutions to be relevant to the related PDE models.

5.1.2. Inhibition of self-focusing by sufficient noise, without damping

The results here are much as seen in the simulations by various previous authors discussed in Section 3.2. With low levels of noise $\gamma \lesssim 0.5$, focusing of energy to a single node

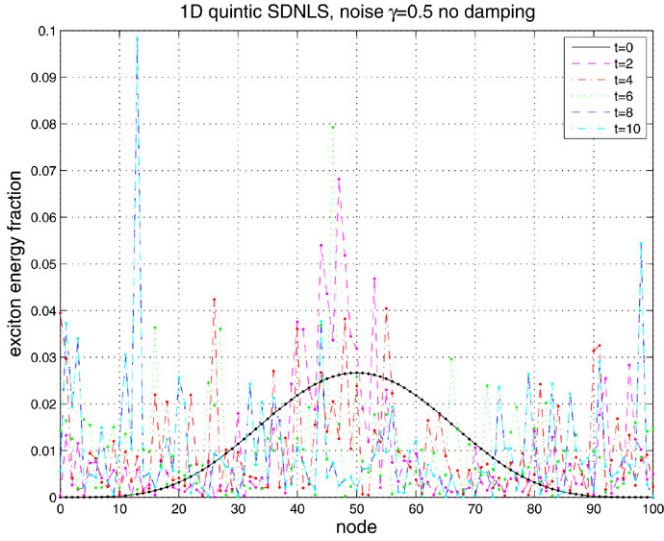


Fig. 4. Exciton energy distribution for 1D quintic, noise $\gamma = 0.5$, no damping.

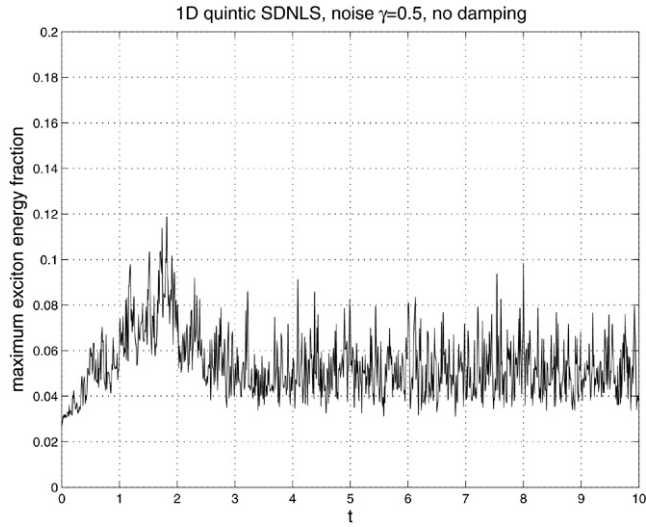


Fig. 5. Maximum single node exciton energy fraction for 1D quintic, noise $\gamma = 0.5$, no damping.

followed by persistent self-trapping still occurs. Higher noise levels of $\gamma \geq 0.5$ inhibit self-focusing and energy self-trapping, as shown in Fig. 4 for the single standard noise realization, and confirmed in all other noise realizations computed.

Another notable feature is the loss of the spatial smoothness that would be needed for continuum limit PDE modeling. It seems likely that this spatial disorder has the effect of inhibiting exciton wave propagation, and that this is the mechanism which prevents energy self-trapping, by preventing the needed energy flux.

The evolution of the degree of self-trapping, or lack thereof, is shown in Fig. 5. Note that transient spikes to values considerably greater than the initial value occur, above all close to the focusing time $t^* \approx 1.3$ noted above, but these are not indications of focusing towards self-trapping. Continuing this solution for considerably more time never again reaches the maximum of about 0.12 seen at $t \approx 1.8$.

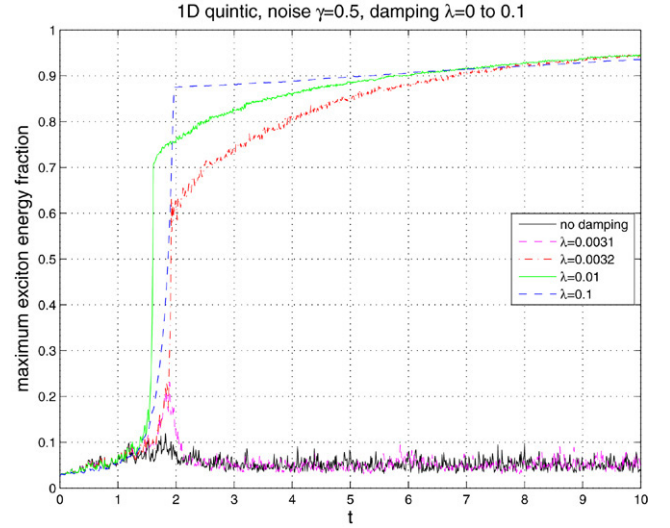


Fig. 6. Maximum single node exciton energy fraction for 1D quintic, noise $\gamma = 0.5$, damping from none to $\lambda = 0.1$.

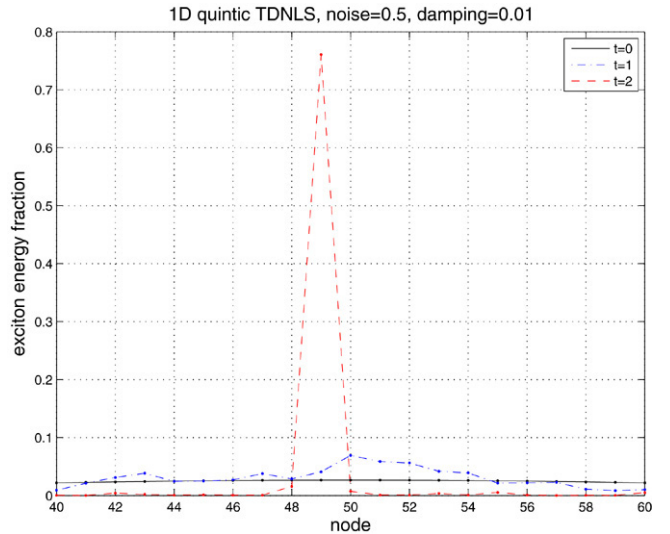


Fig. 7. Exciton energy distribution for 1D quintic, noise $\gamma = 0.5$, damping $\lambda = 0.01$, early times.

5.1.3. Effects of adding both damping and noise

The effect of adding damping at various strengths while maintaining the noise level of $\gamma = 0.5$ is summarized in Fig. 6 in terms of the maximum fraction of total exciton energy at any single node, and spatial structure is shown for the case $\lambda = 0.01$ in Fig. 7.

Small damping values ($\lambda \leq 0.0031$) cause a transient increase in collapse, but not enough to produce self-trapping; instead, one eventually gets dispersion, as with damped noise. With damping above some threshold near $\lambda = 0.0032$, collapse proceeds to persistent self-trapping of over 90% of exciton energy at a single node. Apparently solutions settle into a very close approximation of a steady state that has energy almost completely localized. This is also true at the lower damping values for which self-trapping is seen, but with far slower onset.

This strong spatial self-trapping for $\lambda = 0.01$ is shown in Fig. 8, which gives data for four times after the onset of

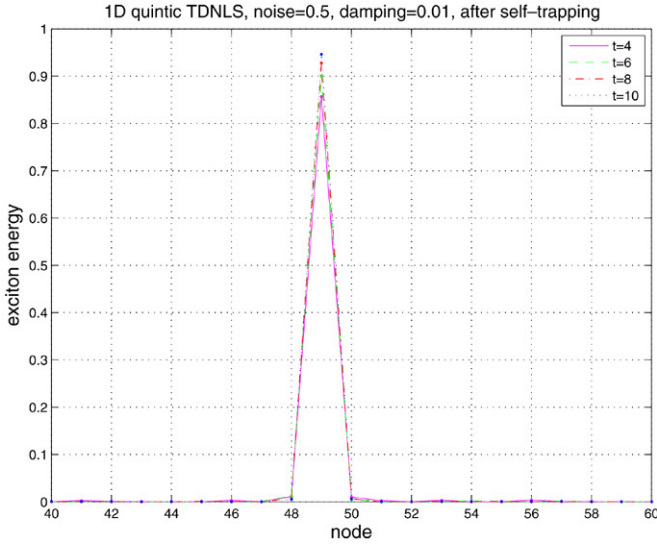


Fig. 8. As above but for times after the onset of self-trapping, showing the persistence of a near steady state.

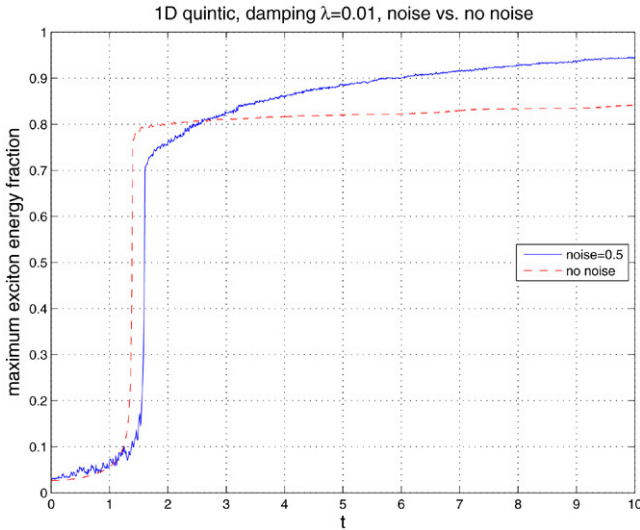


Fig. 9. Maximum single node exciton energy fraction for 1D quintic, damping $\lambda = 0.01$, for both noise $\lambda = 0.5$ and no noise.

self-trapping. This and the previous graph show a form far closer to a steady state than for the undamped, noiseless case above. The strong oscillations seen previously are absent here, replaced only by far smaller fluctuations, perhaps just those inevitably caused by the noise.

Fig. 9 compares the approach to a nearly stationary state to a solution with the same damping but no noise: there is relatively little difference, indicating that damping is the dominant mechanism driving the solution towards a steady state, and that this mechanism is robust enough to be little perturbed by noise.

5.1.4. Connections to evolution of the Hamiltonian

There are indications in Eqs. (10)–(14) that the evolution of the Hamiltonian \mathcal{H} could be related to the occurrence of self-focusing and self-trapping of energy, as it is for the NLS, so this will be examined.

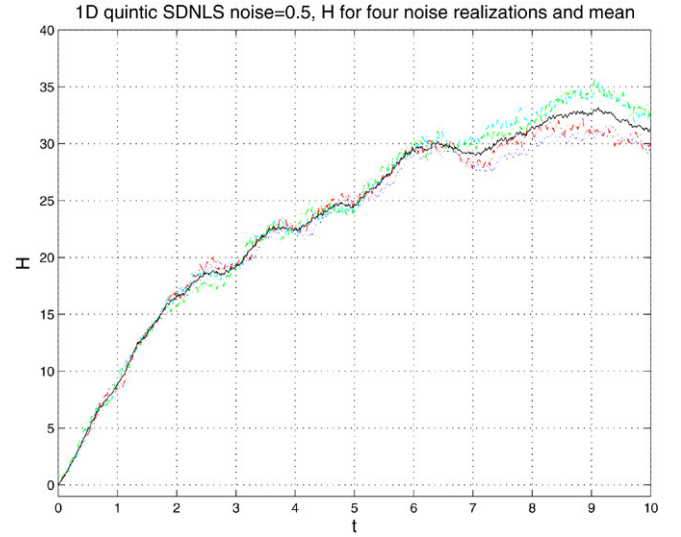


Fig. 10. Hamiltonian for 1D quintic, noise $\gamma = 0.5$, no damping.

First, it can be shown that the results of Eqs. (11) and (13) apply at least qualitatively to the discrete system with noise but no damping, by considering the latter as a discretization of the stochastic NLS with noise having correlation length scale proportional to the lattice spacing l . Since the precise constant of proportionality is not known, this will be done by checking first that $\langle \mathcal{H} \rangle$ grows roughly linearly in time, and then by observing that this linear growth rate is roughly proportional to N^3 , as suggested by Eq. (13).

The evolution of $\langle \mathcal{H} \rangle$ is approximated by the black curve in Fig. 10. This is the average of results for four noise realizations shown by the colored curves, of which the blue curve corresponds to the single realization used in earlier graphs. It is seen that there is indeed a roughly linear growth in time up to about $t = 2$, and at a rate that is very consistent between realizations.

Increasing N with initial data and noise adjusted as for grid refinement in discretization of the SNLS, the initial approximately linear growth rate of the Hamiltonian varies roughly as N^3 , which is consistent with the suggestion of Eqs. (11) and (13). This indicates that in the continuum limit $N \rightarrow \infty$ of SNLS with uncorrelated noise, \mathcal{H} would become infinite instantly, and so that this equation is ill-posed in H^1 .

Eq. (14) suggests that the addition of damping might at least partially offset the growth of \mathcal{H} caused by noise. It is natural to ask under what circumstances this effect is sufficient to bring \mathcal{H} back to negative values, and how the restoration of negative \mathcal{H} is related to the restoration of energy self-trapping, and the answers appear to be positive.

In the less interesting case of damping insufficient to restore energy self-trapping, \mathcal{H} initially grows roughly linearly as without damping, but then levels out to fluctuation around a significantly positive value.

With damping sufficient to restore self-trapping ($\lambda = 0.01$, $\gamma = 0.5$), Fig. 11 shows for each of four realizations there is initial roughly linear growth of \mathcal{H} at about the same rate as seen above, but this is followed by slowing of the growth, and then a sudden drop to negative values. These negative values quickly

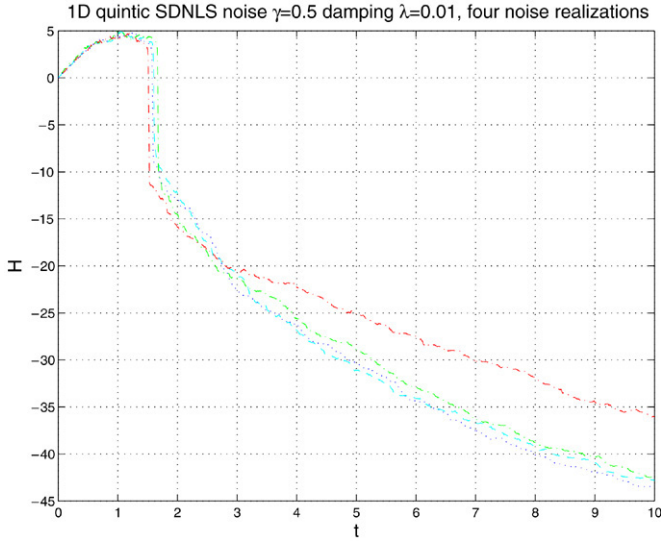


Fig. 11. Hamiltonian for 1D quintic, noise $\gamma = 0.5$, damping $\lambda = 0.01$. Same noise realizations as in Fig. 10.

become very large and remain so, as verified by computation to far longer times, not shown here. For each realization, the time of this drop is fairly close to the time at which self-trapping occurs, and indeed is driven by the sixth power nonlinearity term in \mathcal{H} taking on a large negative value when the energy at any one node is a substantial proportion of the total.

6. Continuum limit approximations and simulations

PDE's such as the DSNLS equation (2) which arise as continuum limits of the discrete model studied here have some potential advantages, such as the greater possibilities for theoretical results (evolution of the “total energy” \mathcal{H} , the variance results for collapse) and for reduced models allowing efficient simulation. One drawback is that the continuum limit is only valid so long as phenomena have a spatial length scale significantly exceeding the node spacing, and thus exceeding the correlation length scale of the noise. Thus continuum models are not valid in the regimes seen above where energy is concentrated at a single node (Figs. 1 and 7) or where noise produces non-smoothness in the form of significant variations in value of ψ_n at neighboring nodes (Fig. 4).

Thus such models are at best informative when such fine spatial structure is not present, including at early times in a solution in which fine structure develops later. For example, proofs or numerical evidence of single point blow-up in a continuum approximation can support at least the conclusion that the underlying discrete equations have substantial energy self-trapping, at least down to the length scale of about a dozen nodes at which the continuum approximation breaks down.

Another continuum modeling approach would be to retain higher order terms in approximating the discrete coupling terms by Taylor series expansions, which preserves explicit dependence on a node spacing length l . Returning to the original physical model of a two dimensional lattice with cubic nonlinearity, and assuming sufficient symmetry such as

the dihedral D_2 symmetry of the brick-wall molecular film structure, one gets

$$\sum_m J_{nm} \Psi_m = j_{2,0} \psi_{xx} + j_{0,2} \psi_{yy} + l^2 [j_{4,0} \psi_{xxxx} + j_{2,2} \psi_{xxyy} + j_{0,4} \psi_{yyyy}] + O(l^4). \quad (17)$$

With the physically natural assumption of non-trivial and attractive coupling, meaning that all J_{nm} are non-negative and some are positive, all the new j_{ab} coefficients are non-negative and all j_{a0}, j_{0b} are positive. Discarding terms $o(l)$ gives DSNLS as before, but retaining the next terms of $O(l^2)$ and linear rescaling of the x and y variables then gives the form

$$i \frac{\partial \psi}{\partial t} + \Delta \psi + l^2 [j_{4,0} (\psi_{xxxx} + \psi_{yyyy}) + j_{2,2} \psi_{xxyy}] + |\psi|^2 \psi + \gamma \sigma \psi - \lambda \frac{\partial (|\psi|^2)}{\partial t} \psi = 0. \quad (18)$$

With nearest neighbor coupling on a rectangular lattice the cross derivative term vanishes ($j_{2,2} = 0$), but that does not fit the brick-wall symmetry observed for cyanine dye Scheibe aggregates.

Another higher order model comes from using Padé fitting to the coupling term instead of Taylor polynomials, giving a pseudo-differential equation. With nearest neighbor coupling on a rectangular lattice one can get

$$i \frac{\partial \psi}{\partial t} + \left[I - \frac{l^2}{12} \Delta \right]^{-1} \Delta \psi + |\psi|^2 \psi + \gamma \sigma \psi - \lambda \frac{\partial (|\psi|^2)}{\partial t} \psi = 0. \quad (19)$$

One potentially advantage is that the pseudo-differential operator is bounded, which explicitly removes the risk of an “ultra-violet catastrophe” and so might facilitate analysis.

6.1. Discrete 2D radially symmetric DSNLS

For numerical simulation, one advantage of a continuum limit is that it allows the use of dimensional reduction of the 2D lattice model through imposition of radial symmetry, as used in conjunction with a further collective coordinates reduction to a single nonlinear ODE in [8]. Note however that this involves the physically unlikely assumption of radially symmetric noise, and so is of primarily mathematical interest, and only for confirmation of the robustness of qualitative features of the inhibition of energy self-trapping by noise and its restoration by damping.

These qualitative features were observed in the single ODE reduction of [8] and corroborated above for the 1D quintic discrete system, and it will now be seen that they are also confirmed in simulations of the radially symmetric 2D cubic case of DSNLS. Such simulations also provide a computationally efficient initial comparison to simulations of the full 2D cubic SNLS model (with noise but no damping) by Bang et al. [1].

These simulations are done with a simple nearest neighbor discretization. Rather than pursue more sophisticated numerical

study of this equation, simulations of the full 2D discrete model are planned for a future paper.

All results are for the initial data from discretization of $\psi(0, r) = 1.65 \operatorname{sech}(r)$ on $0 \leq r \leq 10$ with 256 equally spaced nodes. This function is close to the ground state *Townes soliton*, giving the initial value of the Hamiltonian $\mathcal{H} \approx -0.006$ and $\mathcal{N} \approx 1.8867$, just above the collapse threshold value $N_c \approx 1.87$. Thus singularity formation is ensured in the absence of noise and damping, but only just. The idea of this initial data choice is to maximize the sensitivity of self-focusing effects to the perturbations applied.

Noise without damping inhibits self-trapping of energy if its strength γ exceeds a threshold, between 0.01 and 0.02. The Hamiltonian for each realization \mathcal{H} grows roughly linearly in time, and the approximation of the ensemble average $\langle \mathcal{H} \rangle$ given by averaging even a few realizations grows even faster. If the spatial discretization is refined to more nodes, the rate constant increases rapidly, suggesting the failure of the continuum limit and ill-posedness of this form of SNLS.

With above-threshold noise $\gamma = 0.02$, damping restores energy self-trapping once its strength λ in turn exceeds a threshold, between 0.05 and 0.1. This is related to first slower growth of \mathcal{H} , and then its decrease to substantially negative values at about the same time as the self-trapping.

6.2. The 1D quintic continuum limit solved with spectral spatial discretization

As a final test of the robustness of these phenomena under modeling approximations, the DSNLS continuum limit in the 1D quintic case above has been solved numerically using a discretization very far from the three point scheme corresponding to the discrete system: spectral discretization, with periodic boundary conditions.

Once again, the main qualitative features described above are seen, so details are omitted.

7. Conclusions and plans

Noise without damping has been seen to inhibit self-trapping in the discrete system, and this is related to an increase in the (initially negative) Hamiltonian. There is a minimum noise level needed to do this; with sufficiently low noise levels, self-trapping still occurs. This pattern is as suggested by the theoretical results of [18,13] for the continuum limit case with spatially correlated noise.

With damping as well as noise, self-trapping is seen to be restored, again with a threshold. That is, for a given noise level that without damping would inhibit self-trapping, sufficiently low damping levels still lead to no self-trapping, but stronger damping restores self-trapping. The damping level needed to restore self-trapping is also that which suffices to reverse the noise induced growth of the Hamiltonian, causing it instead to return to negative values.

The continuum limit as a stochastic NLS equation with spatially uncorrelated noise appears to be ill-posed, at least in H^1 : solutions develop substantial differences between the

values at neighboring nodes. When self-trapping occurs, it also involves such substantial differences, so again the phenomenon is outside the realm of the SNLS continuum limit.

Directions for future work include the simulation and analysis of full 2D models; consideration of the 1D cubic case and related models of nonlinear waves in long biomolecules, where energy self-trapping still occurs in discrete NLS models but the NLS continuum limit does not have self-focusing blow-up; analysis of the well-posedness of various PDE and pseudo-differential equation models, including the effects of damping; direct analysis and study of the ODE system (lattice models) with various interaction forms such as longer range; and simulation with time correlation in the noise, as seen in Eq. (7).

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