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MODELING THERMAL EFFECTS ON NONLINEAR WAVE MOTION IN BIOPOLYMERS BY A STOCHASTIC DISCRETE NONLINEAR SCHRÖDINGER EQUATION WITH PHASE DAMPING

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Abstract. A mathematical model is introduced for weakly nonlinear wave phenomena in molecular systems like DNA and protein molecules that includes thermal effects: exchange of heat energy with the surrounding aqueous medium. The resulting equation is a stochastic discrete nonlinear Schrödinger equation with focusing cubic nonlinearity and "Thermal" terms modeling heat input and loss: PDSDNLS.

New numerical methods are introduced to handle the unusual combination of a conservative equation, stochastic, and fully nonlinear terms. Some analysis is given of accuracy needs, and the special issues of time step adjustment in stochastic realizations. Numerical studies are presented of the effects of thermalization on solitons, including damping induced *self-trapping* of wave energy, a discrete counterpart of single-point blowup.

1. **Introduction.** Pulse propagation in bio-polymers is of possibly great significance to energy transmission in protein and conformational change in DNA, and accurate mathematical modeling relies on nonlinear effects and thermal effects: energy input to internal vibrational modes from heat in the aqueous medium of the molecule, and energy loss through radiation from such modes.

The modeling and theory started with the work of Davydov [6, 7, 8] on protein molecules, giving continuum limit equations related to the (one-dimensional, focusing, cubic) nonlinear Schrödinger equation (NLS), with the sech soliton solutions of that equation playing an important role as pulses capable of carrying energy for significant distances along molecules.

Further developments by Scott, Eilbeck and Lomdahl [10, 15] emphasized spatially discrete models rather than continuum limits, and extended such models to other molecules. Indeed, such discrete NLS (DNLS) models seem to arise from a few generic features: dipole coupling along polymers interacting with localized vibration modes with faster time scales. An important feature revealed only by spatially discrete models is *self-trapping* driven by nonlinear self-focusing, in which energy from traveling pulses becomes localized in an oscillation at one or a few spatial nodes.

More recent work by Bang, Christiansen, Giadidei, If, Johansson, Kivshar, Mingaleev, K. Rasmussen, Yakimenko [1, 5, 14] extends such modeling to DNA molecules, and adds thermal effects, modeling thermal energy input and radiation as stochastic

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driving and liner damping respectively of local vibration modes. Discrete models become even more important with stochastic effects, since these violate the smoothness over longer spatial scales need to justify continuum limit, so here Stochastic Discrete NLS (SDNLS) models are considered, with only occasional comparisons to more familiar NLS and Stochastic NLS (SNLS) models for comparisons. Also, previous work shows that modeling thermal energy input by stochastic driving but without a balancing energy loss mechanism leads to unphysical effects: excessive disorder and disruption of pulses, due to *thermal run-away* [1].

Thus a major goal here is proper handling of the internal mode damping, introduced in previous models but not handled in simulations, and direct attention to the discrete model rather than passing to continuum limits and then discretizing for numerical simulations. The internal mode damping means that the equations are no longer semi-linear (or even quasi-linear), and thus their numerical solution requires some refinement of previous numerical methods for NLS and SNLS, refinements first introduced in [13], which deals with a related model of two dimensional molecular lattices.

Numerical studies are then done are then applied to the effects of thermalization on solitons and self-trapping.

2. **Physical modeling and the slowly varying amplitude approximation.** The model used here is introduced in [1, 4], and full details of the derivation can be found there. Without modeling thermal energy input and radiation, a fully quantum mechanical derivation can be made from a Hamiltonian, as done by Bartnick and Tuszyński [2]. In semi-classical reduction, this comes from a Hamiltonian $\mathcal{H} = \mathcal{H}_{co} + \mathcal{H}_{ph} + \mathcal{H}_{int}$ where

- $\mathcal{H}_{co} = -\sum_{n,m\neq n} J_{nm}\overline{\psi}_n\psi_m$ is the energy of coupling between the *exciton* modes ψ_n of nearby molecular subgroups,
- $\mathcal{H}_{ph} = \frac{M}{2}\sum_n \left[(du_n/dt)^2 + (\omega_0 u_n)^2\right]$ is the energy of localized *phonon* modes u_n, such as vibrations of molecular bonds, and
- $\chi|\psi_n|^2 u_n$ is the energy of interaction between the exciton and phonon modes.

The system of ODE's arising from that Hamiltonian can be modified by adding random driving forces on phonon modes from Brownian motion, $\nu\dot{w}_n(t)$ and energy loss from the phonon modes modeled as linear damping, $-M\lambda du_n/dt$, giving the system

$$i\frac{d\psi_n}{dt} + \sum_{m\neq n} J_{nm}\psi_m + \chi u_n\psi_n = 0 \tag{1}$$

$$M\frac{d^2u_n}{dt^2} + M\lambda\frac{du_n}{dt} + M\omega_0^2 u_n = \chi|\psi_n|^2 + \nu\dot{w}_n(t) \tag{2}$$

Molecular bending, stretching and motion are ignored, so we model "straight, stationary" molecules: c.f. [5, 14].

Here, J_{nm} is the strength of the dipole coupling interactions between molecular sub-groups; χ is the strength of exciton-phonon coupling; M is the mass of each molecular sub-group; ω_0 is the frequency of the phonons; $\dot{w}_n(t)$ is the formal derivative of a Wiener process representing random external forces such as collisions with water molecules, uncorrelated in n and t; ν is the strength of the random external forces; and λ is the strength of the phonon damping or radiation rate.

Typically the coupling constants are uniform except at domain boundaries, so that the quantities $J_{nn} := \sum_{m\neq n} J_{nm}$ have a common value J_0 except possibly at some boundary nodes. Then it is convenient to remove a fast phase evolution term e^{itJ_0} by adding $-J_0 \sum_n |\psi_n|^2$ to the coupling energy. Next, the u_n can be eliminated with the variation of parameters formula, giving a time integral expression in terms of the single node exciton energy $\mathcal{E}_n = |\psi_n|^2$ and $\dot{w}_n$. Using the slowly varying amplitude approximation that the exciton amplitudes vary far slower than the phonon frequency, $|(\mathcal{E}_n)_t \ll \omega_0$, and with some rescaling of variables to eliminate various constants, one gets the central object of this study, the *Phase Damped Stochastic Discrete Nonlinear Schrödinger Equation* (PDSDNLS)

$$i\frac{d\psi_n}{dt} = -\mathcal{L}\psi_n + \left[-|\psi_n|^2 - \nu\dot{W}_n(t;\omega) + \lambda\frac{d}{dt}(|\psi_n|^2)\right]\psi_n, \text{ where} \tag{3}$$

$$\dot{W}_n(t) = \int_0^t e^{-\lambda\omega_0^2 s/2}\sin(\omega s)\dot{w}_n(t-s)ds, \quad \mathcal{L}\psi_n = \sum_m J_{nm}\psi_m. \tag{4}$$

The coupling operator $\mathcal{L}$ typically resembles a discrete second derivative: for example with uniform nearest neighbor only interactions and defining $1/\delta x^2$ as the common non-zero coupling strength $J_{n,n\pm1}$, $\mathcal{L}\psi_n = (\psi_{n-1} - 2\psi_n + \psi_{n+1})/\delta x^2$.

The new noise terms $\dot{W}_n(t)$ are still uncorrelated in n, but are now correlated in time through the integral in (4). Note however that the correlation is on a time scale of $1/(\lambda\omega_0^2)$, and since ω_0 gives the fast time scale suppressed by the slowly varying envelope approximation; thus, once the rescaled damping strength λ is sufficient, this temporal correlation time scale will be smaller than the time scale on which the model is valid, rendering the noise effectively uncorrelated again. Thus, temporal noise correlation is ignored below, and the numerical solutions below are done with uncorrelated random values.

It is sometimes useful to eliminate the time derivative from the damping related term. Solving Eq. (3) for $d\psi_n/dt$ and substituting into that term gives

$$i\frac{d\psi_n}{dt} = -\mathcal{L}\psi_n + \left[-|\psi_n|^2 - \nu\dot{W}_n(t;\omega) - 2\lambda\mathrm{Im}\left(\overline{\psi}_n\mathcal{L}\psi_n\right)\right]\psi_n. \tag{5}$$

The resemblance of the coupling term to a discrete second derivative suggests a continuum limit: the *Phase Damped Stochastic Nonlinear Schrödinger equation* (PDSNLS)

$$\begin{aligned} i\frac{\partial\psi}{\partial t} &= -\psi_{xx} + \left[-|\psi|^2 - \nu\dot{W} + \lambda\frac{\partial(|\psi|^2)}{\partial t}\right]\psi, \\ &= -\psi_{xx} + \left[-|\psi|^2 - \nu\dot{W} - 2\lambda\mathrm{Im}\left(\overline{\psi}\psi_{xx}\right)\right]\psi. \end{aligned} \tag{6}$$

Without the phase damping term, this is the much studied 1D Stochastic Nonlinear Schrödinger equation (SNLS). This continuum limit can be useful for comparison to familiar properties of the NLS equation and for describing initial data. However, many interesting phenomena in the PDSDNLS model are at the scale of single nodes and lead to spatial non-smoothness which invalidates such a PDE model.

2.1. **Conserved quantities and energies of PDSDNLS.** The *exciton energy* $\mathcal{E} = \sum_n |\psi_n|^2$ is always conserved. The DNLS (no noise or damping) also conserves

its hamiltonian or *total energy*

$$\mathcal{H}_0 = -\sum_{n,m} J_{nm}\overline{\psi}_n\psi_m - \frac{1}{2}\sum_n |\psi_n|^4 = -\sum_n \overline{\psi}_n \mathcal{L}\psi_n - \frac{1}{2}\sum_n |\psi_n|^4.$$

With noise and damping, the total energy evolves under PDSDNLS as

$$\frac{d\mathcal{H}_0}{dt} = \sum_n \left\{ \nu \dot{W}_n(t;\omega)\frac{d}{dt}|\psi_n|^2 - \lambda\left[\frac{d}{dt}|\psi_n|^2\right]^2 \right\}. \tag{7}$$

Note that the damping term does indeed cause loss of total energy. The effect of noise is less clear, and nothing is proven for the discrete system, but for the SNLS with spatially correlated noise, it is known that the ensemble average of the energy grows linearly in time ([9, 11, 12]), and this is confirmed by the numerical results of [13] and in Fig. 2(c) below.

2.2. **Stratonovic stochastic integral form.** The above equations must be interpreted via stochastic integral equations, and in in order to respect conservation of the exciton energy, the Stratonovic stochastic integral must be used rather than the more common Itô stochastic integral.

An equivalent system of ODE's can be constructed which give the same solutions under the Itô integral interpretation, by adding the so-called Itô correction term to the time derivative:

$$d\psi_n/dt = [\text{as before}] - (\nu^2/2)\psi_n. \tag{8}$$

However, this is unpleasant as it destroys the conservative form with a fast decay factor, needed to counter rapid exponential growth in the Itô interpretation of the uncorrected equation, adversely affecting numerical solution.

3. Numerical methods.

3.1. **A conservative linearly implicit iterative approximation of the trapezoid method.** The fully nonlinear damping term present here prevents the use of Fourier split-step methods popular with NLS type equations. Thus instead, an implicit time discretization based on fixed point iterative solution of the trapezoid rule is used, similar to one analysed by Chang and Xu [3]. This has several virtues:

- it satisfies the needed Stratonovic interpretation,
- it exactly conserves the exciton energy $\mathcal{E}$, and
- with no noise or damping, it exactly conserves the total energy $\mathcal{H}_0$.

The main disadvantage is the need for iterative solution, and the fact that it is difficult to go beyond simple fixed point iteration due to the existence of coupled nonlinear terms, leading to the time step size restrictions typical of an explicit method rather than the underlying implicit method. The exact conservation of exciton energy $\mathcal{E}$ is preserved by using an iterative scheme with linearization of only the *effective potential* $V := -|\psi|^2 - \nu\dot{W} - 2\lambda\mathrm{Im}\left(\overline{\psi}\mathcal{L}\psi\right)$ as detailed below.

3.2. **Trapezoid method: conservative time discretization.** 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

$\dot{W}_n(t)$, constant on $t^j \le t \le t^{j+1}$, the underlying trapezoid method is

$$i\frac{\psi_n^{j+1}-\psi_n^j}{\delta t}+\sum_m J_{mn}\frac{\psi_m^j+\psi_n^{j+1}}{2}+\left[\frac{|\psi_n^j|^2+|\psi_n^{j+1}|^2}{2}+\nu\frac{\delta W_n^j}{\delta t}\right.$$
$$\left.+\lambda\mathrm{Im}\left(\overline{\psi_n^j}\sum_m J_{mn}\psi_m^j+\overline{\psi_n^{j+1}}\sum_m J_{mn}\psi_n^{j+1}\right)\right]\times\frac{\psi_n^j+\psi_n^{j+1}}{2}=0 \qquad (9)$$

For the approximation of totally uncorrelated noise used here, the noise components δW_n^j are independent with normal distribution of standard deviation $\sqrt{\delta t}$, mean 0.

3.3. **Conservative iterative approximation of the trapezoid method.** The nonlinear implicit scheme can be solved by a simple *linearly implicit* fixed point iteration in which the problematic quadratic nonlinear terms in the effective potential are replaced by their most recent iterative approximations. Writing $\psi_n^{j,k}$ for the k-th iterate, the initial approximation used for the new time step is $\psi_n^{j+1,0}=\psi_n^j$, and each subsequent iterate is given by solving for $\psi_n^{j+1,k+1}$ in the simultaneous linear equations

$$i\frac{\psi_n^{j+1,k+1}-\psi_n^j}{\delta t}+\sum_m J_{mn}\frac{\psi_m^j+\psi_n^{j+1,k+1}}{2}+\left[\nu\frac{\delta W_n^j}{\delta t}+\frac{|\psi_n^j|^2+|\psi_n^{j+1,k}|^2}{2}\right.$$
$$\left.+\lambda\mathrm{Im}\left(\overline{\psi_n^j}\sum_m J_{mn}\psi_m^j+\overline{\psi_n^{j+1,k}}\sum_m J_{mn}\psi_n^{j+1,k}\right)\right]\times\frac{\psi_n^j+\psi_n^{j+1,k+1}}{2}=0 \qquad (10)$$

Retaining the unknown values $\psi_n^{j+1,k+1}$ in the final term retains exact conservation of the exciton energy at each iteration, unlike most iterative approaches to solving Eq. (9).

3.4. **Time step refinement with noise.** Accuracy testing by refining time step size has a difficulty with random noise terms: changing the time step size changes the random numbers, so that one is looking at a different realization. To overcome this, noise is generated on the finest anticipated time scale δt_{noise}, with longer computational time step sizes δt accommodated by averaging of these noise values. Time step refinement is then done with $\delta t = 2^p \delta t_{noise}$ for various $p \in \mathbb{N}$, fixed δt_{noise}.

Time step size choice is limited in practice by accuracy restrictions rather than stability issues; both noise and self-trapping generate significant contributions from the highest spatial frequencies and then the error term $O(\|\boldsymbol{\psi}_{ttt}\|\delta t^2)$ includes terms $O(\|\mathcal{L}^3\|\delta t^2)=O(J^3\delta t^2)$, potentially requiring $\delta t \approx \sqrt{tol}J^{-3/2}$ for relative error tol. For the numerical results below, $\delta t_{noise}=10^{-5}$, with the δt needed ranging from 4×10^{-5} to 16×10^{-5}.

3.5. **Three iterations are enough, two are not.** Two iterations will give the same second order accuracy as the trapezoid rule itself. However, a third iteration can lower the coefficient of the error term, and greatly improves conservation of the total energy $\mathcal{H}_0$ for "heatless" case, DNLS. On the other hand, experiments show that whenever there is further significant change after the third iteration, the error in the trapezoid method itself is excessive, and the solution is to reduce δt rather than increase the iteration count.

4. **Numerical results.** All solutions here use the same initial data, based on 1000 interval discretization of a sech pulse of width 2, initial group velocity 5 with a mesh spacing $\delta x = 1/10$, so that $J = 1/(\delta x)^2 = 100$ and the initial group velocity should be 50 nodes per unit time (apart from boundary effects):

$$\psi_n(0) = 2\,\mathrm{sech}\left(\frac{n-200}{10\sqrt{2}}\right)\exp(in/4), 0 \le n \le 1000. \tag{11}$$

This comes from doubling the width of a unit width soliton, allowing phenomena in the discretized NLS such as partial self-focusing and defocusing, production of scattering, and splitting to multiple solitons.

4.1. **DNLS reference cases: cold, rigid biopolymers.** The two graphs in Fig. 1 review some familiar properties of the DNLS equation, related to soliton solutions of NLS. The initial data here has twice the width of the standard sech soliton, leading to pulse propagation akin to that soliton, but with periodic oscillations of the amplitude. Note that there is no splitting into two solitons (as occurs with greater initial amplitude), and little scattering.

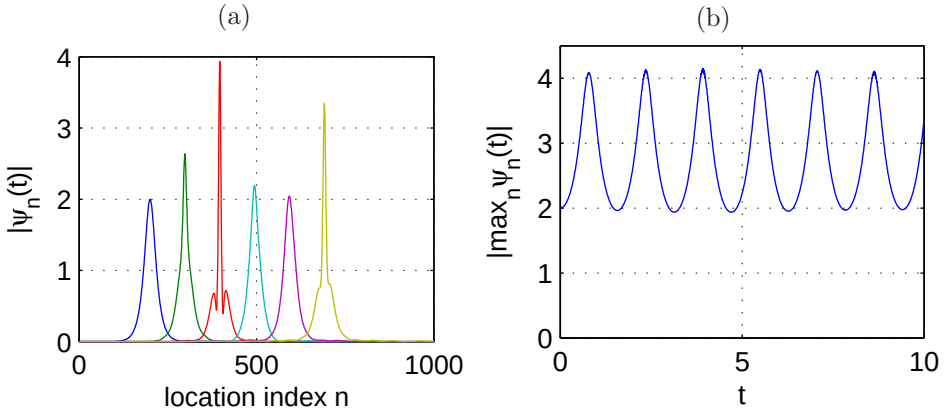

FIGURE 1. DNLS: no noise or damping. (a) Amplitude profiles at times $t = 0, 2...10$. (b) Maximum amplitude oscillations.

4.2. **SDNLS: noise without damping.** Adding noise alone produces fairly predictable results, with pulses somewhat lowered and broadened but maintaining momentum.

- Noise $\nu = 0.01$ produces very little change in propagation or energy.
- Noise $\nu = 0.05$ produces a little spatial symmetry breaking in the pulse, which will in fact lead to separation off of a lower faster peak at later time (Fig. 2). There is also some decay in the strength of the focusing/defocusing oscillations, but no noticeable effect on the mean amplitude of about 3, or on the propagation speed.

However, the total energy shows a linear accumulation of "heat energy", as heuristically predicted from the continuum limit (Fig. 2(c)). This seems unphysical; hence damping is needed to achieve a physically more plausible thermal equilibrium.

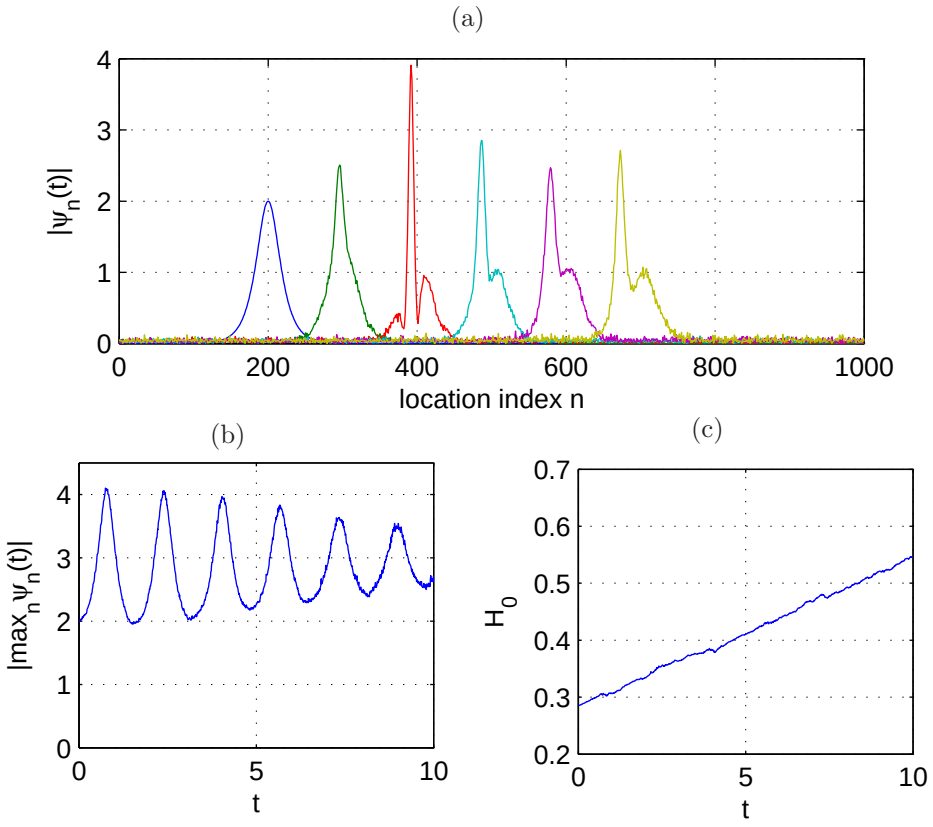

FIGURE 2. Noise $\nu = 0.05$. (a) Amplitude profiles $t = 0, 2...10$. (b) Maximum amplitude oscillations. (c) Total energy.

4.3. **PDSDNLS: seeking thermal equilibrium with noise and damping.** Using the same initial data, noise strength $\nu = 0.05$ and realization as above, with increasing damping strength, three main phenomena are seen (Fig's 3-4):

- The pulse splits into a main pulse which is tall, narrow (strongly self-focused) and slow moving, and a lower faster pulse going off the front.
- The oscillations of maximum pulse width die out with this splitting, so that the main pulse approaches a steady state.
- The main pulse also stops moving almost completely, so become a narrow stationary solution, similar to self-trapping.
- As damping is increased, the growth in total energy $\mathcal{H}_0$ ceases. Instead it becomes less than initially, with the coupling energy coming to rough equilibrium somewhat higher than its initial value.

Damping $\lambda = 0.01$ already produces these effects, but after an initial steep drop in total energy, it seems to be slowly rising, though staying well below its initial value till final computed time $t = 10$ (Fig's 3). With damping $\lambda = 0.05$, total energy growth seems very strongly suppressed: if anything, this is "overdamped" (Fig's 4). With even stronger damping $\lambda = 0.05$ (not shown), the only changes are that the pulse stops moving earlier, and the total energy grows even more slowly after its initial drop.

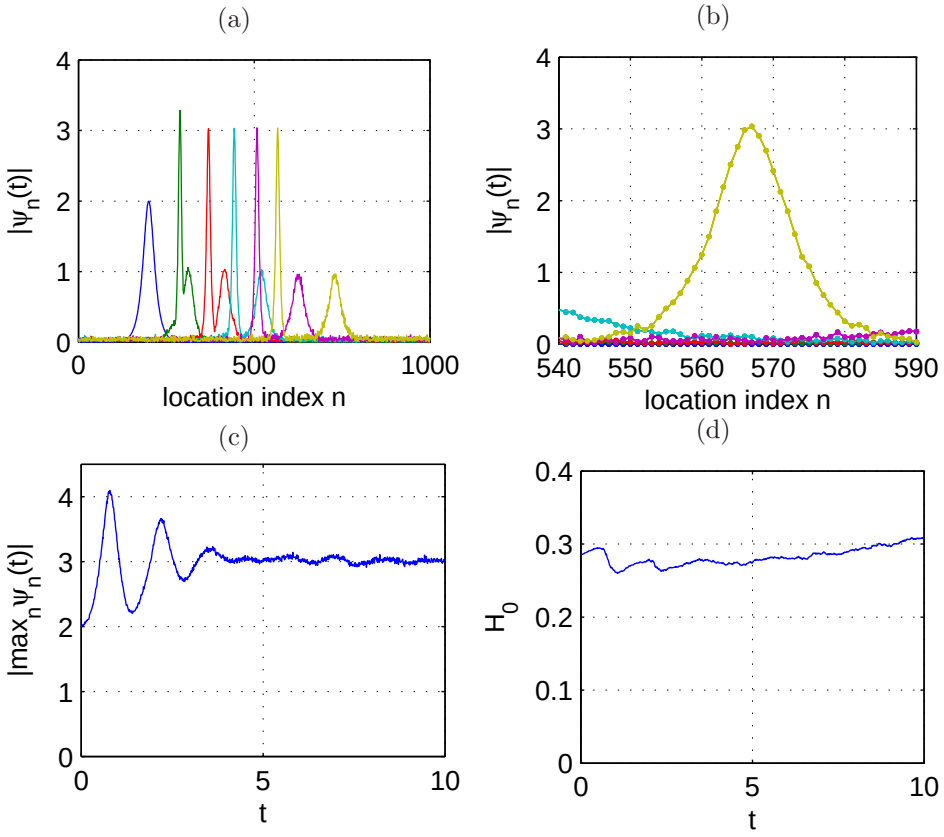

FIGURE 3. Noise and slight damping $\lambda = 0.001$. (a) Amplitude profiles $t = 0, 2...10$. (b) Detail of main pulse at final time (c) Maximum amplitude oscillations. (d) Total energy.

4.4. **The effect of phase damping on DNLS without noise.** It is perhaps physically reasonable to consider phonon damping without noise: the situation where phonons are driven only by coupling to excitons:

$$i\frac{\partial \psi}{\partial t} = -\psi_{xx} + \left[-|\psi|^2 + \lambda \frac{\partial (|\psi|^2)}{\partial t}\right]\psi$$

It is anyway mathematically interesting, as it offers a possible explanation of the effect of phonon damping, which can be seen as an additional self-induced nonlinear potential which is

- repulsive where the intensity is increasing (e.g. the leading edge of a pulse), and
- attractive where intensity is falling (the trailing edge of a pulse).

As seen in Fig's 5,6, the absence of noise has little effect on the pulse behavior, while total energy is now consistently decreasing, consistent with solutions converging to a minimum energy solution in the form of a stationary trapped state related to a discretized stationary soliton.

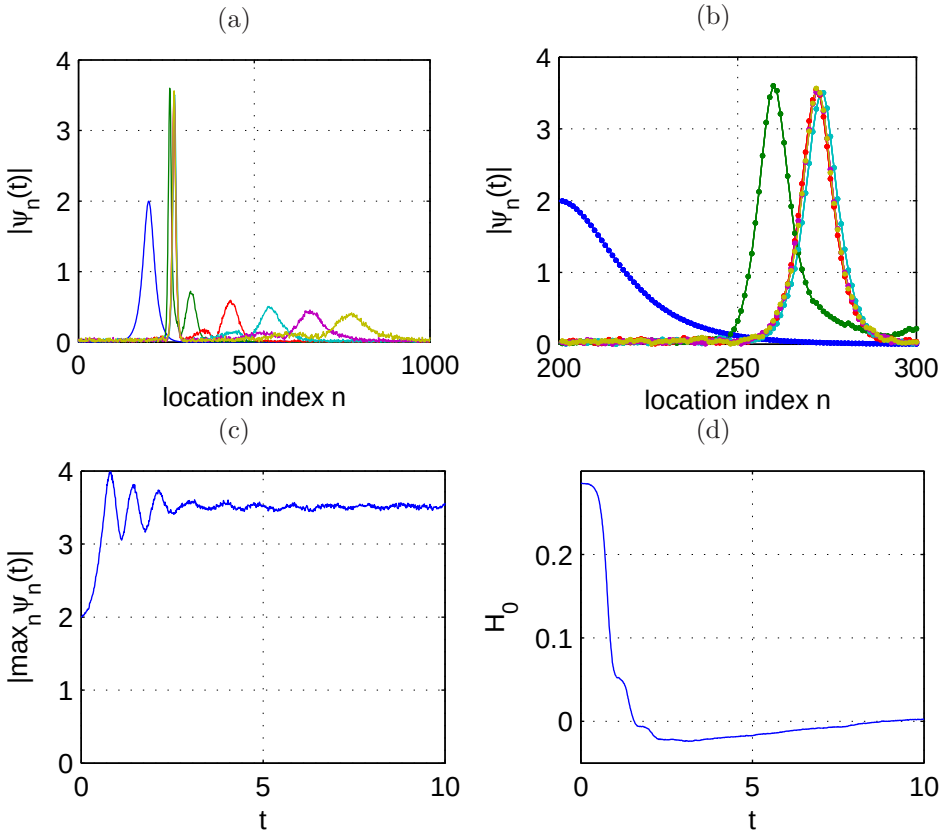

FIGURE 4. Noise and stronger damping $\lambda = 0.01$. (a) Amplitude profiles $t = 0, 2...10$. (b) Detail of trapped main pulse. (c) Maximum amplitude oscillations. (d) Total energy.

5. **Summary.** Damping the internal vibrations of the system of Eq's (1,2), manifested as phase damping in the PDSDNLS approximation of Eq's (3,4) can decelerate and stabilize self-focused pulses, leading to a new variety of *pulse self-trapping*. Damping with noise can prevent or greatly slow the growth of total energy seen with noise alone. Sufficient damping in fact drives the total energy down, perhaps close to the minimum value associated with soliton solutions. Damping without noise has similar effects, and seems to drive the main pulse of the solution to a stationary state (also a steady state of the DNLS), possibly a minimizer of the DNLS Hamiltonian subject to exciton energy constraint.

Further study is needed. Results so far use single realizations, and a number of issues are not addressed, including proper temporal averaging (correlation) in the noise for the case of weak damping; modeling of molecular dynamics (bending, stretching, and other motion); studying the effect of pulses of conformational changes (like DNA strand coiling), seen in models without noise and damping; random variation in the phonon parameters for mass, frequency etc.; and the effects of random initial data.

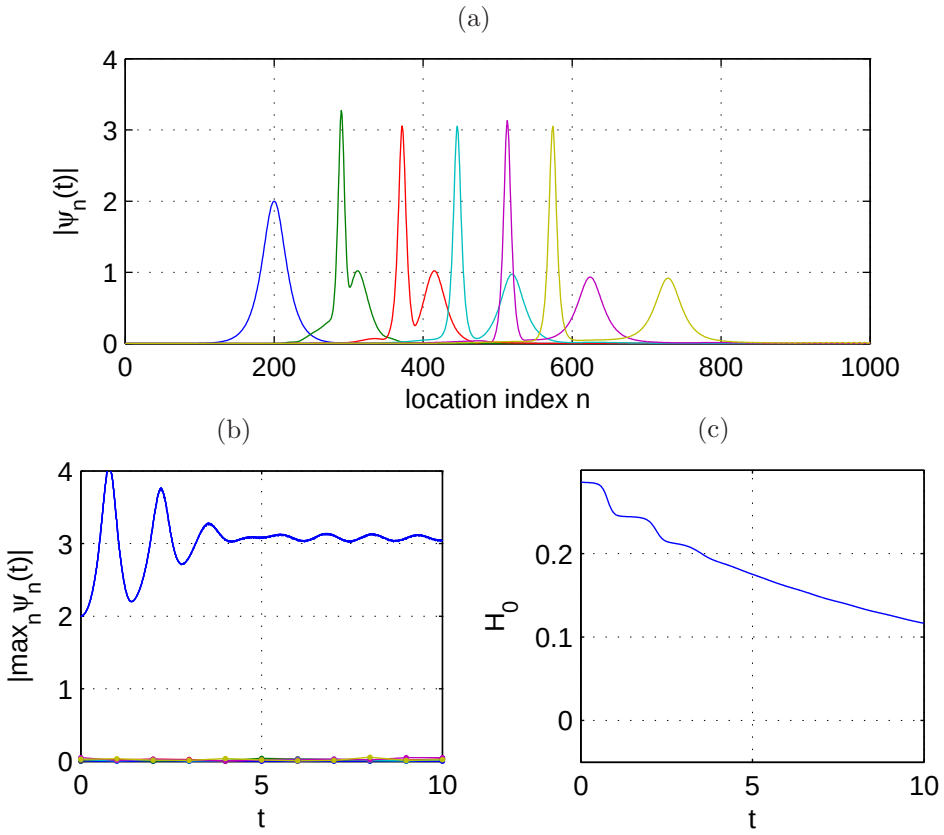

FIGURE 5. No noise, slight damping $\lambda = 0.001$. (a) Amplitude profiles $t = 0, 2...10$. (b) Maximum amplitude oscillations (c) Total energy.

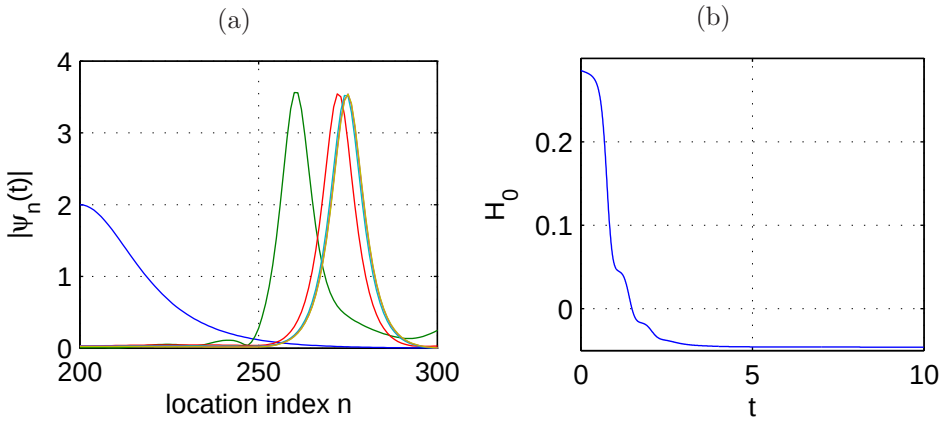

FIGURE 6. No noise, stronger damping $\lambda = 0.01$. (a) Details of main pulse. (b) Total energy.

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