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# Modeling and simulating thin molecular films: a modified 2D nonlinear Schrödinger equation with noise and nonlinear damping

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# ***Exciton-phonon system with noise and damping***

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Vibrations in a thin molecular film can be modelled as an exciton-phonon system, with noise and damping acting on the molecules:

$$(1) \quad i\hbar\dot{\psi}_n + \sum_{m \neq n} J_{nm}\psi_m + \chi u_n \psi_n = 0$$

$$(2) \quad M\ddot{u}_n + M\lambda\dot{u}_n + M\omega_0^2 u_n - \chi|\psi_n|^2 = \gamma\eta_n(t)$$

$\psi_n(t)$  the exciton wave at location  $n$

$u_n(t)$  the elastic d.o.f. of the molecule at location  $n$ ;

$J_{nm}$  the dipole-dipole interaction energy

$\lambda$  the damping coefficient

$\gamma\eta_n$  an external force from white noise of strength  $\gamma$

Each  $\eta_n$  is the derivative of a Wiener process: a normalized random walk.

## Elimination of the $u_n$

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The  $u_n$  can be eliminated with an integral expression in terms of  $\psi_n$ , and then the assumption that the exciton intensity  $|\psi_n(t)|^2$  is slowly varying relative to the phonon frequency gives the approximation

$$(3) \quad i\hbar\dot{\psi}_n + \sum_{m \neq n} J_{nm}\psi_m + V|\psi_n|^2 - \frac{\lambda V}{\omega_0^2}\psi_n \frac{d}{dt}[|\psi_n(t)|^2] + \frac{2k_B T \chi}{\omega}\sigma_n(t)\psi_n = 0,$$

$$\sigma_n(t) = \lambda \int_0^t e^{-\lambda(t-s)/2} \sin(\omega(t-s))\eta_n(s)ds,$$

$$V = \chi^2/M\omega_0^2, \quad \omega^2 = \omega_0^2 - (\lambda/2)^2.$$

# *Continuum limit: a NLS equation*

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With enough symmetry in the lattice and the dipole interaction, the limit as molecular spacing goes to zero gives the PDE

$$\text{(NLSND)} \quad i\psi_t + \nabla^2\psi + |\psi|^2\psi + \Gamma\sigma\psi - \Lambda(|\psi|^2)_t\psi = 0$$

$$\Gamma = \frac{2k_B T \chi}{J\omega}, \quad \Lambda = \frac{\lambda J}{\hbar\omega_0^2}.$$

For numerical solution, the time derivatives can be eliminated from the dissipation term, giving the fully nonlinear form

$$\text{(NLSND')} \quad i\psi_t + \nabla^2\psi + |\psi|^2\psi + \Gamma\sigma\psi - 2\Lambda\text{Im}(\bar{\psi}\nabla^2\psi)\psi = 0$$

# ***The 2D cubic Schrödinger equation [CSE]***

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Without the noise and damping terms, the above model reduces to the well-studied 2D cubic Schrödinger equation

$$i\psi_t + \nabla^2\psi + |\psi|^2\psi = 0, \quad \psi = \psi(t, x, y).$$

This has two important conserved quantities,  $\mathcal{N}$  (exciton energy), and  $\mathcal{H}$ , the hamiltonean

$$\mathcal{N} = \iint |\psi|^2 dx dy, \quad \mathcal{H} = \iint \left\{ |\nabla\psi|^2 - \frac{1}{2}|\psi|^4 \right\} dx dy$$

With noise and damping,  $\mathcal{N}$  is still conserved, but the hamiltonean evolves with

$$\frac{d\mathcal{H}}{dt} = \gamma \iint \sigma(|\psi|^2)_t - \Lambda[(|\psi|^2)_t]^2 dx dy.$$

# ***Beam width evolution, point singularity formation***

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Self-focusing collapse and singularity formation in the CSE are predicted by the evolution of the variance

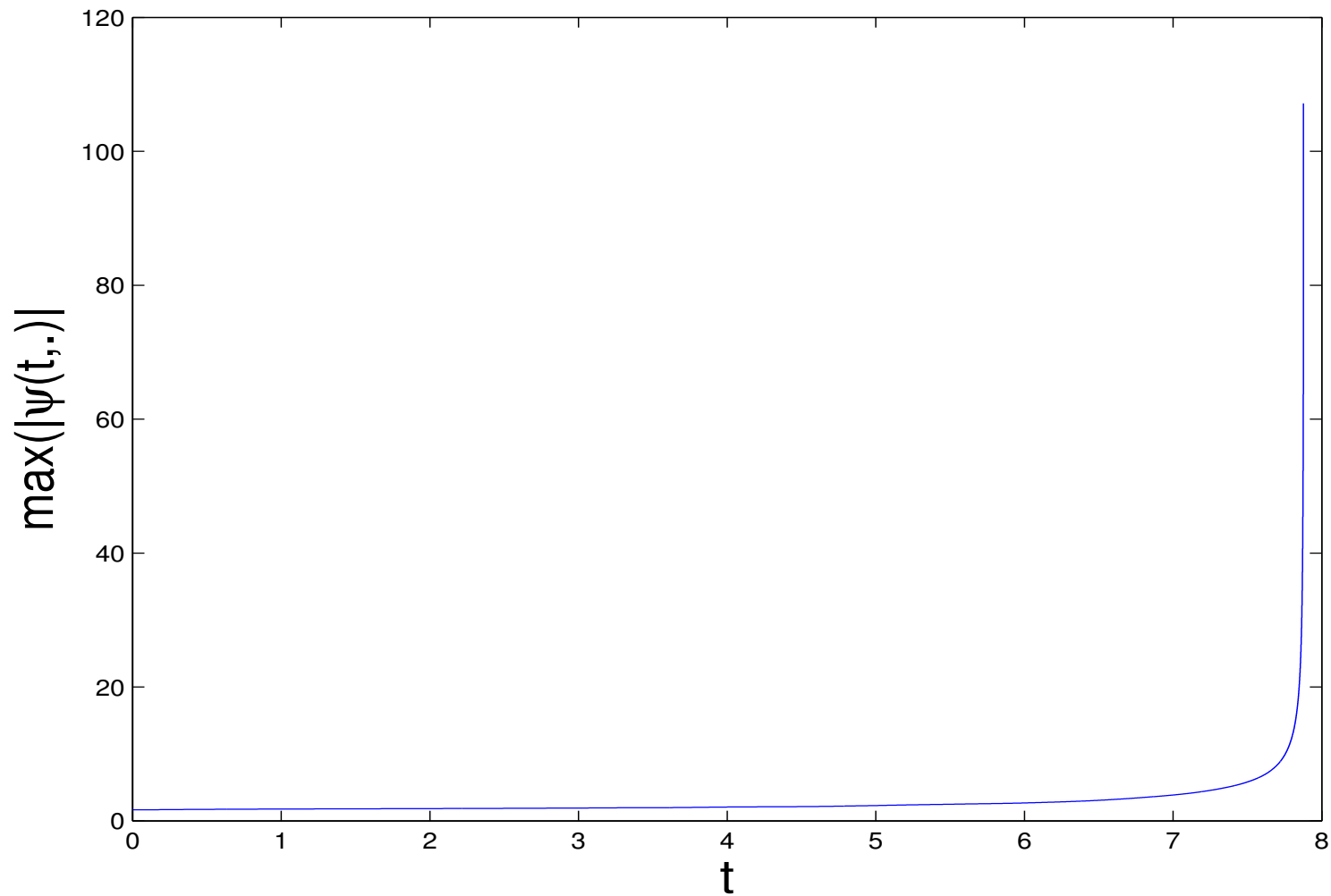
$$V(t) := \iint (x^2 + y^2) |\psi|^2 dx dy$$

which for the 2D CSE obeys

$$V_{tt} = 8\mathcal{H}.$$

# *Self-focusing in the CSE: intensity growth*

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**Figure 1:** Self-focusing collapse for initial data  $\psi(0, r) = 1.65\text{sechr}$

# *Self-focusing in the CSE: intensity cross sections*

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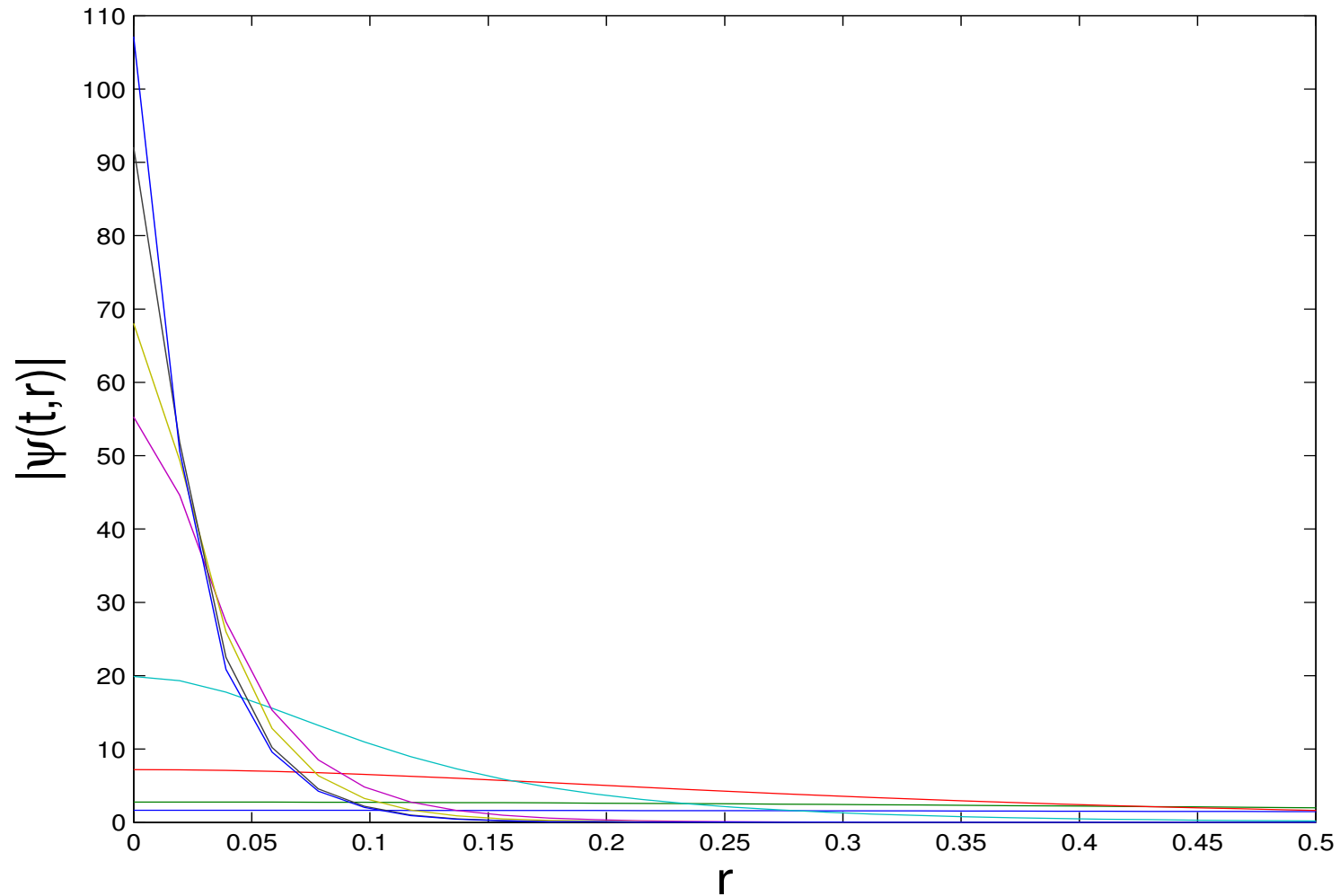


Figure 2: Amplitude cross sections for the case of Fig. ??

# *Further approximations and previous results*

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Numerical solution of the resulting ODE's shows two patterns

- Noise without damping can prevent wave collapse (giving wave dispersion instead) if sufficiently strong.
- Damping can have the opposite effect: increasing damping with a given noise level can lead to collapse where with noise alone there would be dispersion.

These each fit with heuristic predictions on the effect of noise and damping on the evolution of the hamiltonean.

# ***Numerical methods: PCC trapezoid Milstein***

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Separating the deterministic and stochastic parts with the notation

$$\partial\psi/\partial t = \mathcal{D}[\psi] + i\Gamma\sigma\psi$$

we use the trapezoid and Milstein methods, solved by a predictor-corrector iteration.

Predictor:

$$\psi_{n+1}^0 = \psi_n + \mathcal{D}[\psi_n]\delta t + \psi\{i\Gamma\delta W - (\Gamma^2/2)((\delta W)^2 - \delta t)\}$$

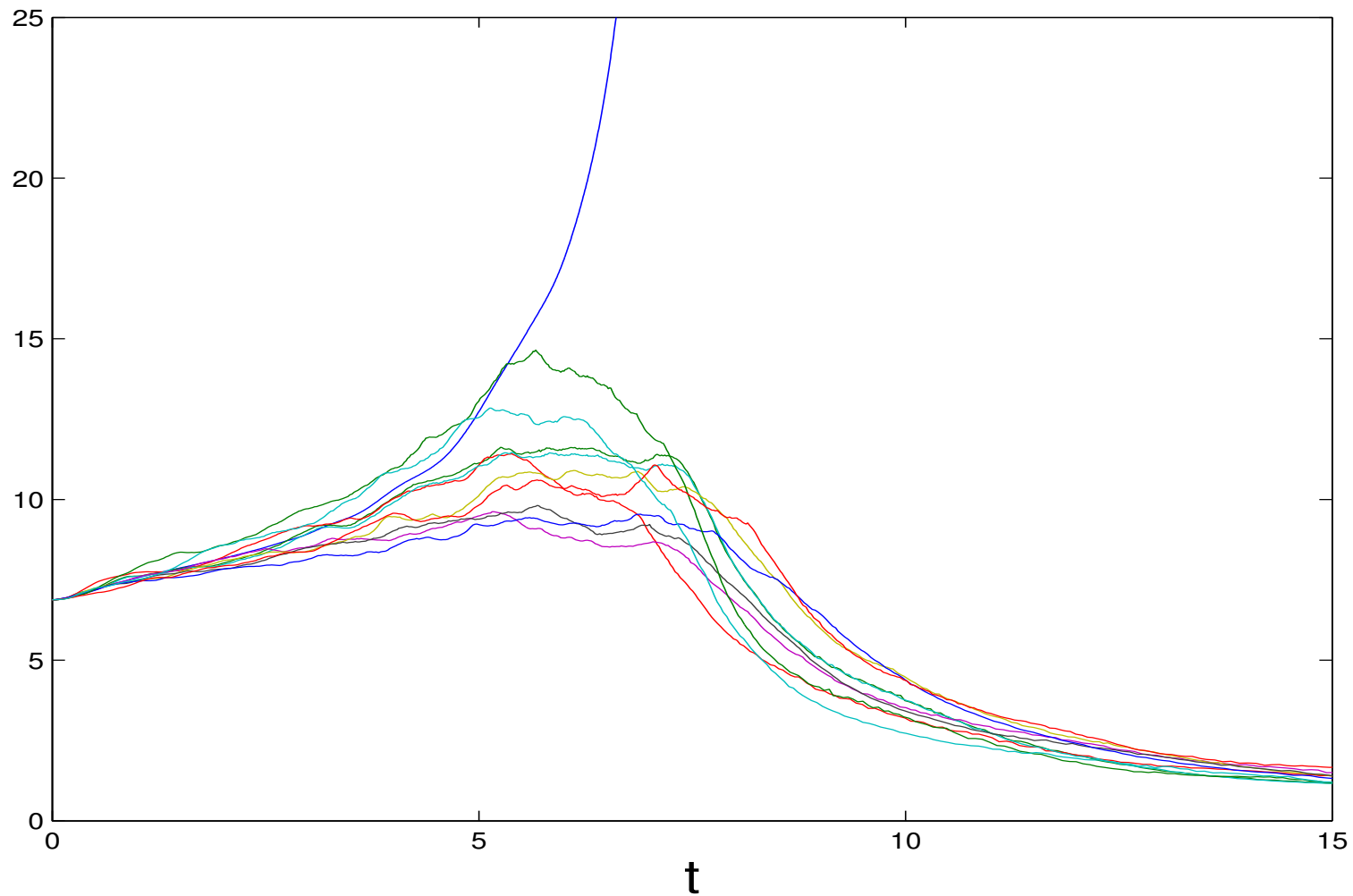
with  $\delta W$  at each position being independent, normally distributed, of variance  $\delta t$ , mean 0.

Corrector:

$$\psi_{n+1}^{k+1} = \psi_n + \frac{1}{2}(\mathcal{D}[\psi_n] + \mathcal{D}[\psi_{n+1}^k])\delta t + \psi\{i\Gamma\delta W - (\Gamma^2/2)((\delta W)^2 - \delta t)\}.$$

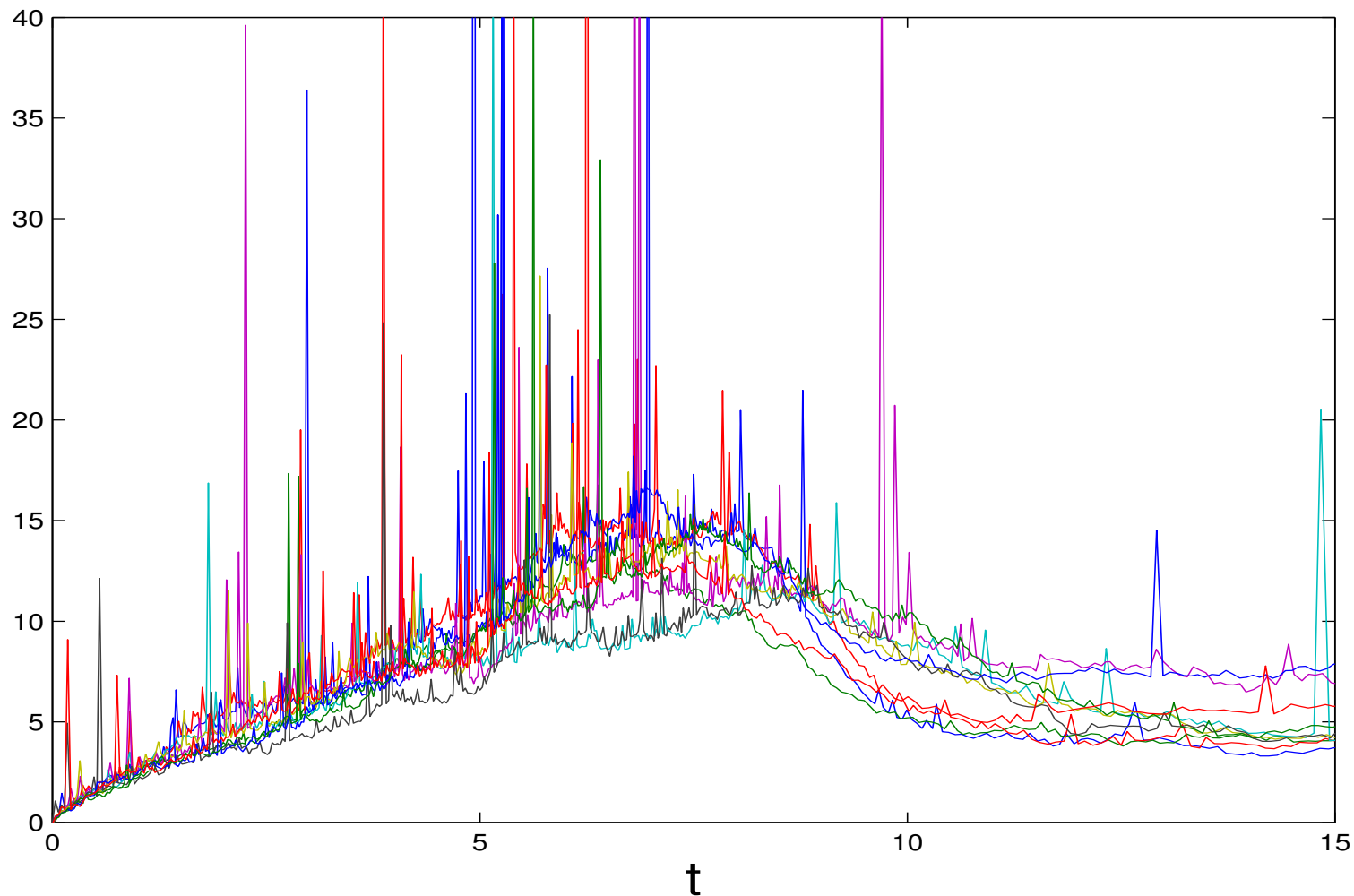
Stability requires two corrector iterations.

# *CSE with noise: intensity evolution*



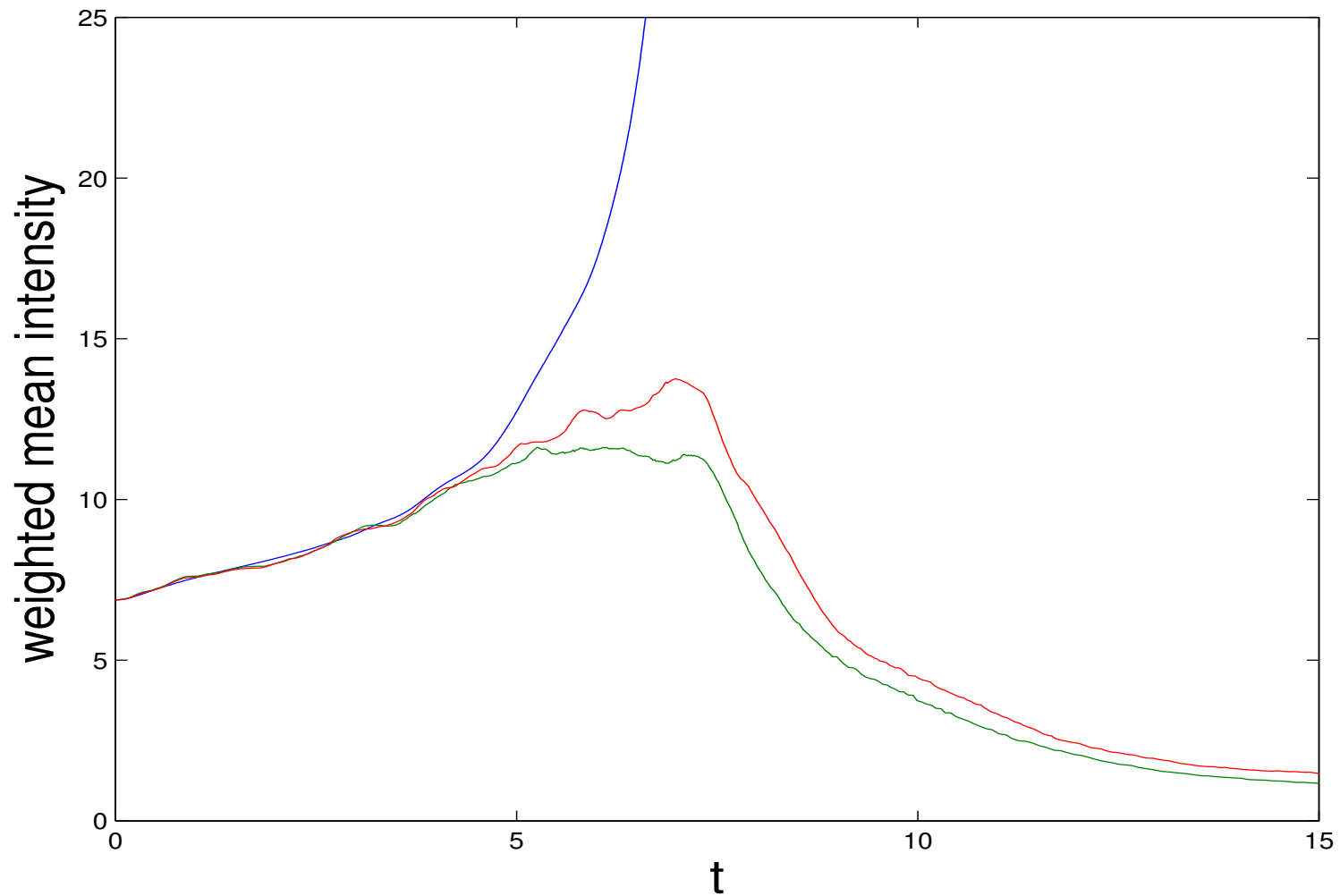
**Figure 3:** Maximum magnitude evolution: the rising blue curve is CSE without noise; other curves are ten noise realizations.

# *CSE with noise: hamiltonean evolution*



**Figure 4:** Note that the rise in hamiltonean (conserved without noise) is due to a rise in the gradient term, and the timing of this coincides with the reversal of beam collapse.

# *CSE with noise, damping: intensity evolution*



**Figure 5:** Blue is CSE, green is with noise, red is with noise and damping.

# *CSE with noise, damping: hamiltonean evolution*

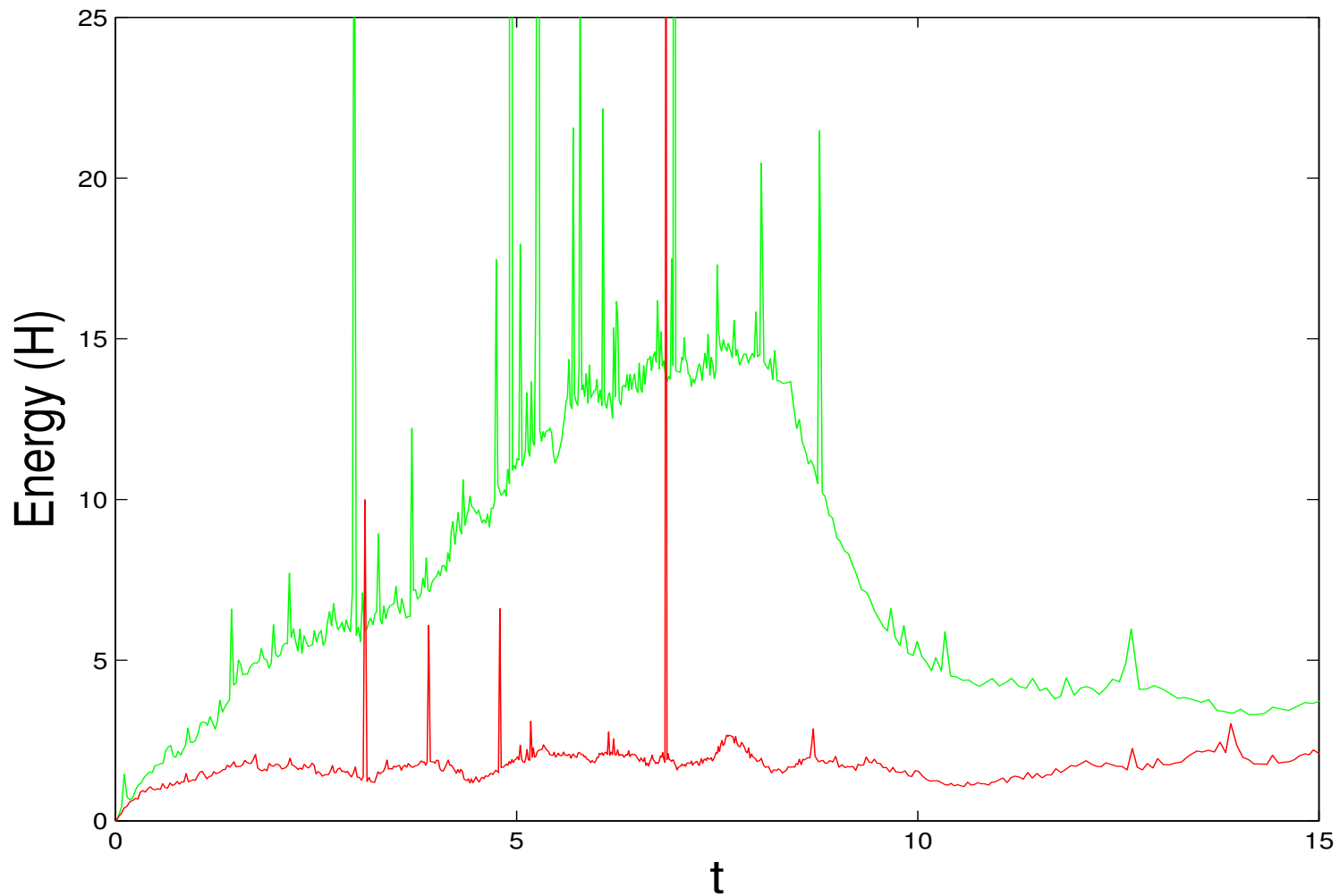


Figure 6: Green is with noise, red is with noise and damping.

- As expected, noise is sometimes seen to inhibit wave collapse, related to an increase in the hamiltonean.
- A small degree of damping greatly reduces the increase in hamiltonean, but collapse is still inhibited in test cases so far.
- Some simulations with larger damping indicate the predicted restoration of wave collapse, but these have not yet been achieved with adequate accuracy.
- Some simulations with damping alone (no noise) show acceleration of wave collapse, but again these have not yet been achieved with adequate accuracy.

# ***Acknowledgements***

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The work was supported in part by the College of Charleston 4th Century Initiative through a Summer Undergraduate Research Grant.