

Modeling thermal effects on nonlinear wave motion in biopolymers by a stochastic discrete nonlinear Schrödinger equation with phase damping

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

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 trapping of wave energy in a very small part of the molecule, a discrete counterpart of NLS single-point blowup.