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Studying Davydov's ODE model of wave motion in α-helix protein using exactly energy–momentum conserving discretizations for Hamiltonian systems

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Abstract

Davydov's modeling of long-range energetic pulse propagation in α-helix protein started with an exciton–phonon ODE system and proceeded to the integrable nonlinear Schrödinger (NLS) equation in the limit of both large pulse width relative to amino acid spacing and high characteristic speed of the "phonon" terms. Soliton solutions of NLS have then been used to propose a mechanism for coherent long-range propagation of energetic pulses in such proteins.

Here ODE models are studied directly, in particular a simplification that considers only coordination bond coupling parallel to the helix axis, discounting interactions along the molecular backbone. The time discretization is constructed by a new method based on discretizing the Hamiltonian using a finite difference calculus for gradients, which ensures exact conservation of both the Hamiltonian and all quadratic and linear conserved quantities, and allows a simple, highly stable iterative method for solving the resulting implicit system.

The simulation results show that as the parameters get further from the continuum limit regime, substantial changes occur in the solution form. For characteristic phonon speed drops below the characteristic speed of the exciton equation, the main exciton pulse slows and narrows, and other faster exciton pulses appear with speeds related to the characteristic phonon speed. This suggests that more careful simulation studies are needed, based on Scott's full model or further refinements.

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1. Introduction and main results

1.1. Energy–momentum conserving and symmetry preserving discretizations

Many models of nonlinear wave motion and pulse propagation have a Hamiltonian form, embodying conservation of energy and other "momenta": Noetherian first integrals related to continuous symmetries in the dependent variables.

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