Davydov soliton dynamics: initial state, boundary conditions, and numerical procedure.

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Abstract

The performance of a Runge-Kutta method of fourth order in dynamic simulations within Davydov's so-called $|D2\rangle$ state ansatz is studied by comparison with anal. solns. available for two special cases. Further, the Runge-Kutta method is compared with the one-step procedure used by Su and Schrieffer. A detailed anal. of the structure and energetics of Davydov solitons is given. The differences in the dynamics between open chain ends and periodic boundary conditions are also discussed. The properties of the soliton detector plot introduced by Lomdahl and Kerr are studied. Finally, three widely used initial states for Davydov soliton dynamics are compared.