Davydov soliton dynamics in proteins: I. Initial states and exactly solvable special cases.

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Abstract

For the Davydov Hamiltonian several special cases are known which can be solved anal. Starting from these cases the authors show that the initial state for a simulation using Davydov's |D1> ansatz the coherent state amplitudes are site dependent. The site dependences evolve from this initial state exclusively via the equations of motion. Starting the |D1> simulation from an ansatz with site dependent coherent state amplitudes leads to an evolution which is different from the anal. solns. for the special cases. Further the authors show that simple construction of such initial states from the expressions for displacements and momenta as functions of the amplitudes leads to results which are inconsistent with the expressions for the lattice energy. The site-dependence of coherent state amplitudes can only evolve through the exciton-phonon interactions and cannot be introduced already in the initial state. Thus also in applications of the |D1> ansatz to polyacetylene always |D2> type initial states have to be used in contrast to the authors' previous suggestion. Further the authors expand the known exact solns. in Taylor series in time and compare expectation values in different orders with the exact results. The authors find that for an approxn. up to third order in time (for the wave function) norm and total energy, as well as displacements and momenta are reasonably correct for a time up to 0.12-0.14 ps, depending somewhat on the coupling strength for the transportless case. For the oscillator system in the decoupled case the norm is correct up to 0.6-0.8 ps, while the expectation values of the no. operators for different sites are reasonably correct up to roughly 0.6 ps, when calcd. from the third order wave function. The most important result for the purpose to use such expansions for controlling the validity of ansatz states is, however, that the accuracy of S(t) and H(t) (const.

in time, exact values known in all cases) is obviously a general indicator for the time region in which a given expansion yields reliable values also for the other, phys. more interesting expectation values.