**Accuracy of Davydov's |D1⟩ approximation for soliton dynamics in proteins.** Foerner, Wolfgang.


**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 |D⟩ approxn. has to be constructed from a given set of initial lattice displacements and momenta in the form of a coherent state with its amplitudes independent of the lattices site, corresponding to Davydov's |D2⟩ approxn. The site dependences in the |D1⟩ ansatz 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. Thus also in applications of the |D1⟩ ansatz to polyacetylene |D2⟩-type initial states always have to be used in contrast to the previous suggestion [W. Foerner, J. Phys. Condens. Matter 6, 9105 (1994)]. 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. The authors performed long-time simulations using the |D1⟩ approxn. where the authors computed expectation values of the relevant operators with the state (H/J)|.tplbond.1⟩ and the deviation |δ⟩ from the exact soln. over long times, namely 10 ns. The authors found that in the very long-time scale the |D1⟩ ansatz is very close to an exact soln. Further the authors report results from an investigation of the very short-time behavior of the |D1⟩ state compared with that of an expansion of the exact soln. in powers of time t. Within a time of roughly 0.10-0.15 ps the second- and third-order corrections turned out to be not very important.

This is due to the fact that the first-order state contains already some terms of the expansion, summed up to infinite order. The authors found good agreement of the results obtained with the expansion and those from the corresponding |D1⟩ simulations within the time of about 0.10 ps. Altogether the authors have shown that the |D1⟩ state, although of approximative nature, is very close to an exact soln. of the Davydov model on time scales from some fs up to ns.