

## **Abstract**

The authors performed long time simulations using the  $|D1\rangle$  approxn. for the soln. of the Davydov Hamiltonian. In addn. the authors computed expectation values of the relevant operators with the state  $(H/J)|D1\rangle$  and the deviation  $|\delta\rangle$  from the exact soln. over long times, namely 10 ns. The authors found that in the very long time scale the  $|D1\rangle$  ansatz is very close to an exact soln., showing expectation values of the relevant phys. observables in the state  $(H/J)|D1\rangle$  being about 5-6 orders of magnitudes larger than in the deviation state  $|\delta\rangle$ . In the intermediate time scale of the ps range such errors, as known from the authors' previous work, are somewhat larger, but still more or less negligibly. Thus the authors also report results from an investigation of the very short time (in the range 0-0.4 ps) behavior of the  $|D1\rangle$  state compared with that of an expansion of the exact soln. in powers of time  $t$ . This expansion is reliable for about 0.12 ps for special cases as shown in the previous paper. However, the accuracy of the exactly known value of the norm and the expectation value of the Hamiltonian finally indicates up to what time a given expansion is valid, as also shown in the preceding paper. The comparison of the expectation values of the operators representing the relevant phys. observables, formed with the third order wave function with the corresponding results of  $|D1\rangle$  simulations has shown, that the authors' expansion is valid up to a time of roughly 0.10-0.15 ps. Within this time the second and third order corrections turned out to be not very important. This is due to the fact that the authors' first order state contains already some terms of the expansion, summed up to infinite order. Further the authors found good agreement of the results obtained with the authors' expansion and those from the corresponding  $|D1\rangle$  simulations within the time of about 0.10 ps.

At later times, the factors with explicit powers of  $t$  in second and third order become dominant, making the expansion meaningless. Possibilities for the use of such expansions for larger times are described. Altogether the authors have shown (together with previous work on medium times), that the  $|D1\rangle$  state, although of approximative nature, is very close to an exact soln. of the Davydov model on time scales from some femtoseconds up to nanoseconds. Esp. the very small time region is of importance, because in this time a possible soliton formation from the initial excitation would start.