Multiquantum states derived from Davydov's |D1⟩ ansatz: II. An exact special case solution for the Su-Schrieffer-Heeger Hamiltonian and its relation to the |Φ 2⟩ state.

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Abstract

We present the derivation of an exact special case soln. (for a classical lattice) for the Su-Schrieffer-Heeger model for the calcn. of soliton dynamics in trans-polyacetylene. Our soln. is exact, in the sense that the ansatz state yields an exact soln. provided that the equations of motion for its parameters are obeyed. However, these equations can be solved only numerically (in principle to any desired accuracy) not anal. The model is applied to time simulations of neutral solitons as a function of temp. We find agreement of the results of our time simulations with exptl. data on the mobility of neutral solitons in the system. Comparative calcns. using the completely adiabatic model indicate that the results of this model are at variance both with expt. and with those of our model. A simple consideration of the potential barriers for soliton displacement leads to an overestimation of the soliton mobility for low temps. and an underestimation for higher ones. In an appendix we discuss in some detail the relationship of this exact soln. with the |Φ2⟩ state ansatz as presented in our previous paper We find that the ansatz and the exact soln. yield identical results for lattice momenta, displacement and site occupancies, but differ in a time dependent phase factor. Thus spectra computed with the dynamic resulting from the exact soln. for the classical lattice on one hand and from the ansatz state on the other would differ from each other.