Abstract

The mechanism for energy and signal transport in proteins as suggested by Davydov is discussed. The idea is based on a coupling of amide-I oscillators to acoustic phonons in a hydrogen-bonded chain. Results as obtained with the usually used ansatze are discussed. The quality of these states for an approx. soln. of the time-dependent Schrodinger equation is investigated. It is found that the semiclassical ansatz is a poor approxn., while the more sophisticated |D1> state seems to represent the exact dynamics quite well. Calcus. at a temp. of 300 K for one chain, as well as for three coupled ones (as they are present in an α -helix), are presented and discussed. From the calcus, it is evident that Davydov solitons are stable for reasonable parameter values at 300 K only for special initial excitations close to the terminal sites of the chain. However, for soliton formation, it is not necessary that the initial excitation occurs at the chain end which has its C=O group directly coupled to the lattice as it is the case for T = 0 K. At higher temps., solitary waves can be formed from both chain ends. Since the model for temp. effects used was criticized from the theor. point of view, we suggest an improved theory for temp. effects. Finally, we discuss recent exptl. findings which indicate that normal modes describing the N-H stretch and its coupling to the hydrogen bonds should be considered in addn. to the amide-I vibration.