Davydov soliton dynamics in proteins: III. Applications and calculation of vibrational spectra. Foerner, Wolfgang

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 ansatz 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. This was shown by extensive calcns., both anal. and numerically in the two preceding papers. Calcns. at 300K for one chain, as well as for three coupled ones (as they are present in an α-helix) are presented and discussed. From the calcns. it is evident, that Davydov solitons are stable for reasonable parameter values at 300K for special initial excitations close to the terminal sites of the chain. Further vibrational spectra are presented and discussed. Our results suggest, that due to their strong dependence on the initial state, the Davydov |D1> model system might be a (quantum) chaotic one.