Thermal stability of protein solitons. Foerner, Wolfgang

Abstract

The thermal stability of Davydov solitons at 300 K is investigated numerically using different ansatz states. Within the classical |D2 > state the dependence of the results on the spring const. W of the hydrogen bonds, the oscillator-phonon coupling const. X and the dipole-dipole coupling const. J between neighboring oscillators is investigated. The results suggest that provided W is larger (W > 40 N/m) than the usually accepted value for proteins around 13 N/m the Davydov soliton could also function at 300 K. Since the value of 13 N/m is taken from cryst. formamide where free mols. vibrate, a more realistic value of the spring const. for the covalently bound peptide units in proteins should be larger. Some of the results obtained are compared to those from other heat bath models advocated in the literature. Further numerical results obtained with the more sophisticated |D1 > ansatz state are discussed. At 300 K solitons also exist in the |D1 > state in proteins if W > 50 N/m.