Effects of temperature and interchain coupling and Davydov solitons. Foerner, Wolfgang

Abstract

After a short review of the authors' previous results on temp. effects on Davydov soliton dynamics, the authors give some comparisons between results with Davydov's av. Hamiltonian method within the |D1> ansatz state in one chain with quantum Monte Carlo results found in the literature. The authors find that Davydov's method leads to quant. incorrect results, but reproduces the qual. trends correctly. The authors' results obtained with different models point to the direction that Davydov solitons should be stable, if the value of the spring const. for hydrogen bonds is larger than usually assumed. Therefore the authors return to Scott's suggestion, that in order to simulate the three coupled hydrogen bonded chains present in protein α-helixes with one chain, the spring const. and the mass should be enlarged. In case of the |D1> state the authors present numerical simulations for three coupled chains including temp. with different initial states and for one chain using Scott's revised parameters at 300 K.