Dinamika Distribusi Energi Pada Protein ?-Helix berdasarkan Model Davydov

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ABSTRACT
A crucial aspect of many biological processes at molecular level is the transfer and storage mechanism of bioenergy released in the reaction of the hydrolysis of Adenosinetriphosphate (ATP) by biomacromolecule especially protein. Model of Soliton Davydov is a new breakthrough that could describe that mechanism. There are two model proposed by Davydov namely that based on: simplified ansatz 2 D and more complicated ansatz 1 D . Here we have reformulated quantum mechanical the Davydov theory, using least action principle. Temperature effect has been inserted using standard method of statistical mechanics for 1 D and using Langevin equation for 2 D . Dynamical aspect of the model is analyzed by numerical calculation. We found two dynamical cases: the traveling and pinning soliton that are related to the energi transfer and storage mechanism in the protein. Traveling and pinning soliton can be controlled by strength of coupling parameter and the appropriate initial condition. In 3- channel (chain) approximation, we found the breather phenomena in which its frequency is determined by interchain coupling parameter. The 1 D and 2 D models have the same dynamical characteristics at zero temperature, but at finite temperature 1 D more reliable than 2 D .