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New Theoretical Approaches to Molecular Systems

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NEW THEORETICAL APPROACHES TO MOLECULAR SYSTEMS

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NONLINEAR BIOENERGETICS^{1,2}

A soliton mechanism for the transfer of the energy of hydrolysis of an ATP molecule along a helical protein molecule is proposed. The transformation of this chemical energy into an energy of mechanical movement in living organisms including both intracellular and intercellular processes, is considered. A new hypothesis describing a mechanism for muscle contraction at a molecular level is discussed.

The soliton concept is applied to explain the mechanism of a radiation effect on living cells as well as the mechanism of anaesthesia.

An electrosoliton model is proposed to describe electron transfer along protein molecules. The transport of an electron from a donor to an acceptor molecule is considered for an alpha-helical section of a protein molecule that might be an ideal guide. Helix segments constitute a considerable part of the protein structure of the cell cytoskeleton, and provide mechanical motion as well as transfer of energy and information from one site of the cell to another. These processes are described by the propagation of soliton excitations.

Transmembrane glycoproteins play an important role in the vitality of a cell. Glycoproteins are formed by covalent bonding of a protein with a carbohydrate residue, or a polysaccharide. The longitudinal protein fractions have a helical structure which spans the whole thickness of the cellular membrane. A polysaccharide component is hydrophilic and is located outside the cell. The interior glycoproteins are strongly coupled with the microfilaments and microtubes of the cell skeleton. Thus glycoproteins provide a coupling of the cell interior and the cell exterior. Based on the nonlinear dynamics of solitons, one can undoubtedly proceed in understanding the mechanism of transduction of information from the exterior to the interior of a cell.

A bisoliton concept is introduced. The high stability of bisoliton

states argue in favour of a bisoliton mechanism for the synthesis of an ATP molecule in living organism when electron transfer through the conjugated membranes of chloroplasts occur. It has been established experimentally³ that electrons moving in such processes are paired.

NONLINEAR RESONANCE TUNNELING AND MOLECULAR ELECTRONICS

Molecular devices formed by macromolecules seem to be a most promising basis for the next generation of computers. The simplest device of this kind is a molecular one-dimensional system described by two identical potential barriers.^{4,5} Ingoing electrons from an external electric circuit are captured in the well when passing through the barriers due to multiple reflection from the barriers. This results in a nonlinear interaction of these electrons with the next ones entering the well, and causes some new nonlinear effects such as bistability and an autooscillating regime of the voltage/current dependence that strongly depend on the current density. This model system is appropriate for a description of the mechanism of switching and/or amplifying of current as well as for generation of electromagnetic radiation.

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