Nonlinear Mechanisms of Energy And Charge Transfer in Biomolecules

Nonlinear and Complex Systems Group Research Programme

Many biological activities, such as photosynthesis, repair mechanism of DNA after radiation damage, metabolism, signal transduction in cells, enzymatic processes and respiration are driven by electron transfer (ET) reactions. In biomolecules ET is assumed to take place via single-step tunneling over distances from donors to acceptors in the range of $5 - 20$ Åwhile the shortest time scale lies in the range of picoseconds. Characteristic for biomolecules is that they exhibit a strong interplay between function and structure. In fact, structural elements such as the protein backbone can serve as effective molecular wires along which electrons tunnel between redox sites in proteins. So has it been shown that in certain protein ET systems the electron tunneling occurs along polypeptide strands with tunneling jumps via hydrogen bonds.

The experimental evidence that polypeptide chains can form an effectively one-dimensional molecular wire appears to be highly promising for applicable molecular electronics offering a way to miniaturization on the nanoscale. From the perspective of using biomaterials in molecular electronics the control of the electron flow is essential for the successful operation of electronic devices on the molecular scale. Such an achievement requests a theoretical understanding of the underlying transfer mechanism.

Attempts to theoretically describe the charge transport invoked from the beginning polaron and soliton models utilizing the idea that the interaction between the charge carrier and vibrational degrees of freedom of the molecular system conspire to form localized compounds. Davydov and co-workers showed that a mobile self-trapped state can travel as a solitary wave along the molecular structure. We investigate a possible ET scenario where supersonic acoustic solitons can capture and transfer self-trapping modes in biomolecular systems and ET can be mediated by supersonic solitons using realistic parameter values of biomolecular systems. The model represents typical polypeptides where neighboring peptide groups are bridged via hydrogen bonds.

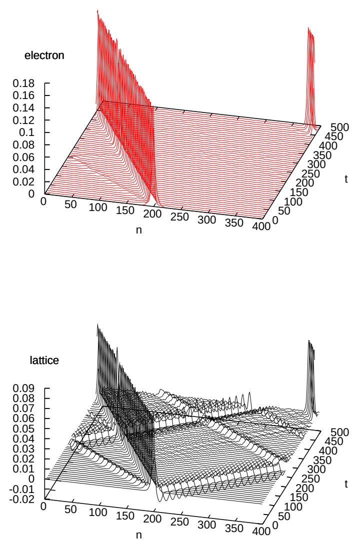

Figure: Coherent motion of an electron (top) with its accompanying localised lattice deformation (bottom).

The Nonlinear and Complex Systems Group welcomes enquiries regarding job vacancies, Ph.D. and Postdoctoral study, and academic and industrial collaboration on its research programmes.
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