

Comment

The modeling of energy transport for life goes on Comment on “The theory of bio-energy transport in the protein molecules and its properties” by Xiao-feng Pang

Philip W.T. Pong

Department of Electrical and Electronic Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong

Received 24 July 2011; accepted 26 July 2011

Available online 30 July 2011

Communicated by L. Perlovsky

There is absolutely no doubt that bio-energy transport in protein molecules plays a key role in understanding various basic problems in life science. This topic, regarded as a “crisis in bioenergetics”, was discussed in depth in a symposium of the New York Academy of Sciences in 1973. Since the first quantum mechanical model for vibrational energy propagation down the α helix of a protein proposed by Davydov and Kislukha [1], various models have been developed to unwind this mystery in biological systems. A soliton, a localized and dynamically self-sufficient solitary wave, is believed to be the energy carrier through the α -helical protein structures. Started from the discovery of the “wave of translation” by John Scott Russell in 1834, this interesting phenomenon is also observed in other fluid-like systems such as plasmas and flowing sand, and in many other areas of physics involving nonlinear partial differential equations, for example, the FitzHugh–Nagumo equations of nerve impulse propagation [2], and the sine–Gordon equation in solid state physics and nonlinear optics [3]. Recently, great interest in this research area has been further strengthened because of its applications in nanotechnologies, microelectronics, information storage devices, and biosensors. The significance of this scientific topic has stretched beyond fundamental science into practical utilizations.

One of the critical questions to ask about these energy transport models for protein is whether a soliton has a sufficiently long lifetime to carry out the energy transfer along the polypeptide chains of the protein structure. Are solitons really too delicate to survive in biology? Like other nonlinear scientific phenomenon, the system behavior is relatively unpredictable and the solution is relatively hard to obtain. Yet scientists spared no effort in solving the energy transport mechanism based on the soliton model. While biological solitons remain an abstruse concept and their observation in protein is experimentally difficult (if not impossible), the theoretical framework may enable us to gradually unveil the mysterious process of energy transport in life. Proteins are the major workers within the cells and carrying out the functions described by the genetic codes: providing structural support, transmitting signals, catalyzing reactions, and transporting molecules. Thus the fundamental understanding on the energy transport mechanism in protein will also have great values to protein folding, conformational changes, and misfolding disease research.

Experimental data are needed to verify the mathematical modeling of the energy transport [4,5]. The first evidence for the soliton-like state was obtained in the crystal of acetanilide [6,7]. Further evidence for self-trapped states was observed in the organic crystal of N-methylacetamide (NMA) [8] and even in a small polypeptide

DOI of original article: [10.1016/j.plrev.2011.06.001](https://doi.org/10.1016/j.plrev.2011.06.001).

E-mail address: ppong@eee.hku.hk.

poly- γ -benzyl-L-glutamate (PBLG) [9]. However, experimental evidences demonstrating the lifetimes of the vibrational states on various systems are in dire need. The direct evidence of the soliton stability at physiological temperature is still scarce. Advanced experimental techniques and instruments such as the pump-and-probe experiment [10], nanoscale calorimetry, and vibrational echo technique [11], are being developed for investigating vibration solitons in protein molecules. The competition among different models has been going on over a couple of decades. Probably, only experiments can resolve the difference and integrate them into a single comprehensive paradigm for analyzing protein energy transport. The Pang's review [12] provides an overview of this research area and gives an in-depth comparison over all the proposed models. Moreover, it is suggested that the Pang's model could deduce a carrier soliton with higher binding energy, higher thermal stability, and longer lifetime of the order of 100 ps at 300 K. If this is verified by future scientific developments, it will be a breakthrough for the vibrational excited states hypothesis.

Today, the "crisis in bioenergetics", in fact, still goes on. No definite solution has emerged yet. The Pang's review may, after all, help to offer a survey and analysis of this whole "crisis" from the theoretical perspective.

References

- [1] Davydov AS, Kislukha NI. Solitary excitons in one-dimensional molecular chains. *Phys Status Solidi B* 1973;59:465.
- [2] Volpert V, Petrovskii S. Reaction-diffusion waves in biology. *Phys Life Rev* 2009;6:267.
- [3] Barone A, Esposito F, Magee C, Scott A. Theory and applications of the sine-Gordon equation. *Riv Nuovo Cimento* 1971;1:227.
- [4] Berlin Y, Burin A, Friedrich J, Köhler J. Spectroscopy of proteins at low temperature. Part I: Experiments with molecular ensembles. *Phys Life Rev* 2006;3:262.
- [5] Berlin Y, Burin A, Friedrich J, Köhler J. Low temperature spectroscopy of proteins. Part II: Experiments with single protein complexes. *Phys Life Rev* 2007;4:64.
- [6] Edler J, Hamm P. Two-dimensional vibrational spectroscopy of the amide I band of crystalline acetanilide: Fermi resonance, conformational substates or vibrational self-trapping? *J Chem Phys* 2003;119:2709.
- [7] Scott A. Davydov's soliton. *Phys Rep* 1992;217:1.
- [8] Edler J, Hamm P. Spectral response of crystalline acetanilide and N-methylacetamide: Vibrational self-trapping in hydrogen-bonded crystals. *Phys Rev B* 2004;69:214301.
- [9] Edler J, Pfister R, Pouthier V, Falvo C, Hamm P. Direct observation of self-trapped vibrational states in alpha-helices. *Phys Rev Lett* 2004;93:106405.
- [10] Hamm P. Femtosecond IR pump-probe spectroscopy of nonlinear energy localization in protein models and model proteins. *J Biol Phys* 2009;35:17.
- [11] Bodis P, Yeremenko S, Berná J, Buma WJ, Leigh DA, Woutersen S. Bimodal dynamics of mechanically constrained hydrogen bonds revealed by vibrational photon echoes. *J Chem Phys* 2011;134:134504.
- [12] Pang X-f. The theory of bio-energy transport in the protein molecules and its properties. *Phys Life Rev* 2011;8(3):264–86 [in this issue].