

Protein dynamics from a quantum energy landscape perspective – a facette of quantum biology

Gerald Kneller

Centre de Biophysique Moléculaire UPR4301 CNRS / Université d'Orléans

In different fields of science and technology quantum physics is currently perceived as a key element for substantial progress. Although quantum effects are usually experimentally observed at extremely low temperatures and clean laboratory conditions, they are believed to play also an essential role in biological systems, going beyond quantum chemistry [1]. An example is presented in this lecture, which shows that a wave mechanical description of proteins as quantum many-body systems leads to a conceptually very simple interpretation of protein dynamics probed through neutron scattering experiments and naturally to a space-resolved energy landscape picture of protein dynamics [2]. A semiclassical interpretation is obtained for the quasielastic regime, which reflects the slow relaxation dynamics of proteins, and a corresponding a "minimalistic" three-parameter model is proposed for the observed scattering functions. The relaxation dynamics is here accounted for by a stretched Mittag-Leffler function, $\phi(t) \equiv E_\alpha(-[t/\tau]^\alpha)$ ($0 < \alpha < 1$), where α can be related to the "roughness" of the protein energy landscape. Several applications are presented [3, 4].

References

- [1] Philip Ball. The Dawn of Quantum Biology. *Nature*, 474(7351):272–274, 2011.
- [2] Gerald R. Kneller. *Proceedings of the National Academy of Sciences USA*, 115(38):9450–9455, 2018.
- [3] Melek Saouessi, Judith Peters, and Gerald R. Kneller. *J. Chem. Phys.*, 150(16):161104, 2019.
- [4] Abir N. Hassani, Luman Haris, Markus Appel, Tilo Seydel, Andreas M. Stadler, and Gerald R. Kneller. *J. Chem. Phys.*, 156(2):025102, 2022.