

Exploring the Quantum Realm of Proteins: The Interplay of Quantum Criticality, Landauer Formula, and High Conductance

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Abstract

Electron transport is a pivotal process in biology, with far-reaching implications for nanobiotechnology, biosensors, and biofuels. While microbial nanowires and DNA molecules are known for their high conductivity, recent findings have shown that single proteins, even without metal ion cofactors, can exhibit remarkable conductive properties akin to semiconductors. The conductance of these proteins displays a slow decay over distance and reveals a complex spatial structure with highly conductive and insulating domains. However, a comprehensive theory to explain these phenomena still needs to be discovered. In this colloquium, we present a novel approach that integrates the density matrix of the Liouville-Master Equation, initially developed for quantum transport in nanoscale devices, with a phenomenological model of electronic conductance in molecules. This combination allows us to calculate and visualize the electronic wiring of biomolecules, providing insights into the intricate spatial structure and longrange high conductance. The underlying mechanism can be attributed to the highly correlated quantum mechanical wave functions near the critical point of the metal-insulator transition. By incorporating novel AI-based protein structure prediction methods, our computational technique has the potential to accelerate the design of protein-based nanoelectronic devices and enable the exploration of electron transfer properties in mutated protein structures.