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Statistical mechanics of non-equilibrium steady state systems

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One of the important classes of non-equilibrium systems is the systems, which are maintained in non-equilibrium steady state by the contact with several external macroscopic reservoirs. These systems are ubiquitous and their theoretical description has been a challenging fundamental scientific problem for many years. They are also of significant practical interest for various nanotechnological and biological applications, such as quantum contacts, molecular motors, nanowires, and molecular junctions. There is no unique theoretical approach to wide variety of non-equilibrium steady state systems. General theoretical description of non-equilibrium steady states has not been developed yet and many fundamental theoretical questions are yet to be answered. For example, how to include many-particle correlation effects into theoretical treatment, is there exist a general variational principle for non-equilibrium steady state, do we enforce by the choice of a particular theoretical treatment a specific non-equilibrium steady state which is not the same as the real system would establish under the same boundary conditions, do we have a unique steady state in a system of non-equilibrium interacting particles for given boundary conditions? In my talk, I will review these questions and their relevance to electron transport through molecules. I will also give account of our recent computational and theoretical work on non-equilibrium quantum transport through molecular nanostructures.