Quantum thermodynamics of single particle systems

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Thermodynamics is built with the concept of equilibrium states. However, it is less clear how equilibrium thermodynamics emerges through the dynamics that follows the principle of quantum mechanics. In this paper, we develop a theory of quantum thermodynamics that is applicable for arbitrary small systems, even for single particle systems, in contact with a reservoir. We generalize the concept of temperature into non-equilibrium regime that depends on the detailed dynamics of quantum states. We apply the theory to a single-mode cavity system and a two-level atomic system interacting with a reservoir, the results unravels (1) the emergence of thermodynamics naturally from the exact quantum dynamics in the weak system-reservoir coupling regime without introducing the hypothesis of equilibrium between the system and the reservoir from the beginning; (2) the emergence of thermodynamics in the intermediate system-reservoir coupling regime where the Born-Markovian approximation is broken down; (3) the breakdown of thermodynamics in the strong coupling regime due to the long-time non-Markovian memory effect; (4) the occurrence of dynamical quantum phase transition characterized by inflationary dynamics associated with negative non-equilibrium temperature. The corresponding dynamical criticality provides a border separating classical and quantum thermodynamics. The inflationary dynamics may also provide a simple picture for the origin of big bang and universe inflation; (5) the third law of thermodynamics, allocated in the deep quantum realm, is naturally proved.

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