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Kinetic and thermodynamic temperatures in quantum systems

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Non equilibrium thermodynamics is intimately linked to the concept of non-equilibrium

temperature which in turn tights to the concept of non-equilibrium entropy. Several attempts have been made in the past in order to provide a consistent definition of all these concepts and the field is still reach of fruitful debates.

One of such attempts can be called informational thermodynamics, resting on the extension of the Gibbs-Shannon entropy to non-equilibrium conditions. This encounters the difficulty of assigning probabilities to microstates which is solved, for instance, using the debated postulate of maximal entropy or maximal entropy production rate. However, for many non-equilibrium systems, maximal entropy principle fails, signifying that fast evolving dynamics prevent any meaningful definition of such probabilities.

Nonetheless, in non-equilibrium systems under steady-state conditions the concept of a probability distribution is meaningful. Such systems are characterized by steady-state fluxes of energy, mass or charges driven by non-equilibrium distributions of phase-space degrees of freedom. To this class belongs a broad range of interesting physical systems ranging from electronic devices, electrochemical cells, catalytic systems, photochemical steady state reactions. Many assumptions widely used in the simulation of macroscopic or mesoscopic scales often assume local quasi-equilibrium, with a well defined local electrochemical potential controlling state occupancy and densities and a local equilibrium temperature. However, this approximation fails when the perturbation cannot be considered small with respect to the characteristic length scale. On the other hand, in a non-equilibrium theory, it would be useful to retain as much as possible those concepts that have provided so deep insights in systems close to equilibrium [1].

In this work [2] we present a formalism to describe non equilibrium conditions in systems with a discretized energy spectrum, such as quantum systems. We develop a formalism based on a combination of Gibbs-Shannon entropy and information thermodynamics that arrives to a generalization of the De-Brujin identity applicable to discrete and non-symmetric distributions. This allows to define the concept of a thermodynamic temperature with a different, albeit complementary meaning to the equilibrium kinetic temperature of a system. The theory is applied to Bosonic and Fermionic cases represented by an harmonic oscillator and a single energy state, respectively. We show that the formalism correctly recovers known results at equilibrium, then we demonstrate an application to a genuine non equilibrium state: a coherent quantum oscillator.

A. Gagliardi and A. Di Carlo, arXiv:submit/0713552 [cond-mat.stat-mech] (2013).
A. Gagliardi, A. Pecchia and A. Di Carlo, arXiv:submit/0713577 [cond-mat.stat-mech] (2013).