A General Non-equilibrium Thermodynamic Approach Applicable at Any Scale and Throughout the Non-equilibrium Realm

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This seminar provides a brief introduction to a novel general first-principle, non-equilibrium thermodynamic-ensemble based framework, called steepest-entropy-ascent quantum thermodynamics (SEAQT), able to describe quantum mechanically or classically the single and coupled non-equilibrium phenomena occurring in reactive and non-reactive systems. Unlike other approaches, SEAQT is not phenomenological nor does it require detailed information about the particle mechanics involved (e.g., the collision of particles) but instead models the kinetics and dynamics of the relaxation process based on the principle of steepest-entropy ascent (SEA) or maximum-entropy production (MEP), suggesting a constrained gradient dynamics in state space. This framework is based on general definitions for energy and entropy and at least theoretically has from its inception enabled the prediction of the nonequilibrium relaxation of system state at all temporal and spatial scales. However, to make this not just theoretically but computationally possible, recent developments of our research group have introduced the concept of density of states to simplify the application of this relaxation model, which effectively extends its application to infinite-dimensional state spaces. Associated system energy eigenstructures on the order of 10^{130} and yielding to the quasicontinuous assumption have been modeled. The principle of SEA results in a unique trajectory of system thermodynamic state evolution in Hilbert space in the nonequilibrium realm, even that far from equilibrium. To describe this trajectory, our research group has developed the concepts of subsystem hypoequilibrium state and definitions of intensive properties (e.g., temperature, pressure, chemical potential, etc.) able to characterize each system-level, nonequilibrium state. These definitions are fundamental rather than phenomenological and are a generalization of those defined at stable equilibrium. In fact, with this generalization, the Onsager relations and the Casimir condition can be derived without any of the limiting assumptions required by the traditional derivation. In addition, to deal with the large number of energy eigenlevels (i.e., finite as well as infinite-dimensional state spaces), the equation of motion is formulated on the basis of the density of states and a set of associated degeneracies. This seminar provides a brief introduction to this framework; experimental validations at the atomistic level, which suggest the reasonableness of this approach; and results from a number of applications ranging from the nanoscale to the mesoscale to the macroscale.