From Hamilton to Boltzmann: The dynamical road toward equilibrium

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Can Hamiltonian dynamics explain the ubiquity of the Boltzmann factor? That isolated systems with many degrees of freedom evolve asymptotically in time towards thermal equilibrium lies at the heart of classical thermodynamics. Statistical mechanics teaches that for systems described by a Hamiltonian H, the thermal states are those described by the canonical Boltzmann relation $\rho = Z^{-1} \exp(-\beta H)$. This follows from original arguments of Maxwell, marginal distributions that arise from microcanonical ensembles, and the properties of the maximum entropy states to which systems thermodynamically tend. While such statistical arguments identify the thermal state, they provide no insight into the problem of how the microscopic dynamics of diverse large systems each lead towards equilibrium from an arbitrary initial state. Demonstrating how microscopic dynamics cause large systems to approach thermal equilibrium remains an elusive, longstanding, and actively pursued goal of statistical mechanics.

We explore this issue by studying the convergence toward thermal equilibrium of Hamiltonian (and mechanical) systems of interacting particles in contact to a bath of other systems. We focus on interactions that occur through collisions and explore the conditions under which the system reaches equilibrium after repeated and random interactions with the bath's degrees of freedom.

We identify a dynamical mechanism for thermalisation in a general class of two-component dynamical Lorentz gases and prove that each component, even when maintained in a nonequilibrium state itself, can drive the other to a thermal state with a well-defined effective temperature, yielding a two-stage process for the thermalization of all the degrees of freedom. If the system is in contact with a bath out of equilibrium, equilibration of the system is always attained when the coupling with the bath is weak. Beyond the weak-coupling limit, equilibration is not always attained and it strongly depends on the details of the bath's energy distribution.

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