Boltzmann subspaces and temperatures in systems driven far from equilibrium

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Out-of-equilibrium many-body quantum systems are generally not associated with a thermal state. Yet, inspecting single molecule junctions in different scenarios, we found non-trivial clustering of steady state populations into distinctive subspaces with Boltzmann-like statistics, which persist far from equilibrium. The existence of Boltzmann subspaces simplifies our understanding of transport in open quantum systems and holds promise for reducing the numerical effort in simulations of driven molecular junctions which are otherwise beyond reach of current computations. In this lecture we focus on molecules under a thermal bias imposed by coupling to two electrodes at different temperatures. We demonstrate that within the realm of weak electrode-molecule coupling (Pauli master equations), even far from equilibrium, Boltzmann subspaces do emerge and the system can be assigned (at least approximately) an effective temperature. We demonstrate the emergence of Boltzmann subspaces under thermal bias and identify the corresponding effective temperature in a variety of molecular junction models, including account for electron-electron interaction, molecular disorder, asymmetric coupling to the electrodes, and the orbital energy density. The relation of the Boltzmann subspaces temperature to other definitions of a temperature in non equilibrium conditions, e.g., in terms of external probes, is discussed. Our results draw guidelines for controlling the effective temperature of single-molecule electronic devices operating far from equilibrium.

[1] M. Iv, S. Rahav and U. Peskin, Phys. Rev. Lett. 132, 110401 (2024)

[2] Y. Gomeh and U. Peskin, J. Chem. Phys. 163, 034122 (2025)