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Integrability and KAM Non-Ergodicity in the Thermostated Hamiltonian Systems

In this talk I will discuss Hamiltonian systems that are thermostated using the Jellinek–Berry (JB) thermostat (J. Phys. Chem. 1988; Phys. Rev. A 1988). Jellinek and Berry proposed this model as a functional extension of Nosé’s thermostat (J. Chem. Phys. 1984), introducing several functional parameters that generalize the coupling between the physical system and the thermal reservoir. In molecular dynamics, the JB family aims to generate the canonical ensemble of a Hamiltonian H by coupling H to a one-dimensional heat reservoir with potential energy $v(s)$ and kinetic energy $\frac{1}{2Q}(p_s/u(s))^2$; i.e.,

$$G(x, s, p_s) := \underbrace{H(a(s) \cdot x)}_{\text{Physical system}} + \underbrace{\frac{p_s^2}{2Q u(s)^2} + gkT v(s)}_{\text{Thermostat}}.$$

I will describe when the JB–thermostated periodic ideal gas is Liouville completely integrable and satisfies a KAM twist condition known as Rüssmann non-degeneracy. This property ensures that the system admits action–angle variables and a nondegenerate frequency map. Using these results, one can show that a thermostated, collisionless, non-ideal gas—that is, a smooth perturbation of the ideal case—possesses a positive-measure set of invariant tori at sufficiently high reservoir temperatures. Consequently, the thermostated dynamics remain non-ergodic in this regime.

The talk will emphasize the geometric structure underlying these results, including the role of symplectic transformations, the existence and persistence of invariant tori, highlighting the connection between thermostat design and classical problems of integrability and ergodicity in Hamiltonian systems.