Deterministic dynamical systems for sampling the canonical ensemble

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The Nose-Hoover thermostat is a deterministic dynamical system designed for computing phase space integrals for the canonical Gibbs distribution. Newton's equations are modified by coupling an additional reservoir variable to the physical variables. The correct sampling of the phase space according to the Gibbs measure is dependent on the Nose-Hoover dynamics being ergodic. Hoover presented numerical experiments that show the Nose-Hoover dynamics to be non-ergodic when applied to the harmonic oscillator. We have proven that the Nose-Hoover thermostat does not give an ergodic dynamics for the one-dimensional harmonic oscillator when the "mass" of the reservoir is large. Our proof of non-ergodicity uses KAM theory to demonstrate the existence of invariant tori for the Nose-Hoover dynamical system.

We present numerical experiments motivated by our analysis that seem to show that the dynamics is not ergodic even for a moderate thermostat mass. We also give numerical experiments of the Nose-Hoover chain (proposed by Martyna, Klein, and Tuckerman) with two thermostats applied to the one-dimensional harmonic oscillator. These experiments seem to support the non-ergodicity of the dynamics if the masses of the reservoirs are large enough and are consistent with ergodicity for more moderate masses.

Joint work with Frederic Legoll and Richard Moeckel

The talk will be in Vincent Hall 570 at 3:35 pm