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Role of ergodicity in molecular dynamics

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Abstract

The role of ergodity is discussed in the context of computational molecular biophysics. Ergodicity does not seem essential for basic statistical mechanics, since one can apply plausible maximum entropy arguments. Nor is ergodicity essential for computing ensemble averages, since it is not necessary to use strictly deterministic sampling methods. However, explaining the effect of perturbations on time-dependent properties may require not only the assumption of ergodicity but also the stronger assumption of mixing. A plausible formal perturbation analysis for time-dependent properties is presented which requires the assumption of mixing.