UNIVERSITÄT LEIPZIG

Fakultät für Physik und Geowissenschaften

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Physics Colloquium

Thursday, 3 December 2020 at **17:15**

Prof. Dr. Alexander K. Hartmann

Universität Oldenburg

Simulation of extremely rare ultra-fast non-equilibrium processes close to equilibrium

Fluctuation theorems like those of Crooks or Jarzynski allow to obtain equilibrium quantities from non-equilibrium processes. For example, the distribution $P(W)$ of the work allows to extract the free energy difference ΔF between equilibrium starting state and final state, after hypothetical final equilibration. The region of $P(W)$ where $W \approx \Delta F$ holds is most relevant to obtain ΔF. But $P(W)$ may be extremly small in this region. In the case of computer simulations this requires sophisticated large-deviation algorithms. As example, the Ising model with work performed by changing the external field is shown, where probabilities as small as 10^{-50} and lower must be reached.

Going beyond the calculation of ΔF, we ask, how similar are the non-equilibrium processes in this rare-event tail to the equilibrium ones that determine ΔF? Here, this question is investigated for the unfolding and refolding of RNA secondary structures under influence of an external force f. Indeed the extreme low-probability trajectories, which exhibit $W \approx \Delta F$ and thus contribute most to the determination of ΔF via Crooks equation, are most similar to the equilibrium trajectories.
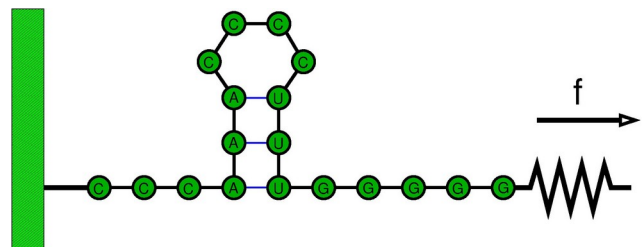
Joint Colloquium with *CompPhys20,* Leipzig, 3–5 December 2020

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