Physics Colloquium

Thursday, 3 December 2020 at 17:15

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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 $\Delta F$ 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 $\Delta F$. But $P(W)$ may be extremely 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 $\Delta F$, we ask, how similar are the non-equilibrium processes in this rare-event tail to the equilibrium ones that determine $\Delta F$? 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 $\Delta F$ via Crooks equation, are most similar to the equilibrium trajectories.

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