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Modified kinetic Monte-Carlo algorithm based on fluctuation theorem

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Kinetic Monte Carlo (KMC) is an algorithm which finds transitions between states during an evolution of a system out of equilibrium according to the prescribed transition rate probabilities. One Major caveat with the original KMC is no attention that is given to how the system interacts with the environment. In particular, it is not known how the transition rate probability matrix plays a role in determining the heat exchange with the environment. To improve upon KMC, a fluctuation theorem is applied to KMC that connects the ratio of transition rate probability and its time conjugate to the entropy change of the environment. Our Modified Kinetic Monte Carlo (MKMC) algorithm chooses the next state in such a way as to obey the second law of thermodynamics. We apply the algorithm to solve the problem of Brownian heat engine operating between two heat baths. The result of the simulation is consistent with the analytic solution and the second law of thermodynamics.

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