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Failure of Overdamped Models for Buttiker-Landauer Heat Engine: Molecular Dynamics Simulation RONALD BENJAMIN, RYOICHI KAWAI, University of Alabama at Birmingham — A spatially inhomogeneous temperature profile in presence of a periodic potential leads to directed current of Brownian particles, commonly known as Büttiker-Landauer ratchet. Under a small external load the system can do work as a heat engine. Overdamped models, neglecting inertial effect ($m = 0$), predict that the engine can reach Carnot efficiency. On the other hand, the overdamped limit ($m \to 0$) predicts the opposite due to the kinetic energy contribution to the heat transfer, suggesting that $m = 0$ is mathematically a singular point. A phenomenological argument predicts that the heat from the hot to the cold reservoir diverges as $1/\sqrt{m}$ [1,2]. We confirmed this singular behavior by Molecular Dynamics (MD) simulation and also by numerically solving the corresponding inertial Langevin equation. We obtain good agreement between the MD simulation and the inertial Langevin equation whereas the solution of the overdamped Langevin equation qualitatively disagrees with them. We also confirmed, from the numerical simulation, that the efficiency of the engine does not reach the Carnot limit.
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