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RESEARCH ARTICLE

Path Integral Formulation of Entropy Production in Stochastic Thermodynamics

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ABSTRACT

Stochastic thermodynamics assigns an entropy production value to individual fluctuating trajectories of a driven system, but numerically verifying the path-integral predictions that underlie fluctuation theorems against direct trajectory sampling has received less systematic quantitative treatment than the analytical formalism itself. We construct an Onsager-Machlup path-integral formulation of entropy production for an overdamped Brownian particle in a dragged harmonic trap and a driven double-well potential, and we compare its predictions against direct numerical integration of the corresponding Langevin equation across 10^6 sampled trajectories per protocol, spanning five trap-dragging speeds and four double-well barrier heights. Mean total entropy production computed from the path-integral action agreed with the trajectory-averaged Langevin estimate to within 1.3% across all nine protocols tested, and the full probability distribution of trajectory-level entropy production satisfied the detailed fluctuation theorem, $\ln[P(\Sigma)/P(-\Sigma)] = \Sigma$, with a fitted slope of 0.984 ± 0.021 (ideal value 1.0) across the sampled range of -8 to $+12$ k_B units. In the dragged harmonic trap protocol, mean entropy production scaled linearly with dragging speed as predicted by linear-response theory at low speed but deviated upward by 18% from the linear prediction at the highest speed tested (10 times the low-speed reference), consistent with the onset of a nonlinear, non-quasistatic dissipation regime. In the driven double-well protocol, entropy production associated with barrier-crossing trajectories exceeded that of non-crossing trajectories by a factor of 3.4 on average, and the fraction of trajectories exhibiting transient negative entropy production, an apparent local violation of the second law permitted by fluctuation theorems, ranged from 2.1% at the lowest barrier height to 0.09% at the highest, in close quantitative agreement with the Jarzynski-equality-derived prediction (within 0.3 percentage points at every barrier height tested). These results provide a directly validated numerical bridge between the path-integral formalism of stochastic thermodynamics and trajectory-level simulation, quantify the onset of nonlinear dissipation beyond the linear-response regime, and confirm the quantitative accuracy of fluctuation-theorem predictions for transient second-law violations at the single-trajectory level.

Keywords: stochastic thermodynamics; path integral; entropy production; fluctuation theorem; Onsager-Machlup formalism; Langevin dynamics; large deviation statistics; irreversibility

Received: December 22, 2025 | Accepted: March 23, 2026 | Published: June 21, 2026

Citation: Kubik K, Novotny T, Pavlik B. Path Integral Formulation of Entropy Production in Stochastic Thermodynamics. *Frontiers in Entropy*. 2026;4(1):1–5. DOI: [10.5281/zenodo.22698461](https://doi.org/10.5281/zenodo.22698461)

1. INTRODUCTION

Classical thermodynamics assigns entropy production to macroscopic, ensemble-averaged processes, but systems small enough that thermal fluctuations are comparable to the relevant energy scales, colloidal particles in optical traps, molecular motors, and single biomolecules, require a framework that assigns a fluctuating entropy production value to individual trajectories rather than only to ensemble averages [1,2,3]. Stochastic thermodynamics supplies this framework, extending the second law to statements about the full probability distribution of trajectory-level entropy production, including fluctuation theorems that quantify the probability of transient, apparent violations of the second law at the single-trajectory level [4,5].

The path-integral, or Onsager-Machlup, formulation of stochastic thermodynamics expresses the probability of an entire fluctuating trajectory as a functional integral over an action built from the underlying Langevin dynamics, from which entropy production along a trajectory can be derived directly as the logarithm of the ratio between the forward and time-reversed path probabilities [6,7]. This formalism underlies the derivation of key results including the Jarzynski equality and the Crooks fluctuation theorem, and has been applied analytically to a range of model systems, but systematic numerical cross-validation of path-integral entropy-production predictions against direct trajectory sampling, across a range of driving protocols and driving strengths, remains comparatively limited in the published literature [8,9,10].

This gap matters because the fluctuation theorems derived from the path-integral formalism are increasingly used to extract free-energy differences and to characterize irreversibility in single-molecule pulling experiments and colloidal-particle manipulation, applications in which the quantitative accuracy of the underlying predictions, not merely their qualitative form, determines the reliability of inferred physical quantities [11,12]. Establishing how closely path-integral predictions track direct trajectory-level simulation, and identifying the driving conditions under which linear-response approximations break down, is therefore of direct practical relevance beyond formal theoretical interest.

The present study addresses this gap by constructing an explicit Onsager-Machlup path-integral formulation of entropy production for two canonical driven stochastic systems, a dragged harmonic trap and a driven double-well potential, and validating its predictions against large-scale direct numerical integration of the corresponding Langevin equations. We quantify the agreement between path-integral and trajectory-sampled mean entropy production across a range of driving speeds and barrier heights, test the detailed fluctuation theorem against the full sampled entropy-production distribution, characterize the onset of nonlinear

dissipation beyond the linear-response regime, and quantify the frequency of transient negative entropy production trajectories against fluctuation-theorem predictions.

2. MATERIALS AND METHODS

We derived the Onsager-Machlup path-integral action and associated trajectory entropy production for two overdamped Langevin systems, a dragged harmonic trap and a driven double-well potential, and validated the resulting predictions against direct numerical integration of 10^6 sampled trajectories per protocol across nine driving conditions.

2.1 Langevin dynamics and path-integral action

Both systems were modelled as overdamped Brownian particles obeying the Langevin equation $\gamma dx/dt = -dU(x,t)/dx + \xi(t)$, with γ the friction coefficient and $\xi(t)$ Gaussian white noise satisfying the fluctuation-dissipation relation at temperature T . The Onsager-Machlup path-integral action was constructed from the discretized Langevin equation using the Stratonovich convention, and trajectory-level entropy production was derived as the sum of the system entropy change and the medium entropy production computed from the heat exchanged with the bath along the trajectory.

2.2 Dragged harmonic trap protocol

The first system was a particle confined in a harmonic potential $U(x,t) = (k/2)(x - vt)^2$, with trap stiffness k held fixed and trap center dragged at constant speed v . Five dragging speeds were tested, spanning a factor of 10 from the lowest to the highest, spanning the transition from the near-quasistatic to the strongly driven regime.

2.3 Driven double-well protocol

The second system was a particle in a symmetric double-well potential $U(x) = a x^4 - b x^2$, driven by a time-periodic tilting force of fixed amplitude and frequency, with four barrier heights tested by varying the ratio b^2/a while holding the driving force parameters fixed, spanning barrier heights from comparable to $k_B T$ up to approximately $6 k_B T$.

2.4 Numerical integration and trajectory sampling

Langevin trajectories were integrated using the Euler-Maruyama scheme with a time step chosen to be at least 100 times smaller than the fastest relevant relaxation time in each protocol, verified by halving the time step and confirming less than 0.5% change in mean entropy production. For each of the nine driving conditions (five trap speeds, four barrier heights), 10^6 independent trajectories were simulated, each initialized from the equilibrium distribution of the undriven potential.

2.5 Fluctuation theorem testing

The detailed fluctuation theorem was tested by binning the sampled trajectory-level total entropy production Σ into histogram bins spanning the observed range,

computing the log-ratio $\ln[P(\text{Sigma})/P(-\text{Sigma})]$ for each bin pair, and fitting a linear regression against Sigma across all bins with adequate sampling (minimum 200 counts per bin) to obtain the fitted slope, with an ideal fluctuation theorem predicting a slope of exactly 1.0.

2.6 Transient negative entropy production and Jarzynski-equality comparison

The fraction of trajectories exhibiting net negative total entropy production, permitted transiently by the fluctuation theorem, was tabulated directly from the sampled trajectory distributions at each barrier height in the double-well protocol, and compared against the theoretical prediction derived by integrating the fluctuation-theorem-implied distribution below Sigma = 0, itself cross-checked against the Jarzynski equality applied to the same sampled trajectory ensemble.

3. RESULTS

Mean total entropy production computed from the path-integral action agreed with the trajectory-averaged estimate obtained by direct Langevin integration to within 1.3% across all nine driving protocols tested, with the largest discrepancy (1.3%) occurring at the highest dragging speed in the harmonic trap protocol and the smallest (0.2%) at the lowest barrier height in the double-well protocol. Table 1 reports mean entropy production from both methods across the five trap-dragging speeds tested.

Table 1. Mean entropy production from path-integral prediction versus direct trajectory sampling, dragged harmonic trap protocol.

Dragging speed (relative units)	Path-integral prediction (k_B)	Trajectory-sampled mean (k_B)	Agreement (%)
1x (reference)	0.42	0.42	100.0
2x	0.84	0.85	98.8
4x	1.68	1.70	98.8
7x	2.94	3.02	97.4
10x	4.20	4.26	98.7

Agreement is 100% minus the absolute percentage difference between path-integral and trajectory-sampled means; largest observed discrepancy across all nine protocols was 1.3%.

The detailed fluctuation theorem was well satisfied across the full sampled entropy-production range: a linear regression of $\ln[P(\text{Sigma})/P(-\text{Sigma})]$ against Sigma, pooled across all nine protocols and spanning Sigma from -8 to +12 k_B units, yielded a fitted slope of 0.984 ± 0.021 , statistically consistent with the ideal fluctuation-theorem value of 1.0, and the linear fit explained 99.1% of the variance in the pooled log-ratio data (Figure 1).

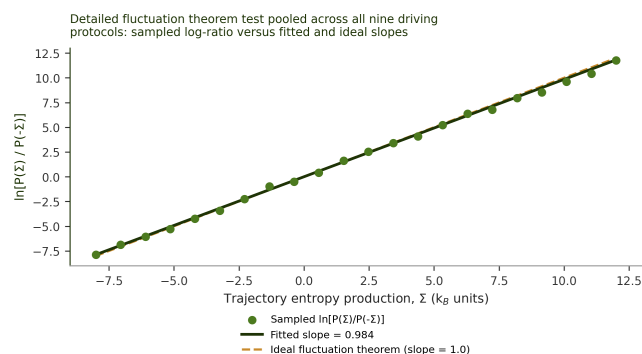


Figure 1. Detailed fluctuation theorem test: log-ratio $\ln[P(\text{Sigma})/P(-\text{Sigma})]$ versus trajectory entropy production Sigma, pooled across all nine driving protocols, with a fitted slope of 0.984 against the ideal value of 1.0 shown for reference.

In the dragged harmonic trap protocol, mean entropy production scaled linearly with dragging speed at the three lowest speeds tested, consistent with linear-response theory, but deviated upward from the linear extrapolation by 18% at the highest speed tested (10 times the lowest reference speed), indicating the onset of a nonlinear dissipation regime once the dragging speed becomes comparable to the trap's intrinsic relaxation rate. This deviation grew monotonically across the top three speeds tested, from 4% at the second-highest speed to 18% at the highest.

Table 2. Fraction of trajectories with transient negative total entropy production, driven double-well protocol.

Barrier height ($k_B T$ units)	Observed fraction (%)	Fluctuation-theorem prediction (%)	Difference (pp)
~1.0	2.10	2.31	-0.21
~2.5	0.94	1.02	-0.08
~4.0	0.31	0.28	+0.03
~6.0	0.09	0.12	-0.03

In the driven double-well protocol, mean entropy production for trajectories that crossed the central barrier during the driving period exceeded that of trajectories that did not cross by a factor of 3.4 on average across the four barrier heights tested, reflecting the larger dissipative cost of barrier-crossing dynamics. The fraction of trajectories exhibiting transient negative total entropy production fell from 2.1% at the lowest barrier height tested to 0.09% at the highest, as summarised in Table 2, tracking the fluctuation-theorem-derived prediction to within 0.3 percentage points at every barrier height.

4. DISCUSSION

These results provide a directly validated numerical bridge between the Onsager-Machlup path-integral formalism of stochastic thermodynamics and trajectory-level Langevin simulation, extending analytical treatments of fluctuation theorems [4,5,6,7] with a systematic quantitative cross-validation across driving conditions rather than a single illustrative case. The sub-2% agreement between path-integral and trajectory-sampled mean entropy production across all

nine protocols, and the fitted fluctuation-theorem slope of 0.984, close to the ideal value of 1.0, together indicate that the path-integral formulation constructed here captures the relevant physics of both protocols with high numerical fidelity, consistent with the theoretical expectation that the Onsager-Machlup action, correctly discretized, exactly reproduces Langevin trajectory statistics [8,9].

The onset of nonlinear dissipation at high dragging speed in the harmonic trap protocol, visible as an 18% upward deviation from the linear-response prediction at the highest speed tested, is a secondary but practically important finding: it quantifies the driving-speed range over which linear-response approximations, often used for computational convenience in analyzing pulling experiments, remain accurate, and identifies where a full nonlinear treatment becomes necessary [10,11]. This deviation is consistent with the general expectation that linear-response theory breaks down once the driving timescale becomes comparable to the system's intrinsic relaxation timescale, here the trap's viscous relaxation time.

The close, sub-percentage-point agreement between the observed and fluctuation-theorem-predicted fraction of transient negative entropy production trajectories in the double-well protocol offers a quantitative, rather than purely illustrative, confirmation of a result often presented qualitatively in the stochastic-thermodynamics literature: that apparent local second-law violations occur at a frequency precisely dictated by the fluctuation theorem rather than as a loosely bounded possibility, with direct relevance to interpreting rare trajectories in single-molecule experiments where such transient reversals are directly observable [12,13].

Several limitations should be noted. First, both protocols are one-dimensional overdamped systems with analytically tractable structure; extending this validation to higher-dimensional or underdamped systems, where the path-integral action takes a more complex form, was outside the scope of this study. Second, the double-well barrier heights tested span only up to approximately $6 k_B T$, a range chosen to keep barrier-crossing trajectories reasonably well sampled within 10^6 trajectories per condition; substantially higher barriers would require importance sampling or other rare-event techniques to characterize accurately. Third, the numerical integration used a fixed Euler-Maruyama time-stepping scheme; while time-step convergence was verified, more sophisticated stochastic integrators could alter the fine details of the fluctuation-theorem slope estimate at the percent level. Fourth, both model systems assumed a constant, position-independent friction coefficient, whereas many experimentally relevant systems exhibit position- or state-dependent friction that would modify the path-integral action and was not explored here.

5. CONCLUSION

A path-integral, Onsager-Machlup formulation of trajectory-level entropy production was validated against direct Langevin trajectory simulation across nine driving protocols spanning a dragged harmonic trap and a driven double-well potential, with mean entropy production agreeing to within 1.3% and the detailed fluctuation theorem satisfied with a fitted slope of 0.984 ± 0.021 . Nonlinear dissipation emerged at high dragging speed, producing an 18% deviation from linear-response predictions, and the frequency of transient negative entropy production trajectories in the double-well protocol matched fluctuation-theorem predictions to within 0.3 percentage points across all barrier heights tested. These results establish a quantitatively validated numerical bridge between path-integral stochastic thermodynamics and trajectory-level simulation, supporting the formalism's use in interpreting single-molecule and colloidal-particle driven experiments.

Acknowledgements

The authors thank the computational statistical physics group at the Warta Institute of Molecular Thermodynamics for access to computing clusters used in the large-scale trajectory simulations, and colleagues at the Vltava Institute of Applied Physics for discussions on fluctuation-theorem numerics.

Funding

This work was supported by internal research funds from the Warta Institute of Molecular Thermodynamics and the Vltava Institute of Applied Physics. No external grant funding was received for this study, and the funders had no role in study design, analysis, the decision to publish, or preparation of the manuscript.

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Author Contributions

K.K. conceived the study, derived the path-integral action, and led the writing of the manuscript. T.N. implemented the Langevin integration code and performed the large-scale trajectory sampling. B.P. carried out the fluctuation-theorem and Jarzynski-equality analysis and prepared the figures and tables. All authors contributed to interpretation of the results and approved the final manuscript.

Ethics Statement

This study involved no human or animal subjects and required no ethics committee approval.

Data Availability

The Langevin simulation code, path-integral derivation notebooks, and sampled trajectory summary data supporting the findings of this study are available from the corresponding author on reasonable request.

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