

8.808/8.308 IAP 2026 Recitation 3: Operator TRS, simulating a polymer

Jessica Metzger

jessmetz@mit.edu | Office hours: 1/9, 1/14, 1/20, 1/27 11am-12pm (8-320)

January 14, 2026

Contents

1	TRS for Brownian particles in spatially-varying T	1
2	Ideal polymer	2
2.1	Average energy	2
2.2	End-to-end separation	2
3	Numerics	3

1 TRS for Brownian particles in spatially-varying T

First, we will show using the operator identity

$$\text{time-reversal symmetry} \iff H_{\text{FP}}^\dagger = P_S^{-1} H_{\text{FP}} P_S \quad (1)$$

that an overdamped Brownian particle with spatially-varying temperature obeys time-reversal symmetry.

We showed in the previous recitation that an overdamped Brownian particle with spatially-varying temperature and discretization α evolves according to the Fokker-Planck equation

$$\dot{P} = \nabla \cdot [T^\alpha \nabla (T^{1-\alpha} P)] \equiv -H_{\text{FP}} P \quad (2)$$

so that the Fokker-Planck operator is

$$H_{\text{FP}} = -\nabla \cdot T^\alpha \nabla T^{1-\alpha} . \quad (3)$$

Its adjoint can be calculated using

$$\langle H_{\text{FP}}^\dagger f | g \rangle = \langle f | H_{\text{FP}} g \rangle^* = \langle f | H_{\text{FP}} g \rangle \quad (4)$$

$$= \int d^d \mathbf{r} f(\mathbf{r}) H_{\text{FP}} g(\mathbf{r}) = - \int d^d \mathbf{r} f(\mathbf{r}) \nabla \cdot \{ T^\alpha \nabla [T^{1-\alpha} g(\mathbf{r})] \} \quad (5)$$

$$= \int d^d \mathbf{r} \nabla f(\mathbf{r}) \cdot \{ T^\alpha \nabla [T^{1-\alpha} g(\mathbf{r})] \} \quad (6)$$

$$= - \int d^d \mathbf{r} \nabla \cdot \{ T^\alpha \nabla f(\mathbf{r}) \} T^{1-\alpha} g(\mathbf{r}) \quad (7)$$

$$\implies H_{\text{FP}}^\dagger = -T^{1-\alpha} \nabla \cdot T^\alpha \nabla . \quad (8)$$

Next, we can use the steady-state probability distribution

$$P_S(\mathbf{r}) = \frac{C}{T(\mathbf{r})^{1-\alpha}} \quad (9)$$

(for some normalization constant C) to calculate

$$P_S^{-1} H_{\text{FP}} P_S = -\frac{T^{1-\alpha}}{C} \nabla \cdot T^\alpha \nabla T^{1-\alpha} \frac{C}{T^{1-\alpha}} = -T^{1-\alpha} \nabla \cdot T^\alpha \nabla = H_{\text{FP}}^\dagger . \quad (10)$$

Thus, time-reversal symmetry is satisfied.

This seems contradictory, because a real system with inhomogeneous temperature is out of thermal equilibrium. However, the above model is a subsystem of the real system: it only accounts for the position degrees of freedom of the Brownian colloid, having coarse-grained out its momentum degrees of freedom along with all bath degrees of freedom. Violation of TRS in the overall system doesn't preclude a hidden TRS in the colloidal subsystem.

2 Ideal polymer

The simplest model of a polymer consists of N identical beads of mass m connected by springs of stiffness k . This has Hamiltonian

$$H[\{\mathbf{r}_n\}] = \sum_{n=1}^N \frac{|\mathbf{p}_n|^2}{2m} + \sum_{n=1}^{N-1} \frac{k}{2} |\mathbf{r}_{n+1} - \mathbf{r}_n|^2 . \quad (11)$$

In the large-damping limit, the dynamics are

$$\dot{\mathbf{r}}_n = \mu \mathbf{f}_n + \sqrt{2\mu k_B T} \boldsymbol{\eta}_n(t) = -\mu \frac{\partial H}{\partial \mathbf{r}_n} + \sqrt{2\mu k_B T} \boldsymbol{\eta}_n(t) \quad (12)$$

where

$$\mathbf{f}_n = \begin{cases} k(\mathbf{r}_2 - \mathbf{r}_1) , & n = 1 \\ k(\mathbf{r}_{n+1} - \mathbf{r}_n) - k(\mathbf{r}_n - \mathbf{r}_{n-1}) , & 2 \leq n \leq N-1 \\ -k(\mathbf{r}_N - \mathbf{r}_{N-1}) , & n = N \end{cases} . \quad (13)$$

We will simulate this model of a polymer.

2.1 Average energy

One observable we can use to validate our simulation is the average potential energy of the polymer. Because the system follows the Boltzmann distribution, we can explicitly calculate this:

$$\langle V[\{\mathbf{r}_n\}] \rangle = \frac{1}{Z} \int \prod_{n=1}^N (d^d \mathbf{r}_n d^d \mathbf{p}_n) \left(\sum_{n=1}^{N-1} \frac{k}{2} |\Delta \mathbf{r}_n|^2 \right) \exp(-\beta H[\{\mathbf{r}_n\}]) \quad (14)$$

$$= (N-1) \frac{d}{2} k_B T , \quad (\text{Gaussian integration}) . \quad (15)$$

2.2 End-to-end separation

One important question in polymer science is how the end-to-end separation of the polymer, $\mathbf{R} \equiv \mathbf{r}_N - \mathbf{r}_1$, scales with the number N of monomers. We define the exponent ν such that

$$R \sim N^\nu , \quad (16)$$

and develop theory to estimate ν .

For the ideal polymer, it is easy to calculate ν . Because each $\Delta \mathbf{r}_n$ is an independent d -dimensional Gaussian random variable, $\mathbf{R} = \sum_{n=1}^{N-1} \Delta \mathbf{r}_n$ is also a d -dimensional Gaussian random variable. We know that it has zero mean, and can calculate the variance

$$\langle |\mathbf{R}|^2 \rangle = \left\langle \left| \sum_{n=1}^{N-1} \Delta \mathbf{r}_n \right|^2 \right\rangle \quad (17)$$

$$= \sum_{n=1}^{N-1} \sum_{m=1}^{N-1} \langle \Delta \mathbf{r}_n \cdot \Delta \mathbf{r}_m \rangle \quad (18)$$

$$= \sum_{n=1}^{N-1} \frac{dk_B T}{2} = \frac{dk_B T}{2} (N-1) . \quad (19)$$

Thus

$$R^2 \sim N \quad \implies \quad R \sim N^{1/2} \quad \implies \quad \nu = \frac{1}{2} . \quad (20)$$

3 Numerics

You will simulate an ideal polymer using the code `Rec3_Polymer.jl` which uses `Rec3_module.jl` (both on the website). Your task is to

1. Fill in the missing code to simulate the polymer
2. Make sure your polymer is well-behaved and check if the energy matches expectation
3. (if done early) Check that the end-to-end distance distribution matches expectation
4. (if you still have time) Check the N -dependence of the end-to-end distance.