Supplementary Material for:

Gaussian fluctuations of spatially inhomogeneous polymers

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This document is meant to provide additional technical details related to results reported on in the manuscript.

I. FREE ENERGY IN THE CONTINUUM THEORY

Consider a general one-dimensional system whose energy is treated to quadratic order. The continuum energy takes the form

$$U^{\rm CT}(w(x)) = \frac{1}{2}\langle w(x)|\mathfrak{L}|w(x)\rangle \equiv \frac{1}{2L}\int_0^L w(x)\,\mathfrak{L}\,w(x)\,dx\ ,$$

where $\mathfrak{L}$ is a self-adjoint real differential operator. Our convention is that the eigenvalues of $\mathfrak{L}$ are of energy dimensions, and thus $w(x)$ is dimensionless. We work in the eigenbasis of $\mathfrak{L}$, which we denote by $w_{q_1}(x),\ldots,w_{q_N}(x)$. These functions are orthonormal, i.e.

$$\frac{1}{L}\int_0^L w_q w_{q'}\,dx = \delta_{qq'}\ ,\quad \text{and} \qquad \langle w_q|\mathfrak{L}|w_{q'}\rangle = \lambda_q\delta_{qq'}\ , \tag{S1}$$

where λ_q is the eigenvalue associated with w_q. The eigenmodes span the functional space and a general configuration $w(x)$ can be written as $w(x) = \sum_q a_q w_q(x)$ where $a_q \equiv \langle w(x)|w_q\rangle$. The energy is thus written as $U^{\rm CT} = \frac{1}{2}\sum_q \lambda_q\, a_q^2$, and the partition function, defined in Eq. (26) of the main text, reads

$$\begin{aligned} Z^{\rm CT} &= \int Dw\, e^{-\beta\langle w|\mathfrak{L}|w\rangle}\Theta\Big(\varepsilon - w(L)\Big) \\ &= \int d^N a_q\, \exp\left[-\beta\sum_q \tfrac{1}{2}\lambda_q a_q^2\right]\Theta\Big(\varepsilon - \sum_q a_q w_q(L)\Big)\ . \end{aligned} \tag{S2}$$

This is a multivariate Gaussian integral over a half-space. In Sec. IV of this file we derive a general formula for integrals of this type (Eq. (S25)). Applying this formula to Eq. (S2) yields

$$Z^{\rm CT} = \frac{1}{2}\left(\frac{(2\pi)^N}{\beta^N \det\mathfrak{L}}\right)^{1/2}\left(1+\mathrm{erf}\left[\varepsilon\sqrt{\frac{\beta\kappa_h}{\ell^{\rm CT}}}\right]\right) \tag{S3}$$

$$\ell^{\rm CT} \equiv 2L\sum_q\left(\frac{w_q(L)}{qL}\right)^2\ . \tag{S4}$$

where $\mathrm{erf}(\cdot)$ is the standard error function and the relation $\lambda_q = \kappa_h L q^2$ was used. $\det\mathfrak{L}$ is defined as $\prod_q \lambda_q$. The factor $\frac{1}{2}(2\pi)^{N/2}$ is of no physical importance and will be omitted in what follows.

Note that here we take into account exactly N continuum modes, which is basically a choice of an ultraviolet cutoff on q. The results presented here do not depend qualitatively on the choice of the ultraviolet cutoff, as long as the number of modes scales with N, which is anyway a trivial requirement from any reasonable cutoff scheme.

The free energy is thus given by

$$\begin{aligned} F^{\rm CT} &\equiv -k_BT\log Z^{\rm CT} = F^{\rm CT}_{\rm uc} + F^{\rm CT}_{\varepsilon}\ , \\ F^{\rm CT}_{\rm uc} &\equiv \tfrac{1}{2}k_BT\log\left(\beta^N\det\mathfrak{L}\right)\ , \\ F^{\rm CT}_{\varepsilon} &\equiv -\tfrac{1}{2}k_BT\log\left(1+\mathrm{erf}\left[\varepsilon\sqrt{\frac{\beta\kappa_h}{\ell^{\rm CT}}}\right]\right)\ . \end{aligned} \tag{S5}$$

We now turn to calculate $\det\mathfrak{L}$, which is done by explicit calculation of the eigenmodes. Since the wavenumbers are given approximately by Eqs. (19)-(20) of the main text, the calculation of $F^{\rm CT}$ is straightforward. The eigenvalue associated with the wavenumber q is $\lambda_q = L\,\kappa_h\,q^2$ and thus

$$\det\mathfrak{L} = \prod_q\lambda_q = \prod_n \kappa_h L q_n^2 = \left(\frac{\kappa_h}{L}\right)^N C^{2N}(N!)^2\ .$$

This immediately leads to

$$\begin{aligned} F^{\rm CT} &= \frac{1}{2}k_BT\log\left[\beta^N\det\mathfrak{L}\right] = \\ & Nk_BT\left[\tfrac{1}{2}\log\left(\frac{\beta\kappa_h}{L}\right) - \log\left(\frac{\phi\Delta+1-\phi}{\pi}\right) + \frac{1}{N}\log N!\right]. \end{aligned} \tag{S6}$$

We now apply Stirling's approximation, which we write as $\log(N!)\approx N\log\left(\frac{N}{e}\right)$ and after some rearrangement we obtain

$$\begin{aligned} F^{\rm CT} \approx Nk_BT\Bigg[&\tfrac{1}{2}\log\left(\frac{\beta\kappa_h}{L/N}\right) \\ &- \log\left(\Delta\phi+1-\phi\right) + \log\left(\sqrt{N}\frac{\pi}{e}\right)\Bigg]\ . \end{aligned} \tag{S7}$$

The free energy of a homogeneous polymer, $f^{\rm CT}$ is immediately obtained by setting $\phi = 0$.

II. FREE ENERGY IN THE DISCRETE THEORY

Here we present the calculation of the free energy associated with $\boldsymbol{H}^{(1)}$ in the discrete formalism. We want to calculate the partition function

$$Z^{\rm DT} = \int_{-\infty}^{\infty} d^N\boldsymbol{w}\, e^{-\beta U^{\rm DT}(\boldsymbol{w})}\Theta(\varepsilon - w_N)\ , \tag{S8}$$

with

$$U^{\rm DT}(\boldsymbol{w}) = \sum_{i=1}^{N}\frac{1}{2}\kappa_i\left(\frac{w_i - w_{i-1}}{\Delta x}\right)^2 \Delta x\ . \tag{S9}$$

Unlike the continuum case described in the previous section, here the calculation can be performed without explicit reference to the eigenmodes. The trick is to use the non-orthogonal change of variables

$$y_i \equiv \sqrt{\frac{\kappa_i}{\Delta x}}(w_i - w_{i-1})\ , \quad w_i = \sum_{j=1}^{i} y_j\sqrt{\frac{\Delta x}{\kappa_j}}\ . \tag{S10}$$

The Jacobian of this transformation is $\prod_i \sqrt{\frac{\kappa_i}{\Delta x}} = \sqrt{\det \boldsymbol{H}}$. With the new variables y_i the energy takes the simple form $U = \frac{1}{2}||\boldsymbol{y}||^2$. The partition function is thus

$$Z^{\rm DT} = \sqrt{\frac{1}{\det \boldsymbol{H}}}\int_{-\infty}^{\infty} d^N\boldsymbol{y}\, e^{-\frac{\beta}{2}|\boldsymbol{y}|^2}\Theta\left(\varepsilon - \sum_j y_j\sqrt{\frac{\Delta x}{\kappa_j}}\right)\ .$$

This is a Gaussian integral over a half-space, for which we derive an explicit formula in Sec. IV of this file (Eq. (S25)). The result is

$$Z^{\rm DT} = \frac{1}{2}\sqrt{\frac{(2\pi)^N}{\beta^N \det \boldsymbol{H}}}\left(1 + {\rm erf}\left[\varepsilon\sqrt{\frac{\beta\kappa_{\rm eff}}{2\Delta x}}\right]\right)\ , \tag{S11}$$

where we introduced the notation $\kappa_{\rm eff} \equiv \left(\sum \kappa_i^{-1}\right)^{-1}$, i.e. the effective spring constant of the chain.

Note that this expression holds for an arbitrary choice of κ_i, and also that it is invariant to permutations in the order of the κ_i's (since $\det \boldsymbol{H}$ is). If we assume $\kappa(x)$ has the form described in the main text, i.e. $N\phi$ springs have a spring constant of κ_s and $N(1-\phi)$ have a spring constant of κ_h, we have

$$\kappa_{\rm eff} = \left(\frac{N\phi}{\kappa_s} + \frac{N(1-\phi)}{\kappa_h}\right)^{-1} = \frac{\kappa_h/N}{\Delta^2\phi + (1-\phi)}\ , \tag{S12}$$

$$\det \boldsymbol{H} = \prod_i \frac{\kappa_i}{\Delta x} = \left(\frac{\kappa_h}{\Delta x}\right)^N \Delta^{-2N\phi}\ . \tag{S13}$$

Thus, the free energy is

$$\begin{aligned} F^{\rm DT} &\equiv -k_BT\log Z^{\rm DT} = F_i^{\rm DT} + F_\varepsilon^{\rm DT}\ ,\\ F_{\rm uc}^{\rm DT} &\equiv \tfrac{1}{2}k_BT\log\left(\beta^N\det \boldsymbol{H}\right)\\ &= \tfrac{N}{2}k_BT\left[\log\left(\frac{\beta\kappa_h}{L/N}\right) - \phi\log\Delta\right]\ , \qquad \text{(S14)}\\ F_\varepsilon^{\rm CT} &\equiv -\tfrac{1}{2}k_BT\log\left(1 + {\rm erf}\left[\varepsilon\sqrt{\frac{\beta\kappa_h}{\ell^{\rm DT}}}\right]\right)\ ,\\ \ell^{\rm DT} &= 2L\Big(\Delta^2\phi + (1-\phi)\Big)\ . \qquad \text{(S15)} \end{aligned}$$

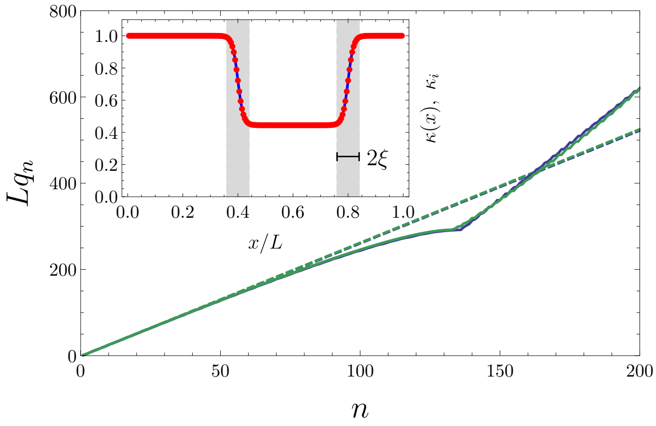

FIG. S1. The spectrum of the SFT operator (dashed lines) and the discrete operator (solid lines) for the case $\xi = L/25$ (green) and $\xi = 0$ (blue) which is discussed in the manuscript. Inset: The smoothed $\kappa(x)$ (solid line) and the discrete κ_i (points). The parameters used are the same as those of Fig. 1 of the main text, together with $\xi = L/25$. The shaded regions, each of width 2ξ, show the region where κ varies.

III. SMOOTH VARIATION OF $\kappa(x)$

The continuum eigenmodes of a system with a smoothly varying $\kappa(x)$ can be obtained using a straightforward shooting method. The Sturm-Liouville problem associated with $\mathfrak{L}^{(1)}$, namely

$$\frac{\partial}{\partial x}\left(\kappa(x)\frac{\partial w}{\partial x}\right) = \lambda\, w(x) \tag{S16}$$

is interpreted as a differential equation which is integrated with the initial conditions $w(0)=0$ and $w'(0)=1$. The equation is integrated up to $x = L$ and the value $w'(L;\lambda)$ is obtained as a function of λ. The eigenvalues are those λ for which $w'(L;\lambda)=0$. These are found using standard root-finding methods.

To explore the effect of the smoothness of $\kappa(x)$ on the results, we chose a specific form of smoothing. Instead of a sharp step function, defined as

$$\Theta(x) = \begin{cases} 0 & x < 0\\ 1 & x > 0\end{cases}\ , \tag{S17}$$

we use a hyperbolic tangent function that varies over a finite lengthscale ξ

$$\Theta(x;\xi) = \frac{1}{2}\left[1 + \tanh\left(\frac{2x}{\xi}\right)\right]\ . \tag{S18}$$

ξ can be significantly larger than the monomeric lengthscale. Equation (S17) in recovered in the limit $\xi \to 0$. An example of a smoothed $\kappa(x)$ with $\xi = L/25$ is shown in Fig. S1. The computed spectra are also shown and it is seen that the effect of ξ on the spectrum is small and the qualitative discrepancies between the continuum and discrete theories persist. Moreover, the qualitative discrepancies between the continuum and discrete theories are independent of ξ, at least as long as $\xi \ll L$.

IV. HALF-SPACE GAUSSIAN INTEGRALS

The partition function, defined in Eq. (26) of the main text, is a multivariate Gaussian integral over a half space. In this section we calculate such an integral in a general manner, to be used in calculations of Z^{DT} and Z^{CT}.

We want to calculate the integral

$$I(\boldsymbol{A},\boldsymbol{v}) = \int_{-\infty}^{\infty} d^N\boldsymbol{x}\, e^{-\frac{1}{2}\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x}}\Theta\left(b-\boldsymbol{v}\cdot\boldsymbol{x}\right) \ . \quad \text{(S19)}$$

That is, the integral of a multivariate Gaussian over the half space defined by $\boldsymbol{v}\cdot\boldsymbol{x} < b$. $\boldsymbol{v}$ is an arbitrary real vector and $\boldsymbol{A}$ is a strictly positive-definite symmetric matrix. We begin with the simpler case where $\boldsymbol{A}$ is diagonal. The generalization for the non-diagonal case will be immediate. The integral is then

$$I(\boldsymbol{A},\boldsymbol{v}) = \int_{-\infty}^{\infty} d^N\boldsymbol{x}\, e^{-\frac{1}{2}\sum_i \lambda_i x_i^2}\Theta\left(b-\boldsymbol{v}\cdot\boldsymbol{x}\right) \ ,$$

where the λ_i's are the eigenvalues of $\boldsymbol{A}$. We replace the Heaviside function by the integral identity

$$\Theta(b-x) = \int_{-\infty}^{b} \delta(z-x)dz = \int_{-\infty}^{b}\frac{dz}{2\pi}\int_{-\infty}^{\infty} d\omega\, \exp[i\omega(z-x)] \ ,$$

where two auxiliary variables, ω and z, were introduced. This identity holds for arbitrary $x, b \in \mathbb{R}$. With this replacement, after simple rearrangement the integral is written as

$$I = \int_{-\infty}^{b}\frac{dz}{2\pi}\int_{-\infty}^{\infty} e^{i\omega z} \times \left(\prod_{j=1}^{N}\int_{-\infty}^{\infty} dx_j\, \exp\left[-\left(\frac{1}{2}\lambda_j x_j^2 + i\omega v_j x_j\right)\right]\right) d\omega \ . \quad \text{(S20)}$$

This is a product of Gaussian integrals, for each of which we can use the integral identity

$$\int_{-\infty}^{\infty} \exp\left[-\frac{1}{2}az^2 \pm i\omega z\right] dz = \sqrt{\frac{2\pi}{a}}\exp\left[-\frac{\omega^2}{2a}\right] \ , \quad \text{(S21)}$$

which holds for any $\omega \in \mathbb{C}$ and real $a > 0$. Thus,

$$I = \int_{-\infty}^{b}\frac{dz}{2\pi}\int_{-\infty}^{\infty} d\omega e^{i\omega z}\prod_{i=1}^{N}\sqrt{\frac{2\pi}{\lambda_i}}\exp\left[-\frac{\omega^2 v_i^2}{2\lambda_i}\right] \quad \text{(S22)}$$
$$= \sqrt{\frac{(2\pi)^N}{\det\boldsymbol{A}}}\int_{-\infty}^{b}\frac{dz}{2\pi}\int_{-\infty}^{\infty} d\omega e^{-\frac{1}{2}\left(\sum\frac{v_i^2}{\lambda_i}\right)\omega^2 + i\omega b} \ .$$

The latter is again a Gaussian integral of the form of Eq. (S21), and denoting $D \equiv \sum_i \frac{v_i^2}{\lambda_i} = \boldsymbol{v}^T\boldsymbol{A}^{-1}\boldsymbol{v}$ we get

$$I = \sqrt{\frac{(2\pi)^N}{\det\boldsymbol{A}}}\int_{-\infty}^{b} dz\sqrt{\frac{2\pi}{D}}\exp\left[-\frac{z^2}{2D}\right] \ . \quad \text{(S23)}$$

The last integral is expressed in terms of the standard error function

$$\mathrm{erf}(z) \equiv \frac{2}{\sqrt{\pi}}\int_0^z e^{-x^2}dx \ , \quad \text{(S24)}$$

such that

$$I(\boldsymbol{A},\boldsymbol{v}) = \frac{1}{2}\sqrt{\frac{(2\pi)^N}{\det\boldsymbol{A}}}\left[1+\mathrm{erf}\left(\frac{b}{\sqrt{2D}}\right)\right] \ , \quad D \equiv \boldsymbol{v}^T\boldsymbol{A}^{-1}\boldsymbol{v} \ . \quad \text{(S25)}$$

This completes the derivation. While this is not necessary for the present needs, we note that the formula (S25) is valid also when $\boldsymbol{A}$ is not diagonal. This can be seen by a simple change of variables.