Supporting information for:

Influence of topology on the free energy and metric properties of an ideal ring polymer confined in a slit

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Autocorrelation time of an unknotted ring in simulation

To ensure the conformations generated by our biased Monte Carlo are fully equilibrated, we calculate the autocorrelation time of an unknotted ring by analyzing the autocorrelation function for the square radius of gyration R_g^2:

$$C(t) = \frac{< A_m A_{m+t} > - < A_m >^2}{< A_m^2 > - < A_m >^2} \sim \exp(-t/\tau) \tag{1}$$

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where the observable A is R_g^2, m indicates any point in the time series and τ is the autocorrelation time. Fig. 1 shows the autocorrelation function for an unknotted ring with bias potential parameter $K = 0$ for four different chain lengths. The correlation vanishes after 2×10^5 MCS even for the largest ring. The autocorrelation time for the different chain lengths and K are estimated by fitting to an exponential; the results are presented in Table 1. In our simulation, we collect conformations every 2×10^5 MCS, which is longer than the autocorrelation time even for the largest ring size at the largest value of the bias potential parameter, as shown in Table 1.

Table 1: The autocorrelation time τ for different ring chain lengths N and bias potential parameters K.

	$K=0$	$K=4$	$K=8$	$K=16$	$K=32$	$K=64$
$\tau(N=100)$	504	569	695	782	948	
$\tau(N=250)$	2336	3052	3275	3719	4350	5220
$\tau(N=500)$	10370	12786	14417	15200	17200	19500
$\tau(N=1000)$	33110	34900	48110	50870	95780	117900

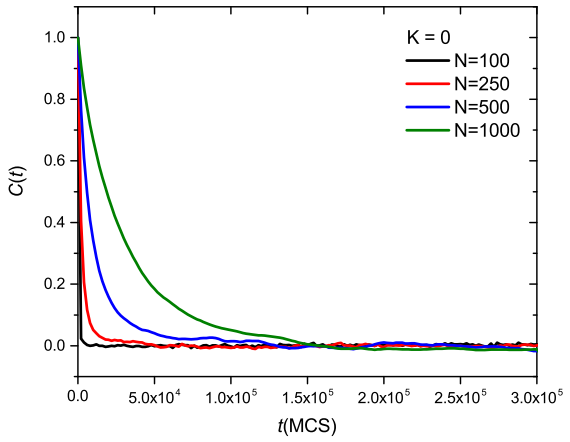

Figure 1: Autocorrelation function $C(t)$ for the square radius of gyration R_g^2 as a function of MC step t for an unknotted ring with bias potential parameter $K = 0$ and ring sizes: $N = 100$, 250, 500 and 1000.