Supplemental Material for: "Equilibrium organization, conformation, and dynamics of two polymers under box-like confinement"

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I. CENTRE-OF-MASS POSITION PROBABILITY DISTRIBUTIONS

Figure 1 in the article shows centre-of-mass position probability distributions for systems of one and two polymers confined to a box-like cavity for the case of polymer chain length $N = 60$ and box height $h = 4$. A value of $N = 60$ was chosen because most of the results for the dynamics presented in Section 4.2 were limited to polymers of this length, and it was convenient for showing how the dynamics were related to the organization of the polymers in the cavity. While using longer polymers would make the model system better resemble the λ DNA system examined experimentally by Capaldi *et al.*[1], the dynamics simulations become infeasibly time consuming. On the other hand, the centre-of-mass distribution functions, as well as other quantities considered in Section 4.1, can be calculated using Monte Carlo (MC) simulations, for which much larger systems are more easily simulated. Below, we present results for polymers of length $N = 300$. In addition, we also consider the effect of varying the box height h.

Figure 1 shows 2-D probability distributions that characterize the position of the polymers inside the the box-like cavity in the transverse plane. Results are shown $N = 300$, $h = 4$, and for a wide range of box widths. The top row shows the probability of the centre of mass of a polymer at any position in the $x - y$ plane for the case where just a single polymer is confined to the cavity. The middle row shows the same probability distribution for the case where two identical polymers are confined to the box. As in the article, we label these distributions $\mathcal{P}_1(x, y)$, where the subscript denotes the single-polymer aspect of the distribution. The bottom row shows probability distributions for the difference in the centre-of-mass coordinates, δx and δy, of the polymers in the two-polymer system. As in the article, we label these distributions $\mathcal{P}_2(\delta x, \delta y)$, where the subscript denotes the fact that this is a 2-polymer property.

The qualitative behaviour of the distributions as the box width L changes are exactly the same as in Fig. 1 of the article for a system with two $N = 60$ chains in a box of the same height. Note

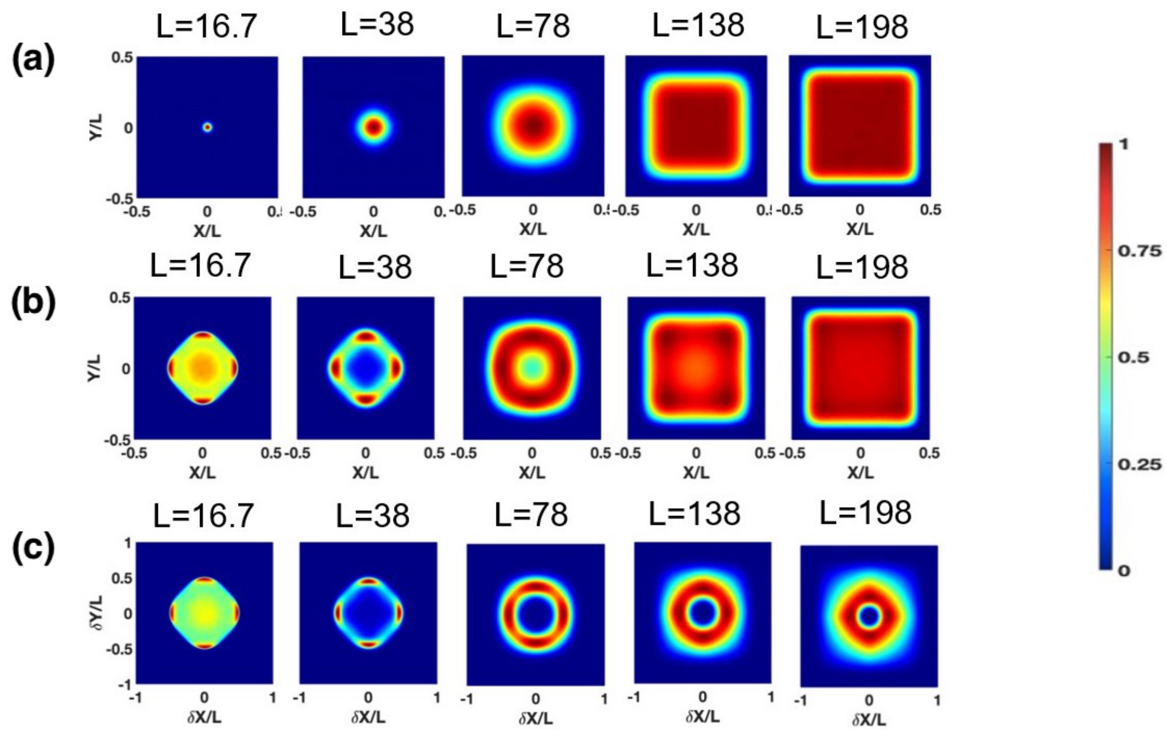

FIG. 1. Probability distributions for a system of one and two polymers of length N=300 confined to a box of height h=4. Results for various box widths are shown. Row (a) shows results for the distribution $\mathcal{P}_1(x, y)$ for a single-polymer system. Row (b) shows distribution $\mathcal{P}_1(x, y)$ for a two-polymer system. Row (c) shows $\mathcal{P}_2(\delta x, \delta y)$, the probability distributions for the difference in the centre-of-mass coordinates, δx and δy of the polymers in the two-polymer system. In all cases, the axes are scaled by the box width, L, and the colour intensity maximum corresponds to the maximum value of the probability for each graph.

that a probability distribution for a given L for N=300 tends to resemble one for N=60 that with a smaller L. For example, the distributions for $L = 38$ for $N = 300$ closely resemble those for $L = 13$ for $N = 60$, and so on. This arises from the fact that larger polymers experience the combined effects of confinement and crowding at larger box sizes than is the case for small polymers.

For the results presented in the article, all of the simulations used a box height of h=4. As noted, this value was chosen to be small enough to compress the polymer along that direction (as was the case in the experiments for confinement of λ DNA) but not so small as to create artifacts as a result of using such a small h/w ratio (where $w = \sigma = 1$ is the width of the polymer). Here we show that small changes to h in this regime do not significantly change the qualitative behaviour of the system.

Figures 2 and 3 show the effects of varying the box height h on the distributions $\mathcal{P}_1(x, y)$ and $\mathcal{P}_2(\delta x, \delta y)$, respectively. For two different box widths ($L = 38$ and 78), results are shown for the three box heights of h=4, 6, and 8. In each case, the chain length is $N = 300$. In the case of $\mathcal{P}_1(x, y)$, there is a slight reduction of the probability depletion in the centre of the box as h decreases. Thus, there is a slightly greater probability that the centres of mass of the polymer will be located at the box centre. However, the basic structure of the distributions is not affected: four symmetrically spaced quasi-discrete states are present for L=38 for all three values of h, and the ring-like structure for L=78 is likewise preserved. In the case of $\mathcal{P}_2(\delta x, \delta y)$, the qualitative appearance of the distributions is likewise unaffected by small changes to h.

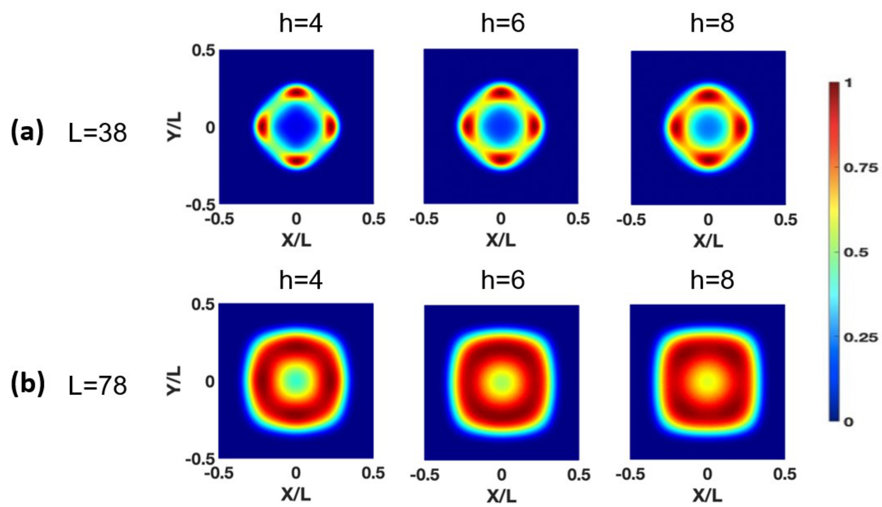

FIG. 2. Probability distributions $\mathcal{P}_1(x, y)$ for a two-polymer system with chain length N=300. (a) The top three panels show distributions for $L = 38$ for three different values of box height h. (b) The bottom three panels show distributions for $L = 78$ and for the same values of h.

In the article, the observed dynamics of the system were interpreted using the qualitative behaviour of the centre-of-mass probability distributions. The qualitative agreement between the results for the distributions for $N = 60$ and $N = 300$ suggest that the tends in the dynamics for the smaller system are likely to be relevant to larger systems, for which simulations using the Brownian dynamics method are currently too computationally demanding to examine directly. Likewise, small changes in the box height h will also not likely change the dynamics in any significant way.

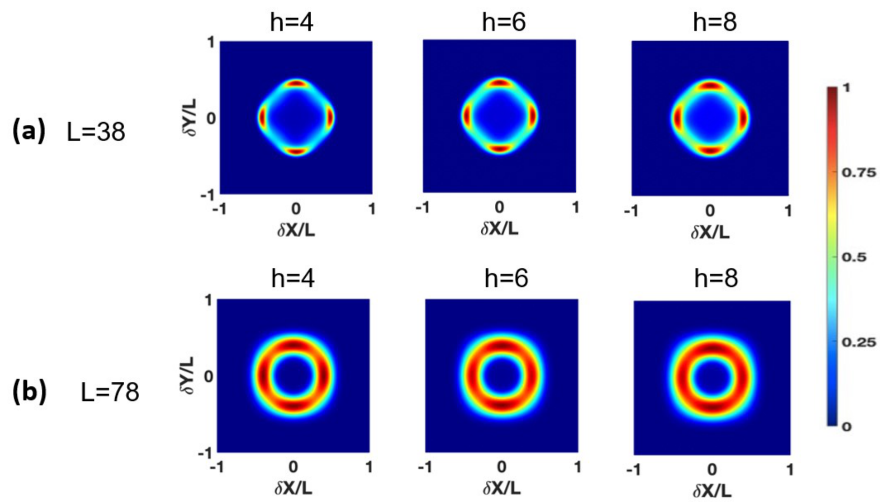

FIG. 3. Probability distributions $\mathcal{P}_2(\delta x, \delta y)$ for a two-polymer system with chain length N=300. (a) The top three panels show distributions for $L = 38$ for three different values of box height h. (b) The bottom three panels show distributions for $L = 78$ and for the same values of h.

II. POLYMER OVERLAP

Figure 4 in the article illustrates the effects of increasing lateral confinement on the degree of overlap between the two polymers. The overlap was quantified using the parameter $\chi_{\rm ov} \equiv N_{\rm ov}/N$, where $N_{\rm ov}$ is the mean number of monomers per polymer that lie inside the overlapping region of the two equivalent ellipses describing the instantaneous size and shape of the polymers. (See Section 3.3 for further details.) The ratio of the overlap for systems where the polymers interact and where the interactions between the polymers are omitted reveal that the regime $L/R^*_{{\rm g},xy} \lesssim 5$ corresponds to systems where the overlap of the polymers is appreciable.

In this section of the ESI, we carry out similar measurements using an alternative measure of overlap: $N_{\rm con}$, the mean number of pairs of monomers on separate polymers that lie within a distance of 1.5σ in the $x-y$ plane, where σ is the monomer diameter. Figure 4(a) below shows the variation of $N_{\rm con}$ with respect to the box width. Figure 4(b) shows the ratio of the degree of overlap for interacting (I) and noninteracting (NI) polymer systems. Results are shown for polymer lengths of N=40, 60, and 300. Although the data for different N do not overlap as was the case for the results of $\chi_{\rm ov}$ in Fig. 4 of the article, the trends are otherwise the same. Most significantly, the ratio is invariant with respect to box width for $L/R^*_{\mathrm{g},xy} \gtrsim 5$, and it decreases rapidly with decreasing L for $L/R^*_{\mathrm{g},xy} \lesssim 5$. Thus, both measures of polymer overlap suggest that overlap becomes appreciable in the latter regime.

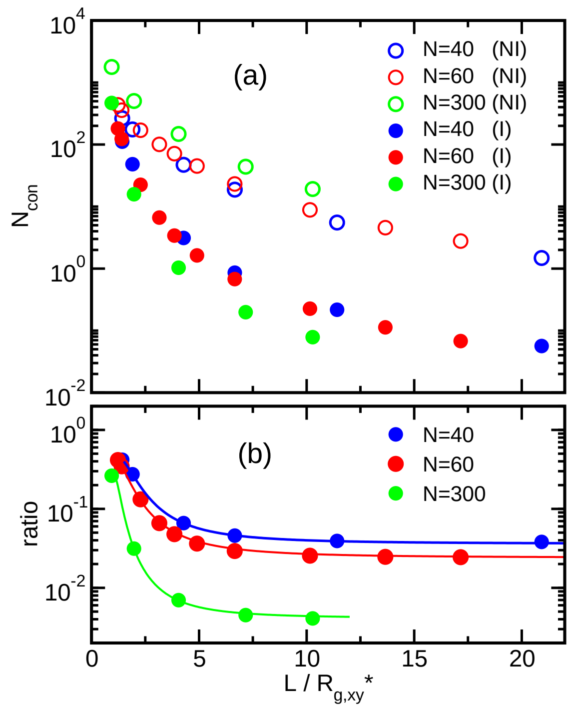

FIG. 4. (a) N_{con} vs. $L/R^*_{\mathrm{g},xy}$ for polymer lengths of N=40, 60 and 300. Results are shown for a 2-polymer system in which interactions between monomers on different polymers are either included (I) or not included (NI). (b) Ratio of of the overlap parameters for the I and NI systems vs. $L/R^*_{\mathrm{g},xy}$. The solid curves are guides for the eye.

[1] X. Capaldi, Z. Liu, Y. Zhang, L. Zeng, R. Reyes-Lamothe, and W. Reisner, Soft matter **14**, 8455 (2018).