# Distance measures and evolution of polymer chains in their topological space (Supplementary Material) 

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## Appendix A: Details of the minimum assignment algorithm

Consider two $M \times M$ matrices $\mathrm{A}^{1}$ and $\mathrm{A}^{2}$ with elements $\mathrm{A}_{l l^{\prime}}^{1,2} \in\{p, s, x\}$ defining the relative position of links $l$ and $l^{\prime}$. The aim is to find a one-to-one assignment $k(l)$ of the links from $\mathbf{l} \rightarrow \mathbf{k}$ minimizing the Hamming distance $D\left(\mathrm{~A}^{1}, \mathrm{~A}^{2}\right)=\sum_{l<l^{\prime}}\left(1-\delta_{\mathrm{A}_{l l^{\prime}}^{1}, \mathrm{~A}_{k k^{\prime}}^{2}}\right)$. Here, to shorten the notation, we use $k, k^{\prime}$ for $k(l), k\left(l^{\prime}\right)$.

We start from the local marginals $\mu_{l}(k)$ of the probability measure $\mu(\mathbf{k}) \propto e^{-\beta D\left(\mathrm{~A}^{1}, \mathrm{~A}^{2}\right)}$ of the assignments written in the Bethe approximation for a finite $\beta$ [1],

$$
\begin{equation*}
\mu_{l}(k) \propto \prod_{l^{\prime} \neq l}\left(\sum_{k^{\prime} \neq k} e^{-\beta\left(1-\delta_{A_{l l^{\prime}}, \mathrm{A}_{k k^{\prime}}^{2}}\right)} \mu_{l^{\prime} \rightarrow l}\left(k^{\prime}\right)\right) . \tag{A1}
\end{equation*}
$$

The cavity marginals $\mu_{l^{\prime} \rightarrow l}\left(k^{\prime}\right)$ give the probability of assigning $l^{\prime} \rightarrow k^{\prime}$ in the absence of link $l$. The recursive equations governing these cavity marginals are called the belief propagation equations [1, 2],

$$
\begin{equation*}
\mu_{l^{\prime} \rightarrow l}\left(k^{\prime}\right) \propto \prod_{l^{\prime \prime} \neq l l^{\prime}}\left(\sum_{k^{\prime \prime} \neq k^{\prime}} e^{-\beta\left(1-\delta_{A_{l^{\prime} l^{\prime}}^{\prime}}, A_{k^{\prime} k^{\prime \prime}}^{2}\right)} \mu_{l^{\prime \prime} \rightarrow l^{\prime}}\left(k^{\prime \prime}\right)\right) . \tag{A2}
\end{equation*}
$$

We can solve the equations by iteration starting from a random initial condition.
But we are interested in the limit $\beta \rightarrow \infty$ of the equations concentrating on the optimal assignments minimizing $D\left(\mathrm{~A}^{1}, \mathrm{~A}^{2}\right)$. Assuming the scaling $\mu_{l \rightarrow l^{\prime}}(k)=e^{-\beta h_{l \rightarrow l^{\prime}}(k)}$ for the cavity marginals, the limit $\beta \rightarrow \infty$ of the BP equations read

$$
\begin{equation*}
h_{l^{\prime} \rightarrow l}\left(k^{\prime}\right)=\sum_{l^{\prime \prime} \neq l, l^{\prime}} \min _{k^{\prime \prime} \neq k^{\prime}}\left\{\left(1-\delta_{\mathrm{A}_{l^{\prime} l^{\prime \prime}}^{1}, \mathrm{~A}_{k^{\prime} k^{\prime \prime}}^{2}}\right)+h_{l^{\prime \prime} \rightarrow l^{\prime}}\left(k^{\prime \prime}\right)\right\}-C_{l^{\prime} \rightarrow l} . \tag{A3}
\end{equation*}
$$

Here $C_{l^{\prime} \rightarrow l}$ is a constant to make $\min _{k^{\prime}} h_{l^{\prime} \rightarrow l}\left(k^{\prime}\right)=0$. These equations are called minsum equations [2].

We use the above equations in a reinforcement algorithm to fix smoothly the assignment variables [3]. To this end, we use the information in the local marginals $\mu_{l}(k)=e^{-\beta h_{l}(k)}$ to increase slowly an external field acting on the variables. The aim is to concentrate more and more the cavity and local marginals on a minimum assignment as the algorithm proceeds. More precisely, we start from random initial messages $h_{l}^{0}(k), h_{l \rightarrow l^{\prime}}^{0}(k)$, and in each step we update the message in the following way:

$$
\begin{equation*}
h_{l \rightarrow l^{\prime}}^{t+1}(k)=\eta_{l}(k)+r(t) h_{l}^{t}(k)+\sum_{l^{\prime \prime} \neq l, l^{l^{\prime}}} \min _{k^{\prime \prime} \neq k}\left\{\left(1-\delta_{\mathrm{A}_{l l^{\prime \prime}}^{1}, \mathrm{~A}_{k k^{\prime \prime}}^{2}}\right)+h_{l^{\prime \prime} \rightarrow l}^{t}\left(k^{\prime \prime}\right)\right\}-C_{l \rightarrow l^{\prime}} \tag{A4}
\end{equation*}
$$

In the same way, we update the local messages

$$
\begin{equation*}
h_{l}^{t+1}(k)=\eta_{l}(k)+r(t) h_{l}^{t}(k)+\sum_{l^{\prime \prime} \neq l} \min _{k^{\prime \prime} \neq k}\left\{\left(1-\delta_{\mathrm{A}_{l l^{\prime \prime}}^{1}, \mathrm{~A}_{k k^{\prime \prime}}^{2}}\right)+h_{l^{\prime \prime} \rightarrow l}^{t}\left(k^{\prime \prime}\right)\right\}-C_{l} . \tag{A5}
\end{equation*}
$$

Here $r(t)$ is the reinforcement parameter; it is zero at the beginning and increases slowly by time as $r(t+1)=r(t)+\delta r$, for a small $\delta r \simeq 0.01$. In addition, we introduced a small noise $\eta_{l}(k)$ to the equations to reduce the number of possible minimum assignments. In each iteration one updates all the local and cavity messages selected in a random sequential way, according to the above equations. In the end, one obtains an assignment by looking at the local messages; that is $l \rightarrow k=\arg \min h_{l}^{t}(k)$.

## Appendix B: Ordering statistics of the local changes

Consider two link configurations $\mathrm{L}_{0}, \mathrm{~L}_{T}$ connected by a sequence of local changes, that is $\mathrm{L}_{T}=\mathbf{u}_{T} \cdots \mathbf{u}_{1} \mathrm{~L}_{0}$. To be specific, we assume the $\mathbf{u s}$ are local changes (LC) of type II, where $\mathbf{u}$ is an elementary permutation of the neighboring endpoints $\left(i_{u}, i_{u}+1\right)$. There could be different orderings of the LCs connecting the same boundary configurations. The question is how these different orderings affect on a macroscopic behavior (phenotype) of the chain, for example a monotonically increasing (fitness) function of the $N_{p, s, x}$.

For simplicity, let us ignore the link labels and work with the connectivity patterns of the endpoints $C$. We will also focus on the simple case of two local changes $\mathbf{u}, \mathbf{v}$ of type II. The local change $\mathbf{u}$ commutes with $\mathbf{v}$ in the context of C if $\mathbf{v u C}=\mathbf{u v C}$. Note that the transformations are reversible, that is from $\mathrm{C}^{\prime}=\mathbf{v u C}$ we obtain $\mathrm{C}=\mathbf{u v} \mathbf{C}^{\prime}$. The definitions can readily be extended to link configurations with distinguishable links as well.

The two local changes $\mathbf{u}, \mathbf{v}$ may involve two, three, or four distinct links; we will not consider permutation of neighboring endpoints that belong to a single link, because it has no effect. In table I we summarize the possible effects of two commutative local changes on a contact configuration, considering only the nontrivial case of three links. One can easily construct the other cases with two or four links, following the above rules. Note that each transformation in the table can also happen in the reverse direction. As the table shows, the changes in numbers $N_{p, s, x}$ in the two paths are correlated depending on how that quantity changes form C to $\mathrm{C}^{\prime}$. In particular, when $N_{q}$ increases (or decreases) the corresponding changes in the two paths do not have different signs; a LC-II only changes

| $p^{N_{p}} S^{N_{s}} x^{N_{x}}$ | $N_{p}$ | $N_{s}$ | $N_{x}$ | $p^{N_{p}} s^{N_{s}} x^{N_{x}}$ | $N_{p}$ | $N_{s}$ | $N_{x}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $p^{3} \rightarrow\left(p^{2} x, p^{2} x\right) \rightarrow p x^{2}$ | $(\downarrow, \downarrow)$ | $(-,-)$ | $(\uparrow, \uparrow)$ | $s^{3} \rightarrow\left(s^{2} x, s^{2} x\right) \rightarrow s x^{2}$ | $(-,-)$ | $(\downarrow, \downarrow)$ | $(\uparrow, \uparrow)$ |
| $x^{3} \rightarrow\left(p x^{2}, s x^{2}\right) \rightarrow p s x$ | $(\uparrow,-)$ | $(-, \uparrow)$ | $(\downarrow, \downarrow)$ | $x^{3} \rightarrow\left(p x^{2}, p x^{2}\right) \rightarrow p^{2} x$ | $(\uparrow, \uparrow)$ | $(-,-)$ | $(\downarrow, \downarrow)$ |
| $p s^{2} \rightarrow\left(p s x, s^{2} x\right) \rightarrow s x^{2}$ | $(-, \downarrow)$ | $(\downarrow,-)$ | $(\uparrow, \uparrow)$ | $p x^{2} \rightarrow\left(p^{2} x, p s x\right) \rightarrow p^{2} s$ | $(\uparrow,-)$ | $(-, \uparrow)$ | $(\downarrow, \downarrow)$ |
| $p x^{2} \rightarrow\left(p s x, x^{3}\right) \rightarrow s x^{2}$ | $(-, \downarrow)$ | $(\uparrow,-)$ | $(\downarrow, \uparrow)$ | $p x^{2} \rightarrow\left(p^{2} x, x^{3}\right) \rightarrow p x^{2}$ | $(\uparrow, \downarrow)$ | $(-,-)$ | $(\downarrow, \uparrow)$ |
| $p^{2} s \rightarrow(p s x, p s x) \rightarrow s x^{2}$ | $(\downarrow, \downarrow)$ | $(-,-)$ | $(\uparrow, \uparrow)$ | $p^{2} s \rightarrow\left(p s x, p^{2} x\right) \rightarrow p x^{2}$ | $(\downarrow,-)$ | $(-, \downarrow)$ | $(\uparrow, \uparrow)$ |
| $p^{2} x \rightarrow\left(p x^{2}, p^{2} s\right) \rightarrow p s x$ | $(\downarrow,-)$ | $(-, \uparrow)$ | $(\uparrow, \downarrow)$ | $p^{2} x \rightarrow\left(p x^{2}, p^{3}\right) \rightarrow p^{2} x$ | $(\downarrow, \uparrow)$ | $(-,-)$ | $(\uparrow, \downarrow)$ |
| $s^{2} x \rightarrow\left(p s^{2}, s x^{2}\right) \rightarrow p s x$ | $(\uparrow,-)$ | $(-, \downarrow)$ | $(\downarrow, \uparrow)$ | $s^{2} x \rightarrow\left(s^{3}, s x^{2}\right) \rightarrow s^{2} x$ | $(-,-)$ | $(\uparrow, \downarrow)$ | $(\downarrow, \uparrow)$ |
| $p s x \rightarrow\left(s x^{2}, p^{2} s\right) \rightarrow p s x$ | $(\downarrow, \uparrow)$ | $(-,-)$ | $(\uparrow, \downarrow)$ |  |  |  |  |

TABLE I. The set of distinct transformations $C \rightarrow(\mathbf{u C}, \mathbf{v C}) \rightarrow \mathrm{C}^{\prime}=\mathbf{u v C}=\mathbf{v u C}$ obtained by two commutative local changes of type II applied on three links. The arrows in each column show the change in the numbers $N_{p, s, x}$ : positive ( $\uparrow$ ) or negative ( $\downarrow$ ). The first (second) arrow in the parenthesis corresponds to the first (second) transition. Here $p^{N_{p}} s^{N_{s}} x^{N_{x}}$ shows a configuration of $N_{q}$ contact pairs of type $q=p, s, x$.
the state of two links from x to ( $\mathrm{p}, \mathrm{s}$ ), or from ( $\mathrm{p}, \mathrm{s}$ ) to x . This means that in a LC-II we have $\delta N_{p, s}=-\delta N_{x}= \pm 1$, and two LC-II can at most change $N_{p, s, x}$ by two. Consequently, if $N_{q}$ increases (decreases), the changes $\delta N_{q}$ resulted by the two LC-II can not have different signs, because they can not give the expected total variation in $N_{q}$.

## Appendix C: Details of the minimum evolution algorithm

Let us start from the dynamical partition function

$$
\begin{equation*}
\mathcal{Z}\left(\mathrm{L}_{0} \rightarrow \mathrm{~L}_{T}\right)=\sum_{\mathbf{u}(1), \mathbf{u}(2), \ldots, \mathbf{u}(T)} e^{-\beta \mathcal{E}} \delta_{\mathrm{L}\left(\mathbf{u}(1), \mathbf{u}(2), \ldots, \mathbf{u}(T) \mid \mathrm{L}_{0}\right), \mathrm{L}_{T}}, \tag{C1}
\end{equation*}
$$

where $\mathrm{L}_{t}=\mathrm{L}\left(\mathbf{u}(1), \mathbf{u}(2), \ldots, \mathbf{u}(t) \mid \mathrm{L}_{0}\right)$ is the link configuration at time step $t$, and $\mathbf{u}(t)$ defines the position of the possible local changes. In the following, we assume the local changes are of type II. Here $\mathcal{E}=\sum_{t=1}^{T-1} E(t)+\sum_{t=1}^{T} E(t-1, t)$ with $E(t)=-N_{p}(t)$, and $E(t-1, t)=$ $-\sum_{q<q^{\prime}} \lambda_{q \rightarrow q^{\prime}} N_{q \rightarrow q^{\prime}}(t-1, t)$ for $q=p, s, x$. We recall that a link configuration is defined by the endpoints of all the links, and any two links have different endpoints. A local-change
configuration $\mathbf{u}(t)=\left\{u_{l l^{\prime}}(t)=0,1 \mid \sum_{l^{\prime} \neq l} u_{l l^{\prime}}(t) \leq 1\right\}$ is a matching of neighboring links with adjacent endpoints along the contact chain.

We solve the above problem by a dynamic programming (message-passing) algorithm: Define the cavity messages $\mu_{t \rightarrow t+1}\left(\mathrm{~L}_{t}\right)$ and $\mu_{t \rightarrow t-1}\left(\mathrm{~L}_{t}\right)$ as the probability of having link configuration $L_{t}$ in the absence of the energy terms and constraints imposed by the other part of the system; i.e. the segment $(t, T]$ for the forward message $\mu_{t \rightarrow t+1}$, and $[0, t)$ for the backward message $\mu_{t \rightarrow t-1}$. From the above partition function we can easily write the equations for these cavity marginals

$$
\begin{align*}
\mu_{t \rightarrow t+1}\left(\mathrm{~L}_{t}\right) & =\frac{1}{z_{t \rightarrow t+1}} e^{-\beta E(t)} \sum_{\mathbf{u}(t)} \delta_{\mathrm{L}\left(\mathbf{u}(t) \mid \mathrm{L}_{t-1}\right), \mathrm{L}_{t}} e^{-\beta E(t-1, t)} \mu_{t-1 \rightarrow t}\left(\mathrm{~L}_{t-1}\right),  \tag{C2}\\
\mu_{t \rightarrow t-1}\left(\mathrm{~L}_{t}\right) & =\frac{1}{z_{t \rightarrow t-1}} e^{-\beta E(t)} \sum_{\mathbf{u}(t+1)} \delta_{\mathrm{L}\left(\mathbf{u}(t+1) \mid \mathrm{L}_{t}\right), \mathrm{L}_{t+1}} e^{-\beta E(t, t+1)} \mu_{t+1 \rightarrow t}\left(\mathrm{~L}_{t+1}\right) . \tag{C3}
\end{align*}
$$

Then the total marginal at time step $t$ is given by

$$
\begin{equation*}
\mu_{t}\left(\mathrm{~L}_{t}\right)=\frac{1}{z_{t}} e^{\beta E(t)} \mu_{t \rightarrow t+1}\left(\mathrm{~L}_{t}\right) \mu_{t \rightarrow t-1}\left(\mathrm{~L}_{t}\right) \tag{C4}
\end{equation*}
$$

The $z_{t \rightarrow t \pm 1}$ and $z_{t}$ are normalization constants.

## 1. Approximating the messages

We represent a link configuration L by the set of endpoints $e_{l}=\left(i_{l}, j_{l}\right)$, and label the links according to the order of their first endpoints. We also approximate the cavity messages by a Bethe distribution

$$
\begin{equation*}
\mu_{t-1 \rightarrow t}(\mathrm{~L}) \approx \prod_{l} \mu_{t-1 \rightarrow t}^{l}\left(e_{l}\right) \prod_{l<l^{\prime}} \frac{\mu_{t-1 \rightarrow t}^{l l^{\prime}}\left(e_{l}, e_{l^{\prime}}\right)}{\mu_{t-1 \rightarrow t}^{l}\left(e_{l}\right) \mu_{t-1 \rightarrow t}^{\prime \prime}\left(e_{l^{\prime}}\right)} \tag{C5}
\end{equation*}
$$

Using this structure for the cavity messages in the right hand side of the equations, we obtain the equations for the two-link marginals $\mu_{t \rightarrow t+1}^{l l^{\prime}}\left(e_{l}, e_{l^{\prime}}\right)$,

$$
\begin{align*}
\mu_{t \rightarrow t+1}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right) \propto & \sum_{\left\{e_{l^{\prime \prime}}(t)\left[l^{\prime \prime} \neq l, l^{\prime}\right\}\right.} e^{-\beta E(t)} \sum_{\mathbf{u}(t)} \delta_{\mathrm{L}\left(\mathbf{u}(t) \mid \mathrm{L}_{t-1}\right), \mathrm{L}_{t}} e^{-\beta E(t-1, t)} \\
& \times \prod_{k} \mu_{t-1 \rightarrow t}^{k}\left(e_{k}(t-1)\right) \prod_{k<k^{\prime}} \frac{\mu_{t-1 \rightarrow t}^{k k^{\prime}}\left(e_{k}(t-1), e_{k^{\prime}}(t-1)\right)}{\mu_{t-1 \rightarrow t}^{k}\left(e_{k}(t-1)\right) \mu_{t-1 \rightarrow t}^{k^{\prime}}\left(e_{k^{\prime}}(t-1)\right)} . \tag{C6}
\end{align*}
$$

We compute the sum in the right hand side of the above equation using the Bethe approximation [1]. To this end, we introduce auxiliary variables $\delta l$ to see how the local
changes affect link $l$. More precisely, given $e_{l}(t)$ and $\delta l$ we can recover the endpoints and the link label $e_{k}(t-1)$ in previous step. Note that $\delta l$ takes a small number of values as the number of possible local changes of type II are small; the endpoints and the label of a link can at most change by $\pm 1$. The approximate two-link marginal $\mu_{t \rightarrow t+1}^{l l^{\prime}}\left(e_{l}, e_{l^{\prime}}\right)$ can be obtained by considering the constraints involving $\left(e_{l}, e_{l^{\prime}}\right)$, and by taking into account the effect of the remaining degrees of freedom. The latter is provided by a new set of cavity marginals $\nu_{l \rightarrow l^{\prime}}\left(e_{l}(t) ; \delta l ; u_{l l^{\prime}}(t)\right)$ giving the probability of indicated variables in the absence of $l^{\prime}$. Putting all together, we obtain

$$
\begin{align*}
\mu_{t \rightarrow t+1}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right) \propto \sum_{\delta l, \delta l^{\prime}, u_{l^{\prime}}(t)} w_{l l^{\prime}}\left(e_{l}(t)\right. & \left., e_{l^{\prime}}(t) ; \delta l, \delta l^{\prime} ; u_{l l^{\prime}}(t)\right) \\
& \times \nu_{l \rightarrow l^{\prime}}\left(e_{l}(t) ; \delta l ; u_{l l^{\prime}}(t)\right) \nu_{l^{\prime} \rightarrow l}\left(e_{l^{\prime}}(t) ; \delta l^{\prime} ; u_{l l^{\prime}}(t)\right), \tag{C7}
\end{align*}
$$

where we defined

$$
\begin{equation*}
w_{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t) ; \delta l, \delta l^{\prime} ; u_{l l^{\prime}}(t)\right)=w_{l^{\prime} \rightarrow l}\left(e_{l}(t), e_{l^{\prime}}(t) ; \delta l, \delta l^{\prime} ; u_{l l^{\prime}}(t)\right) \mu_{t-1 \rightarrow t}^{k}\left(e_{k}(t-1)\right), \tag{C8}
\end{equation*}
$$

with

$$
\begin{align*}
& w_{l^{\prime} \rightarrow l}\left(e_{l}(t), e_{l^{\prime}}(t) ; \delta l, \delta l^{\prime}\right.\left.; u_{l l^{\prime}}(t)\right)=\mathbb{I}\left(\delta l, \delta l^{\prime}, u_{l l^{\prime}}(t) \mid e_{l}(t), e_{l^{\prime}}(t)\right) e^{\beta \delta_{q\left(e e_{l}(t), e_{l^{\prime}}(t)\right), p}} \\
& \times e^{u_{l^{\prime}}(t) \beta \lambda_{q}\left(e_{k}(t-1), e_{k^{\prime}}(t-1)\right) \rightarrow q\left(e_{l}(t), e_{l^{\prime}}(t)\right)} \mu_{t-1 \rightarrow t}^{k k^{\prime}}\left(e_{k^{\prime}}(t-1) \mid e_{k}(t-1)\right) . \tag{C9}
\end{align*}
$$

Here $\mathbb{I}\left(\delta l, \delta l^{\prime}, u_{l l^{\prime}}(t) \mid e_{l}(t), e_{l^{\prime}}(t)\right)$ is an indicator function to ensure that: (i) $e_{l}(t) \neq e_{l^{\prime}}(t)$, (ii) the links are labeled from left to right according to their first endpoints, and (iii) to check for the possibility of a local change given the endpoints and the $\delta l, \delta l^{\prime}, u_{l l^{\prime}}(t)$. Moreover, $\mu_{t-1 \rightarrow t}^{k k^{\prime}}\left(e_{k^{\prime}}(t-1) \mid e_{k}(t-1)\right)=\mu_{t-1 \rightarrow t}^{k k^{\prime}}\left(e_{k^{\prime}}(t-1), e_{k}(t-1)\right) / \mu_{t-1 \rightarrow t}^{k}\left(e_{k}(t-1)\right)$ is the conditional probability of $e_{k^{\prime}}(t-1)$ given $e_{k}(t-1)$, and $\mathbf{q}\left(e_{l}, e_{l^{\prime}}\right) \in\{p, s, x\}$ depending on the link endpoints.

The $\nu_{l \rightarrow l^{\prime}}\left(e_{l}(t) ; \delta l ; u_{l l^{\prime}}(t)\right)$ are determined by the following Bethe equations:

$$
\begin{align*}
\nu_{l \rightarrow l^{\prime}}\left(e_{l}(t) ; \delta l ; 0\right) & \propto \prod_{l^{\prime \prime} \neq l, l^{\prime}}\left(\sum_{e_{l^{\prime \prime}}(t), \delta l^{\prime \prime}} w_{l^{\prime \prime} \rightarrow l}\left(e_{l}(t), e_{l^{\prime \prime}}(t) ; \delta l, \delta l^{\prime \prime} ; 0\right) \nu_{l^{\prime \prime} \rightarrow l}\left(e_{l^{\prime \prime}}(t) ; \delta l^{\prime \prime} ; 0\right)\right) \\
& +\sum_{l^{\prime \prime} \neq l, l^{\prime}}\left(\sum_{e_{l^{\prime \prime}}(t), \delta l^{\prime \prime}} w_{l^{\prime \prime} \rightarrow l}\left(e_{l}(t), e_{l^{\prime \prime}}(t) ; \delta l, \delta l^{\prime \prime} ; 1\right) \nu_{l^{\prime \prime} \rightarrow l}\left(e_{l^{\prime \prime}}(t) ; \delta l^{\prime \prime} ; 1\right)\right) \\
& \times \prod_{l^{\prime \prime \prime} \neq l, l^{\prime}, l^{\prime \prime}}\left(\sum_{e_{l^{\prime \prime \prime}}(t), \delta l^{\prime \prime \prime}} w_{l^{\prime \prime \prime} \rightarrow l}\left(e_{l}(t), e_{l^{\prime \prime \prime}}(t) ; \delta l, \delta l^{l^{\prime \prime} ;} ; 0\right) \nu_{l^{\prime \prime \prime} \rightarrow l}\left(e_{l^{\prime \prime \prime}}(t) ; \delta l^{\prime \prime \prime} ; 0\right)\right), \tag{C10}
\end{align*}
$$

and,

$$
\begin{equation*}
\nu_{l \rightarrow l^{\prime}}\left(e_{l}(t) ; \delta l ; 1\right) \propto \prod_{l^{\prime \prime} \neq l l^{\prime}}\left(\sum_{e_{l^{\prime \prime}}(t), \delta l^{\prime \prime}} w_{l^{\prime \prime} \rightarrow l}\left(e_{l}(t), e_{l^{\prime \prime}}(t) ; \delta l, \delta l^{\prime \prime} ; 0\right) \nu_{l^{\prime \prime} \rightarrow l}\left(e_{l^{\prime \prime}}(t) ; \delta l^{\prime \prime} ; 0\right)\right) . \tag{C11}
\end{equation*}
$$

Similarly, we obtain the cavity marginals $\mu_{t \rightarrow t-1}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right)$, and finally the local marginals read

$$
\begin{equation*}
\mu_{t}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right) \propto \nu_{l \rightarrow l^{\prime}}\left(e_{l}(t)\right) \tilde{w}_{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right) \nu_{l^{\prime} \rightarrow l}\left(e_{l^{\prime}}(t)\right), \tag{C12}
\end{equation*}
$$

where now

$$
\begin{equation*}
\tilde{w}_{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right)=\tilde{w}_{l^{\prime} \rightarrow l}\left(e_{l}(t), e_{l^{\prime}}(t)\right) \mu_{t \rightarrow t+1}^{l}\left(e_{l}(t)\right) \mu_{t \rightarrow t-1}^{l}\left(e_{l}(t)\right), \tag{C13}
\end{equation*}
$$

with

$$
\begin{equation*}
\tilde{w}_{l^{\prime} \rightarrow l}\left(e_{l}(t), e_{l^{\prime}}(t)\right)=e^{-\beta \delta_{q\left(e_{l}(t), e_{l}(t)\right), p}} \mu_{t \rightarrow t+1}^{l l^{\prime}}\left(e_{l^{\prime}}(t) \mid e_{l}(t)\right) \mu_{t \rightarrow t-1}^{l l^{\prime}}\left(e_{l^{\prime}}(t) \mid e_{l}(t)\right), \tag{C14}
\end{equation*}
$$

and,

$$
\begin{equation*}
\nu_{l \rightarrow l^{\prime}}\left(e_{l}(t)\right) \propto \prod_{l^{\prime \prime} \neq l l^{\prime}}\left(\sum_{e_{l^{\prime \prime}}(t)} \tilde{w}_{l^{\prime \prime} \rightarrow l}\left(e_{l}(t), e_{l^{\prime \prime}}(t)\right) \nu_{l^{\prime \prime} \rightarrow l}\left(e_{l^{\prime \prime}}(t)\right)\right) . \tag{C15}
\end{equation*}
$$

Given the local marginals $\mu_{t}^{l}\left(e_{l}(t)\right)$ and $\mu_{t}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right)$, an estimation of the entropy at time step $t$ can be obtained by the Bethe entropy [1],

$$
\begin{equation*}
S(t)=\frac{1}{M \ln M}\left(\sum_{l<l^{\prime}} \Delta S_{l l^{\prime}}-(M-2) \sum_{l=1}^{M} \Delta S_{l}\right) \tag{C16}
\end{equation*}
$$

where

$$
\begin{align*}
\Delta S_{l} & =-\sum_{e_{l}} \mu_{t}^{l}\left(e_{l}\right) \ln \mu_{t}^{l}\left(e_{l}\right)  \tag{C17}\\
\Delta S_{l l^{\prime}} & =-\sum_{e_{l}, e_{l^{\prime}}} \mu_{t}^{l l^{\prime}}\left(e_{l}, e_{l^{\prime}}\right) \ln \mu_{t}^{l^{\prime}}\left(e_{l}, e_{l^{\prime}}\right) \tag{C18}
\end{align*}
$$

In summary, from Eq. C7 we obtain the cavity marginals $\mu_{t \rightarrow t+1}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right)$, and similarly for $\mu_{t \rightarrow t-1}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right)$. Then, Eq. C12 gives the local marginals $\mu_{t}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right)$, which are used in Eq. C16 to compute the Bethe entropy.

## 2. The zero temperature limit $\beta \rightarrow \infty$

To take the limit $\beta \rightarrow \infty$, we assume the above probability distributions scale as

$$
\begin{align*}
\mu_{t \rightarrow t+1}^{l}\left(e_{l}(t)\right) & =e^{-\beta h_{t \rightarrow t+1}^{l}\left(e_{l}(t)\right)}  \tag{C19}\\
\mu_{t \rightarrow t+1}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right) & =e^{-\beta h_{t \rightarrow t+1}^{l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right)} \tag{C20}
\end{align*}
$$

and similarly for the messages from $t$ to $t-1$. In addition, we define

$$
\begin{align*}
\nu_{l \rightarrow l^{\prime}}\left(e_{l}(t) ; \delta l ; u_{l l^{\prime}}(t)\right) & =e^{-\beta g_{l \rightarrow l^{\prime}}\left(e_{l}(t) ; \delta l ; u_{l l^{\prime}}(t)\right)},  \tag{C21}\\
\nu_{l \rightarrow l^{\prime}}\left(e_{l}(t)\right) & =e^{-\beta g_{l \rightarrow l^{\prime}}\left(e_{l}(t)\right)} . \tag{C22}
\end{align*}
$$

Now the zero temperature (minsum) equations read [1, 2],

$$
\begin{align*}
& h_{t \rightarrow t+1}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right)= \min _{\delta l, \delta l^{\prime}, u_{l^{\prime}}(t): \mathbb{I}}\{ \\
&-\delta_{\mathbf{q}\left(e_{l}(t), e_{l^{\prime}}(t)\right), p}+h_{l-1 \rightarrow t}(t) \lambda_{\mathbf{q}\left(e_{k}(t-1), e_{k^{\prime}}(t-1)\right) \rightarrow \mathbf{q}\left(e_{l}(t), e_{l^{\prime}}(t)\right)}\left(e_{k}(t-1), e_{k^{\prime}}(t-1)\right) \\
&\left.+g_{l \rightarrow l^{\prime}}\left(e_{l}(t) ; \delta l ; u_{l l^{\prime}}(t)\right)+g_{l^{\prime} \rightarrow l}\left(e_{l^{\prime}}(t) ; \delta l^{\prime} ; u_{l l^{\prime}}(t)\right)\right\}, \tag{C23}
\end{align*}
$$

where the minimum is subject to the constraints in $\mathbb{I}\left(\delta l, \delta l^{\prime}, u_{l l^{\prime}}(t) \mid e_{l}(t), e_{l^{\prime}}(t)\right)$, and

$$
\begin{align*}
& g_{l \rightarrow l^{\prime}}\left(e_{l}(t) ; \delta l ; 0\right)=\min \left\{F_{l \rightarrow l^{\prime}}^{0}\left(e_{l}(t), \delta l\right), \min _{l^{\prime \prime} \neq l, l^{\prime}} F_{l \rightarrow l^{\prime}}^{l^{\prime \prime}}\left(e_{l}(t), \delta l\right)\right\},  \tag{C24}\\
& g_{l \rightarrow l^{\prime}}\left(e_{l}(t) ; \delta l ; 1\right)=F_{l \rightarrow l^{\prime}}^{0}\left(e_{l}(t), \delta l\right) . \tag{C25}
\end{align*}
$$

Here we defined

$$
\begin{align*}
& F_{l \rightarrow l^{\prime}}^{0}\left(e_{l}(t), \delta l\right)=\sum_{l^{\prime \prime} \neq l, l^{\prime}} f_{l^{\prime \prime} \rightarrow l}^{0}\left(e_{l}(t), \delta l\right),  \tag{C26}\\
& F_{l \rightarrow l^{\prime}}^{l^{\prime \prime}}\left(e_{l}(t), \delta l\right)=f_{l^{\prime \prime} \rightarrow l}^{1}\left(e_{l}(t), \delta l\right)+\sum_{l^{\prime \prime \prime} \neq l, l^{\prime}, l^{\prime \prime}} f_{l^{\prime \prime \prime} \rightarrow l}^{0}\left(e_{l}(t), \delta l\right), \tag{C27}
\end{align*}
$$

with

$$
\begin{align*}
& f_{l^{\prime \prime} \rightarrow l}^{0}\left(e_{l}(t), \delta l\right)=\min _{e_{l^{\prime \prime}}(t), \delta l^{\prime \prime}: I, u_{l^{\prime \prime}}(t)=0}\left\{-\delta_{\mathbf{q}\left(e_{l}(t), e_{l^{\prime \prime}}(t)\right), p}\right. \\
& \left.\quad+h_{t-1 \rightarrow t}^{k k^{\prime \prime}}\left(e_{k}(t-1), e_{k^{\prime \prime}}(t-1)\right)-h_{t-1 \rightarrow t}^{k}\left(e_{k}(t-1)\right)+g_{l^{\prime \prime} \rightarrow l}\left(e_{l^{\prime \prime}}(t) ; \delta l^{\prime \prime} ; 0\right)\right\}, \tag{C29}
\end{align*}
$$

and

$$
\begin{align*}
& f_{l^{\prime \prime} \rightarrow l}^{1}\left(e_{l}(t),\right.\delta l)=\min _{e_{l^{\prime \prime}}(t), \delta l^{\prime \prime} \mathbb{I}, u_{l^{\prime \prime}}(t)=1}\left\{-\lambda_{\mathbf{q}\left(e_{k}(t-1), e_{k^{\prime \prime}}(t-1)\right) \rightarrow \mathbf{q}\left(e_{l}(t), e_{l^{\prime \prime}}(t)\right)}-\delta_{\mathbf{q}\left(e_{l}(t), e_{l^{\prime \prime}}(t)\right), p}\right. \\
&\left.+h_{t-1 \rightarrow t}^{k k^{\prime \prime}}\left(e_{k}(t-1), e_{k^{\prime \prime}}(t-1)\right)-h_{t-1 \rightarrow t}^{k}\left(e_{k}(t-1)\right)+g_{l^{\prime \prime} \rightarrow l}\left(e_{l^{\prime \prime}}(t) ; \delta l^{\prime \prime} ; 1\right)\right\} . \tag{C30}
\end{align*}
$$

Similarly we obtain the minsum messages $h_{t \rightarrow t-1}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right)$, and finally the local messages read

$$
\begin{align*}
h_{t}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right)=\delta_{\mathbf{q}\left(e_{l}(t), e_{l^{\prime}}(t)\right), p}+h_{t \rightarrow t+1}^{l l^{\prime}}\left(e_{l^{\prime}}(t), e_{l}(t)\right)+ & h_{t \rightarrow t-1}^{l l^{\prime}}\left(e_{l^{\prime}}(t), e_{l}(t)\right) \\
& +g_{l \rightarrow l^{\prime}}\left(e_{l}(t)\right)+g_{l^{\prime} \rightarrow l}\left(e_{l^{\prime}}(t)\right) \tag{C31}
\end{align*}
$$

and,

$$
\begin{align*}
g_{l \rightarrow l^{\prime}}\left(e_{l}(t)\right)= & \sum_{l^{\prime \prime} \neq l, l^{\prime}} \min _{e_{l^{\prime \prime}}(t) \neq e_{l}(t)}\left\{\delta_{\mathbf{q}\left(e_{l}(t), e_{l^{\prime \prime}}(t)\right), p}+h_{t \rightarrow t+1}^{l l^{\prime \prime}}\left(e_{l^{\prime \prime}}(t), e_{l}(t)\right)\right. \\
& \left.-h_{t \rightarrow t+1}^{l}\left(e_{l}(t)\right)+h_{t \rightarrow t-1}^{l^{\prime \prime}}\left(e_{l^{\prime \prime}}(t), e_{l}(t)\right)-h_{t \rightarrow t-1}^{l}\left(e_{l}(t)\right)+g_{l^{\prime \prime} \rightarrow l}\left(e_{l^{\prime \prime}}(t)\right)\right\} . \tag{C32}
\end{align*}
$$

We use the above equations in a reinforcement algorithm to find a minimum evolution path satisfying all the connectivity constraints. In a reinforcement algorithm, we use the information in the local messages $h_{t}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right)$ to slowly polarize the cavity messages $h_{t \rightarrow t \pm 1}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right)$ in the direction favored by the local messages, as we did in Appendix A for the minimum distance algorithm.

In summary, the cavity messages $h_{t \rightarrow t+1}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right)$ are obtained by solving Eq. C23 (similarly for $h_{t \rightarrow t-1}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right)$ ). These messages are used in Eq. C31 to compute the local messages $h_{t}^{l l^{\prime}}\left(e_{l}(t), e_{l^{\prime}}(t)\right)$ which are utilized in a reinforcement algorithm to find an approximate optimal pathway.

## Appendix D: More details and figures

In this section, we give more details of the numerical data and figures obtained in this study.

We are interested in topological evolutions connecting two boundary contact configurations $\left(\mathrm{L}_{0}, \mathrm{~L}_{T}\right)$ by a sequence of local changes in the link arrangements. More specifically, we look for optimal pathways of length $T$ minimizing the energy functional $\mathcal{E}=-\sum_{t=1}^{T-1} N_{p}(t) \equiv$


FIG. 1. Examples of contact configurations of $M=6$ links used as boundary configurations in the minimum evolution algorithm: $x 6$ (top), $x 3 x 3$ (middle), and $p 3 x 3$ (bottom).
$-\mathcal{N}_{p}$, or $\mathcal{E}=-\sum_{t=1}^{T}\left[N_{x \rightarrow p}(t-1, t)+N_{x \rightarrow s}(t-1, t)\right] \equiv-\mathcal{N}_{x \rightarrow p, s}$. Here $\mathcal{N}_{p}$ is the total number of contact pairs of type $p$, and $\mathcal{N}_{x \rightarrow p, s}$ gives the total number of contact pairs changed from $x$ to $p, s$ during the evolution. Figure 1 shows some boundary contact configurations we use in the following examples. For now, we assume the paths are simple with no loops, that is each configuration in the path is visited only once.

Figure 2 shows the optimal pathways from the all- $x(x 6)$ configuration of $M=6$ links to the modular structure $p 3 x 3$, following the local changes of type I. The results have been obtained by an exact algorithm searching in the space of all paths connecting the two boundary configurations. In Fig. 3, we compare the optimal paths connecting two random link configurations of $M=5$ links with local changes of type II and (II $+M^{*}$ ). In the latter case, two link configurations are connected if they are related either by LC-II or LC- $M^{*}$. Figure 4 displays an example of evolution with variable number of links from $x 4$ to $p 2 x 2$.

So far we have considered simple paths with no loops (also called off-pathways). The off-pathways can localize the dynamics in a small region of the configuration space wasting the evolution time. To escape from these traps, one may increase the path length $T$ in the hope of finding another path dominating the off-pathways, but probably another set of offpathways would appear. Another strategy is to perturb the system, for example, by adding the transition rates $\mathcal{N}_{x \rightarrow p, s}$ to the original energy function $\mathcal{E}=-\sum_{t=1}^{T-1} N_{p}(t)$. However, we observe that in this case the off-pathways are very robust. The reason is that the offpathways that maximize $\mathcal{N}_{p}$, maximize also the number of these transitions making the above perturbations ineffective. Table II shows some examples of evolution in the presence of off-pathways.


FIG. 2. Evolution with local changes of type I: (top) $N_{p, s, x}(t)$, and (bottom) $D_{I}(t)$ of the intermediate link configurations from the boundary configurations in the paths obtained by the exact algorithm for $M=6$ links. The paths connect the all-x (x6) configuration to a modular structure of two components $(p 3 x 3)$ at shortest distance $D_{I}=5$. Besides the shortest path (a), we display the path maximizing $\mathcal{N}_{p}(\mathrm{~b})$, and the path maximizing $\mathcal{N}_{x \rightarrow p, s}$ for $x 6 \rightarrow p 3 x 3$ (c) and $p 3 x 3 \rightarrow x 6$ (d). Here $t$ denotes the number of local changes of type I. The path degeneracy $g$ and energy gap $\Delta$ are: $(g=2, \Delta=2)_{a},(g=8, \Delta=2)_{b},(g=1, \Delta=4)_{c},(g=1, \Delta=4)_{d}$.

| $T$ | $\mathcal{N}_{p}$ | $(g, \Delta)$ | $N_{p}^{\text {off }}$ | $(g, \Delta)^{\text {off }}$ | off-pathway |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 4 | 31 | $(1,1)$ | 31 | $(1,1)$ | - |
| 6 | 58 | $(3,1)$ | 58 | $(3,1)$ | - |
| 8 | 86 | $(24,1)$ | 86 | $(24,1)$ | - |
| 10 | 113 | $(48,1)$ | 114 | $(24,1)$ | $\rightarrow$ loop |
| 12 | 142 | $(48,1)$ | 143 | $(24,1)$ | $\rightarrow$ loop $\rightarrow$ loop |
| 14 | 169 | $(372,1)$ | 172 | $(120,1)$ | $\rightarrow$ loop $\rightarrow$ loop $\rightarrow$ loop |

TABLE II. The total number of parallel two-links $\mathcal{N}_{p}$, degeneracy of the optimal paths $g$, and energy gap $\Delta$ obtained by an exhaustive search algorithm with local changes of type II. The optimal paths maximizing $\mathcal{N}_{p}$ connect tow boundary configurations of $M=6$ links at shortest distance $D_{I I}=4$. We compare the cases with and without off-pathways. An off-pathway which is a single loop appears for the first time at $T=10$. By increasing the path length $T$, we observe that more loops appear following each other.


FIG. 3. Evolution with local changes of type II (a,b) and (II $+M^{*}$ ) ( $\mathrm{c}, \mathrm{d}$ ): ( top ) $N_{p, s, x}(t)$, and (bottom) distance $D(t)$ of the intermediate link configurations from two random boundary configurations of $M=5$ links. The boundary configurations have shortest distance $D_{I I}=3$, and the optimal paths are obtained by the exact algorithm maximizing $\mathcal{N}_{p}$. Besides the optimal shortest paths ( $\mathrm{a}, \mathrm{c}$ ), we display the results for a larger evolution time $T=9(\mathrm{~b}, \mathrm{~d})$. Here $t$ denotes the number of local changes of type II (a,b) or II $+M^{*}(\mathrm{c}, \mathrm{d})$. The path degeneracy $g$ and energy gap $\Delta$ are: $(g=1, \Delta=14)_{a},(g=78, \Delta=1)_{b},(g=1, \Delta=2)_{c},(g=64, \Delta=1)_{d}$.

Figure 5 display the results we obtained by the approximate minimum-evolution algorithm for paths minimizing $\mathcal{E}=-\sum_{t=1}^{T-1} N_{p}(t)$. In this figure, we show instances of evolution paths between two random link configurations for a larger number of links $M=10$ and steps $T=9$.
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FIG. 4. Evolution with local changes of type $\mathrm{I}+M^{ \pm}$(a) and $\mathrm{II}+M^{ \pm}$(b): (top) $N_{p, s, x}(t)$, and (bottom) distance $D(t)$ of the intermediate link configurations from the boundary configurations for $T=10$ steps. The boundary configurations $(x 6, p 2 x 2)$ have different number of links with shortest distances 4 (a) and 6(b). The optimal paths are obtained by the exact algorithm maximizing $\mathcal{N}_{p}$. Here $t$ denotes the number of local changes of type $\mathrm{I}+M^{ \pm}$(a) or $\mathrm{II}+M^{ \pm}(\mathrm{b})$. The path degeneracy $g$ and energy gap $\Delta$ are: $(g=1, \Delta=1)_{a},(g=3, \Delta=1)_{b}$.


FIG. 5. Evolution paths of $M=10$ links for $T=9$ coarse-grained steps from a random link configuration to another random configuration obtained by the approximate minimum evolution algorithm minimizing $\mathcal{E}=-\sum_{t=1}^{T-1} N_{p}(t)$. The endpoints on the chain start from $i=0$ (at the bottom of the circle) and increase to $i=2 M-1$ in the counter-clockwise direction.


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