Monte Carlo simulations of circular supercoiled polymers

César L. Pastrana

1 Energy

The total energy of the system is given by,

$$E = E_b + E_s + E_t \tag{1}$$

where the first terms

2 Trial movements

2.1 Procedure

Rodrigue's rotation

2.2 Intersections

Monte Carlo moves can result in regions of the polymer intersecting between each other. To prevent this movement to occurs we need to check if the resulting trial configuration is intersecting. Then, a pair of edges of the polymer is defined by the following equations:

$$\vec{r} = \vec{r}_0 + \delta_1 \hat{t} \tag{2}$$

$$\vec{u} = \vec{u}_0 + \delta_2 \hat{v} \tag{3}$$

where $\vec{r}_0$ and $\vec{u}_0$ are the coordinates of the two points of the polymer and $\hat{t}$ and $\hat{v}$ are the local and unitary direction vectors. The squared distance between the two lines is $d(\vec{r}, \vec{u}) = \|\vec{r} - \vec{u}\|^2$ and we look for the δ_1 and δ_2 minimising the distance d,

$$\frac{\partial d(\vec{r}, \vec{u})}{\partial \delta_1} \stackrel{!}{=} 0, \qquad \frac{\partial d(\vec{r}, \vec{u})}{\partial \delta_2} \stackrel{!}{=} 0 \tag{4}$$

Evaluating the derivatives and solving for δ_i, we find,

$$\boxed{\delta_2 = \frac{(\vec{r}_0 - \vec{u}_0) \cdot \hat{v} - [(\vec{r}_0 - \vec{u}_0) \cdot \hat{v}](\hat{t} \cdot \hat{v})}{(\hat{t} \cdot \hat{v})^2 - 1}} \tag{5}$$

and

$$\boxed{\delta_1 = \delta_2(\hat{t} \cdot \hat{v}) - (\vec{r}_0 - \vec{u}_0) \cdot \hat{t}} \tag{6}$$

We check if $0 < \delta_1 < s_1$ and $0 < \delta_2 < s_2$, with s_i the length of the edges. If δ_1 and δ_2 are in the indicated range, then the minimum distance between points is occuring at some point along the edges defined at $\vec{r}_0$ and $\vec{u}_0$. In such scenario, we check if $d(\vec{r}, \vec{u})\big|_{\delta_1, \delta_2} < 2R$, with R the (effective) polymer radius: in affirmative case, there is an intersection at the edge.

The indicated procedure is repeated for every possible pair of edges. Hence, this is a complex step of the code, with a complexity order $\mathcal{O} \sim N^2$, where N the number of edges/particles. We can reduce the complexity by considering the intereaction between the N edges with the K edges involved in the monte carlo trial.

2.3 Knots

The rotation of a set of edges can result in a knotted configuration. This configurations are an artifact of the mechanism followed to generate the trial configuration and this is not a real effect. We exclude knotted conigurations of the XXX Fáry–Milnor theorem