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LINKING MATRICES IN SYSTEMS WITH PERIODIC BOUNDARY CONDITIONS

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Abstract. Using the Gauss linking number, we define a new measure of entanglement, the *linking matrix*, for a collection of closed or open chains in 3-space. Periodic Boundary Conditions (PBC) are often used in the simulation of physical systems of filaments. Using the periodic linking number, defined in [24], we define the *periodic linking matrix* to study entanglement of closed or open chains in systems employing PBC. We study the properties of the periodic linking matrix as a function of cell size. We provide analytical results concerning the eigenvalues of the periodic linking matrix and show that some of them are invariant of cell-size.

Key words. linking matrix, linking number, periodic boundary conditions, entanglement

AMS subject classifications. 57M99,57M25,15B99,0072,00A69,68U20

1. Introduction. [1]

The entanglement of open or closed filaments arises in many physical systems, such as polymers, biopolymers, fluid flows, textile weaves etc. Often, these systems consist of a large collection of filaments which interlace and cannot cross each other without breaking their constituent bonds. For the study of the conformational properties of these systems, computer simulations are necessary. The computer simulations require the use of Periodic Boundary Conditions (PBC) to avoid having boundary effects.

The uncrossability of the chains gives rise to entanglement. The degree of complexity of the entanglement of the chains dramatically affects their mechanical and dynamical properties. In determining the degree of entanglement in physical systems is therefore very important to understand their properties [11, 12, 10, 7, 32, 36, 34].

Edwards first pointed out that in the case of ring polymers, the global entanglement of the chains can be studied by using tools from mathematical topology, such as the Gauss linking number [11, 12]. Since Edwards, many studies have been devoted to the topology of polymer rings and its relation to physical properties [14, 30, 20, 33, 13]. However, in the case of linear polymers, the notion of topological invariant does not apply since topological open curves can be continuously deformed to attain any configuration [14, 21, 35]. A measure of global entanglement, that is meaningful both for closed or open chains, is the *Gauss linking integral.* For two closed chains (ring polymers) the Gauss linking integral is a topological invariant that measures the algebraic number of times one chain turns around the other. For two open chains (linear polymers), it is a real number that is a continuous function of the chain coordinates. The Gauss linking integral can be also applied to one chain in order to provide measures of global self-entanglement of a chain, called the *writhe* and the *self-linking number* [1, 18, 4]. Computer experiments indicate that the linking number and the writhe are effective indirect measures of global entanglement in systems of random filaments [3, 16, 20, 22, 23]. Analytical and numerical results have shown that the writhe of random walks and polygons depends on their length and that it follows a different scaling

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[1] Preliminary results on the periodic linking matrix can be found in [27]

for random walks in a lattice, or under confinement [20, 8, 26]. In [28, 27, 25, 24] the linking integral was applied to polymer melts to study their entanglement and it was shown that it can give physically relevant information about polymer properties. In this work, we provide a more refined tool for measuring entanglement in polymers or collections of filaments, by taking into consideration all the pairwise linking in the system.

The PBC impose further complexity in measuring the entanglement both for open and closed chains. In order to study entanglement in systems with PBC, in [24] we defined the *periodic linking number* and showed that it is well defined both for open and closed chains. In a periodic system, the periodic linking number measures the degree of entanglement of one filament in the periodic system with an entire collection of filaments in the periodic system. For closed chains the periodic linking number is a finite sum and it is an integer topological invariant. For open chains, the periodic linking number is an infinite summation, which we proved converges and is a continuous function of the chains' coordinates. In this work, we provide a measure of all the pairwise entanglement in a system with PBC.

More precisely, we propose that one may strengthen the measures of entanglement used so far by using a matrix containing all the pairwise entanglement information of the many components of the system. The eigenvalues of this matrix are indicative of the pairwise entanglement information in the system and provide more information than the average (absolute) linking of the chains in the system. An important advantage of using the linking matrix of a collection of chains is that its eigenvalues can detect inhomogeneities in the entanglement of the system. The material properties of polymeric systems, textiles, or wire weaves, all rely on homogeneous structures. The existence of inhomogeneities therein can result in undesired properties such as breakage of the corresponding material under deformation or, on the other hand, provide advantageous features of the system that can be exploited in novel applications.

In this work we study the *linking matrix* of chains in 3-space and in systems employing one Periodic Boundary Condition. One reason to study systems in one PBC is that the results presented therein will be used as a basis to extend to the case of two and three PBC. More importantly, systems employing one PBC occur very often in applications, usually to simulate physical filaments confined to a tubular structure. Systems which employ PBC generate infinite systems of chains. To study entanglement in those systems we define the *periodic linking matrix*. We also examine how the periodic linking matrix changes with respect to the size of the simulation cell. There are several reasons to study this:

(1) The properties of the linking matrix that are invariant of cell-size characterize the infinite periodic system and, therefore, are of particular importance.

(2) Topologically, the larger cell-sizes correspond to different topological objects in the corresponding *identification space*, the space that results from gluing the opposite faces of the cell according to the PBC. In the case of a systems with 1,2 or 3 PBC the identification space is the solid torus, ST, the thickened torus. $T \times I$ or the 3-torus, T^3, respectively. In our study we analyze how these are related.

This manuscript is organized as follows: In Section 2 we define the linking matrix and in section 3 we give the definitions necessary to study entanglement in systems employing PBC (as they were initially defined in [24]). In Section 4 we define the periodic linking matrix of filaments in PBC and discuss its properties. In Section 5 we study the properties of the periodic linking matrix for chains in one PBC as a function of cell-size.

2. The linking matrix.

In this section we define the linking matrix as a measure of entanglement that contains all the pairwise and self-entanglement of the chains that compose a system. For its definition, the definitions of the linking and self-linking number are necessary.

2.1. The Gauss linking number and the self-linking number.

The Gauss linking number is a classical measure of the algebraic entanglement of two disjoint oriented closed curves that extends directly to disjoint oriented open chains [9, 26, 11].

DEFINITION 1. *The Gauss linking number of two disjoint (closed or open) oriented curves l_1 and l_2, whose arc-length parametrizations are $\gamma_1(t), \gamma_2(s)$ respectively, is defined as a double integral over l_1 and l_2 [15]:*

$$L(l_1, l_2) = \frac{1}{4\pi} \int_{[0,1]} \int_{[0,1]} \frac{(\dot{\gamma}_1(t), \dot{\gamma}_2(s), \gamma_1(t) - \gamma_2(s))}{||\gamma_1(t) - \gamma_2(s)||^3} dtds, \tag{1}$$

where $(\dot{\gamma}_1(t), \dot{\gamma}_2(s), \gamma_1(t) - \gamma_2(s))$ is the triple product of $\dot{\gamma}_1(t), \dot{\gamma}_2(s)$ and $\gamma_1(t) - \gamma_2(s)$.

In the case of closed chains the Gauss linking number is an integer and a topological invariant, equal to zero when the two chains are algebraically unlinked. The Gauss linking number can be computed for a fixed configuration of two open chains to give a real number that is equal to half the average algebraic sum of crossings between the two chains over all projection directions.

For two open chains, the Gauss linking number may be non-zero, even if their convex hulls do not intersect. But as the distance between their convex hulls increases, the Gauss linking number tends to zero.

The Gauss linking integral can be applied to one chain to measure its entanglement with itself. The *self-linking number* is defined as the linking number between a curve l and a translated image of that curve l_ϵ at a small distance ϵ, called the *normal variation curve* of l, that is, $Sl\,(l) = L\,(l, l_\epsilon)$ [5]. This can be expressed by the Gauss integral over $[0,1]^* \times [0,1]^* = \{(x,y) \in [0,1] \times [0,1]\,|x \neq y\}$ by adding to it a correction term, so that it is a topological invariant of closed curves [2] under regular isotopy,

$$\begin{aligned} Sl\,(l) = {} & \frac{1}{4\pi} \int_{[0,1]^*} \int_{[0,1]^*} \frac{(\dot{\gamma}\,(t)\,, \dot{\gamma}\,(s)\,, \gamma\,(t) - \gamma\,(s))}{||\gamma\,(t) - \gamma\,(s)\,||^3} dtds \\ & + \frac{1}{2\pi} \int_{[0,1]} \frac{(\gamma'(t) \times \gamma''(t)) \cdot \gamma'''(t)}{||\gamma'(t) \times \gamma''(t)||^2} dt. \end{aligned} \tag{2}$$

2.2. The Linking Matrix.

We use the linking and self-linking number to define a measure of entanglement of an entire collection of closed or open chains. We define the *Linking Matrix*, LM, of a collection of chains, say $H1, H2, \ldots, Hn$, to be the $n \times n$ matrix with elements $a_{ij} = L(Hi, Hj)$ if $i \neq j$ and $a_{ii} = Sl(Hi)$, etc. The linking matrix collects together all the linking information of the system.

The following properties derive from the properties of the Gauss linking number and the self-linking number:
(i) Since the linking number is symmetric, this is a real symmetric matrix and therefore has n real eigenvalues, representantive of the pairwise entanglement of the system.
(ii) For closed chains, the eigenvalues are link-homotopy invariants, i.e. does not change under continuous deformations of the system that allows intersections of a

chain with itself but not between distinct chains, and they change when torsion of the chains changes. Notice that if the diagonal elements were 0 (so, suppressing the self-linking of the chains), the eigenvalues are invariants under link-homotopy).
(iii) For open chains, the eigenvalues are real numbers that change continuously with the motion of the chains.

The largest eigenvalue increases with increasing entanglement complexity and, indeed, is a principal measure of this. We apply the methods of graph theory to derive pairwise entanglement properties relevant to physical properties. A physical system of filaments is represented by a weighted graph as follows: We represent each chain in the melt by a vertex, $i = 1, \ldots, n$. Then two vertices are connected with an edge if their absolute linking number is greater than zero. Also, there is an edge of a vertex to itself if the chain has absolute self-linking number greater than zero. Thus we have related the polymeric system to a graph. Each edge of this graph has an associated weight function, w, that is defined as $w(i,j) = |L(Hi, Hj)|$ and $w(i,i) = |Sl(Hi)|$.

The homogeneity of the entanglement in a polymer melt is related to the connectivity of the corresponding weighted graph. For example, let us consider the extreme case where all the chains are self-entangled but not at all entangled with each other. The linking matrix will be a diagonal matrix, and the melt consists of n isolated chains. Also, the corresponding weighted graph will be disconnected and the number of its components is the number of polymers. In general if the linking matrix has the form of a block diagonal matrix, then there exist collections of chains that are linked with each other and not at all linked with the chains that belong to the other collections. That is, there exist isolated collections of chains, and the corresponding graph is disconnected and the number of its components is equal to the number of collections. The linking matrix allows one to detect such situations. Moreover, the graph theoretic approach can be useful to determine which collections of chains are important in maintaining the homogeneity of the system, or, in other words, whether or not there are chains whose removal would result in a drastic change of the entanglement of the chains and therefore change the properties of the material. In a graph, a subset of edges that disconnects a graph is called a *cut set*. Cut sets arise naturally in the study of connectivity of graphs and the sizes of the connected components are an important consideration. Isoperimetric problems examine optimal relations between the size of the cut set and the sizes of the separated parts. Roughly speaking, isoperimetric problems involving edge-cuts correspond in a natural way to Cheeger constants in spectral geometry. If the gap between the first and second eigenvalue of a regular graph is large then the graph has good connectivity, expansion and randomness properties. Therefore, when none of the entries of the periodic linking matrix are zero, then the gap between the two eigenvalues is a measure of the homogeneity of their entanglement. Notice that for open chains, none of the entries is exactly zero with probability one, therefore, the gap between its first two eigenvalues is also a measure of its homogeneity. One can use thresholds to the entries of the linking matrix of open chains to relate the strength of linking to the structure of the material as expressed in the quantities derived via the graph. More precisely, one can set to zero all entries less than a given thresshold value which represents low linking. Then some entries of the matrix may become zero and reveal interesting properties of the system.

3. Entanglement in systems with PBC.

3.1. Systems in PBC. In this section we give some definitions that form the basis for our study of entanglement in PBC. They were originally defined and discussed

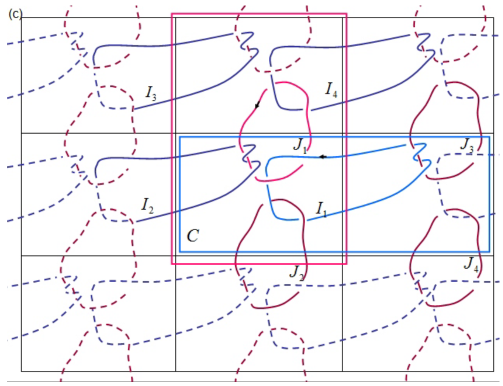

FIG. 1. *The central cell C and the periodic system it generates in the case of closed free chains. The generating chain i (resp. j) is composed by the blue (resp. red) arcs in C. The free chain I (resp. J) is the set of blue (resp. red) chains in the periodic system. Highlighted are the minimal unfoldings of the images I_1 and J_1.*

in [24].

We study a system consisting of a collection of polygonal chains of length n (ie. of n edges), by dividing the space into a family of cubic boxes of volume l^3, where l is the edge length of the cube, so that the structure of the filaments in each cube is identical, i.e. we impose PBC on the system [32]. Specifically, we make the following definition:

DEFINITION 2. *A cell consists of a cube with embedded arcs (ie. parts of curves) whose endpoints lie only in the interior of the cube or on the interior of one of its faces, but not on an edge or corner, and those arcs which meet a face satisfy the PBC requirement. That is, to each ending point corresponds a starting point at exactly the same position on the opposite face of the cube. See Figure 1 for an illustrative example.*

A cell generates a *periodic system* in 3-space by tiling 3-space with the cubes so that they fill space and only intersect on their faces. This allows an arc in one cube to be continued across a face into an adjacent cube and so on. Notice that the resulting chains may be closed, open or infinite.

Without loss of generality, we choose a cell of the periodic system that we call *generating cell*. A *generating chain* is the union of all the arcs inside the cell the translations of which define a connected component in the periodic system. For each arc of a generating chain we choose an orientation such that the translations of all the arcs would define an oriented curve in the periodic system. For each generating chain we choose without loss of generality an arc and a point on it to be its *base point* in the generating cell. For generating chains we shall use the symbols $i, j, \ldots$. For the arcs of a generating chain, say i, we use the symbols $i_1, \ldots, i_k$. An *unfolding* of a generating chain is a connected arc in the periodic system composed by exactly one translation of each arc of the generating chain. Then an unfolding contains exactly one translation of the base point of the generating chain. Without loss of generality, let us make the convention that the base point of each image lies in the leftmost cell of its minimal unfolding. A generating chain is said to be closed (resp. open) when its unfolding is a closed (resp. open) chain. The smallest union of the copies of the cell needed for one unfolding of a generating chain shall be called the *minimal unfolding*.

The smaller number of copies of the cell whose union contains the convex hull of the complete unfolding of a generating chain shall be called the *minimal topological cell*.

The collection of all translations of the same generating chain i shall be called a *free chain*, denoted I. A free chain is a union of connected components, each of which is equivalent to any other under translation. For free chains we will use the symbols $I, J, \ldots$. An *image* of a free chain is any arc of a free chain that is the unfolding of a generating chain. The minimal unfolding of I containing an image I_u of I, will be denoted $mu(I_u)$. For example, in Figure 1, the blue closed curves are some of the images of the free chain I and the highlighted blue cells compose $mu(I_0)$. In the particular case where the images of a free chain form infinite components in the periodic system, this free chain shall be called *infinite free chain*. We call an infinite connected component of an infinite free chain I an *infinite image* of I. Note that an image of an infinite free chain is still a finite arc, an unfolding of a generating chain, lying on an infinite image of I. For example in Fig. 1 the infinite curve on which the image I_0 lies is an infinite image of I, called $\mathcal{I}_0$. The image of I whose base point lies in the generating cell shall be called the *parent image* and it shall be denoted I_0. Then any other image of I can be defined as a translation of I_0 by a vector $\vec{v}$ based on the base point of the parent image. That is:

$$I_v = I_0 + \vec{v}. \tag{3}$$

Also, we denote $i^{(0)}$ the generating chain whose base pont is that of $I^{(0)}$ and any translation of it is denoted $i^{(m)} = i^{(0)} + \vec{m}$. Similarly, we define a base point for every cell in the periodic system (say to be its central point). Let us denote by C_0 the simulation cell. Then any cell, C_u, in the periodic system is a translation of it, $C_u = C_0 + \vec{u}$.

3.2. The periodic linking number. In a periodic system we must define linking at the level of free chains (see [24] for an analysis of the motivation for this definition). Given that two free chains are two infinite collections of chains, how can we measure the linking of only the different pairs of chains? Looking at the periodic system we notice that, due to the periodicity, the linking imposed by all the images of one free chain, say J, to one image of another free chain, say I, are the same for any image of I. Based on this observation in [24] we gave the following definition of a measure of entanglement between two free chains:

Definition 3 (Periodic linking number). *Let I and J denote two (closed, open or infinite) free chains in a periodic system. Suppose that I_0 is the parent image of the free chain I in the periodic system. The periodic linking number, LK_P, between two free chains I and J is defined as:*

$$LK_P(I,J) = \sum_v L(I_0, J_0 + \vec{v}), \tag{4}$$

where the sum is taken over all the images $J_v = J_0 + \vec{v}$ of the free chain J in the periodic system.

The periodic linking number has the following properties with respect to the structure of the cell, which follow directly by its definition:
(i) LK_P captures all the linking that all the images of a free chain impose to an image of the other.

(ii) LK_P is independent of the choice of the image I_0 of the free chain I in the periodic system.
(iii) LK_P is independent of the choice, the size and the shape of the generating cell.
(iv) LK_P is symmetric.

We notice that the periodic linking number is an infinite summation of Gauss linking numbers (see Fig. 1 for an illustrative example). In the case of closed chains, LK_P is reduced to a finite summation and in [24] we show that it is equal to the linking number of two chains in a manifold. However, the periodic linking number of open or infinite chains is an infinite summation since the Gauss linking number is in general non-zero even if the chains are far from each other. In [24] we show that LK_P indeed converges and that it is a continuous function of the chain coordinates. Also in [24] we defined the *local* and *cell periodic linking number* as cut-offs of the periodic linking number.

3.2.1. The periodic self-linking number. Inspired by the definition of the periodic linking number at the level of free chains in [24] we defined a measure of self-linking number at the level of free chains. We notice that an image of a free chain may be entangled with other images of itself (see Fig. 1 for an illustrative example). Thus a measure of self-entanglement of a free chain must capture this information. In [24] we introduced the following definition of self-linking for chains in PBC:

Definition 4 (Periodic self-linking number). *Let I denote a free chain in a periodic system and let I_0 be the parent image of I, then the periodic self-linking number of I is defined as:*

$$SL_P(I) = Sl(I_0) + \sum_{\vec{v}} L(I_0, I_0 + \vec{v}), \tag{5}$$

where the index v runs over all the images of I, except $I_v = I_0 + \vec{v}$, in the periodic system.

The periodic self-linking number has the following properties with respect to the structure of the cell, which follow directly by its definition:
(i) SL_P captures the linking that all the images of a free chain impose to one image of it.
(ii) SL_P is independent of the choice of the image I_u of the free chain I in the periodic system.
(iii) SL_P is independent of the choice, the size and the shape of the generating cell.
(iv) SL_P is invariant under regular isotopy of the corresponding diagrams (If we ignore the self-linking number in SL_P, we obtain the periodic linking number with self-images, which is invariant under link homotopy).

4. Periodic Linking Matrix. In order to capture all the pairwise and self-entanglement in a periodic system generated by a cell C with free chains $H1, H2, \ldots,$ Hn, we define the *periodic linking matrix*, LM_C, as the matrix with elements $a_{ij} = LK_P(Hi, Hj)$ if $i \neq j$ and $a_{ii} = SL_P(Hi)$. Therefore, LM_C has size $n \times n$. Thus the periodic linking number enables us to reduce the study of the entanglement of an infinite collection of chains that compose the periodic system to the study of a finite dimensional matrix.

The periodic linking matrix has the following properties deriving from its definition:
(i) LM_C is a real symmetric $n \times n$, thus has n real eigenvalues.

(ii) For closed chains, the eigenvalues are a finite summation and are topological invariants up to regular isotopy of the corresponding diagram. If we suppress the self-linking number from the periodic self-linking number in the diagonal entries, the eigenvalues are topological invariants under link-homotopy.
(iii) For open chains, the eigenvalues are infinite summations which converge and are continuous functions of the chains coordinates.

Our next goal is the extraction of quantities characterizing a polymer system from the associated periodic linking matrix.

We also expect the largest eigenvalue of the periodic linking matrix to increase for increasing entanglement complexity. Similarly with the case of chains in 3-space, we can use tools from graph theory to derive pairwise entanglement properties relevant to physical properties. In [27] our numerical results showed that the asphericity of the eigenvalues of the periodic linking matrix, the Cheeger constant and the Laplacian matrix of the corresponding graphs can provide measures of the homogeneity of the entanglement of a collection of chains. Our numerical results also suggest that the homogeneity of the entanglement depends on chain length.

5. The Periodic Linking Matrix as a function of the cell size. In this section we will consider systems employing one PBC. This situation is often encountered in applications in the simulation of polymers in confinement, as for example tubular geometries, or grafted polymers.

By concatenating m cells we obtain a larger cell that we denote mC, which applies PBC to the chains that touch its faces in the $x-$direction. We can concatenate cells of the type mC by gluing their $x-$faces with respect to the PBC, in order to create the same periodic system that is generated by the cell C. In this section we study the periodic linking matrix of a periodic system as the size of the cell used for its simulation, characterized by m, increases. We will see that the linking matrix depends on the size of the cell used for the simulation of a system. Since the periodic system simulated is the same, one would expect the periodic linking matrix to retain certain entanglement information. However, we will see that in a topological sense, these systems are different. With our study we extract entanglement information that is invariant of the cell size as well as information that depends on it.

Let C denote a cell composed by n generating chains, and let LM_C denote the corresponding periodic linking matrix of size $n \times n$. Without loss of generality we will concatenate cells always to the positive direction of the $x-$axis. Let mC denote the cell that results by gluing m copies of C respecting the PBC. Let us denote the cells that compose mC as follows: $C_j = C_0 + \vec{v}_j$, where $C_0 = C$, $\vec{v_j} = (lj, 0, 0)$, $j = 1, \ldots, m-1$ and l is the length of the edge of the simulation cell in the x-direction. By Lemma 5 in [24] there are m generating chains in the cell mC. Then mC has more chains. More precisely:

Lemma 5. *Let C be a cell with n generating chains. Then the cell mC that results by gluing m copies of C respecting the PBC, has mn generating chains.*

Proof. Let C_0 denote the simulation cell. Let $i_1, i_2, \ldots, i_w$ denote the arcs of the generating chain i in C_0. Let $i_r + \vec{v}_j, i_r + \vec{v}_h$, where $j > h$, be two translations of the arc i_r in mC. Then $\vec{v}_j - \vec{v}_h = (l(j-h), 0, 0)$, where $j - h \in \mathbb{Z}$, $0 < j - h < m$. In the periodic system generated by mC, these two arcs generate the translations $i_r + \vec{v}_j + \vec{u}$ and $i_r + \vec{v}_h + \vec{u'}$, where $\vec{u} = (mlu, 0, 0), \vec{u'} = (mlu', 0, 0)$, $u, u' \in \mathbb{Z}$. Since $jl + mlu \mod ml = jl \neq hl = hl + mlu' \mod ml$, any two translations of these arcs are different arcs in the periodic system generated by mC. Thus, $i_r + \vec{v}_j, i_r + \vec{v}_h$

belong to different generating chains in mC. Therefore, the generating chains $i^{(j)} = i^{(0)} + \vec{v}_j, i^{(h)} = i^{(0)} + \vec{v}_h$ are different for all $0 < j \neq h < m, j, h \in \mathbb{Z}$.

REMARK 6. The different generating chains in mC generate different free chains in the periodic system. We denote the free chains in mC generated by $i^{(j)}$, $j = 0, \ldots, m-1$, as $I^{(j)} = I^{(0)} + \vec{v}_j$.

Thus the corresponding periodic linking matrix, LM_{mC} has size $mn \times mn$. Indeed, the cells C and mC describe different topological objects. If we identify the faces of the cell, then we will get an $n-$component link in the solid torus in the first case and a $mn-$component link in the second case. The 3-manifolds are the same in both cases even though the links that they contain are different, related by an $m-$fold covering space of the second manifold over the first. So, we notice that the linking matrices LM_C and LM_{mC} are different, but the periodic system that the cells generate and whose entanglement we wish to measure, is the same. For this purpose, we will study the dependence of the periodic linking matrix on the cell size and we will look for quantities that remain invariant of cell size.

In the next sections, we will prove that some of the eigenvalues of the periodic linking matrix are independent of cell size. First we will study the simplest case of the periodic linking matrix of a single chain in a cell with one PBC. Next, we will generalize this to the case of n chains in a cell with one PBC. This case will facilitate the understanding of the general case of systems employing one PBC. The methods presented here can also be used to obtain similar results in 2 and 3 PBC.

The following result will be helpful in our analysis:

LEMMA 7. *If an image of a free chain I intersects k cells C, then there are k images of I that intersect a cell C.*

Proof. Let $C_0, C_1, \ldots, C_{k-1}$ denote the cells that belong to $mu(I_0)$. Let i_w denote an arc of I_0 that lies in the cell $C_w = C_0 + (w, 0, 0)$. Then the arc $i_w - (w, 0, 0)$ lies in C_0 and belongs to $I_{-w} = I_0 + (-w, 0, 0)$. Thus I_{-w} intersects C_0. Any other arc of I_0 in C_w gets translated by $(-w, 0, 0)$ to C_0 and belongs to I_{-w}. On the other hand, if $I_{-n} = I_0 - \vec{v}_n$ intersects C_0 and i_{-n} is an arc of I_{-n} in C_0, then the arc $i_{-n} + \vec{v_n}$ belongs to I_0 and lies in the cell $C_n = C_0 + \vec{v_n}$. Similarly, all the arcs of I_{-n} in C_0 correspond to arcs of I_0 in the cell C_n. Thus, the number of images of I intersecting C is equal to the number of cells in the minimal unfolding of I_0.

COROLLARY 8. *Let I denote a free chain in a system with one PBC generated by the cell C. Suppose that the minimal unfolding of an image of I is formed by k cells. Let mC denote the new cell that is created by gluing m copies of C, where $m = ak+b$, $a, b \in \mathbb{N}$ and $b < k$. Then there are m free chains in mC; for $((a-1)k + b + 1) = c$ of those free chains, their images do not touch the boundary of mC, and for the rest $k-1$ free chains there are exactly two images of each intersecting mC.*

Proof. All the images $I_w = I_0 + (w, 0, 0)$ with $m - w \geq k - 1$ unfold in mC and belong to different free chains in mC by Lemma 5. There are $c = (a-1)k + b + 1$ such chains. The rest $m - c = k - 1$ free chains intersect mC and unfold in two copies of mC (since mC contains m cells and $mu(I_0)$ contains $k < m$ cells), thus have two images intersecting mC by Lemma 7.

5.1. One chain in a cell with one PBC. We will next study the case of a cell with one PBC that contains one generating chain that unfolds in k cells. The periodic linking matrix of that system has size 1×1, $LM_C = SL_P(I) = Sl(I_0) + \sum_i L(I_0, I_i)$.

If we concatenate m cells to create a larger cell mC, then by Lemma 5 there are m generating chains in k_1C, we denote $I^{(0)}, I^{(1)} = I^{(0)} + (1,0,0), \ldots, I^{(m)} = I^{(0)} + (m,0,0)$. The linking matrix for this cell has size $m \times m$ and is defined as $(LM_{mC})_{(i,j)} = LK_P(I^{(i)}, I^{(j)})$, when $i \neq j$ and $(LM_{mC})_{(i,i)} = SL_P(I^{(i)})$.

Lemma 9. *Let C denote a cell with one PBC that consists of only one chain, I. Let mC denote the cell that results after gluing m copies of C, then LM_{mC} is a symmetric centrosymmetric matrix.*

Proof. We notice that $Sl(I_0) = Sl(I_u)$ for all u. Also, we notice that the images $I_i + (mrl, 0, 0))$ and I_i are in the same relative positions as $I_0 + (mrl, 0, 0)$ and I_0, so $L(I_0, I_0 + (mrl, 0, 0)) = L(I_i, I_i + (mrl, 0, 0))$, $i = 1, \ldots, k-1$. Thus, $L(I_h, I_l) = L(I_u, I_v)$ when $|h - l| = |u - v|$. Therefore,

$$
\begin{aligned}
SL_P(I^{(i)}) &= Sl(I_i) + \sum_{r \in \mathbb{Z}} L(I_i, I_i + (mrl, 0, 0)) \\
&= Sl(I_0) + \sum_{r \in \mathbb{Z}} L(I_0, I_0 + l(r, 0, 0)) = SL_P(I^{(0)})
\end{aligned}
\tag{6}
$$

for $i = 1, \ldots, m-1$.

Similarly, we notice that $|(m - i) - (m - (j + j_1)| = |i - (j + j_1)|$, so

$$
\begin{aligned}
LK_P(I^{(i)}, I^{(j)}) &= \sum_{j_1} L(I_0 + (i, 0, 0), I_0 + (j + j_1, 0, 0)) \\
&= \sum_{j_1} L(I_0 + (m - i, 0, 0), I_0 + (m - j + j_1, 0, 0)) = LK_P(I^{(m-i)}, I^{(m-j)})
\end{aligned}
\tag{7}
$$

Thus, the entries of the periodic linking matrix, $LM = (l_{i,j})$, satisfy the relations $l_{i,j} = l_{m-i,m-j}$ for $0 \leq i, j \leq m-1$. Thus, the periodic linking matrix is a symmetric centrosymmetric matrix [6, 31]. ∎

Remark 10. For closed chains and for $m > 2|mu(I_0)|$, the linking matrix obtains a simpler expression. When $m > 2|mu(I_0)|$, any image of $I^{(u)}$ will link with at most one image of any $I^{(v)}$, since any two images of $I^{(u)}$ are further that $2|mu(I_0)|$ cells apart, and any image of $I^{(v)}$ occupies $|mu(I_0)|$ cells. Therefore, $SL_P(I^{(j)}) = Sl(I_0)$ for all j, $LK_P(I^{(j)}, I^{(k)}) = L(I_j, I_k)$, for $|j - k| \leq 2|mu(I_0)|$, and $LK_P(I^{(j)}, I^{(k)}) = 0$, for $|j - k| > 2|mu(I_0)|$. Thus, as $m \to \infty$, LM_{mC} becomes an $m \times m$ sparse matrix, where each row has at most $2|mu(I_0)|$ non-zero entries.

Proposition 11. *Let I denote a chain in a cell C with one PBC. Let mC denote the cell that results after gluing m copies of C. Then the j-th eigenvalue of LM_{mC} is given by:*

$$
\lambda_j = SL_P(I^{(0)}) + 2 \sum_{k=1}^{\frac{m-1}{2}} LK_P(I^{(0)}, I^{(k)}) \cos\Big(\frac{2\pi}{m} k(j-1)\Big)
\tag{8}
$$

for m odd and

$$\lambda_j = SL_P(I^{(0)}) + (-1)^{(j-1)} LK_P(I^{(0)}, I^{(\lfloor \frac{m-1}{2} \rfloor + 1)}) + 2 \sum_{k=1}^{\lfloor \frac{m-1}{2} \rfloor} LK_P(I^{(0)}, I^{(k)}) \cos\Big(\frac{2\pi}{m} k(j-1)\Big) \tag{9}$$

for m even.

Proof. By Lemma 9, LM_{mC} is a real symmetric circulant matrix. Its j-th eigenvalue is [31]:

$$\lambda_j = SL_P(I^{(0)}) + LK_P(I^{(0)}, I^{(1)})\omega^{j-1} + LK_P(I^{(0)}, I^{(2)})\omega^{2(j-1)} + \dots + LK_P(I^{(0)}, I^{(m-2)})\bar{\omega}^{2(j-1)} + LK_P(I^{(0)}, I^{(m-1)})\bar{\omega}^{j-1} \tag{10}$$

where $\omega = \exp\Big(\frac{2\pi i}{m}\Big)$, $j = 1, \dots, m$.

Since $LK_P(I^{(0)}, I^{(k)}) = LK_P(I^{(0)}, I^{(m-k)})$ and $\overline{\omega^k} = \bar{\omega}^k$, the eigenvalues can be expressed as:

$$\begin{aligned}
\lambda_j &= SL_P(I^{(0)}) + LK_P(I^{(0)}, I^{(1)})\omega^{(j-1)} + LK_P(I^{(0)}, I^{(2)})\omega^{2(j-1)} \\
&+ \dots + LK_P(I^{(0)}, I^{(m-1)/2})\omega^{\frac{m-1}{2}(j-1)} + LK_P(I^{(0)}, I^{(m+1)/2})\bar{\omega}^{\frac{m-1}{2}(j-1)} \\
&+ \dots + LK_P(I^{(0)}, I^{(m-2)})\bar{\omega}^{2(j-1)} + LK_P(I^{(0)}, I^{(m-1)})\bar{\omega}^{(j-1)} \\
&= SL_P(I^{(0)}) + 2LK_P(I^{(0)}, I^{(1)}) \cos\Big(\frac{2\pi}{m}(j-1)\Big) \\
&+ 2LK_P(I^{(0)}, I^{(2)}) \cos\Big(\frac{2\pi}{m}2(j-1)\Big) \\
&+ \dots + 2LK_P(I^{(0)}, I^{(m-1)/2}) \cos\Big(\frac{2\pi}{m}\frac{m-1}{2}(j-1)\Big)
\end{aligned} \tag{11}$$

for m odd, and as:

$$\begin{aligned}
\lambda_j &= SL_P(I^{(0)}) + LK_P(I^{(0)}, I^{(1)})\omega^{j-1} + LK_P(I^{(0)}, I^{(2)})\omega^{2(j-1)} + \dots \\
&+ LK_P(I^{(0)}, I^{(\lfloor \frac{m-1}{2} \rfloor)})\omega^{\lfloor \frac{m-1}{2} \rfloor (j-1)} \\
&+ LK_P(I^{(0)}, I^{(\lfloor \frac{m-1}{2} \rfloor + 1)})\omega^{(\lfloor \frac{m-1}{2} \rfloor + 1)(j-1)} + LK_P(I^{(0)}, I^{(\lfloor \frac{m-1}{2} \rfloor + 2)})\bar{\omega}^{\lfloor \frac{m-1}{2} \rfloor j} + \\
&\dots + LK_P(I^{(0)}, I^{(m-2)})\bar{\omega}^{2(j-1)} + LK_P(I^{(0)}, I^{(m-1)})\bar{\omega}^{j-1} \\
&= SL_P(I^{(0)}) + 2LK_P(I^{(0)}, I^{(1)}) \cos\Big(\frac{2\pi}{m}(j-1)\Big) \\
&+ 2LK_P(I^{(0)}, I^{(2)}) \cos\Big(\frac{2\pi}{m}2(j-1)\Big) \\
&+ \dots + 2LK_P(I^{(0)}, I^{\lfloor \frac{m-1}{2} \rfloor}) \cos\Big(\frac{2\pi}{m}\lfloor\frac{m-1}{2}\rfloor(j-1)\Big) \\
&+ (-1)^{(j-1)} LK_P(I^{(0)}, I^{(\lfloor \frac{m-1}{2} \rfloor + 1)})
\end{aligned} \tag{12}$$

∎

for m even. In the last equality we noticed that $\omega^{(\lfloor \frac{m-1}{2} \rfloor + 1)} = -1$ for m even.

REMARK 12. . (i) λ_1 is independent of cell-size, m and $\lambda_1 = SL_P(I)$ for all m.

(ii) There are at most $1+\lfloor \frac{m-1}{2} \rfloor$ distinct eigenvalues, as expected for real circulant matrices [31]. Therefore, $\lambda_j = \lambda_{m-j+2}$ for all $j > 1$.

(iii) For closed chains and for $m > 2|mu(I_0)|$, the j-th eigenvalue of the linking matrix has a simpler formula which can be obtained by Eq. 8,9 by replacing the periodic linking and self-linking numbers by the classical linking and self-linking numbers.

REMARK 13. The difference between the first two eigenvalues of LM_{mC} is:

$$\lambda_1 - \lambda_2 = 2 \sum_{k=1}^{\frac{m-1}{2}} LK_P(I^{(0)}, I^{(k)})(1 - \cos\Big(\frac{2\pi}{m}k\Big)) \tag{13}$$

for m odd and

$$\lambda_1 - \lambda_2 = 2 \sum_{k=1}^{\lfloor \frac{m-1}{2} \rfloor} LK_P(I^{(0)}, I^{(k)})(1 - \cos\Big(\frac{2\pi}{m}k\Big)) \tag{14}$$

for m even.

The above formula shows that the difference between the first eigenvalues does not depend on the self-linking number of the chain. The formula indicates that the difference, which is a measure of the homogeneity of the entanglement, is a weighted function of the linking numbers of the chain with its images. Interestingly, for large m, the linking with the nearest images contributes less than the linking with further images.

REMARK 14. Often in applications one is interested in the average properties of filaments. Cancellations may occur when using the Gauss and periodic linking number. For this reason, one may want to use the absolute values of all the entries of the periodic linking matrix, we call the resulting matrix the *absolute periodic linking matrix*. The absolute periodic linking matrix is also symmetric centrosymmetric. Lower bounds on the maximum eigenvalue of nonnegative real symmetric centrosymmetric matrices can be found in [31].

LEMMA 15. *Let C denote a cell with one PBC that consists of only one chain. Let mC denote the cell that results after gluing m copies of C, then the sum of all the entries of a row of LM_{mC} is equal to $SL_P(I)$, for any m.*

Proof. Let us compute the total sum of the elements of the first row:

$$\begin{aligned}
&SL_P(I^{(0)}) + LK_P(I^{(0)}, I^{(1)}) + \ldots + LK_P(I^{(0)}, I^{(m-1)}) \\
&= Sl(I_0) + \sum_{r\in\mathbb{Z}} L(I_0, I_0 + rml(1,0,0)) + \sum_{r\in\mathbb{Z}} L(I_0, I_0 + (1+rm)l(1,0,0)) + \\
&+ \ldots + \sum_{r\in\mathbb{Z}} L(I_0, I_0 + (m-1+rm)l(1,0,0)) \\
&= Sl(I_0) + \sum_{r\in\mathbb{Z}} L(I_0, I_0 + rl(1,0,0)) = SL_P(I)
\end{aligned} \tag{15}$$

∎

By Lemma 9, the sum of the elements of each row is $SL_P(I)$.

REMARK 16. Exactly the same holds for the sum of all the terms of each column, since the matrix is symmetric.

REMARK 17. [Consequences of Lemma 15]
(i) The total linking applied to a chain remains constant and is independent of the size of the cell, as expected from the structure of the periodic system.
(ii) The total sum of the elements of the linking matrix depends linearly on the size of the cell. Let $Total(LM_C)$ denote the total sum of the elements of the periodic linking matrix LM_C. Then, $Total(LM_{mC}) = mTotal(LM_C) = mSL_P(I)$.

In the following we will use matrices that result from products of simple matrices. We denote Q the $m \times m$ matrix for which $[Q]_{ij} = 1$ for $j \leq i$ and $[Q]_{ij} = 0, j > i$, and Q^{-1} its inverse, ie. the matrix for which $[Q^{-1}]_{ii} = 1$, $[Q^{-1}]_{i,i-1} = -1$ and $[Q^{-1}]_{ij} = 0$ for $j \neq i, i-1$.

These matrices can be expressed as

$$Q = \prod_{0 \leq l \leq m-1} Q^{(m-l)} \text{ and } Q^{-1} = \prod_{0 \leq l \leq m-1} (Q^{(m-l)})^{-1}, \tag{16}$$

where $Q^{(k)}$ is the matrix whose elements are $[Q^{(k)}]_{ii} = 1$ and $[Q^{(k)}]_{ij} = 0$ for all $j \neq i$ except for the element $[Q^{(k)}]_{k,k-1} = 1$.

Accordingly, $(Q^{(k)})^{-1}$ is the matrix whose elements are $[(Q^{(k)})^{-1}]_{ii} = 1$ and $[(Q^{(k)})^{-1}]_{ij} = 0$ for all $j \neq i$ except for the element $[(Q^{(k)})^{-1}]^{-1}_{k,k-1} = -1$.

PROPOSITION 18. *Consider one free chain I in the periodic system formed by a cell with one PBC. Then the periodic linking matrix LM_{mC} of the periodic system generated by a larger cell made from m concatenated cells, mC, is similar to the matrix:*

$$LM'_{mC} = \begin{bmatrix} SL_P(I) & C \\ 0 & D \end{bmatrix} \tag{17}$$

where C and D are real matrices of size $1 \times (m-1)$ and $(m-1) \times (m-1)$ respectively.

Proof. We will show that

$$LM'_{mC} = Q^{-1} LM_{mC} Q = \begin{bmatrix} SL_P(I) & C \\ 0 & D \end{bmatrix} \tag{18}$$

where Q and Q^{-1} are products of simple matrices.

The multiplication $LM_{mC}Q^{(k)}$ performs the addition of all the elements of the k-th column of LM_{mC} to the elements of the $(k-1)$-th column. The multiplication $(Q^{(k)})^{-1} LM_{mC}$ performs the subtraction of all the elements of the $(k-1)$-th row of LM_{mC} from the elements of the k-th row.

The element $[LM'_{mC}]_{ij}$ can be expressed as:

$$\begin{aligned} [LM'_{mC}]_{ij} &= \sum_{1 \leq r \leq m} [Q^{-1}]_{ir} \big[\sum_{1 \leq v \leq m} [LM_{mC}]_{rv} [Q]_{vj} \big] \\ &= \sum_{j \leq v \leq m} ([LM_{mC}]_{iv} - [LM_{mC}]_{i+1,v}) \end{aligned} \tag{19}$$

where we noticed that $[Q]_{vj} = 0$ for $v < j$, and $[Q]_{vj} = 1$ for $v \geq j$. Also, $[Q^{-1}]_{ir} = 0$ for all $r \neq i-1, i$ and $[Q]_{i,i-1} = -1, [Q]_{ii} = 1$.
Thus, by Lemma 15 for $i > 1, j = 1$:

$$[LM'_{mC}]_{i1} = \sum_{1 \leq v \leq m} [LM_{mC}]_{iv} - \sum_{1 \leq v \leq m} [LM_{mC}]_{i+1,v} = SL_P(I) - SL_P(I) = 0 \quad (20)$$

∎

Remark 19. [Consequences of Proposition 18] (i) From this result, follows that the eigenvalue of LM_C, $SL_P(I)$, is among the eigenvalues of LM_{mC} for all m, as we also derived from Proposition 11.
(ii) By the Proof of Lemma 18 we can construct the ij-th element of D as

$$[D]_{ij} = \sum_{j \leq v \leq m} LK_P(I^{(i-1)}, I^{(v-1)}) - LK_P(I^{(i)}, I^{(v-1)}) \quad (21)$$

5.1.1. n Chains in one PBC. In this subsection we will extend our previous results to the case of n chains in a system with one PBC.

Let us consider n chains, say $H1, H2, \ldots, Hn$ in a system with one PBC that unfold in $k_i, i = 1, \ldots, n$ cells each. The periodic linking matrix of that system has size $n \times n$ abd is defined as $(LM_C)_{(i,j)} = LK_P(Hi, Hj)$, when $i \neq j$ and $(LM_C)_{(i,i)} = SL_P(Hi)$.

Then the matrix LM_{mC} has size $mn \times mn$, since to each free chain, Hj, of the cell C, correspond m free chains, $Hj^{(i)}$, $i = 0, \ldots, m-1$, in the cell mC (see Lemma 5). We make the convention that the u-th row of LM_{mC}, where $u = rm + l$ corresponds to the free chain $H(r+1)^{(l-1)}$. Therefore, the (q, w)-th element of LM_{mC}, where $q = q_1 m + q_2, w = w_1 m + w_2$, is: $LK_P(H(q_1+1)^{(q_2-1)}, H(w_1+1)^{(w_2-1)})$.

Lemma 20. *Let C denote a cell with one PBC that consists of n chains. Let mC denote the cell that results after gluing m copies of C, then the sum of all the elements of the $(u-1)m + v$-th row of LM_{mC} is equal to to the sum of all the elements of the $u-$th row of LM_C, for $v = 1, \ldots, m$.*

Proof. Let us consider the q-th row of LM_{mC}, where $q = q_1 m + q_2$.
The sum of the elements $q_1 m + 1$ to $q_1 m + m$ in that row is equal to

$$\begin{aligned}
&\sum_{i=1}^{m} LK_P(H(q_1+1)^{(q_2-1)}, H(q_1+1)^{(i-1)}) \\
&= SL_P(H(q_1+1)^{(q_2-1)}) + LK_P(H(q_1+1)^{(q_2-1)}, H(q_1+1)^{(0)}) + \ldots \\
&+ LK_P(H(q_1+1)^{(q_2-1)}, H(q_1+1)^{(m-1)}) = SL_P(H(q_1+1))
\end{aligned} \quad (22)$$

The sum of the elements h to $h + (m-1)$ of the same row, for $h \in \{1, m+1, \ldots, (q_1-1)m+1\} \cup \{(q_1+1)m+1, \ldots, (n-1)m+1\}$ corresponds to the linking of the free chain $H(q_1+1)^{(q_2-1)}$ with the free chains generated by Hj, where $j = \frac{h-1}{m} + 1$:

$$
\begin{aligned}
&\sum_{i=1}^{m} LK_P(H(q_1+1)^{(q_2-1)}, Hj^{(i-1)}) = LK_P(H(q_1+1)^{(q_2-1)}, Hj^{(0)}) \\
&+ \ldots + LK_P(H(q_1+1)^{(q_2-1)}, Hj^{(m-1)}) \\
&= \sum_{u\in\mathbb{Z}} L(H(q_1+1)_0^{(q_2-1)}, Hj_0^{(0)} + uml(1,0,0)) \\
&+ \sum_{u\in\mathbb{Z}} L(H(q_1+1)_0^{(q_2-1)}, Hj^{(0)} + (um+1)l(1,0,0)) \\
&+ \ldots + \sum_{u\in\mathbb{Z}} L(H(q_1+1)_0^{(q_2-1)}, Hj_0^{(0)} + (um+m-1)l(1,0,0)) \\
&= \sum_{u\in\mathbb{Z}} L(H(q_1+1)_0^{(q_2-1)}, Hj_0^{(0)} + ul(1,0,0)) = LK_P(H(q_1+1), Hj)
\end{aligned} \tag{23}
$$

where in the last equality we noticed that, by definition, the periodic linking number does not depend on the image of $H(q_1+1)$ used for its computation.

Thus, the total sum of the elements of the q-th row, where $q = q_1m + q_2$, is

$$
\begin{aligned}
&LK_P(H(q_1+1), H(1)) + \ldots + LK_P(H(q_1+1), H(q_1)) \\
&+ SL_P(H(q_1+1)) + LK_P(H(q_1+1), H(q_1+2)) + \ldots + LK_P(H(q_1+1), H(n))
\end{aligned} \tag{24}
$$

$\square$

Exactly the same considerations apply for the sum of the rows q_1m to $(q_1+1)m-1$.

Remark 21. [Consequences of Lemma 20] (i) The total sum of the elements of a row measures the total linking applied to a free chain in the system. This suggests that the total linking applied to a chain remains constant, and is independent of the size of the cell, as expected due to the structure of the periodic system.
(ii) The total sum of the elements of the linking matrix depends linearly on the size of the cell.

Remark 22. For closed chains and for $m > 2\max_i\{|mu(Hi)|\}$, the linking matrix obtains a simpler expression. Then any image of $Hj^{(u)}$ will link with at most one image of any $Hj^{(v)}$ or $Hk^{(d)}$. Therefore, $SL_P(Hj^{(u)}) = Sl(Hj_0)$ for all j. Also, $LK_P(Hj^{(u)}, Hj^{(v)}) = L(Hj_u, Hk_v)$, for $|u-v| \leq 2\max_i\{|mu(Hi)|\}$, and $LK_P(Hj^{(u)}, Hk^{(v)}) = 0$, for $|u-v| > 2\max_i\{|mu(Hi)|\}$. Thus, as $m \to \infty$, LM_{mC} becomes an $mn \times mn$ sparse matrix, where each row has at most $2n\max_i\{|mu(Hi)|\}$ non-zero entries.

Proposition 23. *Let C denote a cell with one PBC that consists of n chains. Let mC denote the cell that results after gluing m copies of C, then LM_{mC} can be expressed as an $n \times n$ block matrix of $m \times m$ symmetric circulant matrices. Moreover, the diagonal block matrices are symmetric centrosymmetric matrices. The eigenvalues of the (i,i)-th block of LM_{mC}, $i = 1, \ldots, n$, are:*

$$
\lambda_s = SL_P(Hi^{(0)}) + 2\sum_{k=1}^{\frac{m-1}{2}} LK_P(Hi^{(0)}, Hi^{(k)}) \cos\Big(\frac{2\pi}{m}k(s-1)\Big) \tag{25}
$$

for m odd and

$$\lambda_s = SL_P(Hi^{(0)}) + (-1)^{(s-1)} LK_P(Hi^{(0)}, Hi^{(\lfloor \frac{m-1}{2} \rfloor + 1)}) + 2 \sum_{k=1}^{\lfloor \frac{m-1}{2} \rfloor} LK_P(Hi^{(0)}, Hi^{(k)}) \cos\Big(\frac{2\pi}{m} k(s-1)\Big) \tag{26}$$

for m even, $s = 1, \dots, m$.

The eigenvalues of the (i,j)-th block of LM_{mC}, $1 \leq i < j \leq n$, are:

$$\lambda_s = LK_P(Hi^{(0)}, Hj^{(0)}) + 2 \sum_{k=1}^{\frac{m-1}{2}} LK_P(Hi^{(0)}, Hj^{(k)}) \cos\Big(\frac{2\pi}{m} k(s-1)\Big), \tag{27}$$

for m odd and

$$\lambda_s = LK_P(Hi^{(0)}, Hj^{(0)}) + (-1)^{(s-1)} LK_P(Hi^{(0)}, Hj^{(\lfloor \frac{m-1}{2} \rfloor + 1)}) + 2 \sum_{k=1}^{\lfloor \frac{m-1}{2} \rfloor} LK_P(Hi^{(0)}, Hj^{(k)}) \cos\Big(\frac{2\pi}{m} k(s-1)\Big) \tag{28}$$

for m even, $s = 1, \dots, m$.

Proof. By its definition, LM_{mC} can be expressed as a block matrix of $m \times m$ symmetric matrices, $(LM_{mC})^{i,j}$, where (k,l)-th element of $(LM_{mC})^{i,j}$ is equal to $LK_P(Hi^{(k-1)}, Hj^{(l-1)})$.

We notice that, when $|k_1 - l_1| = |k_2 - l_2| \mod m$,

$$\begin{aligned} &LK_P(Hi^{(k_1)}, Hj^{(l_1)}) = LK_P(Hi + (k_1, 0, 0), Hj + (l_1, 0, 0)) \\ &= \sum_{r \in \mathbb{Z}} L(Hi_0 + (k_1, 0, 0), Hj_0 + (l_1 + mrl, 0, 0)) \\ &= \sum_{r \in \mathbb{Z}} L(Hi_0 + (k_2, 0, 0), Hj_0 + (l_2 + mL, 0, 0)) \\ &= LK_P(Hi + (k_2, 0, 0), Hj + (l_2, 0, 0)) = LK_P(Hi^{(k_2)}, Hj^{(l_2)}) \end{aligned} \tag{29}$$

Thus, each matrix $(LM_{mC})^{i,j}$ is symmetric circulant.

A matrix, $(LM_{mC})^{i,i}$, on the diagonal of LM_{mC} corresponds to the self-image linking of the chain Hi, which by Proposition 9, it is a symmetric centrosymmetric matrix.

The eigenvalues of the block matrices are obtained by Proposition 11. ∎

REMARK 24. When $m > 2 \max_j \{|mu(Hj)|\}$, the eigenvalues of the (i,i)-th and (i,j)-th block, $i = 1, \dots, n$, obtain a simpler expression, which can be obtained by Eq. 25,26,27,28, by replacing the periodic linking and self-linking numbers by the classical linking and self-linking numbers.

REMARK 25. From Proposition 23 follows that $SL_P(Hi)$ is an eigenvalue of the (i,i)-th block of LM_{mC} and $LK_P(Hi, Hj)$ is an eigenvalue of the (i,j)-th block

Notice that in the case of n chains in a system with 1 PBC the periodic linking matrix is no longer a circulant matrix and its eigenvalues are not known. However, the eigenvalues of its block matrices are known. More precisely, LM_{mC} can be expressed as

$$LM_{mC} = \Sigma M + \Lambda M \tag{30}$$

where $\Sigma M, \Lambda M$ are $m \times m$ block matrices. ΣM is a diagonal block matrix, whose blocks represent the linking of a chain Hi with its own images and are symmetric centrosymmetric. ΛM is a block matrix whose diagonal matrices are zero and its off-diagonal matrices represent the linking between different generating chains, and are symmetric circulant matrices

One could use methods such as the ones in [29] to find the determinant of LM_{mC} in terms of the determinants of the block matrices. However, its computation is cumbersome and the eigenvalues of LM_{mC} remain unknown. The following Proposition shows that some of the eigenvalues of the periodic linking matrix are invariant of cell-size, m.

Proposition 26. *Let LM_C be the periodic linking matrix of a periodic system generated by the cell C with one PBC, which contains n chains. Then any other periodic linking matrix LM_{mC} of the same periodic system generated by the cell mC is of the form*

$$LM_{mC} = \begin{bmatrix} LM_C & E \\ 0 & F \end{bmatrix} \tag{31}$$

where E has size $1 \times (m-1)$ and F has size $(m-1) \times (m-1)$.

Proof. Let us multiply LM_{mC} by the matrices $Q' = Q \oplus Q \oplus \ldots \oplus Q$ and $(Q')^{-1} = Q^{-1} \oplus Q^{-1} \oplus \ldots \oplus Q^{-1}$, ($n$ direct sums in each term). Let $i = k_1 m + l_1$, $j = k_2 m + l_2$. The diagonal elements of $(Q')^1 LM_{mC} Q'$ are

$$[(Q')^{-1} LM_{mC} Q']_{ii} = \sum_{1 \le u \le n} [(Q')^{-1}]_{i,u} \sum_{1 \le v \le n} (LM_{mC})^{u,v} [Q']_{v,j} \tag{32}$$

where $[Q']_{v,j} = O$ if $v \neq j$, $[Q']_{j,j} = Q$, $[(Q')^{-1}]_{v,j} = O$ if $v \neq j$, and $[(Q')^{-1}]_{j,j} = Q^{-1}$. Thus,

$$[Q^{-1} LM_{mC} Q]_{ij} = [(Q')^{-1}]_{i,i} (LM_{mC})^{u,j} [Q']_{j,j} = Q^{-1} (LM_{mC})^{i,j} Q \tag{33}$$

Then for the diagonal elements, we showed in the proof of Proposition 18 that

$$Q^{-1} (LM_{mC})_{i,i} Q = \begin{bmatrix} SL_P(H(k_1+1)) & C_i \\ 0 & D_i \end{bmatrix} \tag{34}$$

for $i \neq j$, then in the proof of Lemma 15 we proved that the sum of all the elements of a row of $(LM_{mC})^{i,j}$ is equal to $LK_P(H(k_1), H(k_2))$. Then we compute

$$\begin{aligned} [Q^{-1}(LM_{mC})^{i,j} Q]_{u,v} &= \sum_{1 \le s \le m} [Q^{-1}]_{u,s} \big[\sum_{1 \le t \le m} [(LM_{mC})^{i,j}]_{v,t} [Q]_{t,s} \big] \\ &= \sum_{v \le s \le m} ([(LM_{mC})^{i,j}]_{s,v} - [(LM_{mC})^{i,j}]_{s+1,v}) \end{aligned} \tag{35}$$

where we notice that $[Q]_{t,s} = 0$ for $t < s$, and $[Q]_{t,s} = 1$ for $t \geq s$. Also, $[Q]^{-1}_{t,s} = 0$ for all $s \neq t-1, t$ and $[Q^{-1}]_{t,t-1} = -1, [Q^{-1}]_{t,t} = 1$.
Thus, by Lemma 20, for $u > 1, v = 1$, the sum of each row of $(LM_{mC})^{i,j}$ is $LK_P(H(k_1+1), H(k_2+1))$:

$$\begin{aligned} &[Q^{-1}(LM_{mC})^{i,j}Q]_{u1} \\ &= \sum_{1\leq s\leq m} [(LM_{mC})^{i,j}]_{u,s} - \sum_{1\leq s\leq m} [(LM_{mC})^{i,j}]_{u+1,s} \\ &= LK_P(H(k_1+1), H(k_2+1)) - LK_P(H(k_1+1), H(k_2+1)) = 0 \end{aligned} \tag{36}$$

Thus we have proved that each block is similar to a matrix of the form:

$$Q^{-1}(LM_{mC})^{i,j}Q = \begin{bmatrix} LK_P(H(k_1), H(k_2)) & C_{ij} \\ 0 & D_{ij} \end{bmatrix} \tag{37}$$

Next, let e_i denote the i-th vector of the standard basis of $\mathbb{R}^{mn}$. Let E denote the $mn \times mn$ matrix whose j-th column is $e_{(j-1)m+1}$, for $j \leq n$, e_k when $j = km+1, j > n$ and e_j if $j \mod m \neq 1, j > n$. Then

$$LM_{mC} \sim E^{-1}(Q')^{-1} LM_{mC} Q' E = \begin{bmatrix} LM_C & G \\ 0 & F \end{bmatrix} \tag{38}$$

$\square$

REMARK 27. From Proposition 26 it follows that the eigenvalues of LM_C are among the eigenvalues of LM_{mC}, for all m.

6. Conclusion. The entanglement in polymer melts is a many body problem. Our goal is to provide a measure of entanglement that takes into consideration the overall conformation of a melt. For this purpose we defined the linking matrix. For systems employing PBC we defined the periodic linking matrix using the periodic linking and self-linking measures. In the simulation of a polymer system, the size of the cell may vary. It is necessary to know how the data obtained from different cell sizes are related. By focusing on an arbitrary fixed periodic system simulated by a varying cell-size simulation box with one PBC, we proved that some of the eigenvalues of the periodic linking matrix are invariant of cell size. This information can be used to characterize a periodic system. On the other hand, the rest of the eigenvalues change with the cell-size, as does the topology in the identification space.

More precisely, the size of the periodic linking matrix and the total sum of its entries increase linearly with the size of the cell. Also, the number of eigenvalues increases linearly with cell size. For systems generated by only one chain, we provided analytical formulas for the eigenvalues as a function of cell-size. In the case of systems generated by many chains, we proved that the periodic linking matrix can be expressed as a sum of a block symmetric centrosymmetric matrix, whose eigenvalues are known analytically, and a block symmetric circulant matrix, for which the eigenvalues of each block are known analytically. We also proved that some of the eigenvalues are invariant of cell-size, therefore, they represent properties of the periodic system. In fact, for closed chains, all the eigenvalues are invariant under isotopy of the chains that compose the melt. But some of the eigenvalues change with the size of the cell, which determines the number of components in the identification space, ie. the solid torus in the case of systems with one PBC. This suggests that the periodic linking matrix can be used to study both the periodic system and the identification space.

One could think of physical experiments that would simulate the effect of cell-size to the periodic linking matrix. Our results could apply to experiments where the cell size increases and the number of chains in the cell also increases with chains of the same molecular weight. This is not the same as using copies of the same cell, but we can expect that, on average, the linking of the different chains will be the same and, therefore, we can expect, on average, to have similar results. Another physical experiment that would simulate the effect of cell-size would be the following: One can use the same simulation cell, but increase the number of components. In order to keep the same density for the systems (as is the case in our analysis), while increasing the number of components, one should decrease their molecular weight. Chains of molecular weight may not be able to form links of the same type as the longer chains if they are not flexible enough. Therefore, one should use more chains that are more flexible and of smaller molecular weight. Then we expect that, on average, our analytical results would hold among the different systems.

We have demonstrated that the Gauss linking integral, the periodic linking number and the periodic linking matrix provide fundamental information concerning the structure of polymeric systems. Moreover, they are mathematically well-defined and provide continuous measures in the space of configurations. Thus their properties make them good candidates for the use in thermodynamic equations. In the formulation of evolution equations for polymer melts, there is a need for variables that capture the conformational properties of polymers that are related to entanglement [19, 17]. The radius of gyration tensor, or end-to-end distance, or the number of entanglements per chain are used in these formulations. It would be interesting to use the linking and self-linking measures in these formulations. Furthermore the linking matrix and the Laplacian of the corresponding graph describe the entire melt in one measure and could also be useful in these formulations. Moreover, our results can be extended to any other measures of pairwise interactions in systems with PBC that depend on the relative positions of the chains.

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