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Computing the writhe on lattices

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Abstract

Given a polygonal closed curve on a lattice or space group, we describe a method for computing the writhe of the curve as the average of weighted projected writhing numbers of the polygon in a few directions. These directions are determined by the lattice geometry, the weights are determined by areas of regions on the unit 2-sphere, and the regions are formed by the tangent indicatrix to the polygonal curve. We give a new formula for the writhe of polygons on the face centred cubic lattice and prove that the writhe of polygons on the body centred cubic lattice, the hexagonal simple lattice, and the diamond space group is always a rational number, and discuss applications to ring polymers.

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1. Introduction

Lattice models of self-avoiding random walks have been extensively used to simulate polymer chains with volume exclusion (Fuller 1962, Garcia *et al* 1999, Howard and Duan 1998, 1999, Janse van Rensburg *et al* 1993, 1997, Kennedy *et al* 1994, Lacher and Sumners 1991). These models are useful in understanding biological and chemical properties of polymer molecules which are self-entangled or entangled with neighboring molecules. Topological entanglement (knotting and linking) restricts the number of configurations available to a macromolecule, and is thus a measure of configurational entropy. It has been found that chemical and rheological properties such as the quality of crystal molecules and viscosity of polymer fluids are related to the molecular entanglement (Edwards 1967, Lucas *et al* 1995, Mandelkern *et al* 1993, Moroz and Kamien 1997, Popli and Mandelkern 1987, Vologodskii *et al* 1974), and while a polymer ensemble may behave like a gel, a different ensemble may behave like an oil. It is then of great interest to quantify microscopic entanglement, and if possible, relate it to macroscopic physical properties of the polymer ensemble, such as the stress–strain curve, rubber elasticity and various phase change phenomena. The writhing number (or just writhe), which will be described in the next section, is a geometric measure of self-entanglement. Although this property was named by Fuller (1971), following the definition of writhing (verb, to twist into coils or folds), it was Calugareanu (1961) and White (1969) who presented the mathematical treatment of this measure and its relation between the geometrical and topological properties of a closed ribbon ($Lk = Tw + Wr$). Writhe has been used to understand the geometry and topology of DNA (Arsuaga *et al* 2005, Bauer *et al* 1980, Crick 1976, Fuller 1978). Writhe can indicate chirality of knots, and the presence of knots in a closed circular DNA plasmid can give information about the mechanism of action of enzymes on the DNA molecule (Sumners 1995). The packing geometry of DNA in bacteriophage capsids is believed to be writhe-directed and non-random (Arsuaga *et al* 2005). The writhe has also been useful in the classification of protein folds (Rogen and Fain 2003). This paper will focus on computational methods for the writhe of polygonal closed curves on lattices and space groups.

There are a number interesting results regarding the writhe and spatial conformation of lattice polygons. For example, the knotting probability of a polygon on the simple cubic lattice Z^3 has exponential approach to unity as the length goes to infinity (Pippenger 1989, Sumners and Whittington 1988). Janse van Rensburg *et al* (1993) showed that the expectation of the absolute value of the writhe $\langle |Wr| \rangle$ of polygons in Z^3 increases at least as rapidly as $\sqrt{n}$., where n is the length of the polygon. In addition, Janse van Rensburg *et al* (1997) investigated the mean writhe of a random sample of polygons of fixed knot type in Z^3, finding that if the expected value of the writhe is not zero, then the knot is chiral.

Approximating the writhe of a space curve in general requires choosing a number of planar projections, computing the projected writhe for each of these projections, and averaging the results. For polygons on lattices and space groups, the restricted geometry of the lattice or space group leads to simplification of the writhe calculation, and provides an exact calculation for the writhe. Lacher and Sumners (1991) provided the first exact computation for the writhe of closed curves on Z^3 as the average of four linking numbers of the polygon with pushoffs in four specific directions, proving that four times the writhe for closed curves on Z^3 is an integer; Cimasoni (2001) arrived at the same result, and Garcia *et al* (1999) produced a writhe formula for the face centred cubic lattice (FCC), proving also that the probability that a polygon on FCC of length n has irrational writhe tends to one as n tends to infinity. Also Garcia *et al* (1999) sketched a proof that for the body centred cubic lattice (BCC), 24 times the writhe is an integer, and also made comments related to the hexagonal close packing (HCP) space group.

In this paper, we compute the writhe of a polygon on any lattice or space group. The method is based on the analysis of the tangent indicatrix of the polygonal curve.

Fundamental concepts for this paper as well as the description of the methods and central theorem are described in section 2. Section 3 gives several results illustrating the writhe of closed curves on some important lattices and space groups. In section 4, questions and future directions are proposed.

2. Definitions and known results

A three-dimensional *lattice* can be defined as an arrangement of points or vertices in a regular periodic pattern in space, and the combination of all available symmetry operations on lattices leads to *space groups*. A *simple closed curve* (*lattice polygon*) K on a lattice L is the union of a finite number of edges $e_1 = v_1v_2, e_2 = v_2v_3, \ldots, e_n = v_nv_{n+1}$ $(v_{n+1} = v_1)$ for $v_i \in L$. The edges of a lattice polygon overlap at most in endpoints and each vertex lies on exactly two edges.

Given an oriented polygon (knot) K in R^3, consider its projection into R^2 in the direction of the vector $u \in R^3$. In general, almost all projections will be *regular*, where at most two projected edges intersect, and that intersection is transverse. For any regular projection, each crossing x can be assigned a value of $x(u) = \pm 1$ according to the right-hand rule (see figure 1). Note that the sign of the crossing x does not depend on the orientation chosen for the polygon,

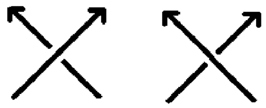


Figure 1. Positive and negative crossings are determined by the right-hand rule.

because reversing the orientation of the polygon reverses both of the arrows at crossing x, leaving the sign unchanged. For each vector u, the *projected writhing number* of K, denoted by $Wr(K, u)$, is defined as the sum of all values $x(u)$ of the projection of K by u. The *writhe* is the average of the projected writhing number of K over every projection and is defined as

$$Wr(K) = \frac{1}{4\pi} \int_{u \in S} Wr(K, u), \tag{2.1}$$

where S is the unit 2-sphere.

Note that for every crossing x, $x(u) = x(-u)$, so for every regular projection over u, $Wr(K, u) = Wr(K, -u)$, and we can compute the writhe as the average over any hemisphere:

$$Wr(K) = \frac{1}{2\pi} \int_{u \in \frac{1}{2}S} Wr(K, u). \tag{2.2}$$

For an oriented polygon K with edges $e_1, e_2, \ldots, e_n$, each oriented edge e_i determines a direction. These directions can be interpreted as points $e'_1, e'_2, \ldots, e'_n$ on S. Given any pair of distinct consecutive points e'_i, e'_{i+1} on S, consider the arc of great circle G_i on S generated by the exterior angle formed by edges e_i and e_{i+1}. If K is a closed curve then $H = \cup G_i$ is also a closed curve, and if we reverse the orientation of K, we obtain another closed curve H', which is the antipodal curve of H. The *indicatrix* I_K of a closed curve K is defined as $I_K = H \cup H'$, and the complement of the indicatrix $S \backslash I_K$ is a finite number of antipodal pairs of open disjoint connected regions $R_1, R'_1, R_2, R'_2, \ldots, R_m, R'_m$.

Although the indicatrix can be defined for smooth closed curves (Fuller 1971), in this paper, we discuss only the writhe of polygonal curves on lattices.

The indicatrix of the closed curve K plays an important role in the calculation of the writhe because it helps to greatly reduce the number of directions u where the writhe changes value. The importance of the indicatrix is given in the following theorem by Cimasoni (2001).

Theorem 2.1 (Cimasoni)**.** *If u_1 and u_2 are two regular directions which belong to the same complementary region R_i, then*

$$Wr(K, u_1) = Wr(K, u_2). \tag{2.3}$$

Now suppose that $R_1, R'_1, R_2, R'_2, \ldots, R_m, R'_m$ are the regions bounded by $S \backslash I_K$ with area A_i respectively. Then for $u_i \in R_i$,

$$Wr(K) = \frac{1}{2\pi} \sum_{i=1}^{m} Wr(K, u_i) A_i. \tag{2.4}$$

Definition 2.2. *Let L be a lattice or space group in space. The lattice indicatrix I_L is defined as the union of all arcs on great circles on S generated by all the pairs of adjacent oriented edges e_i, e_{i+1} in L.*

Note that the indicatrix of any closed curve in the lattice is contained in the lattice indicatrix, that is, $K \subset L \Rightarrow I_K \subset I_L$.

We can also think of I_L as a set of vertices and edges on S, where the vertices are given by the different directions of the edges of L, and the edges on I_L are the arcs of great circles on S produced by the directions of any pair of edges on L. Since the set of edges of a lattice (space group) generate only a small number of different directions, the corresponding lattice indicatrix has only a small number of vertices. Now we proceed to discuss the method to compute the lattice indicatrix for a given lattice.

Let v be a vertex on a lattice L, then the degree m of v is the same as the degree of every other vertex in L because any element of L is invariant under translation by the primitive unit vectors. Therefore the lattice indicatrix I_L consist of m vertices. To find the edges of I_L, we need to consider all the arcs of great circle produced by the directions of any two adjacent oriented edges e_i, e_j of L, where e_i starts at v. Given an edge $e_i = vv_i$ on L, then by excluding e_i, there are $m - 1$ edges incident to v_i, but when two adjacent edges have the same direction, this results in a single vertex on I_L. Hence, for every vertex e'_i on I_L, there are $m - 2$ edges incident to e'_i. Note that if some vertices e'_i, e'_j, e'_k are on the same arc of great circle, then the edges (if any) between them can overlap.

A difference between lattices and space groups is that a lattice preserves orientation under translations by its unit vectors, and this property of invariance makes easier to find I_L, but on a space group the orientations can be reversed (see diamond structure in table 1(E)), rotated or reflected. However, it is known that any space group contains a lattice, hence space groups preserve repetitive patterns as well, and there are only a finite number of directions that an edge of any polygonal closed curve in L can take, and this translates into a finite number of vertices on I_L. A similar affirmation follows for a finite and equal number of edges at every vertex of I_L. Once I_L is drawn and the regions $R_1, R_2, \ldots, R_m$, which constitute half of the sphere, have been identified, we proceed to compute the writhe by using formula (2.4).

3. The writhe of a polygon for some important lattices and a space group

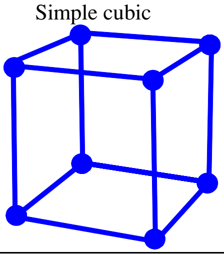
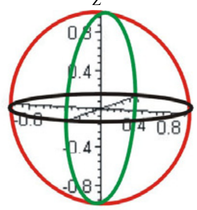
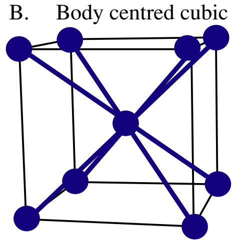
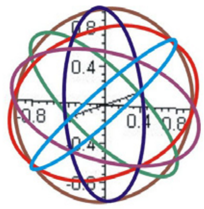
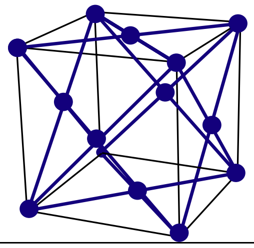
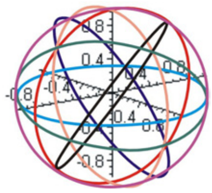
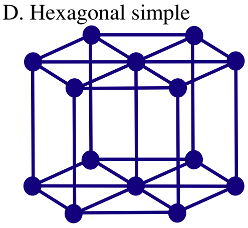
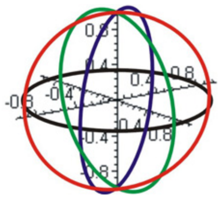
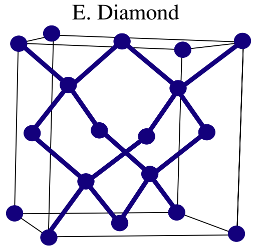
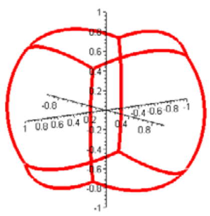
We now produce formulae for the calculation of writhe for a number of lattices and a space group. The first formula computes the writhe of a polygon in the simple cubic lattice Z^3, a case first solved by Lacher and Sumners (1991) and later by Cimasoni (2001). Because of its simplicity, it makes an instructive example. The writhe of polygons on the face centred cubic lattice was studied by Garcia *et al* (1999), who gave a formula for the writhe and proved that the writhe can be irrational. We produce a different formula for the writhe on the FCC lattice, and formulae for the writhe on the body centred cubic lattice, the hexagonal simple lattice and the diamond space group, proving that the writhe on each of the last three is rational. We describe the corresponding unit cells (also known as crystallographic unit cell) and their primitive unit vectors.

3.1. The simple cubic lattice

The unit cell of Z^3 consists of a unit cube with vertices at its corners (see table 1(A). The primitive vectors are given by $a = (1, 0, 0)$, $b = (0, 1, 0)$, $c = (0, 0, 1)$. Since at every vertex of Z^3 there are six different edges with directions $\pm a, \pm b, \pm c$, the lattice indicatrix has six vertices at $\pm a, \pm b, \pm c$. Consider the pair of any two adjacent edges on Z^3, where the first edge starts at the origin. It can be found that I_{Z^3} consists of three great circles on S passing thought the planes XY, YZ and XZ, respectively, which divide the sphere into eight octants of equal area $A = \pi/2$. Because half of those regions are antipodal to the other half, it is enough to consider the four upper octants, then by theorem 2.3

$$Wr(K) = \frac{1}{2\pi}\sum_{i=1}^{4} Wr(K, u_i)\pi/2 = \frac{1}{4}\sum_{i=1}^{4} Wr(K, u_i), \tag{3.1}$$

Table 1. Lattice structures and space groups with their corresponding lattice indicatrices and writhe formulae.

Lattice or space group unit cell	Lattice indicatrix	Writhe formula
A. Simple cubic 	I_{Z^3} 	$Wr(K)=\frac{1}{4}\sum_{i=1}^{4}Wr(K,u_i)$
B. Body centred cubic 	I_{BCC} 	$Wr(K)=\frac{1}{12}\sum_{i=1}^{12}Wr(K,u_i)$
C. Face centred cubic 	I_{FCC} 	$Wr(K)=\frac{\alpha}{2\pi}\sum_{i=1}^{4}Wr(K,u_i),$ $+\frac{\beta}{2\pi}\sum_{j=1}^{12}Wr(K,v_j)$ where $\alpha=3\sec^{-1}3-\pi$ and $3\beta+\alpha=\pi/2$
D. Hexagonal simple 	I_{HS} 	$Wr(K)=\frac{1}{6}\sum_{i=1}^{6}Wr(K,u_i)$
E. Diamond 	I_D 	$Wr(K)=\frac{1}{3}\sum_{i=1}^{3}Wr(K,u_i)$

where u_i are directions taken from vectors on the four upper octants, respectively. The values of u_i as $(\pm 1/\sqrt{3}, \pm 1/\sqrt{3}, 1/\sqrt{3})$ will work. From here we conclude that for any closed curve K on Z^3, $4Wr(K)$ is an integer.

3.2. Body centred cubic lattice

In the BCC, a unit cell is characterized by a unit cube with each corner vertex adjacent to a vertex on the centre of the cube (table 1(B)). The primitive vectors are $a = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$, $b = \left(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right)$, $c = \left(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$ and $d = \left(-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right)$, each edge has length $\sqrt{3}/2$, thus the vertices at each corner do not touch each other by an edge. Because at each vertex there are edges in the directions of $\pm a, \pm b, \pm c$ and $\pm d$. The lattice indicatrix then has eight vertices $\pm\frac{a}{\|a\|}, \pm\frac{b}{\|b\|}, \pm\frac{c}{\|c\|}$ and $\pm\frac{d}{\|d\|}$, each vertex has $8 - 2 = 6$ edges, so each vertex connects to every other except its antipodal and itself. Therefore, I_{BCC} consists of six great circles on S. The lattice indicatrix I_{BCC} divides half of S into 12 spherical triangles of equal area $\pi/6$, and the writhe formula is the following:

Theorem 3.2.1. *The writhe of a polygon K on the BCC lattice is given by*

$$Wr(K) = \frac{1}{12}\sum_{i=1}^{12} Wr(K, u_i), \tag{3.2}$$

where the vectors u_i are taken from the regions R_i on a half of the sphere. A choice of the vectors u_i is $\left(\pm\frac{\sqrt{10}}{10}, 0, \frac{3\sqrt{10}}{10}\right)$, $\left(0, \pm\frac{\sqrt{10}}{10}, \frac{3\sqrt{10}}{10}\right)$, $\left(\frac{3\sqrt{10}}{10}, 0, \pm\frac{\sqrt{10}}{10}\right)$, $\left(\frac{3\sqrt{10}}{10}, \pm\frac{\sqrt{10}}{10}, 0\right)$, $\left(\pm\frac{\sqrt{10}}{10}, \frac{3\sqrt{10}}{10}, 0\right)$, $\left(0, \frac{3\sqrt{10}}{10}, \pm\frac{\sqrt{10}}{10}\right)$.

Thus, $12Wr(K)$ is an integer. Note that this is an improvement to the result from Garcia et al (1999), who proved that $24Wr(K)$ is an integer.

3.3. Face centred cubic lattice

The FCC is composed of a unit cube with vertices at each corner and at the centre of each face (table 1(C)). A unit cell is characterized by the vectors $a_1 = \left(\frac{1}{2}, \frac{1}{2}, 0\right)$, $a_2 = \left(-\frac{1}{2}, \frac{1}{2}, 0\right)$, $a_3 = \left(\frac{1}{2}, 0, \frac{1}{2}\right)$, $a_4 = \left(-\frac{1}{2}, 0, \frac{1}{2}\right)$, $a_5 = \left(0, \frac{1}{2}, \frac{1}{2}\right)$, and $a_6 = \left(0, -\frac{1}{2}, \frac{1}{2}\right)$. Every vertex on the FCC has 12 edges in the directions $\pm a_i$, $1 \leqslant i \leqslant 6$, and therefore the lattice indicatrix contains 12 vertices given by $\pm\frac{a_i}{\|a_i\|}$. To find the edges we consider the directions of any pair of consecutive edges e_k, e_{k+1}, where e_k starts at the origin. The result is a set of seven great circles that divides every octant of the sphere into four triangles, one of area $\alpha = 3\sec^{-1}3 - \pi$ and the other three of equal area β, where $3\beta + \alpha = \pi/2$.

Theorem 3.3.1. *The writhe of any polygon K on the FCC lattice is given by*

$$Wr(K) = \frac{1}{2\pi}\left(\alpha\sum_{i=1}^{4} Wr(K, u_i) + \beta\sum_{j=1}^{12} Wr(K, v_j)\right), \tag{3.3}$$

where the vectors u_i and v_i are taken from the regions (on the upper half sphere) R_i and R_j of area α and β, respectively.

For instance, we can take $\left(\pm\frac{3\sqrt{22}}{22}, \pm\frac{3\sqrt{22}}{22}, \frac{\sqrt{22}}{11}\right)$ for the vectors u_i, for the vectors v_j, $\left(\pm\frac{\sqrt{30}}{6}, \pm\frac{\sqrt{30}}{30}, \frac{\sqrt{30}}{15}\right)$, $\left(\pm\frac{\sqrt{30}}{30}, \pm\frac{\sqrt{30}}{6}, \frac{\sqrt{30}}{15}\right)$, and $\left(\pm\frac{\sqrt{38}}{38}, \pm\frac{\sqrt{38}}{38}, \frac{3\sqrt{38}}{19}\right)$. An interesting fact is that since α is an irrational number that is not a multiple of π (Garcia et al 1999), then the writhe can have an irrational value. Although this improved writhe formula is different from the formula found by Garcia et al (1999), both formulae give the same result for the writhe.

3.4. Hexagonal simple lattice

The unit cell is characterized by the vectors $a = (2, 0, 0)$, $b = (1, \sqrt{3}, 0)$, $c = (-1, \sqrt{3}, 0)$, $d = (0, 0, 2)$. Every vertex on the lattice HS has eight edges with directions. The lattice indicatrix I_{HS} consist of one great circle C_1 on the plane XY, and three great circles C_2, C_3, C_4 perpendicular to XY passing through the point $\frac{a}{\|a\|}, \frac{b}{\|b\|}$ and $\frac{c}{\|c\|}$, respectively and passing all through the point $\frac{d}{\|d\|}$ (table 1(D)). I_{HS} divides the upper half of S into six regions of equal area $A = \pi/3$ and the writhe formula is the following.

Theorem 3.4.1. *The writhe of any polygon K on the HS lattice is given by*

$$Wr(K) = \frac{1}{6}\sum_{i=1}^{6} Wr(K, u_i), \tag{3.4}$$

where u_i are directions taken from the six upper regions of the sphere, respectively.

The choice of the vectors u_i as $\left(\pm\frac{3\sqrt{7}}{14}, \frac{\sqrt{21}}{14}, \frac{2\sqrt{7}}{7}\right)$, $\left(0, \pm\frac{\sqrt{21}}{7}, \frac{2\sqrt{7}}{7}\right)$ and $\left(\pm\frac{3\sqrt{7}}{14}, -\frac{\sqrt{21}}{14}, \frac{2\sqrt{7}}{7}\right)$, *will work. Also, $6Wr(K)$ is an integer.*

3.5. Diamond space group

The diamond space group (D) consists of two interpenetrating FCCs, displayed along the body diagonal of the cubic cell by one quarter of the length of the diagonal (table 1(E)). The space is characterized by the vectors $a = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$, $b = \left(-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$, $c = \left(\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$ and $d = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}\right)$. Every vertex has four edges in the directions a, b, c, d or $-a, -b, -c, -d$, and every pair of adjacent vertices have the edges in inverted directions from each other, therefore D is not a lattice but a space group. However, note that for every curve in D, the closed curve H' (described in section 2) is antipodal to the curve H that runs in the opposite direction, therefore its indicatrix is still $I = H \cup H'$. In general, the lattice indicatrix consists of eight vertices $\pm a, \pm b, \pm c, \pm d$, and together with the set of edges on I_L, makes a spherical cube as shown in table 1(E). Therefore, S is divided into six regions R_i each of equal area $2\pi/3$, and the writhe formula is the following.

Theorem 3.5.1. *The writhe of any polygon K on the diamond structure D is given by*

$$Wr(K) = \frac{1}{3}\sum_{i=1}^{3} Wr(K, u_i). \tag{3.5}$$

For instance, the vectors $u_1 = (1, 0, 0)$, $u_2 = (0, 1, 0)$ and $u_3 = (0, 0, 1)$ can be chosen. Also, $3Wr(K)$ is an integer.

4. Conclusions and future directions

Table 1 shows examples of lattices (and one space group) together with their corresponding lattice indicatrix curves and the formulae which give an exact computation for the writhe of a polygonal closed curve on each lattice (space group). We note that the size and shapes of the regions given by I_L varies among lattices. The FCC lattice, for instance, shows that not every region has the same area, and the diamond space group shows that not every region is a spherical triangle. Garcia *et al* (1999) made interesting comments associated with the regularity of the vertex figure. If the vertex figure is regular, then each vertex will be surrounded by congruent 3-cells (e.g. Z^3, BCC and HS), and this will lead to a lattice indicatrix that will divide the sphere into regions of equal area, hence giving a rational writhe. If the vertex figure is not regular but its lattice indicatrix divides the sphere into two or more sets of regions with areas being a rational multiple of π, then the writhe would still be rational. Otherwise some polygons will have irrational writhe. In addition, combining previous work (Garcia *et al* 1999, Lacher and Sumners 1991) with results from this paper we can see that the vertex transitive property is neither necessary nor sufficient for the rationality of the writhe. We have examples of rational writhe and vertex transitivity (Z^3), irrational writhe and vertex transitivity (FCC), rational writhe and vertex intransitivity (D) and irrational writhe and vertex intransitivity (HCP).

It would be useful to complete the full list of writhe formulae for every lattice and space group. Another problem that should be considered is polygons living in the union of two or more lattices or space groups. If one considers a configuration requiring two or more lattices (or space groups), then the lattice indicatrix of such a configuration would be the union of two or more lattice indicatrices. Another remark is that not every polymer can be represented as a closed curve; there are linear and branched polymers that can be entangled, so it is important to generalize the writhe formula for linear and branched complexes on lattices or space groups (Orlandini *et al* 1993). Important special cases are the calculation of writhe of biopolymers like DNA, RNA and proteins.

Finally, an intriguing geometric problem is to consider the possibility of a duality between lattice spaces and their lattice indicatrices; it would be interesting to explore the geometric relations that both structures can have, and explore possible dual results between lattice theory and spherical geometry.

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