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The writhe of polygons on the face-centred cubic lattice

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Abstract. For polygons on the simple cubic lattice there is an important theorem due to Lacher and Summers which shows that the writhe of a polygon is the average of the linking numbers of the polygon and its pushoffs in four particular directions. This implies that the writhe of a polygon on the simple cubic lattice is always rational. We prove a related theorem for the face-centred cubic (fcc) lattice but show that, on this lattice, the probability that a polygon of length n has irrational writhe tends to unity as n tends to infinity. In addition, we show that the expectation of the absolute value of the writhe increases at least as fast as \sqrt{n} for large n .

1. Introduction

Long polymer molecules can be highly self-entangled and there has been recent interest in describing and quantifying the entanglement complexity of ring polymers. Knotting and linking are features of topological entanglement complexity but polymers can be geometrically entangled even when they are unknotted and unlinked. This paper will be concerned with *writhe* (Wr) which is a useful measure of geometrical entanglement complexity and measures the signed non-planarity of the ring polymer. Writhe has been widely used to describe and understand the geometrical entanglement complexity of DNA (Bauer *et al* 1980, Bates and Maxwell 1993).

The writhe of a simple closed curve in R^3 can be defined as follows. First orient the curve. Choose a direction μ and project the curve in this direction onto a plane. For almost all directions μ the projected curve will have all crossings transverse. The immediate neighbourhood of each crossing will look like two oriented curve segments one of which crosses *over* the other, and each crossing can be assigned a *signed crossing number*, ± 1 , according to a right-hand rule. This signed crossing number encodes information about the relative orientation of the overcrossing and undercrossing curve segments. The writhe of the curve is the sum of these signed crossing numbers, averaged over all projection directions μ . (Directions in which one or more crossings are not transverse have measure zero and do not contribute to the average.)

One of the standard models of ring polymers is lattice polygons. Given a three-dimensional lattice (such as the simple cubic lattice, Z^3) a *lattice polygon* is an embedding of a simple closed curve in this lattice. From the graph-theoretic point of view, a lattice polygon is a connected subgraph of the lattice with all vertices having degree two. If p_n is the number of lattice polygons (modulo translation) with n vertices in the simple cubic lattice, then $p_n = 0$ if n is

odd, $p_4 = 3$, $p_6 = 22$, $p_8 = 207$, etc. Some information is available about the behaviour of p_n for large n and, in particular, Hammersley (1961) showed that the limit

$$0 < \lim_{n \rightarrow \infty} n^{-1} \log p_n = \kappa < \infty \quad (1.1)$$

exists.

Similar results hold for other lattices. For the face-centred cubic (fcc) lattice $p_3 = 8$, $p_4 = 33$, $p_5 = 84$, etc, and (1.1) still holds but with a different value of the connective constant κ .

There are several results available about the writhe of lattice polygons in three dimensions. Janse van Rensburg *et al* (1993) studied the expectation of the absolute value of the writhe $\langle |Wr| \rangle$ of polygons in the simple cubic lattice and showed that there is a positive constant A such that

$$\langle |Wr| \rangle \geq A\sqrt{n} \quad (1.2)$$

for sufficiently large n . Katritch *et al* (1996, 1997) and Janse van Rensburg *et al* (1997) have studied the mean writhe of simple closed curves of fixed knot type, and Vologodskii and Cozzarelli (1993) and Gee and Whittington (1997) have investigated the writhe of the components of a link as a function of link type.

Calculating numerically the writhe of a simple closed curve in R^3 is not easy and, although writhe can be defined as a line integral, its value is usually computed by a stochastic numerical approximation. In an important paper Lacher and Sumners (1991) showed that for polygons in Z^3 the computation of the writhe could be converted into a computation involving only four linking numbers. (Their result implies that four times the writhe is an integer so that all polygons in Z^3 have rational writhe.) Lacher and Sumners made considerable use of pushoffs, and especially of the idea of a *spatial pushoff*, which is a translate of the curve through a small distance in a given direction. We shall also make extensive use of spatial pushoffs. Lacher and Sumners showed that the writhe is the average of the linking number of the polygon with its pushoffs in all possible directions (i.e. all points on a reference 2-sphere). This converts the problem into a topological question. Within any of the eight octants defined by the coordinate planes in Z^3 the linking number is independent of the particular pushoff direction, so the writhe is the mean of the linking numbers of the polygon with pushoffs into the eight octants. Moreover, mutually antipodal octants yield the same linking number so the writhe is given by the mean of the linking numbers with pushoffs into four non-mutually antipodal octants. Since linking number is an integer, four times the writhe is an integer. The Lacher–Sumners theorem plays an important role in the proof by Janse van Rensburg *et al* (1993) of the inequality (1.2), as well as in numerical work on the writhe of polygons in the simple cubic lattice. It has also been used to prove a result about the writhe of closed ribbons in Z^3 (Janse van Rensburg *et al* 1996).

The Lacher–Sumners result raises several interesting questions:

- (1) Can the writhe be calculated for polygons on other lattices by computing linking numbers with a finite number of pushoffs?
- (2) Is the writhe of a lattice polygon always rational for any lattice?

In this paper we shall show that for the fcc lattice the calculation of the writhe can be converted into a calculation of linking numbers with a small number of pushoffs, but that there are polygons with rational writhe and polygons with irrational writhe. Moreover, the probability that a randomly chosen polygon has rational writhe goes to zero as n goes to infinity. We also show that (1.2) holds for the fcc lattice.

2. Computing the writhe of a polygon in the fcc lattice

We first give a description of the fcc lattice which will be needed later. Let $V(Z^3)$ be the vertex set of Z^3 , i.e. the set of points in R^3 with integer coordinates. Alternate vertices of this set comprise the vertices of the fcc lattice. We choose the set $\mathcal{V} \subset V$ which contains

- (1) vertices which have exactly two odd coordinates and
- (2) vertices which have no odd coordinates,

and add edges between nearest-neighbour pairs of vertices in \mathcal{V} . Each vertex has 12 nearest neighbours and the edges are of length $\sqrt{2}$. The vertex figure is a cuboctahedron so that each vertex is surrounded by eight tetrahedra and six octahedra. All faces of the lattice are triangles, each belonging to one tetrahedron and to one octahedron.

Let α_0 be the solid angle at the vertex of a regular tetrahedron and let β_0 be the solid angle at the vertex of an octahedron. Clearly

$$8\alpha_0 + 6\beta_0 = 4\pi. \tag{2.1}$$

The solid angle α_0 can be calculated as the area of the spherical triangle of unit radius whose sides are the arcs of great circles formed by the intersection of the sphere and the tetrahedron. Since the dihedral angle of a regular tetrahedron is $\sec^{-1} 3$, $\alpha_0 = 3 \sec^{-1} 3 - \pi$.

Let S^2 be the 2-sphere in R^3 of radius $\epsilon < 1/2$. S^2 is the space of pushoffs. The writhe $Wr(\omega)$ of a polygon ω is the average over all pushoff directions μ in S^2 of the linking number $Lk(\omega, \omega(\mu))$ of ω and its pushoff $\omega(\mu)$ by a small distance ϵ in direction μ (Lacher and Summers 1991). We shall show that $Lk(\omega, \omega(\mu))$ is independent of μ for certain sets of directions. In fact $Lk(\omega, \omega(\mu))$ is independent of the pushoff direction within each of the solid angles corresponding to the interiors of the eight tetrahedral regions and within each of eight subregions of each of the six octahedra. Moreover, we show that this subdivision is optimal.

A typical octahedral region is defined by the solid angle subtended at the origin by the square whose vertices are the four lattice points $(1, 1, 0)$, $(1, -1, 0)$, $(1, 0, 1)$ and $(1, 0, -1)$. We subdivide this region into eight congruent suboctahedra bounded by four planes defined by the triples of points

- (1) $(0, 0, 0)$, $(1, 0, 1)$ and $(1, 0, -1)$
- (2) $(0, 0, 0)$, $(1, 1, 0)$ and $(1, -1, 0)$
- (3) $(0, 0, 0)$, $(1, 1/2, 1/2)$ and $(1, -1/2, -1/2)$
- (4) $(0, 0, 0)$, $(1, 1/2, -1/2)$ and $(1, -1/2, 1/2)$.

A typical suboctahedral region is defined by the angle subtended at the origin by the triangle with vertices $(1, 0, 0)$, $(1, 1, 0)$ and $(1, 1/2, 1/2)$.

Lemma 2.1. *If μ lies in the interior of any tetrahedral or suboctahedral region on S^2 then ω and $\omega(\mu)$ are disjoint space curves and $Lk(\omega, \omega(\mu))$ is defined.*

Proof. Consider the tetrahedron with vertices $(0, 0, 0)$, $(1, 1, 0)$, $(1, 0, 1)$ and $(0, 1, 1)$. We consider an ϵ -pushoff, $\epsilon < 1/2$, into the interior of this tetrahedral region, T_1 , in a direction from $(0, 0, 0)$ towards the point $(\alpha + \beta, 1 - \alpha, 1 - \beta)$ so that the point (x, y, z) becomes the point $(x + (\alpha + \beta)\delta, y + (1 - \alpha)\delta, z + (1 - \beta)\delta)$, with $\alpha > 0$, $\beta > 0$, $\alpha + \beta < 1$ and

$$\delta < \frac{1}{2} \frac{1}{\sqrt{(\alpha + \beta)^2 + (1 - \alpha)^2 + (1 - \beta)^2}} \leq \frac{\sqrt{3}}{4}. \tag{2.2}$$

Let (x, y, z) be a point on a lattice polygon ω . Then either x, y and z are all integers or one of these is an integer and the other two differ from an integer by the same amount. Without loss of generality, take $x \in Z$ so that $x = a, |y - b| = |z - c| = \eta$ where $a, b, c \in Z$ and $0 \leq \eta < 1$. Now assume, to obtain a contradiction, that the polygon ω and its pushoff $\omega(\mu)$ are not disjoint. That is, at least one point on the pushoff either has all integer coordinates or has one coordinate which is an integer and the other two differ from an integer by the same amount. Each point on the pushoff has coordinates of the form $(a + (\alpha + \beta)\delta, b \pm \eta + (1 - \alpha)\delta, c \pm \eta + (1 - \beta)\delta)$. When $\eta = 0$ none of these coordinates is an integer so we can assume that $\eta > 0$ and, without loss of generality, take $\eta = (1 - \alpha)\delta$ or $\eta + (1 - \alpha)\delta = 1$, so that the y -coordinate is an integer. Then either $(\alpha + \beta)\delta = \pm\eta + (1 - \beta)\delta$ or $1 - (\alpha + \beta)\delta = \pm\eta + (1 - \beta)\delta$. This gives several cases which we handle separately:

- (1) $\eta = (1 - \alpha)\delta$ and $(\alpha + \beta)\delta = \pm\eta + (1 - \beta)\delta$ imply that either $(\alpha + \beta) = 1$ or $\beta = 0$, both of which are impossible;
- (2) $\eta = (1 - \alpha)\delta$ and $1 - (\alpha + \beta)\delta = \pm\eta + (1 - \beta)\delta$ imply that either $\delta = 1/2$ or $\alpha\delta = 1/2$, both of which are impossible;
- (3) $\eta = 1 - (1 - \alpha)\delta$ and $(\alpha + \beta)\delta = \pm\eta + (1 - \beta)\delta$ imply that either $\beta\delta = 1/2$ or $(1 - \alpha - \beta)\delta = 1/2$, both of which are impossible;
- (4) $\eta = 1 - (1 - \alpha)\delta$ and $1 - (\alpha + \beta)\delta = \pm\eta + (1 - \beta)\delta$ imply that either $\alpha\delta = 0$ or $\delta = 1$, both of which are impossible.

This gives the required contradiction and shows that every polygon is disjoint with its ϵ -pushoff into the tetrahedral region T_1 . The remaining tetrahedral regions can be handled by a symmetry argument. Consider a tetrahedral region T_2 . Suppose there exists a direction in T_2 for which the polygon and its pushoff are not disjoint. By a symmetry operation of the lattice this pair can be converted to a (different) polygon and its pushoff into T_1 . Then this pair would not be disjoint and we have a contradiction.

The pushoffs into octahedral regions can be handled similarly. Consider the suboctahedral region defined by the vertices $(0, 0, 0), (1, 0, 0), (1, 1, 0)$ and $(1, 1/2, 1/2)$. Consider a pushoff into the interior of this region towards the point $(1, (1 - \alpha + \beta)/2, (1 - \alpha - \beta)/2)$, so that the point (x, y, z) becomes $(x + \delta, y + \delta(1 - \alpha + \beta)/2, z + \delta((1 - \alpha - \beta)/2))$, with $\alpha, \beta > 0, \alpha + \beta < 1$ and

$$\delta < \frac{1}{2} \frac{\sqrt{2}}{\sqrt{3 + \alpha^2 + \beta^2 - 2\alpha}} \leq \frac{1}{2}. \quad (2.3)$$

Without loss of generality we can take $(a, b \pm \eta, c \pm \eta)$ as a typical point of the polygon ω , and the corresponding point on the pushoff is $(a + \delta, b \pm \eta + \delta(1 - \alpha + \beta)/2, c \pm \eta + \delta(1 - \alpha - \beta)/2)$. To obtain a contradiction we assume that the polygon and its pushoff have at least one common point. If $\eta = 0$ no coordinate on the pushoff is an integer so we can take $\eta > 0$. Without loss of generality, we take $\pm\eta + \delta(1 - \alpha + \beta)/2 \in Z$ so that either $\eta = \delta(1 - \alpha + \beta)/2$ or $\eta = 1 - \delta(1 - \alpha + \beta)/2$. Then, in a similar way to the arguments given above for the tetrahedral case T_1 , one can check that all the possible cases lead to a contradiction, showing that each polygon and its pushoff are disjoint. A symmetry argument extends this to pushoffs in all the remaining suboctahedral regions. \square

The subdivision of the octahedra into eight subcells is optimal since we have found examples of polygons such that the linking number of the polygon and its pushoff changes value when the direction crosses from one subcell to a neighbouring subcell.

Lemma 2.2. *The linking number $Lk(\omega, \omega(\mu))$ is independent of the direction μ for all directions in the interior of a tetrahedral region and for all directions in the interior of a suboctahedral region.*

Proof. Since any two pushoffs, $\omega(\mu_1)$ and $\omega(\mu_2)$, within the interior of a tetrahedral region are ambient isotopic to each other in the complement of the original polygonal curve ω (see Lacher and Sumners 1991), the linking numbers of each of these pushoffs with the polygon ω are equal. A similar argument applies for the interior of a suboctahedral region. \square

Lemma 2.3. *Provided that μ is in the interior of a tetrahedral or suboctahedral region on S^2 , $Lk(\omega, \omega(\mu)) = Lk(\omega, \omega(-\mu))$.*

Proof. The pair of polygons $\{\omega, \omega(\mu)\}$ is ambient isotopic to the pair of polygons $\{\omega(-\mu), \omega\}$. (If ω is translated to $\omega(-\mu)$ the same translation takes $\omega(\mu)$ to ω .) The result then follows from the symmetry of linking numbers in R^3 . \square

If we write $L_i^T, i = 1, \dots, 4$, for $Lk(\omega, \omega(\mu))$ when μ is a direction in the interior of the i th of four non-mutually antipodal tetrahedral regions, and $L_{ij}^O, i = 1, 2, 3, j = 1, \dots, 8$, for $Lk(\omega, \omega(\mu))$ when μ is a direction in the interior of the j th of eight suboctahedral regions of the i th of three non-mutually antipodal octahedral regions, then we have the following theorem.

Theorem 2.4. *The writhe of a polygon ω on the fcc lattice is given by*

$$Wr(\omega) = \frac{\alpha_0 \sum_{i=1}^4 L_i^T + (\beta_0/8) \sum_{i=1}^3 \sum_{j=1}^8 L_{ij}^O}{2\pi}. \tag{2.4}$$

Proof. This follows immediately from lemmas 2.1, 2.2 and 2.3. \square

3. Asymptotic behaviour of the writhe

In this section we examine the behaviour of the writhe of a polygon with n vertices as n goes to infinity and show that the probability that the writhe is rational goes to zero.

We first note the following lemma.

Lemma 3.1. *The angle $\theta = \sec^{-1}3$ is not a rational multiple of π .*

Proof. Suppose the contrary. Define $z = e^{i\theta} = (1 + i2\sqrt{2})/3$. z is an algebraic number satisfying the unique irreducible polynomial equation with integral coefficients, $3z^2 - 2z + 3 = 0$, so that z is not an algebraic integer. However, if θ is a rational multiple of π then z must be a root of unity satisfying an equation $z^N - 1 = 0$ for some positive integer N . This implies that z must be an algebraic integer (Niven *et al* 1991, ch 9, especially theorem 9.10) and we have the required contradiction. \square

From theorem 2.4 it is easy to show that the writhe can be written as

$$Wr(\omega) = \frac{\sec^{-1} 3}{4\pi} \left(6 \sum_{i=1}^4 L_i^T - \sum_{i=1}^3 \sum_{j=1}^8 L_{ij}^O \right) + \frac{1}{8} \left(\sum_{i=1}^3 \sum_{j=1}^8 L_{ij}^O - 4 \sum_{i=1}^4 L_i^T \right). \tag{3.1}$$

Using this, lemma 3.1 implies that $Wr(\omega)$ is rational if

$$\sum_{i=1}^3 \sum_{j=1}^8 L_{ij}^O = 6 \sum_{i=1}^4 L_i^T \tag{3.2}$$

and irrational otherwise. Clearly any planar polygon has rational writhe and we give the following example of a polygon with irrational writhe. Consider the polygon ω_0 with vertices having coordinates $(0, 0, 0)$, $(1, 1, 0)$, $(2, 2, 0)$, $(3, 2, -1)$, $(4, 1, -1)$, $(3, 1, 0)$, $(2, 0, 0)$ and $(1, 0, -1)$. A calculation using (2.4) shows that $Wr(\omega_0) = \alpha_0/2\pi \equiv \psi$. (Since the linking numbers do not satisfy (3.2) ω_0 has irrational writhe.) The polygon ω_0^* which is the reflection of ω_0 in the plane $z = 0$ clearly has writhe equal to $-\psi$. We note that the polygon with vertices $(1, 1, 0)$, $(2, 2, 0)$, $(3, 2, -1)$, $(4, 1, -1)$, $(3, 1, 0)$ and $(2, 0, 0)$ also has writhe ψ and its mirror image has writhe $-\psi$.

We next show that polygons with rational writhe become rare as n goes to infinity. To prove this we need a number of lemmas.

Lemma 3.2. *Any polygon ω containing a translate of the walk w_0 with vertices $(0, 0, 0)$, $(1, 1, 0)$, $(2, 2, 0)$, $(3, 2, -1)$, $(4, 1, -1)$, $(3, 1, 0)$, $(2, 0, 0)$ and $(1, -1, 0)$ has writhe*

$$Wr(\omega) = Wr(\omega_1) + \psi \quad (3.3)$$

where ω_1 is the corresponding polygon with the walk w_0 replaced by the walk with vertices $(0, 0, 0)$, $(1, 1, 0)$, $(2, 0, 0)$ and $(1, -1, 0)$. Similarly, if the walk w_0 is replaced by the walk w_0^* with vertices $(0, 0, 0)$, $(1, 1, 0)$, $(2, 2, 0)$, $(3, 2, 1)$, $(4, 1, 1)$, $(3, 1, 0)$, $(2, 0, 0)$ and $(1, -1, 0)$ then the writhe of ω^* containing a translate of w_0^* is given by

$$Wr(\omega^*) = Wr(\omega_1) - \psi. \quad (3.4)$$

Proof. Consider ω and its pushoff ω' through a small distance in the direction $(-1, -1, 1)$. A calculation shows that the linking number $Lk(\omega, \omega') = +1$. The walk w_0 and its pushoff have three crossings, all of which are the same sign. Take a small 3-ball containing the parts of w_0 and its pushoff forming one of these crossings, and reverse the sign of the crossing by a move lying entirely inside this 3-ball. This move decreases the linking number by 1. The resulting pair of polygons is ambient isotopic to the pair ω_1 and its pushoff ω'_1 so that

$$Lk(\omega, \omega') = Lk(\omega_1, \omega'_1) + 1. \quad (3.5)$$

Similar arguments apply to all the remaining pushoffs where the linking number is non-zero and the result (3.3) is then obtained after application of theorem 2.4. Equation (3.4) follows by an analogous argument. \square

Next we recall an important result due to Kesten (1963). Kesten's original proof is for the cubic lattice but the method can be adapted to work on other lattices, such as the fcc lattice. Let C be a rectangular box with its corners being lattice vertices and let ∂C be its boundary. Let P be a walk contained in C but with its two vertices of degree one in ∂C . Let \mathcal{C} be the ball pair (C, P) in which all vertices of C which are not vertices of P are empty. Let $c_n(\mathcal{C}, \delta)$ be the number of n -edge self-avoiding walks which contain at most $\lfloor \delta n \rfloor$ translates of \mathcal{C} . Then Kesten showed that there is a positive value of δ (which depends on C and P) such that

$$\limsup_{n \rightarrow \infty} n^{-1} \log c_n(\mathcal{C}; \delta) < \kappa. \quad (3.6)$$

That is, all except exponentially few sufficiently long walks contain a positive density of copies of \mathcal{C} . There is a corresponding result for polygons which we state as follows.

Lemma 3.3. *For a fixed rectangular box C and an undirected walk P which is contained in C and has its two vertices of degree one in the boundary of C , let \mathcal{C} be the ball pair (C, P) in which all vertices of C which are not vertices of P are empty. Let $p_n(\mathcal{C}; \delta)$ be the number of n -edge polygons on which translates of \mathcal{C} occur less than $\lfloor \delta n \rfloor$ times. Then there exists a positive value of δ , which depends on C and P , such that*

$$\limsup_{n \rightarrow \infty} n^{-1} \log p_n(\mathcal{C}; \delta) < \kappa. \quad (3.7)$$

Proof. This follows from Kesten's theorem for walks and the fact that polygons are not exponentially rare compared to walks. \square

Theorem 3.4. *The probability that an n -edge polygon on the fcc lattice has rational writhe goes to zero as n goes to infinity.*

Proof. Let C be the rectangular box with corner vertices $(0, 0, \pm 1)$, $(3, 3, \pm 1)$, $(5, 1, \pm 1)$ and $(2, -2, \pm 1)$. Let P be the undirected pattern corresponding to the subwalk w_0 and let \mathcal{C} be the ball pair (C, P) with the remainder of C empty. Let P^* be the pattern consisting of the subwalk w_0^* and let \mathcal{C}^* be the pair (C, P^*) with the remainder of C empty. Then, using Kesten's pattern theorem, for some $\epsilon > 0$ all except exponentially few n -edge polygons contain at least ϵn translates of the patterns P or P^* . These two subwalks are distributed independently (and binomially) in the translates of C . The probability of precisely k occurrences of P among the first ϵn occurrences of P or P^* is bounded above by A/\sqrt{n} for some positive constant A . Consider a randomly chosen polygon with n edges containing at least $\lfloor \epsilon n \rfloor$, the first $\lfloor \epsilon n \rfloor$ of which contain k translates of P and k^* translates of P^* . Lemma 3.3 implies that the writhe of the polygon is given by

$$W = W_0 + k\psi - k^*\psi. \quad (3.8)$$

If W_0 is rational then W is irrational unless $k = k^*$ and this occurs with probability at most A/\sqrt{n} . If W_0 is irrational then there is at most one value of k such that W is rational and again this occurs with probability at most A/\sqrt{n} . Therefore, the probability that a polygon has rational writhe goes to zero as n goes to infinity. \square

Finally, we note the following result which is analogous to the result of Janse van Rensburg *et al* (1993) for the simple cubic lattice.

Lemma 3.5. *For sufficiently long n -edge polygons on the fcc lattice the expectation of the absolute value of the writhe $\langle |Wr| \rangle$ is at least $A\sqrt{n}$ for some positive constant A .*

Proof. The proof follows from theorem 2.4, lemma 3.2 and a coin tossing argument analogous to that given in Janse van Rensburg *et al* (1993). (Each of the two patterns P and P^* (in their respective ball pairs \mathcal{C} , \mathcal{C}^*) will appear with positive density on all except exponentially few polygons. P and P^* will be binomially distributed in the translates of C . The probability that the sum of the writhe contributions from these patterns is within a constant times \sqrt{n} of the writhe of the remainder of the polygon goes to zero as n goes to infinity, and the theorem follows.) \square

4. Discussion

We have shown that the writhe of a polygon on the fcc lattice can be calculated as a suitable weighted average of its linking numbers with pushoffs in certain particular directions. This result is an important tool for the numerical calculation of the writhe of polygons on this lattice and is also useful in proofs of asymptotic results. We have shown that, as for polygons on the simple cubic lattice, the expectation of the absolute value of the writhe of polygons on the fcc lattice increases at least as fast as the square root of the number of edges in the polygon but, unlike polygons on the simple cubic lattice, most polygons on the fcc cubic lattice have irrational writhe.

One can ask similar questions about other lattices. It is clear that if the vertex figure is regular then each vertex of the lattice will be surrounded by congruent 3-cells (just as a vertex of the simple cubic lattice is surrounded by eight congruent cubes). In this case the writhe will be rational although each 3-cell might need to be divided into congruent subcells so that the linking number of the polygon with its pushoff into one such subcell is independent of the pushoff direction within the subcell. The body-centred cubic lattice is an example. Each vertex is surrounded by six octahedra. If each octahedral region is divided into eight congruent right-angled triangles then one can show that when a polygon is pushed off into the interior of any one of these regions, the polygon and its pushoff are disjoint so that the linking number is independent of the pushoff direction within each of these regions. It follows that 24 times the writhe is an integer. If the vertex figure is not regular but has two sets of congruent faces then the writhe would still be rational if the ratio of the solid angles subtended at the centre by the two types of faces were rational. Otherwise some polygons will have irrational writhe and it might be possible to use a pattern theorem argument to show that polygons with rational writhe are rare. For instance, the *hexagonal close packing* of spheres is not a lattice but can be treated using these arguments. The vertex figure has eight triangles and six squares, as does the cuboctahedron, but the relative arrangement of the two types of faces is different. Each vertex is surrounded by eight tetrahedra and six octahedra, so a theorem similar to theorem 2.4 will apply with different pushoff directions. Presumably a pattern theorem could be proved for this system so that we would expect similar results to theorem 3.4 and lemma 3.5, although we have not checked the details. Other lattices (and graphs with some symmetry which are not lattices) could be handled by similar arguments.

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