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Ergodicity of the BFACF algorithm in three dimensions

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Abstract. Let ω be a walk in Z^3. Let the endpoints of ω be fixed at x and y in Z^3. Suppose that $d(x,y) = \max_i\{|X_i(x) - X_i(y)|\}$ where $X_i(x)$ is the ith coordinate of the vertex $x \in Z^3$. Then the BFACF algorithm is ergodic for walks joining x and y, provided that $d(x,y) > 1$.

1. Introduction

The simulation of walks remains an active and interesting activity in Monte Carlo simulations of critical behaviour in statistical models in mathematics, physics and chemistry. Traditionally, walks were studied as a model for polymers in dilute solution (Kuhn and Kuhn 1943, Orr 1947, Montroll 1950). This relation to polymers made walks a much studied subject (Domb 1969, Daoud *et al* 1975, McKenzie 1976, Whittington 1982). Symanzik (1969) discovered a connection between a zero component $g|\phi^2|^2$ field theory ($N \to 0$, where N is the number of components in a real field ϕ) and walks. This connection made walks interesting for the field theorist as well (Emery 1975, Fröhlich 1982, Aragao de Carvalho *et al* 1983), especially because it was hoped that it might provide a proof that the continuum limit of a lattice $g|\phi^2|^2$ theory is trivial.

These facts led to the invention of many algorithms which were used to simulate walks. In the context of a field theory Berg and Foester (1981) invented an algorithm which simulates walks with variable length and fixed endpoints in the hypercubic lattice. They applied this algorithm to 'bosonic' (Brownian) and 'fermionic' walks (walks without 'spikes'). This algorithm was subsequently used to simulate self-avoiding walks in four-dimensions (Aragao de Carvalho *et al* 1983, Aragao de Carvalho and Caracciolo 1983) in an effort to demonstrate that the continuum limit of a lattice $g|\phi^2|^2$ theory is trivial.

In view of all these activities, it remained a remarkable fact that Berg and Foester's algorithm (the BFACF algorithm) remained ill understood, despite numerous applications. The first breakthrough occurred in 1986, when Neal Madras (1986) proved that the algorithm is ergodic in the square lattice (two dimensions). It was later noted that if the endpoints of the simulated walk do not differ by at least 2 in any coordinate in three dimensions, then the algorithm is not ergodic (Madras and Sokal 1987).

A second step in the understanding of the algorithm came with a proof that if the algorithm is applied to *unrooted* lattice polygons in the cubic lattice (three dimensions), then the ergodicity classes are the knot types of the polygons (a polygon

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is a walk which begins and ends at the same lattice site) (Janse van Rensburg and Whittington 1991, hereafter referred to as I). This proof was subsequently used to prove that the algorithm is indeed ergodic in four and more dimensions, if applied to unrooted lattice polygons (Evertz 1991).

In this paper we prove that the BFACF algorithm is ergodic if applied to fixed endpoint walks in three dimensions, provided that the endpoints differ by at least 2 in any one coordinate. We organize the proof as follows: In section 2 we define the algorithm more closely and we consider the projection of a walk and the connection it has to knot projections. In section 3 we prove ergodicity, and we conclude the paper in section 4.

2. The BFACF algorithm and walks

2.1. Definitions

A *self-avoiding walk*, or *walk*, ω, in $\mathcal{Z}^d$, is a sequence of distinct lattice sites ω_0, ω_1, ..., ω_n, and associated edges (ω_i, ω_{i+1}), such that ω_i and ω_{i+1} are nearest neighbours in $\mathcal{Z}^d$. We say that the vertices x and y in $\mathcal{Z}^d$ are the *endpoints* of the walk ω if $x = \omega_0$ and $y = \omega_n$ or $x = \omega_n$ and $y = \omega_0$. Let $\{e_i\}_{i=1}^d$ be the set of d orthogonal unit vectors in $\mathcal{Z}^d$. Let $X_i(x)$ be the ith component of the vertex $x \in \mathcal{Z}^d$. Then $X_j(e_i) = \delta_{ij}$, where δ_{ij} is the Kronecker delta function. Define the metric $\mathrm{d}(x, y)$, where x and y are vertices in $\mathcal{R}^d$, by $\mathrm{d}(x, y) = \max_i\{|X_i(x) - X_i(y)|\}$.

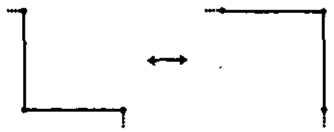
The BFACF algorithm is a local stochastic process which is defined to operate on any sequence of edges in $\mathcal{Z}^d$ (Berg and Foester 1981). It was first applied to the self-avoiding walk by Aragao de Carvalho *et al* (1983) and Aragao de Carvalho and Caracciolo (1983). Let ω be a walk with endpoints x and y. Then the BFACF algorithm operates in the following way: Pick an edge (ω_i, ω_{i+1}) of the current walk with uniform probability. Pick a unit vector e_j which is perpendicular to the vector $(\omega_{i+1} - \omega_i)$. Move the chosen edge one lattice space in the direction e_j, while inserting two new edges at its endpoints to keep the polygon intact. Finally, erase any double edges (spikes) which may result in this process. This recipe results in one of the two possible elementary transitions in figure 1. The total number of edges in the walk can change by 0 or by ± 2. Let the new conformation be ν. If ν is a walk, accept it in the ensemble with probability $p(\omega \to \nu) = Z(\beta)$, and otherwise, reject the transition and read the old conformation again. Here, $Z(\beta) = \beta^2$ if the length of the walk ω increases by 2, where β is the only free parameter in the algorithm, and $Z(\beta) = 1$ otherwise.

This simple Metropolis implementation (Metropolis *et al* 1953) of the algorithm realizes a Markov chain with state space the set of all walks with endpoints x and y. Neal Madras proved that this chain is irreducible (ergodic) in two dimensions (Madras 1986). If we apply this algorithm to unrooted polygons instead, then the chain is reducible in three dimensions (Madras and Sokal 1987). The ergodicity classes are the knot types of the polygons (Janse van Rensburg and Whittington 1991).

2.2. Projections and walks

Let q be an open piecewise linear curve (with two fixed endpoints) in $\mathcal{R}^3$, where $\mathcal{R}$ is the set of all real numbers. Let Pq be the projection of this curve in the subspace

I:



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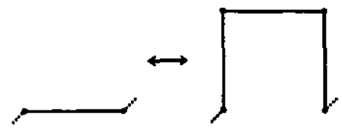

Figure 1. The elementary BFACF moves.

$\mathcal{R}^2 \subset \mathcal{R}^3$. We can borrow ideas from knot theory to characterize the curve in the following way: We call the projection Pq *regular* if all multiple points are double points and if no vertex in q, including the endpoints, are projected into a double point. A vertex in q is defined as a discontinuity in the tangent to the curve. If, in addition, it is indicated in the projection which segment in the double points are the overpassing strand, then a typical regular projection is illustrated in figure 2. This curve has two endpoints, and can therefore not be a knot. We can see this easily; consider the *local* operation on regular projections illustrated in figure 3(a). If we apply one step of this operation to a projection, then we reduce the number of double points by one. If we repeat the operation, then we can remove all double points from the projection, and the projected curve is therefore self-avoiding.

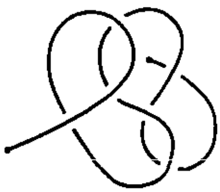

Figure 2. A projected curve. This projection is regular.

We can now apply these ideas to walks in $\mathcal{Z}^3$. Let $\mathcal{P}_a : \mathcal{Z}^d \to \mathcal{Z}^2$, where $d \geqslant 2$, such that $\mathcal{P}_a(x) = \mathcal{P}_a x$ where $\mathcal{P}_a x = (X_1(x), X_2(x), a, a, \ldots, a)$. That is, $\mathcal{P}_a(x)$ is a projection of $x \in \mathcal{Z}^d$ onto its first two coordinates. We can consider the action of $\mathcal{P}_a$ on a walk $\omega \subset \mathcal{Z}^d$. In general $\mathcal{P}_a\omega \in \mathcal{Z}^2 \subset \mathcal{R}^2$, that is, we can think of the walk as a continuous curve projected into the space $\mathcal{R}^2$. Some edges in ω are projected to points in $\mathcal{Z}^2$ (if they are not parallel to either e_1 or e_2). Define the vertices in $\mathcal{P}_a\omega$ to be those points *in the projection* (as opposed to the definition for vertices in the piecewise linear case) where the tangent to the projected curve is discontinuous. Then we can declare the projection regular (in the knot theoretic sense) if all multiple points in the projection are double points, and if no vertex (in $\mathcal{P}_a\omega$) is projected onto a double point. (This definition of vertices is equivalent to noting that vertices are points in the projection where two nearest-neighbour edges make a $90°$ angle, or are one of the endpoints in the projection.)

To proceed, a connection between our projected walk and projected knots must be made. The walk ω can be made into a circle embedded in $\mathcal{R}^3$ if we connect its endpoints by a continuous curve μ in $\mathcal{R}^3$. It is easy to construct this curve such that it *overpasses* any segment of $\mathcal{P}_a\omega$ in its projection. In addition, if $\mathcal{P}_a\omega$ is regular, then it is a simple matter to arrange μ such that the projection $\mathcal{P}_a(\omega \cup \mu)$ is regular. Since $\omega \cup \mu$ is an embedded circle, it is a *knot* (for a review, see the book by Burde and Zieschang (1985)). If the projection $\mathcal{P}_a(\omega \cup \mu)$ is the projection with ascending overpasses, then $\omega \cup \mu$ is the unknot, and there exists consequently a finite sequence of Reidemeister moves (figures 3(*b*)–(*d*)) which will remove all the double points in the projection (Reidemeister 1932) (if we view the knot as a circle in $\mathcal{R}^3$, the lattice is now ignored). The task in the next section is to show that we can perform these moves *in the lattice*, which will prove ergodicity.

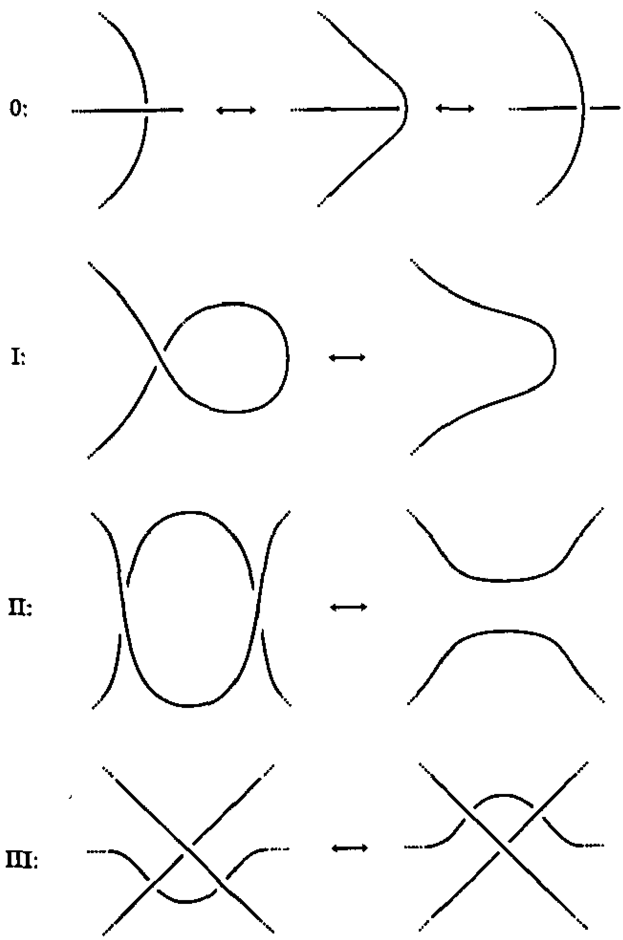

Figure 3. Reidemeister moves.

3. Proof of ergodicity in three dimensions

Let ω be a walk in $\mathcal{Z}^3$, with endpoints x and y. Then we shall need the following definitions:

Definition 3.1. A *segment* $[\omega_i, \omega_j]$ of a walk ω is the set of vertices $\{\omega_i, \omega_{i+1}, \ldots, \omega_j\}$ if $i \leqslant j$, or the set $\{\omega_j, \omega_{j+1}, \ldots, \omega_i\}$, if $j < i$.

Definition 3.2. A segment $[\omega_i, \omega_j]$ is a *side* if the union of all the edges associated with the vertices is a line piece, and if the vertices ω_i and ω_j are either endpoints of ω, or are incident on two edges which make 90° angles in the walk.

A walk ω has at most n sides (if it has n edges) and at least 1 side. Let ω be a walk in $\mathcal{Z}^3$. Consider $\mathcal{P}_a\omega$. If we discard all edges which project to points in $\mathcal{Z}^2$, then $\mathcal{P}_a\omega$ could be a walk in $\mathcal{Z}^2$. If it is a walk, then definitions 3.1 and 3.2 generalize naturally to projected walks. Moreover, if $\mathcal{P}_a\omega$ is a regular projection, then we can easily extend definitions 3.1 and 3.2 to be applicable; the integrity of the walk is preserved by indicating overpasses, but we lose track of the number of edges in the e_3 direction in the walk.

Proposition 3.3. (Janse van Rensburg and Whittington 1991) Let ω be a walk in $\mathcal{Z}^3$ and let $\nu = \mathcal{P}_a\omega$ be its projection. Suppose that ν is a walk in $\mathcal{Z}^2$ with endpoints u and v. Then there exists a sequence of BFACF moves on ω which will change ν into any other walk in $\mathcal{Z}^2$ with endpoints u and v.

This proposition is crucial to the proof of ergodicity, since it allows us to manipulate segments of the projection by using BFACF moves.

Definition 3.4. A *box* $\mathcal{B}(x,y) \subset \mathcal{Z}^d$, where x and y are vertices in $\mathcal{Z}^d$, is the subspace $\mathcal{B}(x,y) = \{z \in \mathcal{Z}^d; |X_i((x+y)/2) - X_i(z)| \leqslant |X_i((x-y)/2)| \forall 0 \leqslant i \leqslant d\}$.

Consider a walk ω with endpoints x and y in $\mathcal{Z}^d$. Let $\mathcal{P}_a(x) = u$ and $\mathcal{P}_a(y) = v$, and let $\nu = \mathcal{P}_a\omega$. Then $\mathcal{B}(u,v) \subset \mathcal{Z}^2$ is the box defined by the vertices u and v. Such a box is indicated in figure 4. If $u = v$, then there is only one point in the box. Since $\mathrm{d}(x,y) > 0$ (ω is a walk), we can always rotate or reflect axes to find a projection ν with $\mathrm{d}(u,v) > 0$. In fact, there exists a rotation or reflection of the axes such that $|X_1(u) - X_1(v)| = \mathrm{d}(u,v) = \mathrm{d}(x,y)$. In the rest of the paper, we can always work on this projection of the walk, without any loss of generality.

Definition 3.5. An open *n-ball* V_r with radius r and centre c is defined by $V_r = \{z \in \mathcal{R}^d | d(z,c) < r\}$.

3.1. Regular projections and walks

In this section we prove that given any walk in $\mathcal{Z}^3$, we can find a sequence of BFACF moves to turn its projection into a regular projection, in the sense defined in section 2.2. We shall need the following notation: Let $\mathcal{T}_i(c) \subset \mathcal{R}^3$ be a plane containing the point $c \in \mathcal{R}^3$ and normal to the vector e_i. In the rest of this section

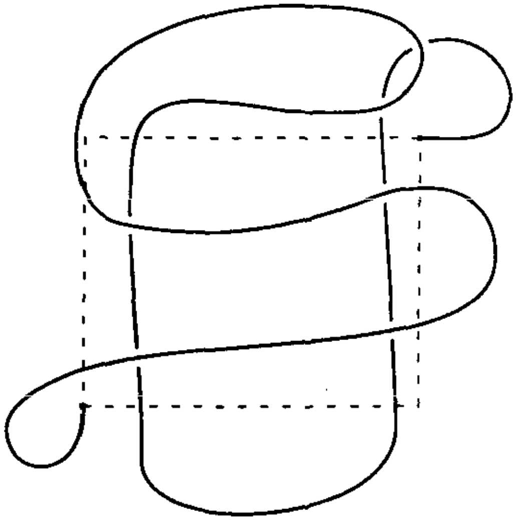

Figure 4. A projected walk.

we use our notation of a walk ω with endpoints x and y, and projection $\nu = \mathcal{P}_a\omega$ with endpoints $u = \mathcal{P}_a x$ and $v = \mathcal{P}_a y$.

To proceed, we need the *shift construction* defined in *I*. For the sake of completeness, we redefine it here. Let $[\omega_i, \omega_j]_s$ be a side, and without loss of generality, suppose that $i < j$. Suppose that e_* is a unit vector, of the form $\pm e_k$, perpendicular to any edge in $[\omega_i, \omega_j]_s$. This side can now be transform into a segment connecting ω_i and ω_j and with vertices $\{\omega_i, \omega_i + e_*, \omega_{i+1} + e_*, \ldots, \omega_j + e_*, \omega_j\}$ using only BFACF moves and without ever using a vertex outside the set of old and new vertices in the side and the segment. We do this as follows: Consider the edge $[e_i, e_{i+1}]$, and operate on it by a BFACF move, whichever is necessary, to shift it to $[\omega_i + e_*, \omega_{i+1} + e_*]$. In succession, perform the same construction on the edges $[\omega_{i+k}, \omega_{i+k+1}]$, for $k = 1, 2, \ldots$, until $i + k = j - 1$. Then $[\omega_i, \omega_j]$ has been 'moved' a unit distance in the e_* direction. Symbolically, we can represent this operation by $\mathcal{M}_{ij}(e_*)$. Then

$$\mathcal{M}_{ij}(e_*)[\omega_i, \omega_j]_s = [\omega_i + e_*, \omega_j + e_*]_s. \tag{3.1}$$

After this operation, we simple relabel the vertices. As in I, we note that we can use this operation in an obvious manner to split any side into smaller segments. We shall now use this construction to prove that we can make the projection ν regular, in the sense explained in section 2.2.

Lemma 3.6. Let ω be any walk with endpoints x and y, and let $\nu = \mathcal{P}_a\omega$. Then we can apply BFACF moves to remove all sides from the planes $\mathcal{T}_i(x)$ and $\mathcal{T}_i(y)$, where $i = 1, 2$ or 3; except for two sides which are incident on the endpoints x and y. One of these two sides will be in the intersection of the two planes $\mathcal{T}_2(x)$ and $\mathcal{T}_3(x)$ and the other will be in the intersection $\mathcal{T}_2(y)$ and $\mathcal{T}_3(y)$.

Proof. Without loss of generality, suppose that $X_i(x) \geqslant X_i(y)$ for each i, and rotate or reflect axes so that $X_1(x) > X_1(y)$. Let $z = (\max_i\{X_1(\omega_i)\}, 0, 0)$.

Consider the intersection $\mathcal{T}_1(z) \cap \omega$. This is a set of sides in ω (some of which projects to points in ν). Label any one of these sides by the integer 1, say $[\omega_i, \omega_j]_s$, and operate on it by $\mathcal{M}_{ij}(e_1)$, its new position is then $[\omega_i + e_1, \omega_j + e_1]_s$. Label a second side now by 2. Operate first on the side labelled 1 by $\mathcal{M}_*(e_1)$, and then on the side 2 with the same construction. Repeat this process until the intersection $\mathcal{T}_1(z) \cap \omega$ contains only one last side, and suppose that it was labelled by an m. Consider the intersection $\mathcal{T}_1(z - e_1) \cap \omega$ then, and perform the same construction as before, starting the labelling now at $m + 1$, and always moving the sides one step at a time, starting at the side labelled 1 with each step in the construction. Finally, we will consider the intersection $\mathcal{T}_1(\zeta) \cap \omega$, where $X_1(\zeta) < X_1(x)$. At this stage, the plane $\mathcal{T}_1(x)$ contains exactly one side. We repeat the construction then once again for this side, which is then moved one step in the e_1 direction. This will remove the last side from $\mathcal{T}_1(x)$. Rotate axes now by $180°$, and repeat the process, this removes all the sides from the plane $\mathcal{T}_1(y)$ by moving them in the $-e_1$ direction. At this stage in the construction, we note that the edges incident on either x or y must be normal to the planes $\mathcal{T}_1(x)$ or $\mathcal{T}_1(y)$ respectively, otherwise they would have been edges in sides which will be moved. Mark these sides incident on x and y for future reference, and note that they are in the intersections $\mathcal{T}_2(x) \cap \mathcal{T}_3(x)$ and $\mathcal{T}_2(y) \cap \mathcal{T}_3(y)$ respectively.

We now repeat this operation, where we probe the walk with $\mathcal{T}_2(*)$ and $\mathcal{T}_3(*)$ instead. At the last application we leave the marked sides incident on x and y alone, but all other sides have now been removed from $\mathcal{T}_i(x)$ and $\mathcal{T}_i(y)$, where $i = 1, 2$ or 3. Note that the segments of the walk inside the box $\mathcal{B}(x, y)$ were left unchanged but the boundary of $\mathcal{B}(x, y)$ contains now only the endpoints of the walk. This completes the proof. □

Lemma 3.7. Let ω be a walk, and suppose that we have applied the construction in lemma 3.6 to ω. Suppose that ω has endpoints x and y, and let $u = \mathcal{P}_a x$, $v = \mathcal{P}_a y$ and suppose that $\nu = \mathcal{P}_a \omega$. Then we can remove all segments of ω which projects into the projected box $\mathcal{B}(u, v)$ by applying the shift operator. In fact, we find that $\mathcal{B}(x, y) \cap \omega = \{x, y\}$ and $\mathcal{B}(u, v) \cap \nu = \{u, v\}$.

Proof. Let the same conditions as in lemma 3.6 be valid. Probe the walk with the plane $\mathcal{T}_1(x - e_1)$. If any sides are in this plane, then we move them by $\mathcal{M}_*(e_1)$ twice to the plane $\mathcal{T}_1(x + e_1)$, in the same manner we did in lemma 3.6. There is no possibility that the moving side will collide with an endpoint; if it does, then the moving side is in the plane $\mathcal{T}_2(x)$ or $\mathcal{T}_3(x)$, which is not true. Repeat this process with all the other sides in the probe $\mathcal{T}_1(x - e_1)$. Once all the sides have been moved, then we look at the plane $\mathcal{T}_1(x - 2e_1)$, and move the sides there out of $\mathcal{B}(u, v)$, and so on. Finally, we will have swept the box $\mathcal{B}(u, v)$, and the only segments which projects into the box are sides in the e_1 direction with endpoints which projects outside the box (by the construction). Rotate axes now and perform the same operation where we probe with $\mathcal{T}_2(*)$ instead. The same conditions are valid here. Finally, the box $\mathcal{B}(u, v)$ have been swept clean. □

If we apply lemmas 3.6 and 3.7 to any given walk, then we note that the result will be a walk in a conformation which has no segments which project to the box $\mathcal{B}(u, v)$ in the projection ν. The next lemma is useful in making a projection regular (as we defined it in section 2.2.)

Lemma 3.8. (Subdivision) Let ω be a walk with endpoints x and y, and suppose that $\mathcal{B}(x,y) \cap \omega = \{x,y\}$. Let $\mathcal{T}_i(z + \frac{1}{2}e_i)$ be a plane where $z \in \mathcal{Z}^3$. Then we can perform a sequence of BFACF moves which will add one edge to each of the sides in ω intersected by the plane. (In other words, we can subdivide each of the edges intersected by the plane into two edges.)

Proof. The construction is similar to that in lemma 3.6. Without loss of generality, let the plane be $\mathcal{T}_1(z + \frac{1}{2}e_1)$. Furthermore, suppose that $X_1(x) \geqslant X_1(y)$. We must consider three possible cases: (i) $(z + \frac{1}{2}e_1) > X_1(x)$, (ii) $X_1(x) > (z + \frac{1}{2}e_1) > X_1(y)$, and (iii) $X_1(y) > (z + \frac{1}{2}e_1)$. The construction is simple in case (i): Probe the walk with the plane $\mathcal{T}_1(p)$, starting at $p = \max_i\{X_1(\omega_i)\}$, as we did in lemma 3.6. Each side encountered in moved one unit step in the e_1 direction. Finally, we will move the sides in the plane $\mathcal{T}_1(z + e_1)$ to the plane $\mathcal{T}_1(z + 2e_1)$. The effect of this is that the sides which penetrate the plane $\mathcal{T}_1(z + \frac{1}{2}e_1)$ are now longer by one edge each. We now first deal with case (3): The construction is identical to that of case (1), we simply rotate axes by $180°$. In the case of (ii) the construction is again similar to that of case (i), the only difference is that the subdivision does not happen inside the box $\mathcal{B}(x,y)$. We note that a new edge is introduced on x in the e_1 direction. This leaves the coordinates of x unchanged. Since $\mathcal{B}(x,y) \cap \omega = \{x,y\}$, there is no possibility of a side colliding with an endpoint. This completes the proof. □

Lemma 3.8 enables us to take a projection and to subdivide the edges (which penetrate a plane $\mathcal{T}_i(*)$) into two edges each, in fact, we are inserting a new two-dimensional layer in our lattice which 'stretch' the walk. The only unaffected region is the box $\mathcal{B}(x,y)$, but since it is empty, it is of no concern here. The subdivision allows an easy construction which will make the projection ν regular. The following result is a direct consequence of the subdivision lemma:

Proposition 3.9. Let ω be a walk with endpoints x and y (which project to the points u and v respectively), and let the projection of ω be ν. Suppose that $\mathcal{B}(u,v) \cap \nu = \{u,v\}$. Let A be an open two-ball in the projection, such that $\mathcal{B}(u,v) \cap A = \emptyset$ and such that $\nu \cap A = \emptyset$. Suppose that the centre of A has half-integer coordinates. Then we can make A arbitrary large, using only BFACF moves.

Proof. This is a direct result of subdivision. Consider the intersection of planes $\mathcal{T}_i(z + \frac{1}{2}e_i)$ and A (where $i = 1$ or $i = 2$), and subdivide the edges which penetrate the plane. (Here we choose z such that the intersection between the plane and A is not empty, and $z \in \mathcal{Z}^3$.) □

Proposition 3.10. Let ω be a walk with endpoints x and y. Let V be an open, connected three-ball in $\mathcal{Z}^3$, such that $\mathcal{B}(x,y) \cap V = \emptyset$ and $\omega \cap V = \emptyset$. Suppose that the centre of V has half-integer coordinates. Then we can make V arbitrary large, using only BFACF moves.

Proof. The proof is a direct consequence of subdivision. □

Proposition 3.11. Let ω be a walk with endpoints x and y (which project to the points u and v respectively), and let ν be the projection of the walk. Then there is a sequence of BFACF moves which will transform ω into a conformation with a regular projection. In addition, $\mathcal{B}(x,y) \cap \omega = \{x,y\}$, and $\mathcal{B}(u,v) \cap \nu = \{u,v\}$.

Proof. The proof is a direct consequence of lemmas 3.6 and 3.7, as well as propositions 3.9 and 3.10. We use the lemmas to empty the boxes of all segments of the walk, and then we turn our attention to unwanted parts in the projection. We can easily rid the projection of these by first applying propositions 3.9 and 3.10, and then we use proposition 3.3 to rearrange the segments in an acceptable fashion, as we did in *I*. □

3.2. Walks and ascending projections

In this section we study the regular projection of a walk. We use the ideas about knot projections and walk projections developed in section 2.2 to prove that we can put our walk in a conformation which has an ascending projection.

In the last section we proved that BFACF moves are sufficient to transform any given walk ω with endpoints x and y, projection $\nu = \mathcal{P}_a\omega$ and projected endpoints u and v into a conformation with a regular projection such that $\mathcal{B}(x,y) \cap \omega = \{x, y\}$ and $\mathcal{B}(u,v) \cap \nu = \{u, v\}$. Since the box $\mathcal{B}(x,y)$ contains at most the endpoints of the walk, we can connect x and y with a line piece μ. The union $\omega \cup \mu$ is now a piecewise linear embedding of the circle S^1 in $\mathcal{R}^3$, and therefore a knot.

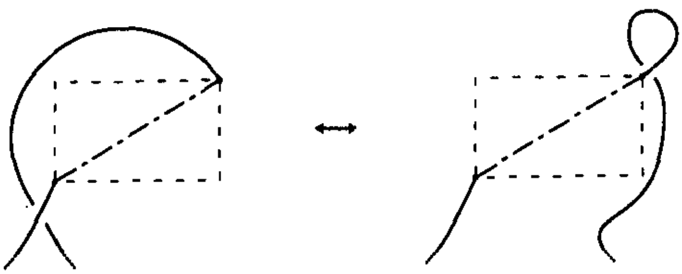

Figure 5. Reidemeister I over the fixed endpoints of the walk.

Note that every double point in ν (which is now redefined as $\mathcal{P}_a(\omega \cap \mu)$) are outside the box $\mathcal{B}(u,v)$. We immediately have the following proposition, which was proven in I:

Proposition 3.12. Let ω be a walk with a regular projection ν, and suppose that $\mathcal{B}(u,v) \cap \nu = \{u, v\}$, where u and v are the projected endpoints of the walk. Then we can perform any Reidemeister move in ν.

Proof. All that we must show is that we can perform these moves if the segments involved are connected to the endpoints of the walk. The easiest case is Reidemeister II (figure 3(*c*)). Two segments are involved, and suppose that one segment contains at least one of the endpoints of the walk. Then we move the segment which does not contain the endpoints and μ, using, as in I, propositions 3.9 and 3.10 to grow space for the move (by subdivision) and proposition 3.3 to move the segment to its new position. The next move we consider is Reidemeister III. Here we move only one segment of the walk (say the segment containing only underpasses), so if it does not contain the endpoints, then we are done, else we move the segment with overpasses, which results in the same configuration (see figure 3(d)). Finally we deal with Reidemeister I (figure 3(b)). If the segment between the overpass and the underpass does not contain one of the endpoints, then we are done, otherwise we perform the move in figure 5 first, this removes the endpoints from the segment we want to readjust. We can always perform the operation in figure 5 (by subdivision and propositions 3.9 and 3.10.) □

There is now one more move that we must consider, the move in figure 3(a). This is the move that we shall use to turn an overpass into an underpass while we manupilate the projection of the walk. We can think of this move as an addition to the Reidemeister moves; we refer to it as Reidemeister 0.

Proposition 3.13. Let ω be a walk with a regular projection ν, and suppose that ω has endpoints x and y. If $\mathrm{d}(x,y) > 1$, and if $\mathcal{B}(x,y)\cap\omega = \{x,y\}$ and $\mathcal{B}(u,v)\cap\nu = \{u,v\}$ (where u and v are the projected images of x and y), then we can perform Reidemeister 0 on the projection of ω.

Proof. Without loss of generality, suppose that $|X_1(x) - X_1(y)| > 1$. Then, if u and v are the projected endpoints, $\mathrm{d}(u,v) > 1$. Without loss of generality, suppose that we must move a segment which overpasses at the double point. In ν, there is a segment of two edges which overpasses the double point (since the projection is regular). Fix this segment at its endpoints; we shall now perform BFACF moves on the segment until it is projected in ν *inside* the box $\mathcal{B}(u,v)$. Determine its new projection and apply propositions 3.9 and 3.10 to sweep all other segment from the projected area to prevent the occurrence of unwanted Reidemeister moves or collisions. Then by proposition 3.3 we can find a conformation of the segment which projects inside $\mathcal{B}(u,v)$. We can now perform BFACF moves in the e_3 direction to push the segment through the box $\mathcal{B}(x,y)$ (we can always do this, since $\mathrm{d}(u,v) > 1$). Since the moves are symmetric, we apply proposition 3.3 again to take the segment back to its original projected position in ν. Then we have changed an overpass into an underpass. Similarly, we can change an underpass into an overpass. □

We can now prove:

Theorem 3.14. Let ω be a walk with endpoints x and y and suppose that $\mathrm{d}(x,y) > 1$. If μ is a line piece which connects the points x and y, then there exists a sequence of BFACF moves which will change the conformation of ω such that the projection $\mathcal{P}_a(\omega\cup\mu)$ is regular and ascending (that is $\omega\cup\mu$ is the unknot).

Proof. The theorem is a direct consequence of propositions 3.11, 3.12 and 3.13, as well as Reidemeister's theorem (Reidemeister 1932). We can always do this by first using a set of moves in the (continuous) plane $\mathcal{R}^2$, which we then approximate arbitrarily close using subdivision in our projected walk. If there is a collision, then we simply subdivide (using propositions 3.9 and 3.10) to avoid it. (In effect, we put our walk on a very fine grid, which looks much like the continuous plane.) □

It is of great importance to note the power of subdivision in all these propositions. In essence, it allows us to approximate an embedding in $\mathcal{R}^3$ arbitrarily close, so that we can perform essentially continuous operations on the polygon (that is we can change the scale such that any move can be made as small as desired, which avoids collisions between different segments).

3.3. Ergodicity

The proof of ergodicity is now an easy consequence of proposition 3.12 and theorem 3.14. Let ω be any given walk with endpoints x and y such that $\mathrm{d}(x, y) > 1$. If μ is a line piece connecting the vertices x and y in $\mathcal{R}^3$, then there is a sequence of BFACF moves which will transform ω such that the projection of $\omega \cup \mu$ is regular and ascending. The following proposition completes the proof:

Proposition 3.15. Let ω be a walk in $\mathcal{Z}^d$ with endpoints x and y, and suppose that μ is a line piece which connects the points x and y in $\mathcal{R}^3$. If in addition there exists a rotation or reflection of the axes such that $\mathcal{P}_a(\omega \cup \mu)$ is a regular and ascending projection, then there exist a sequence of BFACF moves which will remove every double point from the projection.

Proof. This proposition is a direct consequence of Reidemeister's theorem (Reidemeister 1932) and proposition 3.12. □

Therefore, we have the following corollary:

Corollary 3.16. Let ω be a walk with endpoints x and y in $\mathcal{Z}^3$ and suppose that $\mathrm{d}(x, y) = 1$. If x and y are connected by a line piece μ in $\mathcal{R}^3$, and if $\omega \cup \mu$ is the unknot, then the BFACF algorithm is ergodic in the set of all unknots.

In addition, we finally have our main theorem:

Theorem 3.17. The BFACF algorithm is ergodic if we apply it to fixed endpoint walks in three dimensions, provided that the endpoints of the walk differ by at least two units in one coordinate.

Proof. The proof is now easy: First apply theorem 3.14 and proposition 3.15 to the walk, then by proposition 3.3 we can put it in a conformation with a 'standard' self-avoiding projection. The last step is to perform BFACF moves in the e_3 direction, then we can adjust the third component of the coordinates to some prefered value. □

4. Conclusions

The proof provided in section 3 works only in three dimensions. In fact, we do not expect it to generalize to higher dimensions, since it involves the projections of walks in *two* dimensions. It seems likely that the algorithm is ergodic in higher dimensions, independent of the value of $\mathrm{d}(x, y)$, where x and y are the endpoints of the walk. Some progress towards a proof of ergodicity in higher dimensions for polygons and walks has recently been made (Evertz 1991).

In three dimensions a more complicated picture arises. The algorithm is ergodic if $\mathrm{d}(x, y) > 1$, and the ergodicity classes are knot types of the polygons if we apply the algorithm to unrooted polygons (Janse van Rensburg and Whittington 1991). If $\mathrm{d}(x, y) = 1$ and we connect the vertices x and y by a line piece μ, then it seems likely that the ergodicity classes will be defined by the knot types of the embedded circles formed by the union of the walk and the line piece μ, but a proof is elusive.

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