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Entanglement Complexity of Lattice Ribbons

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We consider a discrete ribbon model for double-stranded polymers where the ribbon is constrained to lie in a three-dimensional lattice. The ribbon can be open or closed, and closed ribbons can be orientable or nonorientable. We prove some results about the asymptotic behavior of the numbers of ribbons with n plaquettes, and a theorem about the frequency of occurence of certain patterns in these ribbons. We use this to derive results about the frequency of knots in closed ribbons, the linking of the boundary curves of orientable closed ribbons, and the twist and writhe of ribbons. We show that the centerline and boundary of a closed ribbon are both almost surely knotted in the infinite-n limit. For an orientable ribbon, the expectation of the absolute value of the linking number of the two boundary curves increases at least as fast as $\sqrt{n}$, and similar results hold for the twist and writhe.

KEY WORDS: Ribbon; topological entanglement; knot; link; satellite knot; writhe; double-stranded polymer.

1. INTRODUCTION

Self-avoiding walks have been studied as a model of the conformational properties of linear polymers for many years.[1] Although this model captures faithfully the principal features of connectivity and excluded volume, it cannot be used to examine questions about double-stranded polymers (such as duplex DNA[2] and ι-carageenan[3,4] when one is

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interested in the twisting of one strand about the other. Bauer *et al.*[2] discussed a continuum ribbon model[5] of polymers such as DNA in which each strand of the molecule is a boundary of the ribbon. For this model one can ask about the twist of one boundary curve about the other, or (for closed ribbons) about the linking of the two boundary curves. Recently we introduced a lattice version of this model[6] in which the ribbon is a sequence of plaquettes (the interior and boundary of a unit square) in the cubic lattice Z^3 such that adjacent plaquettes meet at a common edge, and the set of plaquettes obeys some technical geometrical conditions ensuring that the object is a manifold. The ribbon can be open (homeomorphic to a disk) or closed. If it is closed, it can be orientable (homeomorphic to a cylinder, having two boundary curves) or nonorientable (homeomorphic to a Möbius band, having one boundary curve). In the DNA literature[2,7] the interest centers on orientable closed ribbons, but we shall treat all three types in this paper.

Lattice models such as the one discussed here are designed to investigate *universal* properties. That is, they should give a good description of properties which will be the same for all systems which are double-stranded polymers dissolved in good solvents. They are not designed to give a faithful description of small-scale properties which depend on the details of the chemical structure of the polymeric system.

This lattice model can be studied using Monte Carlo methods[6,8] and some asymptotic results can be obtained rigorously. In ref. 6 and 9 we gave sketch proofs of some results about the asymptotic behavior of the numbers of open and closed ribbons, and about the entanglement complexity of the ribbon. These results were confirmed numerically using Monte Carlo methods[8] and the knotting and linking probabilities, as well as the writhe of the boundaries, were estimated.

In this paper we prove several results about the asymptotic behavior of the numbers of ribbons and prove a pattern theorem for ribbons. The pattern theorem establishes that almost all sufficiently long ribbons contain translates of a given subribbon and this allows us to derive rigorous bounds on the knotting and linking probabilities, as well as on the twist and writhe of ribbons. The paper is arranged as follows. In Section 2 we give a definition of a lattice ribbon and prove some theorems about the exponential growth of the numbers of ribbons. In Section 3 we prove the pattern theorem and in Section 4 we use this to prove that the knot probability of each boundary curve of an orientable closed ribbon goes to unity exponentially rapidly as the number of plaquettes goes to infinity. The behavior of the knot probability for the boundary curve of a nonorientable ribbon is more complex, and we also consider this in Section 4. In Section 5 we consider linking of the two boundary curves of an orientable closed ribbon and in Section 6 we discuss geometrical properties such as the twist and writhe. Finally, in Section 7 we discuss some open questions and summarize our results.

2. DEFINITIONS AND ASYMPTOTIC BEHAVIOR

We consider the simple cubic lattice Z^3 in which the vertices are integer points in R^3 and the edges join pairs of vertices which are unit distance apart. We shall write (x_i, y_i, z_i) for the coordinates of a point i. (Throughout the paper we use a right-handed coordinate system.) A *plaquette* is the boundary and interior of a unit square whose vertices are in Z^3. We define an *open ribbon* as an ordered sequence of plaquettes, labeled $i = 1, 2,..., n$, such that:

1. Every two adjacent plaquettes ($|i-j| = 1$) in the sequence have a common edge.
2. Two plaquettes i and j cannot be incident on a common edge unless $|i-j| = 1$.
3. Two nonadjacent plaquettes cannot be incident on a common vertex unless they are also incident on a common plaquette.
4. Not more than three plaquettes can be incident on a common vertex.

We call the number of edges that a plaquette has in common with other plaquettes the *degree* of the plaquette, so that an open ribbon has two plaquettes of degree 1 and all other plaquettes of degree 2. We write w_n for the number of open ribbons with n plaquettes, where two ribbons are considered distinct if they can not be superimposed by translation.

Lemma 2.1. The number of open ribbons obeys the inequalities

$$3 \times 4^{n-1} \leqslant w_n \leqslant 4 \times 9^{n-1} \tag{2.1}$$

Proof. To obtain an upper bound on w_n we consider the set of objects obtained in the following way. The first plaquette is in any of the three coordinate planes, and the second is incident on one of the four edges of the first plaquette, but is not superimposed on the first plaquette. The kth plaquette is added so that it has an edge incident on one of the edges of the $(k-1)$th plaquette, other than the edge on which the $(k-1)$th and $(k-2)$th plaquettes are both incident. In addition the kth and $(k-1)$th plaquettes are not superimposed. This set contains all the open ribbons with n plaquettes, so

$$w_n \leqslant 36(3 \times 3)^{n-2} \tag{2.2}$$

since the first plaquette can be embedded in the lattice in 3 ways, the second can be added to this in 4×3 ways (choose an edge in 4 ways, and an orientation in 3 ways), and subsequent ones in at most 3×3 ways (choose an edge in 3 ways, since one has already been used, and an orientation in 3 ways).

To obtain a lower bound consider the number of open ribbons with n plaquettes which have the property that the barycenter of the ith plaquette has at least one coordinate larger, and no coordinate smaller, than the corresponding coordinate of the barycenter of the $(i-1)$th plaquette. Such objects are certainly examples of open ribbons and give the inequality

$$w_n \geqslant 3(2 \times 2)^{n-1} \tag{2.3}$$

since the first plaquette can be embedded in the lattice in 3 ways and, when adding subsequent plaquettes, the edge to which the next plaquette is to be added can be chosen in 2 ways, and the orientation in 2 ways. ∎

The asymptotic behavior of w_n is given in the next lemma.

Lemma 2.2. The limit

$$\lim_{n \to \infty} n^{-1} \log w_n = \log \rho \tag{2.4}$$

exists with $4 \leqslant \rho \leqslant 9$, and

$$w_n \geqslant \rho^{n-1} \tag{2.5}$$

Proof. Consider two open ribbons with m and n plaquettes, and translate so that the barycenter of the first plaquette of one ribbon is coincident with the barycenter of the last plaquette of the other ribbon. The resulting set of objects will include all open ribbons with $n+m-1$ plaquettes, so that we have

$$w_m w_n \geqslant w_{n+m-1} \tag{2.6}$$

The theorem follows[10] from this inequality together with the bounds (2.2) and (2.3). ∎

A *directed rooted closed ribbon* with n plaquettes is an ordered sequence of n plaquettes, $i = 1, 2,..., n$, obeying the above conditions except that conditions 1 and 2 must be interpreted modulo n. Any cyclic permutation (and the reverse permutation, and any cyclic permutation of the reverse permutation) is also a directed rooted closed ribbon, and the resulting set of ribbons can be regarded as a single geometrical object which we call an undirected unrooted closed ribbon or, simply, a *closed* ribbon. Every plaquette in a closed ribbon has degree 2.

Closed ribbons can be orientable (i.e., having two boundary curves) or nonorientable (having only one boundary curve). We write r_n for the number of closed ribbons with n plaquettes (where two ribbons are considered distinct unless one can be superimposed on the other by translation). We write r_n^o and r_n^u for the numbers of closed ribbons with n plaquettes which are orientable and nonorientable, respectively. Clearly

$$r_n = r_n^o + r_n^u \tag{2.7}$$

We now prove that open and closed ribbons grow at the same exponential rate.

Lemma 2.3. The numbers of open and closed ribbons are related by the inequality

$$2nr_n \leqslant w_{n-1} \tag{2.8}$$

Proof. By deleting any of the n plaquettes in a closed ribbon with n plaquettes, we obtain an open ribbon with $n-1$ plaquettes. The factor of 2 comes from the two possible directions in the resulting open ribbon. ∎

To obtain an inequality in the opposite direction, the idea is to unfold an open ribbon, show that open ribbons and unfolded open ribbons have the same exponential behavior and construct a subset of closed ribbons by a suitable concatenation of unfolded ribbons.

We write (ξ_i, η_i, ζ_i), $i = 1,..., n$, for the coordinates of the barycenter of the ith plaquette in the open ribbon, and (x_k, y_k, z_k), $k = 1,..., 2n+2$, for the coordinates of the kth vertex of the ribbon. Let

$$x^{\min} = \inf x_k \tag{2.9}$$

where the infimum is over all vertices in the ribbon. Similarly let

$$x^{\max} = \sup x_k \tag{2.10}$$

Let j_1 be the smallest index such that the j_1th plaquette contains a vertex with x coordinate equal to $x^{\min}$, and let j_2 be the largest index such that the j_2th plaquette contains a vertex with x coordinate equal to $x^{\max}$. We call the plaquette labeled $j_1(j_2)$ the leftmost (rightmost) plaquette. An open ribbon is *x-unfolded* if the first and last plaquettes are parallel to the xy plane, $\xi_1 < \xi_i$, $\forall i > l_i$, and $\xi_n > \xi_i$, $\forall i < n$, or if the ribbon consists of a single plaquette in an xy plane.

We next describe the progess of x-unfolding an open ribbon. We consider two cases. The leftmost plaquette can lie in the plane $x = x^{\min}$ and in this case $j_1 = 1$. (If j_1 were greater than 1, then an earlier plaquette would have a vertex with x coordinate equal to $x^{\min}$.) One edge in this plaquette is incident on a second plaquette, and we call the edge of j_1 which is opposite to this edge the *first edge*. If the first edge is perpendicular to the xy plane, add three plaquettes parallel to the xy plane with barycenters $(x^{\min} - \frac{1}{2},\ \eta_1,\ \zeta_1 - \frac{1}{2})$, $(x^{\min} - \frac{3}{2},\ \eta_1,\ \zeta_1 - \frac{1}{2})$, and $(x^{\min} - \frac{5}{2},\ \eta_1,\ \zeta_1 - \frac{1}{2})$. Otherwise add a plaquette, incident on the first edge and parallel to the xy plane, with barycenter having ξ coordinate equal to $x^{\min} - \frac{1}{2}$ and two additional plaquettes in the same plane with barycenters having ξ coordinates $x^{\min} - \frac{3}{2}$ and $x^{\min} - \frac{5}{2}$.

If the leftmost plaquette does not lie in the plane $x = x^{\min}$, then $j_1 = 1$ or $j_1 > 1$. If $j_1 > 1$, there are two subcases. If the plaquette $j_1 + 1$ is in the plane $x = x^{\min}$, then we reflect the subribbon composed of the plaquettes $j_l, j_1 - 1, ..., 1$ in the plane $x = x^{\min}$. If the plaquette $j_1 + 1$ is not in the plane $x = x^{\min}$, then we reflect the subribbon composed of the plaquettes $j_1 - 1, j_1 - 2, ..., 1$ in the plane $x = x^{\min} + \frac{1}{2}$. We continue this process until $j_1 = 1$. If after this process the first plaquette lies in the plane $x = x^{\min}$ (where $x^{\min}$ refers to the leftmost plane of the partially unfolded ribbon), then we add the three plaquettes as described above. Otherwise, if the first plaquette lies in the xy plane we add three plaquettes each lying in the xy plane, the ξ coordinates of whose barycenters are $x^{\min} - \frac{1}{2}$, $x^{\min} - \frac{3}{2}$, and $x^{\min} - \frac{5}{2}$. If the first plaquette lies in the xz plane, then add three plaquettes with barycenters at $(\xi_1 - 1, \eta_1, \zeta_1)$, $(\xi_1 - \frac{3}{2}, \eta_1 + \frac{1}{2}, \zeta_1)$, and $(\xi_1 - 2, \eta_1 + \frac{1}{2}, \zeta_1 - \frac{1}{2})$.

We carry out the corresponding process for the rightmost plaquette, and eventually obtain an x-unfolded ribbon with $n + 6$ plaquettes, having the first and last plaquettes in the xy plane.

We next unfold in the z-direction to obtain an (x, z)-*unfolded* ribbon, which we define as follows: The first plaquette is parallel to the yz plane, the last plaquette is parallel to the xy plane, $\xi_1 \leqslant \xi_i < \xi_n$, $\forall i < n$, and $\zeta_1 < \zeta_i \leqslant \zeta_n$, $\forall i > 1$. Write (ξ_i, η_i, ζ_i), $i = 1, ..., n + 6$, for the coordinates of the barycenters of the plaquettes in the x-unfolded ribbon and (x_k, y_k, z_k) for the coordinates of the kth vertex of the x-unfolded ribbon. Let

$$z^{\min} = \inf z_k \tag{2.11}$$

where the infimum is over all vertices in the x-unfolded ribbon. Similarly let

$$z^{\max} = \sup z_k \tag{2.12}$$

By a process of successive reflections in the appropriate planes $x = x^{\min}$ and $x = x^{\max}$ we obtain a ribbon for which $\xi_1 < \xi_i < \xi_{n+6}, \zeta_1 \leqslant \zeta_i \leqslant \zeta_{n+6}$, $1 < i < n+6$, and with the first and last plaquettes in the xy plane. Finally we delete the first plaquette and replace it with a plaquette in the yz plane, with barycenter at $(\xi + \frac{1}{2}, \eta, \zeta - \frac{1}{2})$, where (ξ, η, ζ) are the coordinates of the barycenter of the deleted plaquette. The resulting ribbon is an (x, z)-unfolded ribbon with $n+6$ plaquettes.

Let $w_n^\dagger$ be the number of x-unfolded ribbons with n plaquettes and let $w_n^\ddagger$ be the number of (x, z)-unfolded ribbons with n plaquettes. Then we have the following result.

Lemma 2.4. We have

$$\lim_{n \to \infty} n^{-1} \log w_n^\dagger = \lim_{n \to \infty} n^{-1} \log w_n^\ddagger = \log \rho \tag{2.13}$$

Proof. Clearly $w_n^\ddagger \leqslant w_n^\dagger$, $\forall n > 1$, since an (x, z)-unfolded ribbon can be converted to an x-unfolded ribbon by reorienting the first plaquette so that it lies in the xy plane. In addition, $w_n^\dagger \leqslant w_n$ since every x-unfolded ribbon is an open ribbon. Using arguments analogous to those in ref. 11 we obtain then $w_n \leqslant w_n^\dagger e^{O(\sqrt{n})}$ and $w_n^\dagger \leqslant w_n^\ddagger e^{O(\sqrt{n})}$. The result follows after taking logarithms, dividing n, and letting n go to infinity. ∎

We next concatenate (x, z)-unfolded ribbons to form closed ribbons. Define a *loop* to be an open ribbon in which the first and last plaquettes each lie in a yz plane and whose barycenters have the same ζ coordinate. Let the number of loops with n plaquettes be l_n.

Lemma 2.5. We have

$$\lim_{n \to \infty} n^{-1} \log l_n = \log \rho \tag{2.14}$$

Proof. Clearly

$$l_n \leqslant w_n \tag{2.15}$$

Each (x, z)-unfolded ribbon can be translated so that the barycenter of the first plaquette is at $(0, 1/2, 1/2)$. Then the (x, z)-unfolded ribbons can be separated into classes according to their height, h, the ζ coordinate of the barycenter of their last plaquette. Let $w_n^\ddagger(h)$ be the number of (x, z)-unfolded ribbons with n plaquettes and height h. The number N_c of these classes cannot exceed n, the number of plaquettes. Concatenating (x, z)-unfolded ribbons with $n/2$ plaquettes with height h with members of the same class reflected in the plane $x = x^{\max}$ gives a subset of loops with n plaquettes, so that

$$\begin{aligned} l_n &\geqslant \sum_h w_{n/2}^\ddagger(h)\, w_{n/2}^\ddagger(h) \\ &\geqslant w_{n/2}^\ddagger(h^*)\, w_{n/2}^\ddagger(h^*) \end{aligned} \tag{2.16}$$

where h^* is the value of h corresponding to the most popular class, i.e., the smallest value of h such that $w_{n/2}^\ddagger(h^*) \geqslant w_{n/2}^\ddagger(h)$, $\forall h$. Since the most popular class must contain at least a fraction $1/N_c$ of the objects, we have

$$l_n \geqslant \left(\frac{w_{n/2}^\ddagger}{n/2} \right)^2 \tag{2.17}$$

Taking logarithms, dividing by n and letting $n \to \infty$ in (2.15) and (2.17), and using (2.13) gives (2.14). ▌

Theorem 2.6. We have

$$\lim_{n \to \infty} n^{-1} \log r_n = \log \rho \tag{2.18}$$

Proof. Let $l_n(a, b)$ be the number of loops with n plaquettes, having the barycenter of the first plaquette at $(0, 1/2, 1/2)$ and the barycenter of the last plaquette at $(a, b, 1/2)$. Loops can be subdivided into classes according to a and b, and there are no more than n^2 such classes. Concatenating loops in each class with loops in the same class reflected in the plane $z = 0$ gives

$$r_n \geqslant \sum_{a,b} l_{n/2}(a, b)\, l_{n/2}(a, b) \geqslant \left(\frac{l_{n/2}}{n^2/4} \right)^2 \tag{2.19}$$

Then (2.18) follows from (2.19) and (2.8). ▌

Theorem 2.7. Orientable and nonorientable ribbons grow at the same exponential rate.

Proof. We define the top (bottom) plaquette of a ribbon as that plaquette whose barycenter has lexicographically largest (smallest) coordinate. In general the x coordinate of the barycenter of the top plaquette can be $x^{\max}$ or $x^{\max} - \frac{1}{2}$, depending on whether or not this plaquette lies in the rightmost plane ($x = x^{\max}$) of the ribbon. We define a modified closed ribbon as a closed ribbon which has one and only one plaquette in the plane $x = x^{\min}$, incident on two plaquettes parallel to the xy plane, and one and only one plaquette in the plane $x = x^{\max}$, also incident on two plaquettes parallel to the xy plane. For a modified ribbon, the x coordinate of the barycenter of the top plaquette is $x^{\max}$ and that of the bottom plaquette is $x^{\min}$. Every closed ribbon with n plaquettes can be converted to a unique modified closed ribbon by adding the same number (independent of n) of additional plaquettes, and this construction preserves orientability. That is, every closed ribbon with n plaquettes can be mapped to a modified closed ribbon with $n + 2l$ plaquettes, where l is a constant. Details of this construction are given in the Appendix. Any two nonorientable ribbons ω_n^1 and ω_m^2 can be converted into two modified nonorientable ribbons $\bar{\omega}_{\bar{n}}^1$ and $\bar{\omega}_{\bar{m}}^2$ by this construction. These modified nonorientable ribbons can be concatenated using the construction illustrated in Fig. 1 to form a modified nonorientable ribbon with $\bar{n} + \bar{m} + 8$ plaquettes. Not all such ribbons can be obtained by this construction. If we write $\bar{r}_n^u$ for the number of modified nonorientable ribbons with n plaquettes, we have the inequality

$$\bar{r}_n^u \bar{r}_m^u \leqslant \bar{r}_{n+m+8}^u \tag{2.20}$$

Since $\bar{r}_n^u \leqslant w_{n-1} \leqslant 36 \times 9^{n-3}$, it follows[10] that the limit

$$\lim_{n \to \infty} n^{-1} \log \bar{r}_n^u = \log \bar{\rho} \leqslant \log 9 \tag{2.21}$$

exists. Next we show that

$$\lim_{n \to \infty} n^{-1} \log r_n^u = \log \bar{\rho} \tag{2.22}$$

We have the immediate inequality $\bar{r}_n^u \leqslant r_n^u$ since every modified ribbon is a ribbon. The construction described in the Appendix establishes that $r_n^u \leqslant \bar{r}_{n+2l}^u$ for a fixed value of l, independent of n. Taking logarithms, dividing by n, and letting n go to infinity then establishes (2.22).

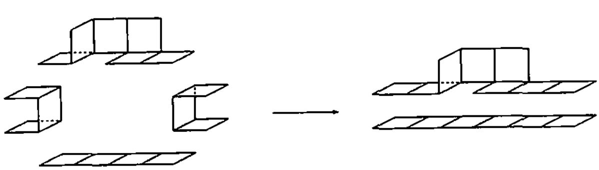

Fig. 1. Concatenation of two nonorientable ribbons to obtain a nonorientable ribbon.

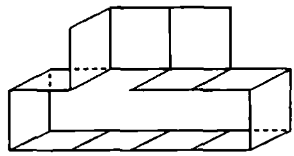

Fig. 2. The nonorientable closed ribbon τ.

Consider the non-orientable ribbon τ with 12 plaquettes shown in Fig. 2. Any modified orientable ribbon $\bar{\omega}_n$ with n plaquettes can be concatenated with this ribbon τ by translating so that the top plaquette of $\bar{\omega}_n$ is coincident with the bottom plaquette of τ and deleting the two coincident plaquettes. The resulting ribbon is nonorientable and has $n+10$ plaquettes. Hence

$$r_n^o \leqslant r_{n+2l+10}^u \tag{2.23}$$

Similarly, every modified nonorientable ribbon can be concatenated with τ to give an orientable ribbon, so that

$$r_n^u \leqslant r_{n+2l+10}^o \tag{2.24}$$

The two inequalities (2.23) and (2.24), together with (2.22), show that $r_n^o = \bar{\rho}^{n+o(n)}$ and, using (2.7) and (2.18), we have

$$\lim_{n\to\infty} n^{-1} \log r_n^o = \lim_{n\to\infty} n^{-1} \log r_n^u = \log \rho \tag{2.25}$$

which concludes the proof. ∎

3. A PATTERN THEOREM

In this section we state and prove a pattern theorem for open ribbons, similar to Kesten's pattern theorem for self-avoiding walks.[12] The proof that we shall give is closely related to an unpublished proof of Kesten's theorem due to Hammersley.[13]

We begin by defining a *factorization* of an x-unfolded ribbon. The ribbon has a *cutting plane* if there are two successive plaquettes k and $k+1$ in the xy plane, such that $\xi_{k+1} = \xi_k \pm 1$, $\eta_{k+1} = \eta_k$, $\zeta_{k+1} = \zeta_k$, and $\xi_l \neq \xi_k, \xi_{k+1}$, $\forall l \neq k, k+1$. The cutting plane is the plane $x = (\xi_k + \xi_{k+1})/2$. If an x-unfolded ribbon has no cutting planes, then it is a *prime ribbon*. Let q_n be the number of prime ribbons with n plaquettes. By factorization at the first available cutting plane we obtain the generalized renewal equation

$$w_n^\dagger = q_n + \sum_{m=1}^{n-1} q_m w_{n-m}^\dagger \tag{3.1}$$

which can be rewritten in terms of the generating functions

$$W^\dagger(x) = \sum_{n>0} w_n^\dagger x^n \tag{3.2}$$

and

$$Q(x) = \sum_{n>0} q_n x^n \tag{3.3}$$

as

$$W^\dagger(x) = \frac{Q(x)}{1 - Q(x)} \tag{3.4}$$

We define an open ribbon to be a *bridge ribbon* if the first plaquette is in either the xy plane or the xz plane, $\xi_1 < \xi_i$, $\forall i > 1$, $\xi_n \geqslant \xi_i$, $\forall i < n$. Let b_n be the number of bridge ribbons (up to translation) with n plaquettes, and notice that $w_n^\dagger \leqslant b_n$. By adding two plaquettes, a bridge ribbon can be converted to one in which the first and last plaquettes are in the same plane (either the xy or xz plane) so that $b_n \leqslant 2w_{n+2}^\dagger$, where the factor of two comes from the possible rotation from the xy to the xz plane. Therefore

$$\lim_{n\to\infty} n^{-1} \log b_n = \log \rho \tag{3.5}$$

Defining the generating function

$$B(x) = \sum_{n>0} b_n x^n \tag{3.6}$$

we also see that if $B(x)$ diverges at $x = 1/\rho$, then $W^\dagger(x)$ also diverges at $x = 1/\rho$. Then it follows from (3.4) that $Q(1/\rho) = 1$.

Defining $W(x) = \sum_{n>0} w_n x^n$, we have the following inequality.

Lemma 3.1. We have

$$W(x) \leqslant \frac{e^{2B(x)}}{x} \tag{3.7}$$

Proof. The proof is almost identical to the proof of Corollary 3.1.8 in ref. 1, p. 61. Note that we define generating functions starting at the $n=1$ term, which leads to minor differences from ref. 1. Alternatively, see ref. 12. ▮

Since $W(x)$ diverges at $x=1/\rho$ [which follows from the inequality (2.5)], $B(x)$ also diverges at $x=1/\rho$, and hence $W^\dagger(x)$ diverges at $x=1/\rho$.

A *pattern* is any finite open ribbon, and a *prime pattern* is any finite prime ribbon. Consider a prime pattern P and the set of open ribbons with n plaquettes, not containing a translate of P. We write $w_n(\bar{P})$, $b_n(\bar{P})$, $w_n^\dagger(\bar{P})$, and $q_n(\bar{P})$ for the numbers of open ribbons, bridge ribbons, x-unfolded ribbons and prime ribbons, respectively, with n plaquettes, not containing the prime pattern P. Similarly we write $W(x;\bar{P})$, $B(x;\bar{P})$, $W^\dagger(x;\bar{P})$, and $Q(x;\bar{P})$ for the corresponding generating functions. We note that

$$w_m(\bar{P})\, w_n(\bar{P}) \geqslant w_{m+n-1}(\bar{P}) \tag{3.8}$$

so that $W(x;\bar{P})$ diverges at $x=1/\rho(\bar{P})$ where $\rho(\bar{P})\leqslant\rho$, since $w_n(\bar{P})\leqslant w_n$. Using the same arguments as in Lemma 3.1, we have

$$W(x;\bar{P})\leqslant\frac{e^{2B(x;\bar{P})}}{x} \tag{3.9}$$

so, since $B(x;\bar{P})\leqslant W(x;\bar{P})$, $\forall x\geqslant 0$, $B(x;\bar{P})$ also diverges at $x=1/\rho(\bar{P})$, and converges for all $x<1/\rho(\bar{P})$. Both $B(x;\bar{P})$ and $W^\dagger(x;\bar{P})$ have the same asymptotic behavior [by an argument exactly similar to that given above for $B(x)$ and $W^\dagger(x)$], so $W^\dagger(x;\bar{P})$ diverges at $x=1/\rho(\bar{P})$ and converges for all $x<1/\rho(\bar{P})$.

Since P is prime, and a prime pattern cannot be split between two prime components of an x-unfolded ribbon, we have

$$W^\dagger(x;\bar{P})=\frac{Q(x;\bar{P})}{1-Q(x;\bar{P})} \tag{3.10}$$

Since $q_m(\bar{P})<q_m$ for at least one value of m, and all q_k are nonnegative, $Q(1/\rho;\bar{P})<1$. This implies that $W^\dagger(1/\rho;\bar{P})$ is finite, and hence that $\rho>\rho(\bar{P})$. This is a key result which we state as follows.

Theorem 3.2. Open ribbons which do not contain the prime pattern P at least once are exponentially rare in the set of open ribbons.

In fact, if a pattern occurs on almost all ribbons, it occurs frequently on almost all ribbons. We state this more precisely in the next theorem:

Theorem 3.3. Let $w_n(P; \varepsilon)$ be the number of open ribbons on which the pattern P occurs at most $\lfloor \varepsilon n \rfloor$ times. Then there exists a positive number $a(P)$ such that

$$\limsup_{n \to \infty} n^{-1} \log w_n(P; \varepsilon) < \log \rho \tag{3.11}$$

for all $\varepsilon < a(P)$.

Proof. The proof of this theorem follows the idea of the proof of Lemma 7.2.5 in ref. 1, p. 236. ∎

There is a corresponding result for closed ribbons, which we state as follows.

Theorem 3.4. Let $r_n^o(P; \varepsilon)$ be the number of orientable closed ribbons on which the pattern P occurs at most $\lfloor \varepsilon n \rfloor$ times. Then there exists a positive number $a(P)$ such that

$$\limsup_{n \to \infty} n^{-1} \log r_n^o(P; \varepsilon) < \log \rho \tag{3.12}$$

for all $\varepsilon < a(P)$.

Proof. Consider any orientable closed ribbon with n plaquettes in which the pattern P occurs at most $\lfloor \varepsilon n \rfloor$ times. Delete the plaquette with lexicographically smallest barycenter, giving an open ribbon with $n-1$ plaquettes. Since deleting a plaquette cannot create a pattern, the number of occurrences of P in the open ribbons is at most $\lfloor \varepsilon n \rfloor \leqslant \lfloor \varepsilon (n-1) \rfloor + 1$. Hence

$$2r_n^o(P; \varepsilon) \leqslant w_{n-1}(P; \varepsilon + (n-1)^{-1}) \tag{3.13}$$

Taking logarithms, dividing by n and letting $n \to \infty$ in (3.13), and using (3.11) gives (3.12). ∎

An exactly analogous theorem holds for the case of nonorientable closed ribbons, and the proof is essentially identical.

4. KNOTS IN CLOSED RIBBONS

In this section we shall be concerned with knots in closed ribbons. Each plaquette in a closed ribbon has four edges, two of which are each incident on two plaquettes (which we call *ribbon edges*) and two of which are incident on only one plaquette (which we call *boundary edges*). We next define the *center line* of the ribbon. This is a piecewise linear simple closed curve composed of line segments joining the barycenters of plaquettes to the midpoints of the two ribbon edges of that plaquette. We prove that, as

n goes to infinity, the probability that the center line of a closed ribbon is knotted goes to unity exponentially rapidly. This implies that each boundary curve of an orientable ribbon is knotted with probability 1, and that the boundary curve of a nonorientable ribbon is a satellite[14] of a nontrivial knot with probability 1, in the $n \to \infty$ limit. (A satellite knot is a simple closed curve in the interior of a solid torus which is embedded in R^3 in such a way that the centerline of the torus is a nontrivial knot, with the restriction that the simple closed curve does not lie in a 3-ball contained in the solid torus. See the figure on p. 111 of ref. 15.)

We first prove a preliminary lemma.

Lemma 4.1. Let $r_n^o(\phi_c)$ be the number of orientable closed ribbons with n plaquettes having unknotted center line. Then the limit

$$\lim_{n\to\infty} n^{-1} \log r_n^o(\phi_c) = \log \rho^o(\phi_c) \leqslant \log \rho \tag{4.1}$$

exists.

Proof. Every orientable closed ribbon with n plaquettes and unknotted centerline can be converted (using the construction described in the Appendix) to a modified orientable ribbon with $\bar{n} = n + 2l$ plaquettes, and the centerline of this modified ribbon is also unknotted. We write $\bar{r}_n^o(\phi_c)$ for the number of modified orientable ribbons with unknotted center line, and n plaquettes. Clearly

$$\bar{r}_n^o(\phi_c) \leqslant r_n^o(\phi_c) \leqslant \bar{r}_{n+2l}^o(\phi_c) \tag{4.2}$$

Every pair of modified orientable ribbons with unknotted centerline can be concatenated to form a modified orientable ribbon with unknotted centerline, as follows. Call the two modified ribbons $\bar{\omega}_n^1$ and $\bar{\omega}_m^2$, where the subscript measures the number of plaquettes. Let (ξ_1, η_1, ζ_1) be the coordinate of the barycenter of the top plaquette of $\bar{\omega}_n^1$. Translate $\bar{\omega}_m^2$ so that the coordinates of the barycenter of its bottom plaquette are $(\xi_1 + 1, \eta_1, \zeta_1)$. Delete the top plaquette of $\bar{\omega}_n^1$ and the bottom plaquette of $\bar{\omega}_m^2$, and add two plaquettes parallel to the xy plane with barycenters at $(\xi_1 + \frac{1}{2}, \eta_1, \zeta_1 + \frac{1}{2})$ and $(\xi_1 + \frac{1}{2}, \eta_1, \zeta_1 - \frac{1}{2})$. The resulting ribbon is orientable and closed, having unknotted centerline, and $n + m$ plaquettes, so that

$$\bar{r}_n^o(\phi_c)\, \bar{r}_m^o(\phi_c) \leqslant \bar{r}_{n+m}^o(\phi_c) \tag{4.3}$$

which implies the existence of the limit

$$\lim_{n\to\infty} n^{-1} \log \bar{r}_n^o(\phi_c) = \log \bar{\rho}^o(\phi_c) \tag{4.4}$$

This, together with the inequalities in (4.2) gives (4.1), with $\bar{\rho}^o(\phi_c) = \rho^o(\phi_c)$. ∎

For nonorientable ribbons the analogue of Lemma 4.1 is as follows.

Lemma 4.2. Let $r_n^u(\phi_c)$ be the number of nonorientable ribbons unith n plaquettes having unknotted centerline. Then the limit

$$\lim_{n \to \infty} n^{-1} \log r_n^u(\phi_c) = \log \rho^u(\phi_c) \leqslant \log \rho \tag{4.5}$$

exists.

Proof. The proof is similar to that of the previous lemma. Each nonorientable ribbon with unknotted centerline can be converted into a corresponding modified ribbon by adding plaquettes as outlined in the Appendix. Two modified nonorientable ribbons with unknotted centerlines can be concatenated, as shown in Fig. 1, to form a modified nonorientable ribbon with unknotted centerline, giving a generalized supermultiplicative inequality. The existence of the limit follows immediately from this inequality. ∎

We now come to the main theorem of this section.

Theorem 4.3. Orientable closed ribbons with unknotted centerline are exponentially rare. That is,

$$\rho^o(\phi_c) < \rho \tag{4.6}$$

Proof. To prove that the centerline of an orientable closed ribbon is knotted it is sufficient(16, 17) to prove that the ribbon contains a prime pattern T, say, such that the centerline of T (suitably extended) and the union of the unit 3-cubes dual to the vertices of T form a knotted ball pair. We call such a pattern a *knotted pattern*. The union of the dual 3-cubes at the vertices of T must form a 3-ball, and the centerline of T must be extended so that its boundary points are in the boundary of the 3-ball. This extension of the centerline of T to meet the boundary of the 3-ball is necessary so that the 1-ball is properly embedded in the 3-ball.

Let i, j, k be unit vectors along the positive x, y, z axes, and consider the sequence of edges T_1 defined as follows:

$$T_1: \quad \{i, i, i, j, k, k, k, -j, -j, -k, -k, -j, -k, -k, j, j, j, -i, k, k, -j, i, i, i, i, -j, i, i\}$$

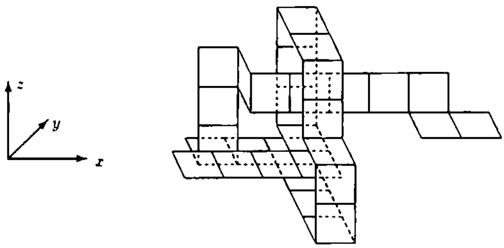

Fig. 3. The prime pattern T. The centerline of this pattern, suitably extended, and the union of the 3-cubes dual to the vertices of T, form a knotted ball pair.

The boundary of the ribbon T, shown in Fig. 3, consists of the edges in T_1 and the edges in a second sequence T_2 defined as follows:

$$T_2 : \quad \{-j, i, i, i, i, j, j, k, k, k, -j, -j, -k, -k, -j, -k, -k, j, j, j, j, -i, -i, -i, -j, k, k, k, i, -j, i, i, i, i, i, -k, i, -j\}$$

Both sequences of edges start at the same point, say the origin. If we construct dual unit 3-cubes at each vertex of T, the union of these 3-cubes is a 3-ball, $B^3(T)$. If the centerline of T is suitably extended it forms a 1-ball $B^1(T)$ properly embedded in the 3-ball $B^3(T)$. The ball pair $(B^3(T), B^1(T))$ is knotted, i.e., it is not homeomorphic to the standard ball pair. If the ribbon contains the prime pattern T, then the prime knot decomposition of the centerline of that ribbon contains a $(+)$ trefoil knot, and hence is knotted.[14, 16]

The set of orientable closed ribbons with n plaquettes whose centerlines are unknotted is a subset of the corresponding ribbons which do not contain the pattern T defined above, i.e., $r_n^o(\phi_c) \leqslant r_n^o(\bar{T})$. Using Theorem 3.4, we have

$$\rho^o(\phi_c) < \rho \tag{4.7}$$

which completes the proof. ▮

In fact, from Theorem 3.4, all except exponentially few orientable closed ribbons contain a positive density of copies of the knotted pattern T in the $n \to \infty$ limit, so that not only the centerline of the ribbon is knotted, but the knot has high complexity, as measured by such *good measures of knot complexity*[17] as crossing number, unknotting number, minor index, braid index minus one, genus, and the spans of knot polynomials. In addition, one can construct patterns corresponding to any knot type, so that one is assured that all knots will eventually appear with positive density in the center lines of sufficiently long ribbons.

There is an exactly analogous result for nonorientable ribbons, which we state as the following Theorem:

Theorem 4.4. Nonorientable closed ribbons with unknotted centerline are exponentially rare. That is,

$$\rho^{n}(\phi_c) < \rho \tag{4.8}$$

Proof. The proof is essentially identical to that for the orientable case, and uses the same pattern T. ∎

Once again the pattern occurs with positive density on almost all ribbons, so the centerline has high knot complexity and, similar arguments can be used to prove that any knot type occurs with positive density for sufficiently long ribbons.

We now consider knots in the boundaries of ribbons, rather than in their centerlines. We first note that each boundary curve, and also the centerline, of an orientable closed ribbon has the same knot type. This is easy to see since the pushoff across the ribbon defines the required ambient isotopy. Hence the probability that each boundary of an orientable closed ribbon is knotted goes to unity exponentially rapidly as n goes to infinity. In addition, the boundary has high knot complexity.

For nonorientable ribbons, if the center line is knotted then the boundary must also be knotted, since it is a $(2, 2k+1)$ satellite (in fact a cable[14, 15]) of the centerline knot. Hence, for sufficiently large n, almost all nonorientable ribbons have boundaries which are satellites of nontrivial knots. Even if the centerline of the ribbon is unknotted, with high probability for large n the boundary is a nontrivial $(2, 2k+1)$ torus knot. This phenomenon is considered in the next section.

If the boundary of a nonorientable ribbon has 12 or fewer crossings, then the centerline must be unknotted, and the boundary knot must be an ordinary $(2, 2k+1)$ torus knot. This is because all torus knots [with the exception of the unknot $(1,1)$] and all $(2, 2k+1)$ satellites of knots are prime knots.[18] In the census of prime knots[19] the first satellite knots are two 13-crossing satellites of the trefoil knot. For orientable ribbons the boundary curves form a $(2, 2k)$ satellite link of the centerline. If this boundary link has eight or fewer crossings then the center line must be unknotted, and the boundary link must be an ordinary $(2, 2k)$ torus link.

5. LINKING OF THE BOUNDARY CURVES AND CENTERLINE OF CLOSED RIBBONS

The boundary curves of orientable closed ribbons can be linked as well as being individually knotted. In this section we first investigate the n dependence of the linking number of these boundary curves. The linking number can be thought of as a three-dimensional analogue of winding number. See ref. 15, pp. 132–133.

Consider an orientable closed ribbon, and orient the two boundary curves in parallel. Project the ribbon onto R^2 in a direction chosen such that all crossings of the boundary curves are transverse. We can associate a sign to each crossing as shown in Fig. 4. The linking number of the two boundary curves is defined as

$$Lk = \tfrac{1}{2} \sum_{k=1}^{N} \sigma_k \tag{5.1}$$

where the sum is over the N transverse crossings between the curves, and $\sigma_k = \pm 1$ is the sign of the kth crossing as determined by the sign convention of Fig. 4.

Consider the pattern P of 31 plaquettes shown in Fig. 5 with subboundaries P_1 and P_2 given by

$$P_1\colon \quad \{i, i, i, i, k, -i, -i, -i, k, i, k, j, i, i, -k, i, i, -j, k, i, -k, \\ i, -k, -i, -i, -i, -k, i, i, i, i\}$$

and

$$P_2\colon \{j, i, i, i, i, k, -i, -i, -i, k, i, i, -j, k, i, -k, i, k, j, i, i, -k, i, \\ -k, -i, -i, -i, -k, i, i, i, i, -j\}$$

both starting at the same point, say the origin. Label the plaquettes sequentially as p_1 to p_{31}. Consider an orientable closed ribbon R which contains

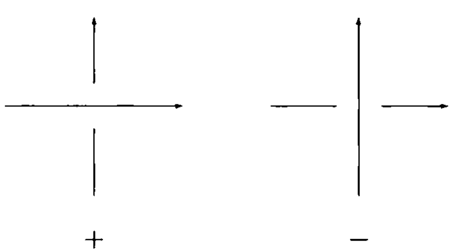

Fig. 4. The sign convention for crossings.

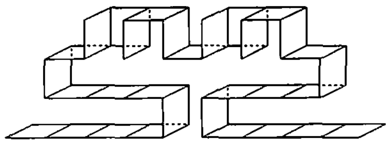

Fig. 5. The prime pattern P.

the pattern P. By deleting the two plaquettes (p_5 and p_{27}) with barycenters having coordinates (with respect to the first vertex being at the origin) $(4, \frac{1}{2}, \frac{1}{2})$ and $(5, \frac{1}{2}, \frac{1}{2})$ and adding the two plaquettes parallel to the xy plane with barycenters at $(\frac{9}{2}, \frac{1}{2}, 0)$ and $(\frac{9}{2}, \frac{1}{2}, 1)$, we obtain two ribbons P' and R', and we say that R has been *decomposed* into P' and R'. The plaquettes labeled p_6 to p_{26} form part of the ribbon P'. We write $\partial_1 R, \partial_2 R$ for the boundaries of R, with similar notation for the boundaries of R' and P'. The linking number of the boundaries of P' is -1.

Lemma 5.1. We have

$$Lk(\partial_1 R, \partial_2 R) = Lk(\partial_1 R', \partial_2 R') + Lk(\partial_1 P', \partial_2 P') \tag{5.2}$$

Proof. In the projection shown in Fig. 5, orient the two ribbon boundaries in parallel, producing two negative crossings formed by the curves $\partial_1 R, \partial_2 R$. By passing $\partial_1 R$ through $\partial_2 R$ locally, change one of these negative crossings to a positive crossing. This removes a full negative twist from the ribbon R producing a ribbon which is ambient isotopic to R'. Hence

$$Lk(\partial_1 R, \partial_2 R) = Lk(\partial_1 R', \partial_2 R') - 1 \tag{5.3}$$

and the lemma follows since $Lk(\partial_1 P', \partial_2 P') = -1$. ∎

Let $\langle |Lk| \rangle_n$ be the expectation of $|Lk|$ over the set of orientable closed ribbons with n plaquettes. Then we have the following result.

Theorem 5.2. We have

$$\langle |Lk(\partial_1 R, \partial_2 R)| \rangle \geqslant A\sqrt{n} \tag{5.4}$$

for some positive constant A, and n sufficiently large.

Proof. The proof is an adaptation of the proof of Theorem 1 in ref. 20. Consider the prime pattern P shown in Fig. 5. By reflecting in the

xz plane we obtain the mirror image pattern P^*. The 3-balls $B^3(P)$ and $B^3(P^*)$ formed by taking the union of the dual 3-cubes to the vertices of each of these patterns are congruent. If the pattern P occurs k times in an orientable closed ribbon R, then the linking number of the boundary curves of R can be written as $l-k$, where l is the linking number of the boundaries of the ribbon obtained from R by k decompositions each of which gives rise to a translate of P'. A similar operation can be carried out for P^*; and the corresponding ribbon $P^{*\prime}$ has linking number $+1$. The two patterns P and P^* are equally likely to occur in a ribbon. Theorem 3.4 implies that there exist positive numbers ε and γ such that, for a fraction 1-exp$(-\gamma n+o(n))$ of the set of orientable closed ribbons with n plaquettes, there are at least $\lfloor \varepsilon n \rfloor$ pairwise disjoint translates of the 3-ball $B^3(P)$ each of which intersects the ribbon in a translate of P or P^*. Since P and P^* are binomially distributed in these 3-balls the probability that P occurs exactly k times among the $\lfloor \varepsilon n \rfloor$ occurences of either P or P^* is bounded above by $1/\sqrt{\lfloor \varepsilon n \rfloor}$, for every $k \leqslant \lfloor \varepsilon n \rfloor$, for sufficiently large n. For each of these ribbons the linking number Lk is the sum of two terms, the first coming from the union of the εn occurrences of P or P^* and the second from the remainder of the ribbon. If the linking number is less than some given number $f(n)$, then the contribution from the $\lfloor \varepsilon n \rfloor$ occurrences of P or P^* must be one of at most $\lceil 2f(n)+1 \rceil$ different values. Hence

$$\operatorname{Prob}(|Lk| < f(n)) \leqslant \frac{(1-e^{-\gamma n+o(n)})\lceil 2f(n)+1 \rceil}{\sqrt{\lfloor \varepsilon n \rfloor}} \tag{5.5}$$

Clearly $\operatorname{Prob}(|Lk| < f(n)) \to 0$ as $n \to \infty$ if $f(n) = o(\sqrt{n})$. The theorem follows immediatley. ▮

The n dependence of the linking number has been investigated using a Monte Carlo approach, and the numerical results suggest that the bound given by Theorem 5.2 may be best-possible.[8]

If the boundaries of the ribbon are unknotted then the only link types of the two boundary curves are the $(2, 2k)$-torus links, and the relative frequency of occurrence of ribbons with linking number 0, 1, and 2 has been investigated numerically.[8] However, if the boundaries are knotted (both with knot type τ), then the link type of the two boundary curves will be a $(2, 2k)$ satellite link of the center knot τ.

We have an analogous result for the linking of a boundary of an orientable ribbon with the centerline of the ribbon. If $Lk(\partial_1 R, C(R))$ is the linking number of the boundary $\partial_1 R$ and the centerline $C(R)$, then we have the following result.

Theorem 5.3. We have

$$\langle |Lk(\partial_1 R, C(R))| \rangle_n \geq A_o \sqrt{n} \tag{5.6}$$

for some positive constant A_o and n sufficiently large.

Proof. The proof follows from Theorem 5.2 by a pushoff of the boundary $\partial_2 R$ to the centerline $C(R)$ across the ribbon. ∎

In the case of a nonorientable ribbon R, the single boundary curve ∂R can also be linked with the centerline $C(R)$, and the corresponding theorem is as follows.

Theorem 5.4. We have

$$\langle |Lk(\partial R, C(R))| \rangle_n \geq A_1 \sqrt{n} \tag{5.7}$$

for some positive constant A_1, and n sufficiently large.

Proof. This can be proved by a similar argument to that used in the proof of Theorem 5.2. ∎

Linking of the boundary curve with the centerline ensures that the boundary of the nonorientable ribbon is knotted even when the center line is unknotted. The knot type of the boundary is then a $(2, 2k+1)$-torus knot. We know from Theorem 4.4 that, for sufficiently large n, the centerline is knotted with high probability, and the linking of the boundary and centerline then determines which satellite of the knot type of the centerline occurs. There are two factors which each lead to increased knot complexity—the knot type of the centerline and the linking of the boundary and the centerline.

6. TWIST AND WRITHE OF ORIENTABLE CLOSED RIBBONS

The linking number considered in the previous section, is a topological quantity, invariant under ambient isotopy. For any smooth orientable closed ribbon the linking number of the two boundary curves can be written as the sum of two geometrical quantities, the twist (Tw) of one boundary curve (A) about the other (B), and the writhe (Wr) of B.[21] Twist characterizes the local crossings between the two boundary curves, and writhe characterizes the distant, or nonlocal crossings of one boundary curve with itself. These quantities have proved useful in describing the conformational properties of duplex DNA molecules.[2,7] In particular, the writhe is a measure of the degree of supercoiling of the DNA molecule.

We first consider the definition of the writhe of a curve. Consider any simple closed curve in R^3, and project it onto R^2 in some direction $\hat{x}$. In general the projection will have crossings and, for almost all projection directions, these crossings will be transverse, so that we can associate a sign $+1$ or -1 with each crossing, as in Fig. 4. For this projection we form the sum of these signed crossing numbers and average over all projection directions $\hat{x}$. This average quantity is the writhe Wr of the curve.[5]

For a smooth ribbon the twist $Tw(A, B)$ of boundary curve A about boundary curve B can be defined as a certain line integral along B.[22] The linking number, twist, and writhe of a smooth ribbon are related by the conservation equation[5, 21, 23]

$$Lk(A, B) = Tw(A, B) + Wr(B) \tag{6.1}$$

For a PL curve in Z^3 the writhe can be defined as above, but its computation is simplified by a theorem of Lacher and Sumners,[24] which reduces the writhe computation to the average of the linking numbers of the given curve with four pushoffs, one into each of four of the eight octants, with no two of the four octants being chosen to be mutually antipodal. For ribbons in Z^3 we define the twist of one boundary (A) about the other (B) to be

$$Tw(A, B) = Lk(A, B) - Wr(B) \tag{6.2}$$

so that White's theorem, Eq. (6.1), is automatically satisfied. In this section we discuss the asymptotics of the twist and writhe of a lattice ribbon.

There is a theorem for the writhe of a boundary curve of a ribbon, corresponding to Theorem 5.2. We consider an orientable closed ribbon R which contains the pattern P defined above. R has two boundary curves, $\partial_1 R$ and $\partial_2 R$. We choose $\partial_1 R$ to be that boundary which contains the subboundary P_1 of P. Decomposing R into P' and R' as described in the previous section, we call $\partial_1 P'$ the boundary of P' consisting of the intersection of P' and R together with the additional edge required to form a polygon. Similarly $\partial_1 R'$ is the boundary of R' consisting of the intersection of R' and R together with the additional edge required to form a polygon.

Lemma 6.1. We have

$$Wr(\partial_1 R) = Wr(\partial_1 R') + Wr(\partial_1 P') \tag{6.3}$$

Proof. The proof is similar to that of Lemma 2 in ref. 20. We compute the writhe of $\partial_1 R$ by considering the linking number of $\partial_1 R$ with its

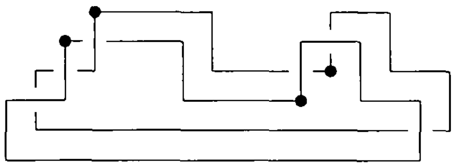

Fig. 6. The boundary $\partial_1 P'$ of the ribbon P', projected in the xz plane, and its pushoff in direction $(1, 1, 1)$. The filled circles indicate a change in the y coordinate.

four pushoffs in directions $(1, 1, 1)$, $(1, -1, 1)$, $(-1, 1, 1)$, and $(-1, -1, 1)$. We first note that the linking number of $\partial_1 P'$ with its pushoff in each of these directions is -1, -1, 0, and 0, respectively. We consider the pushoff $\partial_1 R+$ of $\partial_1 R$ in the direction $(1, 1, 1)$. Inside the 3-ball $B^3(P')$ there are six crossings between $\partial_1 R+$ and $\partial_1 R$, four of which are $(-)$ crossings, and two of which are $(+)$ crossings. By a small move inside $B^3(P')$, which does not change the remainder of $\partial_1 R+$ and $\partial_1 R$, we can change one of the $(-)$ crossings to a $(+)$ crossing. The resulting pair of curves is ambient isotopic to the pair $\{\partial_1 R'+, \partial_1 R'\}$. See Fig. 6. Hence

$$\begin{aligned} Lk(\partial_1 R, \partial_1 R+) &= Lk(\partial_1 R', \partial_1 R'+) - 1 \\ &= Lk(\partial_1 R', \partial_1 R'+) + Lk(\partial_1 P', \partial_1 P'+) \end{aligned} \tag{6.4}$$

We obtain an identical relation by considering a pushoff in direction $(1, -1, 1)$, and when we consider pushoffs in directions $(-1, 1, 1)$ and $(-1, -1, 1)$ we find that the pair $\{\partial_1 R+, \partial_1 R\}$ is ambient isotopic to the pair $\{\partial_1 R'+, \partial_1 R'\}$, without any crossing change being required. Therefore

$$\begin{aligned} Wr(\partial_1 R) &= Wr(\partial_1 R') + \tfrac{1}{4}(-1 - 1 + 0 + 0) \\ &= Wr(\partial_1 R') + Wr(\partial_1 P') \end{aligned} \tag{6.5}$$

which proves the lemma. ∎

Theorem 6.2. We have

$$\langle |Wr| \rangle_n \geqslant B\sqrt{n} \tag{6.6}$$

for some positive constant B, for n sufficiently large.

Proof. The proof follows from Lemma 6.1 and an argument identical to that used in the proof of Theorem 5.2. ∎

The additivity (under decomposition) of the linking number (Lemma 5.1) and the writhe (Lemma 6.1), together with the definition of twist

[Eq. (6.2)], immediately implies the additivity of twist under decomposition. The twist of one boundary of P' about the other can easily be seen to be $-\frac{1}{2}$, so that each occurrence of the pattern P gives a negative contribution to the twist of the ribbon, and each occurrence of the mirror image of P gives a corresponding positive contribution. This leads to a lower bound on the expectation of the absolute value of the twist, analogous to Theorem 5.2 for linking number.

Theorem 6.3. We have

$$\langle |Tw| \rangle_n \geq C\sqrt{n} \tag{6.7}$$

for some positive constant C, and n sufficiently large.

Proof. The proof follows from the additivity of twist, together with the pattern theorem and a coin-tossing argument, as in the proof of Theorem 5.2. ∎

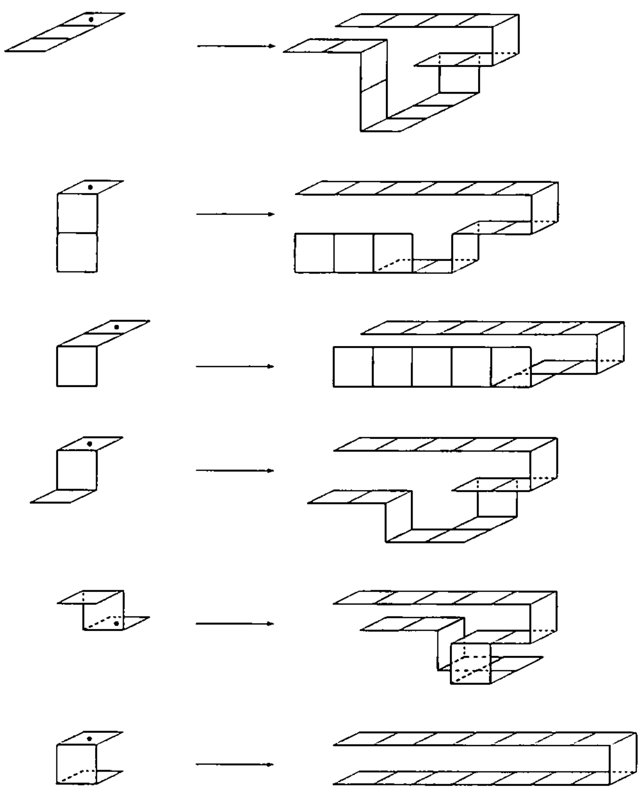

Fig. 7. Cases in which the top plaquette has only one edge in the plane $x = x^{\max}$.

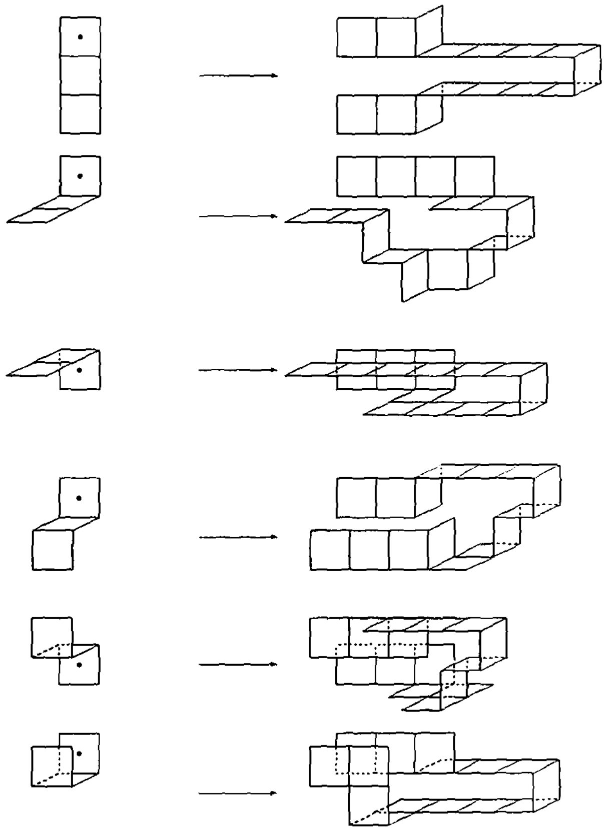

Fig. 7. (*Continued*)

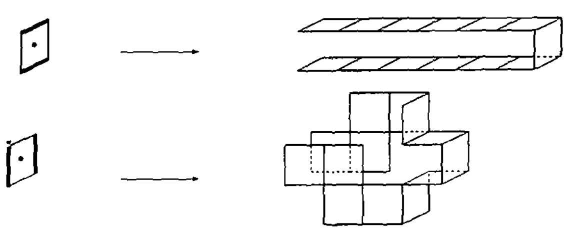

Fig. 8. Cases in which the top plaquette is an ordinary plaquette and lies in the plane $x = x^{\max}$. The bonds marked with a thicker line denote the edges shared by the top plaquette with its neighboring plaquettes. These two constructions are valid regardless of the orientations of the neighboring plaquettes.

Similar theorems to Theorems 6.2 and 6.3 can be proved for the writhe of the centerline and for the twist of one boundary about this centerline, for an orientable ribbon.

7. DISCUSSION

We have discussed the asymptotic behavior of the numbers of lattice ribbons with n plaquettes, where the ribbon is open, or closed and orientable, or closed and nonorientable. We have shown that the numbers of ribbons of these three types grow at the same exponential rate, and have derived bounds on the value of the growth constant ρ. The lower bound is not much smaller than the numerical estimate of $\rho = 4.33 \pm 0.20$.[8]

We have proved a pattern theorem for ribbons, which establishes that certain types of patterns appear with positive density in all except exponentially few sufficiently long ribbons, and we have used this to establish that the boundary curves of closed ribbons are knotted with probability 1 in the $n \to \infty$ limit. In addition, we have shown that the knot complexity (measured in various ways) diverges as n increases.

We have derived lower bounds on the expectation of the absolute value of the linking number and twist of the two boundary curves of an orientable closed ribbon and on the writhe of one of the boundary curves, and showed that the behavior of the lower bounds is asymptotically the same for the three quantities. This was observed numerically[8] for the linking number and the writhe, and the estimated rates of increase were found to be close to the lower bounds which we have derived.

There are a number of interesting open questions. We have no estimate of the constant which appears in the growth rate of the knot probability. It would be useful to have upper and lower bounds on this quantity, and Monte Carlo methods could be used to provide a numerical estimate. In addition, it would be interesting to have upper bounds on the rate of increase of the expectation of the absolute value of the linking number, twist, and writhe.

We have focused on asymptotic properties of the ribbon, but there is an active area of research which addresses questions about knotting, writhing, etc., in models of short DNA rings.[7] There are interesting calculations of knot probability as a function of the effective diameter of the DNA (which is designed to account for electrostatic repulsion),[25] and calculations which take more direct account of ionic strength effects (at the level of a screened Coulomb model).[26,27] In addition there are estimates of the writhe (and of its mean square) as a function of linking deficit[28,29] and ionic strength.[25,27]

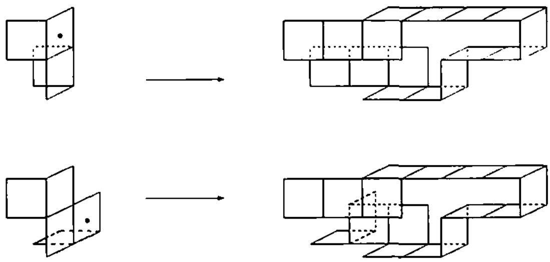

Fig. 9. Cases in which the top plaquette is a corner plaquette and lies in the plane $x = x^{\max}$.

APPENDIX

In this appendix we describe a construction which converts any closed ribbon with n plaquettes into a modified closed ribbon with $n+2l$ plaquettes and which preserves the orientability of the ribbon. The particular construction described requires $l=6$. We concentrate on the rightmost plane of the ribbon and the top plaquette, but an analogous construction applies to the leftmost plane and the bottom plaquette.

The argument is by case analysis. The top plaquette can have either one edge or four edges in the plane $x = x^{\max}$, we consider these cases separately. In the first case we have to consider 24 possible different configurations. For our purposes, configurations obtained by a 180° rotation around an axis perpendicular to the plane are equivalent, so the number of configurations to consider is reduced to 12. These 12 cases are illustrated in Fig. 7. The top plaquette is marked by a dot in the middle of the plaquette. In each case one plaquette is removed, and 13 plaquettes are added. It is easy to check that the orientability of the ribbon is unchanged.

If the top plaquette has four edges in the plane $x = x^{\max}$, we proceed as follows. We define a *corner plaquette* to be a plaquette such that its two neighboring plaquettes share a vertex. Otherwise the plaquette is an *ordinary* plaquette. If the top plaquette is an ordinary plaquette, we have one of the two cases shown in Fig. 8. If the top plaquette is a corner plaquette, then the possible situations are shown in Fig. 9.

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