

# In Search of Minimal Random Braid Configurations

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## **Abstract.**

A geometric braid consists of  $n$  curves stretching between two parallel planes. A group structure may be defined on a geometric braid yielding an algebraic braid. Braids provide information on the structure of knots and links, and have many practical applications, for example in fluid mechanics and astrophysics. A well-known problem in braid theory consists of finding minimal crossing number braids. No efficient algorithm which solves this problem using group theory seems to be possible for  $n > 3$ . Here we investigate several different approaches to obtain minimal configurations: we employ three different relaxation techniques and compare these with each other and with an algebraic heuristic algorithm, in terms of minimization (of energy and crossing number) and time efficiency. By energy we mean total string length of the braid. It is found that more than half of the crossings of a sufficiently large braid (in terms of crossing number and number of strings) are redundant. We analyse the different methods and say in what circumstances which method is to be favoured and conclude that minimum braid energy and minimum braid crossing number are substantially different measures of topological complexity for braids.

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## 1. Introduction

Topological constraints appear in many complex systems. In biology the amount of twisting and knotting of DNA molecules can affect molecular interactions and dynamics [15]. In polymer physics the degree of entanglement of the polymer filaments helps to determine the elastic properties of the polymer [2]. In astrophysics, applications involve the behaviour of magnetic fields (such as those found in stars and accretion disks) with complex topologies [20, 4, 5, 9, 21]. In dynamical systems theory, the time history of the system can be represented by a set of braided particle orbits; the topology of the braid reflects qualitative aspects of the dynamics [11, 8, 19, 16]. In turbulence theory the degree of entanglement of the vortex lines provides a statistical measure of flow properties; this measure is distinguished from most others used in turbulence by being based on the flow in real space rather than on the spectral transform of the flow in Fourier space. In statistical mechanics, braid and knot theory has significantly contributed to exactly solvable models via knot polynomials, for example [27]. Random knotting, as opposed to the random braiding discussed here, has also been investigated [23].

All these applications involve a set of curves (e.g. long molecules, magnetic or vortex lines) which are knotted, linked, or braided. Knot theorists have devoted great effort to classifying such objects. One important part of this effort concerns finding measures of complexity. This idea goes back at least as far as Tait, who first set out tables of different knot types [26]. Tait organized the knot tables according to a simple complexity measure, the minimum crossing number  $C_{min}$ . This number gives the minimum number of crossings of a knot as seen in any two dimensional projection.

There are two types of topological invariants. The first, sometimes called *isotopic invariants*, involve quantities that remain constant if we deform the set of curves. Examples include the Gauss linking integral, helicity integrals, and knot polynomials. The second type involves quantities which do change when the curves deform, but have a lower bound. This second type of invariant can be regarded as a measure of topological complexity [24] of which both crossing number and energy are examples.

This paper investigates the crossing number and energy for random braids. Braids consist of a set of curves stretching between two parallel planes. The endpoints of the curves are fixed but, between the two planes, the curves are free to move so long as they do not cross through each other. Braids are important in knot theory because (unlike knots) they can be readily classified using group theory [7]. They are also important in solar physics, as the field lines within a coronal magnetic loop are braided. (In fact, a coronal loop forms an arch with both ends in the photosphere. But a simple geometrical transformation straightens out the arch into a cylinder with ends on two parallel planes.)

Energy, of course, has the most immediate physical significance. For example, a solar magnetic loop usually stays close to the energy minimum (equilibrium) state consistent with the field topology. Sometimes this equilibrium becomes unstable; a rapid reconnection event changes the topology and energy is released in a flare. Crossing number, on the other hand, relates more directly to the geometry of the field lines. The

state of minimum crossing number may not be exactly the minimum energy state, but one may conjecture that they will be close. We can, in fact, find strict lower bounds for the energy of a magnetic field given its crossing number. This has been done for fields in a spherical geometry with closed field lines [13] and in a cylindrical geometry with braided field lines [4].

We can also consider continuous fields rather than knotted or linked curves, e.g. knotted fluid flows and magnetic configurations [17, 18, 13, 10, 4]. Crossing number can be defined for a continuous field by averaging the crossing number of all pairs of field lines [13, 4]. This average crossing number will have some positive minimum amongst all fields with the same field line topology. Minimum crossing number and minimum field energy will then both measure the topological complexity of the field. For example, a closed, knotted tube of magnetic flux will have a magnetic energy which generally increases with the  $C_{min}$  of the knot (and with internal twist of field lines inside the tube).

There has recently been a major effort to find the ideal shapes of knots. While the definition of "ideal" varies, the ideal shape is mostly obtained by minimizing some form of knot energy. Various energy functionals have been suggested for knotted curves [13, 15, 25]. These energy functionals have a positive minimum depending on the knot type analogous to minimum crossing number. Some theoretical questions arise from this work. For example, are the energy minima found using these approaches local or global minima? One would like an energy such that the minimum is global for any initial configuration. This does not seem to be possible, however [12]. Another important question is whether an energy minimum corresponds to the minimum of a more traditional measure of complexity, for example the crossing number. As mentioned above, it has been implicitly assumed in the literature that this is true, however we argue here on the basis of statistical results that this is not true. As mentioned above, energy can be defined in many ways and different energies behave differently. We consider energy to be the length of the strings in the braid.

The main purpose of this paper is to propose an efficient tool for finding minimal braid configurations. With this in mind, we first demonstrate how to generate random braids both algebraically and geometrically and how to convert between them in §2. In §3 and §4, we introduce the forces which will minimize the crossing number and the elastic energy respectively. An algebraic heuristic minimization is given in §5 and the results of computational experiments of all approaches are discussed in §6 together with theoretical comparisons. We conclude in §7.

## 2. Obtaining and Embedding Random Braids

For the results of our comparison of minimization strategies to be useful we discuss our approach of generating random braids in a way such that we obtain a representative selection of braids. First, we discuss how to obtain a random algebraic braid, then how to convert it into a geometrical braid and finally how to reverse this conversion.

### 2.1. Randomly Generating Algebraic Braids

An algebraic  $n$ -braid is a word over the generators of the braid group  $B_n$ , that is the set  $\{\sigma_i^{\pm 1}\}$  for  $1 \leq i < n$ . Given a number of strings  $n$  and a number of crossings  $c$ , there are clearly  $(2(n-1))^c$  algebraic braids possible. Not all of these braids are necessarily topologically distinct however. Two words in  $B_n$  represent the same braid if and only if one can be transformed into the other using the following relations

$$\sigma_i \sigma_i^{-1} = e, \tag{1}$$

$$\sigma_i \sigma_j = \sigma_j \sigma_i \quad |i - j| > 1, \tag{2}$$

$$\sigma_i \sigma_{i+1} \sigma_i = \sigma_{i+1} \sigma_i \sigma_{i+1} \tag{3}$$

where  $e$  is the identity in  $B_n$  (topologically  $e$  is the braid of no crossings; it consists of  $n$  vertical strings). The problem of determining whether two words are equivalent or not is known as the word problem, the most efficient algorithm for which was found by Birman, Ko and Lee [7] and runs with complexity  $O(nc^2)$ .

We may select a word at random from the  $(2(n-1))^c$  possibilities by choosing each of the  $c$  generators at random from the set  $\{\sigma_i^{\pm 1}\}$  for  $1 \leq i < n$ . The number of words in the set of the  $(2(n-1))^c$  possibilities corresponding to a particular braid will not, on average, depend on this braid; that is, the intersections of the equivalence classes of the represented braids and our set are, on average, of equal size. Thus the uniformly random word corresponds to a uniformly random braid.

### 2.2. Embedding Algebraic Braids

We describe how to determine the geometric braid which an algebraic braid represents in this section. If we select a random braid in the above algebraic manner, we must embed it in three-dimensional Euclidean space in order to use an energy minimizing algorithm on it.

An  $n$ -braid consists of  $n$  strings embedded in  $R^3$  and thus we may describe the braid by giving  $n$  vector functions  $\mathbf{x}_i(z, t)$  parametrised by the vertical  $z$  coordinate and time  $t$ . We construct these functions such that

$$\mathbf{x}_i(z, t) = (x_i(z, t), y_i(z, t), z). \tag{4}$$

The vertical component of the functions is assumed independent of time. This is needed only for efficient computer implementation of the model since it ensures that the points by which the functions would have to be approximated do not collect near the ends of the strings during the simulation, as they would without this constraint. We shall take the braid to lie between  $z = 0$  and  $z = 1$  and, in keeping with the definition of braid isotopy, the points  $\mathbf{x}_i(0, t) = \mathbf{x}_i(0)$  and  $\mathbf{x}_i(1, t) = \mathbf{x}_i(1)$  will be independent of time.

We will generate  $b$  points per crossing and string in order to represent the braid; thus there will be  $bc$  points per string in the braid. The position vector of the  $j^{th}$  point on string  $i$  is  $\mathbf{x}_i(j/bc, t)$ , which must be specified at time  $t = 0$ . If we are given a braid

word in the generators  $\sigma_i$ , we set

$$\mathbf{x}_i(0, 0) = (\delta_x(i - 1), 0, 0) \tag{5}$$

where  $\delta_x$  is a given parameter. The subsequent points will have a  $z$  coordinate between 0 and 1. We then read the first generator in the braid word and add  $b$  points to all strings not involved in the crossing which are vertically above the last set point. For the strings involved in the crossing, the  $x$  and  $z$  coordinates are simply straight lines exchanging the two strings over a vertical region of size  $1/c$ . The  $y$  coordinate is constructed from the Gaussian distribution

$$y_i(j/bc, t) = \pm \frac{\delta_x}{3} \exp\left(-120 \frac{[\alpha/2 - j\alpha/(b - 1)]^2}{\alpha^2}\right) \tag{6}$$

where  $\alpha^2 = \delta_x^2 + 1/c^2$  for  $0 \leq j \leq b - 1$ . The positive  $y$  coordinate is chosen for the overcrossing string and the negative  $y$  coordinate for the undercrossing string. See figure 2 for two examples.

It has been found in practice that this yields an aesthetically pleasing embedding of the braid. Physically, the Gaussian distribution is also intuitive because we assume the string to be elastic later. Numerically, it may be seen that the initial and final points of the Gaussian are always close enough to the straight segments of the braid that this does give a good distribution of points over the braid.

### *2.3. Extracting Geometric Braids*

In this section we describe how to reverse the process described in the last section. In our model, each point will move on a horizontal plane, the original vertical spacing between beads is preserved. Thus we can slice the final braid into  $bc - 1$  slices, which are the segments of the braid strings between two points. Given a position of the observer, it is then easy to extract the left-to-right order of the braid strings for each slice. At the start we label each string with a number increasing from 1 for the leftmost string to  $n$  for the rightmost string. The initial order is thus the identity permutation on  $n$  elements and each slice will have an associated permutation.

In this way we build up a list of permutations from the start to the end of the braid. If the permutation is the same as the one before it, no further generators need to be inserted into the braid word. If it is different, then we must insert a generator into the braid word. Suppose that strings  $i$  and  $j$  are switched in one transition between permutations. We must establish which string is closer to the observer on the current vertical level, which we can readily do. We must also determine which of  $i$  and  $j$  appears first in the permutation structure from the left and in which position it occurs. Suppose that  $i$  is found first in position  $k$  in the permutation and that  $i$  passes over  $j$ , then we must add the generator  $\sigma_k$  to the Artin word. If  $i$  passes under  $j$ , then we must add  $\sigma_k^{-1}$ .

If there is at most one transposition of elements in the permutation at every step, the translation is simple. If there are more than one, we must be careful to assess which

string crossed with which other string. This however may be done simply by checking which string was closest to a given string at the current vertical level. This leaves us with the remote possibility of a triple point, that is three strings crossing at once. This sort of crossing may be removed by a slight shift in the observer's position. However, a repulsive force which we will introduce later and keeps braids from overlapping effectively negates the possibility of triple points and so the only case of complex transitions left is several exchanges, which could be determined from the string positions themselves.

In practice, this recognition algorithm has worked well. For a given embedding of a topological braid, the crossing number depends upon the observer's position, in general. To take this into account, we rotate the observer around the braid and compute the braid word for many observation angles and choose the shortest braid word.

### 3. A Crossing Number Minimizing Force

Here, we will obtain a force which directly minimizes the crossing number of a braid for later comparison with the energy minimizing forces and the algebraic approach.

#### 3.1. Expressions for crossing number

Recall that a braid is represented by a set of  $n$  curves  $(x_i(z, t), y_i(z, t), z), i = 1, \dots, n, 0 \leq z \leq 1$ . By projecting the curves onto a vertical plane we can detect a number of crossings. Let the projection angle be  $\phi$ , with direction vector  $\mathbf{p}(\phi) = (\cos \phi, \sin \phi, 0)$ . Thus for  $\phi = 0$  the projection plane will be the  $x$ - $z$  plane. The crossing number  $C(\phi)$  will then be a function of  $\phi$ . If we distort the braid,  $C(\phi)$  will change. For fixed  $\phi$  we can use group theory to minimize  $C(\phi)$  over all possible deformations of the braid [5]. For  $n \leq 3$  an algorithm linear in the number of initial crossings is known [5] but no efficient algorithm for  $n > 3$  is known (see §5 for more details). Thus, it is worth it to pursue numerical relaxation methods similar to energy relaxation but specifically based on crossing number minimization.

The crossing number dependence on projection angle  $\phi$  can be removed by choosing the minimum all projection angles:

$$C_{min} \equiv \min_{\phi=0}^{\pi} C(\phi). \tag{7}$$

The crossing number is a sum over pairs:

$$C \equiv \sum_{ij} C_{ij} \equiv \sum_{i=1}^n \sum_{j=i+1}^n C_{ij} \tag{8}$$

where  $C_{ij}$  just counts crossings between strings  $i$  and  $j$ .

In addition to decomposing  $C$  into contributions from each  $ij$  pair, we can look at how  $C$  increases with  $z$ . Thus we will let  $C_{ij}(z_0)$  measure the crossings of strings  $i$  and  $j$  between  $z = 0$  and  $z = z_0$ . In this notation  $C_{ij} = C_{ij}(1)$ . Let  $\mathbf{x}_i(z) = (x_i(z), y_i(z), z)$  and define relative position vectors and angles

$$\mathbf{r}_{ij}(z) \equiv \mathbf{x}_j(z) - \mathbf{x}_i(z); \tag{9}$$

$$\theta_{ij}(z) \equiv \tan^{-1} \left( \frac{y_j(z) - y_i(z)}{x_j(z) - x_i(z)} \right). \quad (10)$$

We will let a prime denote differentiation by  $z$ , for example

$$\theta'_{ij}(z) \equiv \frac{d\theta_{ij}(z)}{dz} = \frac{\epsilon_{\alpha\beta} r^{\alpha} r'^{\beta}}{r^2} \quad (11)$$

where  $\epsilon_{\alpha\beta}$  is the Levi-Civita tensor and  $r'^{\beta} = dr^{\beta}/dz$ .

If strings  $i$  and  $j$  wind around each other near some height  $z$  then  $|\theta'_{ij}(z)| > 0$ . Also, there will be some projection angles  $\phi$  where the strings will be seen to cross (in fact, a crossing will be seen at height  $z$  if  $\mathbf{p}(\phi) = \mathbf{r}_{ij}(z)$ ). It can be shown [4] that

$$\frac{dC_{ij}(z)}{dz} = \frac{1}{\pi} |\theta'_{ij}(z)|. \quad (12)$$

We now have

$$C = \frac{1}{\pi} \sum_{ij} \int_0^1 |\theta'_{ij}(z)| dz. \quad (13)$$

### 3.2. Derivation of the crossing number force

Suppose we employ  $C$  as a potential energy term in a Lagrangian for  $n$  strings. Varying the Lagrangian will give an equation of motion with a force corresponding to  $C$ . Adding a strong damping force will then give us dynamics which can be followed numerically to relax the strings to an ‘equilibrium’ state, i.e. a state which is at least a local minimum of  $C$ . Let  $\mu$  be mass per unit length and consider a time interval  $T$ . The Lagrangian action should then be

$$S = \int_0^T (K - \lambda C) dt \quad (14)$$

where

$$K = \frac{1}{2} \int_0^1 \mu \left( \frac{d\mathbf{x}(z, t)}{dt} \right)^2 dz \quad (15)$$

is the kinetic energy term and  $\lambda$  is a constant. The  $K$  variation (at height  $z$ ) gives the usual acceleration term  $\mu d^2\mathbf{x}/dt^2$ .

However, the variation of  $C$  will not work without modification. There are two problems. First, there is the presence of the absolute value in equation (13); derivatives will be ill defined at singular points where  $|\theta'_{ij}(z)| = 0$ . In between these singular points we could replace the absolute value by a factor  $\pm 1$ . However, if we do so an even nastier problem arises:  $\pm d\theta_{ij}(z)/dz$  is a total differential. But the variation of a total differential vanishes apart from boundary terms.

Fortunately, there is a simple way out of these difficulties: replace  $|\theta'_{ij}|$  with

$$X_{ij} = \sqrt{(\theta'_{ij})^2 + \epsilon^2}. \quad (16)$$

Later we can let  $\epsilon \rightarrow 0$ . Let  $\mathbf{F}_{ij}$  be the force on string  $i$  due to string  $j$  associated with the potential  $\lambda X_{ij}$ . A variation in  $\delta\mathbf{x}_i$  and  $d(\delta\mathbf{x}_i)/dz$  leads to

$$\mathbf{F}_{ij} = -\lambda \left( \nabla_i X_{ij} - \frac{d}{dz} \nabla'_i X_{ij} \right); \quad \nabla'_i \equiv \frac{\partial}{\partial \mathbf{x}'_i}. \quad (17)$$

It simplifies the calculation to note that

$$\theta'_{ij} = \mathbf{x}'_i \cdot \nabla_i \theta_{ij} + \mathbf{x}'_j \cdot \nabla_j \theta_{ij}. \quad (18)$$

so, evaluated at the point  $(\mathbf{x}_i, z)$

$$\nabla'_i \theta'_{ij} = \nabla_i \theta_{ij}. \quad (19)$$

Thus, suppressing the  $i, j$  labels,

$$\frac{d}{dz} \nabla' X = \frac{d}{dz} \left( \frac{\theta' \nabla' \theta'}{X} \right) = \frac{d}{dz} \left( \frac{\theta' \nabla \theta}{X} \right) \quad (20)$$

$$= \frac{1}{X} \left( \theta'' \nabla \theta + \theta' \nabla \theta' - \frac{\theta'^2 \theta'' \nabla \theta}{X^2} \right) \quad (21)$$

$$= \frac{\theta' \nabla \theta'}{X} - \epsilon^2 \left( \frac{\theta'' \nabla \theta}{X^3} \right). \quad (22)$$

The first term here cancels the  $\nabla X$  term in (17). Equation (17) becomes

$$\mathbf{F} = -\lambda \epsilon^2 \left( \frac{\theta'' \nabla \theta}{X^3} \right). \quad (23)$$

We let  $\lambda = \epsilon^{-2}$  and let  $\epsilon \rightarrow 0$ . Summing over all strings  $j$  gives the crossing force on string  $i$ ,

$$\mathbf{F}_i = - \sum_{j \neq i} \left( \frac{\theta_{ij}'' \nabla \theta_{ij}}{|\theta'_{ij}|^3} \right). \quad (24)$$

### 3.3. Simulation Considerations

For numerical purposes it may be wise to retain a small  $\epsilon$  as a softening parameter, i.e. replace  $|\theta'_{ij}|^{-3}$  by  $X_{ij}^{-3}$ . This will prevent the force blowing up near  $\theta'_{ij} = 0$ . Being as explicit as possible, the force on the point  $\mathbf{x}_i(z)$  of the braid is

$$\mathbf{F}_i(z) = -\lambda \epsilon^2 \sum_{j \neq i} \frac{[(2r' \mathbf{r}' - r \mathbf{r}'') \cdot (\hat{z} \times \mathbf{r})] (r \hat{z} \times \mathbf{r})}{((\mathbf{r}' \cdot \hat{z} \times \mathbf{r})^2 + r^4 \epsilon^2)^{3/2}} \quad (25)$$

where  $\mathbf{r} = \mathbf{r}_{ij}(z)$ ,  $r = \sqrt{\mathbf{r} \cdot \mathbf{r}}$ ,  $r' = (\mathbf{r}' \cdot \mathbf{r})/r$  and  $\hat{z}$  is the unit vector in the  $z$  direction.

What we observe in practice is that this force causes the strings of the braids to move apart from each other and prevents equilibrium from being reached. Thus we apply the additional constraint that

$$\sum_i \mathbf{x}_i(z) \cdot \mathbf{x}_i(z) \leq R \quad (26)$$

where  $R$  is a parameter of the model. After imposing this we can agree to have reached equilibrium if and only if the maximum distance moved by a point on the braid at any timestep is less than another parameter  $\eta$ . We discuss the consequences of the choices for these two parameters in §6.



#### 4. Energy relaxation

Two energy minimizing approaches were tested with respect to minimizing crossing number. Both minimize elastic energy but they differ essentially in the way the elastic force is implemented: a nearest neighbour approximation (the *constrained* elastic force) versus a tension force depending on the curvature (the *curvature* elastic force). As these forces treat the strings as elastic, they pull the strings closer together and would cause them to intersect and thereby change topology. In order to prevent this, we shall introduce a repulsive force  $\mathbf{F}_i^{(r)}(z, t)$  to the elastic force  $\mathbf{F}_i^{(e)}(z, t)$  to make up the total force which we use to simulate the braids,

$$\mathbf{F}_i(z, t) = \mathbf{F}_i^{(e)}(z, t) + \mathbf{F}_i^{(r)}(z, t). \quad (27)$$

For the purposes of the repulsive force, we imagine the strings to be of circular cross-section with diameter  $d$ . We define this repulsive force by

$$\mathbf{F}_i^{(r)} = \sum_{k \neq i} \begin{cases} 0 & \text{for } |\mathbf{x}_i - \mathbf{x}_k| > d \\ \frac{\mathbf{x}_i - \mathbf{x}_k}{|\mathbf{x}_i - \mathbf{x}_k|} (d - |\mathbf{x}_i - \mathbf{x}_k|) & \text{otherwise.} \end{cases} \quad (28)$$

Since the repulsive force is non-zero in only a limited number of cases, computing it is relatively fast as opposed to using a potential function.

##### 4.1. The Constrained Elastic Force

If we imagine the points of the geometric braid to be beads of mass  $m$  connected by springs of spring constant  $k$  and zero natural length, the elastic force on the  $j^{\text{th}}$  bead due to the two springs attached to it is (considering only nearest neighbour interactions)

$$\mathbf{F}_i^{(e)} \left( \frac{j}{bc}, t \right) = -k \left( 2\mathbf{x}_i \left( \frac{j}{bc}, t \right) - \mathbf{x}_i \left( \frac{j+1}{bc}, t \right) - \mathbf{x}_i \left( \frac{j-1}{bc}, t \right) \right). \quad (29)$$

This is the constrained elastic force. As given in equation (29) the constrained elastic force is a finite difference scheme for the differential equation

$$\mathbf{F}_i^{(e)}(z, t) = \frac{k}{b^2 c^2} \frac{d^2 \mathbf{x}_i(z, t)}{dz^2}. \quad (30)$$

Once the total force is known, we apply it to the beads

$$\mathbf{x}_i(z, t + \delta t) = \mathbf{x}_i(z, t) - \frac{\mathbf{F}_i(z, t)}{2m} (\delta t)^2. \quad (31)$$

We have neglected the fact that beads should acquire a velocity after the force is first applied. Ignoring this velocity serves to heavily damp the system, which is desirable for the simulation. A proof that this is acceptable on a fundamental level is given in [3] and references therein. The force is applied for a duration of  $\delta t$  after which the beads will have moved a certain distance. The maximum distance moved by any bead in the whole braid during any step  $r(t)$  decreases monotonically to zero since the system is heavily damped due to the neglect of the velocity and that fact that the springs have natural length zero. If no bead moves more than a minimum distance of  $\eta$ , we may

terminate the simulation because in all subsequent steps of the simulation no bead will move further than  $\eta$ . Thus the end of the simulation is reached when  $r(t) \leq \eta$ .

A given braid will determine  $n$  and  $c$  but we have endowed the model with a number of parameters: The string diameter  $d$ , the number of beads per crossing  $b$ , the mass of a bead  $m$ , the spring constant  $k$ , the separation of the strings  $\delta_x$ , the duration of the force  $\delta_t$  and the equilibrium distance  $\eta$ . Based on computer experiments we make choices for some of these

$$d = \frac{\delta_x}{6}, \quad \delta_t^2 = 2m, \quad \eta = \frac{\delta_x}{10^5}, \quad (32)$$

$$0.1 \leq k < 0.5, \quad 10 \leq b \leq 50, \quad \delta_x = \frac{1}{n-1}. \quad (33)$$

These values have been found to give good results. With increasing  $k$ , fewer steps are required to reach equilibrium but  $k < 0.5$  must be observed because otherwise the repulsive force will not be very successful. Accuracy increases with  $b$  but so does the computation time. Setting  $b < 10$  will fail because the distances between beads are large enough for the repulsive force not to guarantee isotopy, however  $b > 50$  is unnecessarily expensive in terms of time.

#### 4.2. The Curvature Elastic Energy

The other way of dealing with elastic relaxation is to treat each string in the braid as a bungee cord, subject to a tension force which aims to reduce any curvature and bring back the string to a straight configuration (given the constraint on the end points). Indeed, as already remarked above, a repulsive force among the strings is needed to counteract the tension in order to maintain the topology unchanged.

An expression for the elastic force can be readily obtained by using a variational approach similarly to what has been done in §3. In fact, since this force tends to minimize the length of the bungee cord, we can employ the total length of the strings as a potential energy term in the Lagrangian action  $S$  describing the braid (14)

$$S = \int_0^T (K - \lambda L) dt \quad (34)$$

where

$$K = \frac{1}{2} \int_0^1 \mu \left( \frac{d\mathbf{x}(z, t)}{dt} \right)^2 dz \quad (35)$$

is the kinetic energy term,  $\lambda$  is a constant,

$$L = \int ds, \quad (36)$$

and  $ds$  is the infinitesimal arclength along each string ( $ds^2 = dx^2 + dy^2 + dz^2$ ). The variation of the action (34) provides an equation of motion which is the well-known equation for the vibrating cord. Any perturbation from the equilibrium position is opposed by a restoring force proportional to

$$\mathbf{F} \propto \frac{d^2 \mathbf{x}}{ds^2} \quad (37)$$

and always directed along the radius of curvature. However, we are not allowed to perform any displacement along the  $z$  direction because the braid is represented by a set of curves  $(x_i(z, t), y_i(z, t), z), i = 1, \dots, n, 0 \leq z \leq 1$ . Thus, instead of (37), we use the *horizontal* force

$$\mathbf{F}_i^{(e)} = \frac{d^2 \mathbf{x}_i}{ds^2} - \frac{d^2 z}{ds^2} \frac{d\mathbf{x}_i}{dz}. \quad (38)$$

This is the curvature elastic force. This force moves the curve as the full curvature force would; the second term gives an extra horizontal displacement to the string which compensates for the effect of the missing vertical force. Once its value is known in each point of the braid and cumulated with the repulsive term, advancing in time is achieved according to the same scheme as above (31).

The actual evaluation of the curvature elastic force involves the computation of second and first order spatial derivatives. In this case, then, we found it convenient to use a grid of  $N$  evenly spaced points along the  $z$  axis and ordinary centered difference. Stopping criteria for the numerical simulation of energy relaxation were defined as explained in the previous section. We kept  $N = 200$  in all the cases presented in the following, while the choice of the other parameters was

$$d = \delta_x, \quad \delta_t^2 = 2m, \quad (39)$$

$$\eta = \frac{\delta_x}{10^5}, \quad \delta_x = \frac{1}{20}. \quad (40)$$

## 5. Algebraic Minimization

Recall that the braid group  $B_n$  is defined by

$$B_n = \langle \{\sigma_i\} : 1 \leq i < n; \quad (41)$$

$$\sigma_i \sigma_j = \sigma_j \sigma_i \quad |i - j| > 1; \sigma_i \sigma_{i+1} \sigma_i = \sigma_{i+1} \sigma_i \sigma_{i+1} \rangle. \quad (42)$$

We define the *fundamental braid*  $\Delta_n$  by

$$\Delta_n = \sigma_1 \sigma_2 \cdots \sigma_{n-1} \sigma_1 \sigma_2 \cdots \sigma_{n-2} \cdots \sigma_1 \sigma_2 \sigma_1. \quad (43)$$

The fundamental braid is very important in braid theory and among many properties it has the following

$$\Delta_n \sigma_i \approx \sigma_{n-i} \Delta_n. \quad (44)$$

An  $n$ -braid  $A$  of  $c$  crossings is a word in  $B_n$  of word-length  $c$ , so the general form of  $A$  is

$$A = \sigma_{a_1}^{\epsilon_1} \sigma_{a_2}^{\epsilon_2} \cdots \sigma_{a_c}^{\epsilon_c} \quad \epsilon_k = \pm 1, 1 \leq a_k < n, \forall k : 1 \leq k \leq c. \quad (45)$$

Consider an  $n$ -braid  $A$  of the form given in equation (45). Suppose we wish to find the  $n$ -braid  $A_m$  equivalent to  $A$  such that the length  $L(A_m)$  of  $A_m$  is minimal over the equivalence class of  $A$ . It has been shown [22] that this question is NP-complete and hence computationally difficult (if  $P \neq NP$ , it is intractable). The following presents a heuristic algorithm for getting close to  $A_m$ . We begin with the leftmost generator of  $A$  and attempt to move it to the right using both braid group operations. If we can cancel

it along the way, we do and if we can not, we move it back to where it started. In this way, we proceed to move all the generators as far to the right as possible. Then we begin at the end and move each generator as far to the left as possible in the same manner. This algorithm will always produce an equivalent braid  $A'$  such that  $L(A') \leq L(A)$ . We consider  $L(A)$  generators and move them  $O(L(A))$  moves to the right and left. Thus this algorithm takes  $O(L(A)^2)$  time and constant memory. In fact we move a particular generator at most  $L(A)$  generators and this is only for the case when all the other generators commute with it, thus the average case complexity is likely to be close to linear in  $L(A)$ .

This algorithm will not produce a minimum length representative in all cases because it can not unravel complex crossings. To get to the minimum length would require more subtle transformations than just movements to the right or left, which topologically correspond to pulling the strings apart from underneath the crossing. However, as computer experiments show, it does do quite well.

Let us calculate an upper bound to the reduction ratio obtained by this method as a function of  $n$  and  $c$ . To calculate these, consider the likelihood that a particular generator will be followed by its inverse, which is just  $Q_0 = 1/2(n-1)$ . The probability  $Q_j$  that a generator and its inverse are separated by  $j$  generators through which either can be moved is the corresponding probability for  $j = 1$  to the power  $j$ . We require the number of braids of length 1 which may be generated so as not to contain the generator interfering with the movement of generator  $\sigma_i$ . If  $i = 1$  or  $n - 1$ , this is  $2(n - 3)$  and  $2(n - 4)$  otherwise. Thus

$$Q_j = \left[ \frac{2(n-4) \left( \frac{2(n-1)-2}{2(n-1)} \right) + 2(n-3) \left( \frac{2}{2(n-1)} \right)}{2(n-1)} \right]^j Q_0 \quad (46)$$

$$= \left[ \frac{n^2 - 5n + 5}{(n-1)^2} \right]^j Q_0 \quad (47)$$

The final factor of  $Q_0$  is present because the generator after the sequence of  $j$  generators is required to be inverse of the original generator, an event with probability  $Q_0$ . To get the total probability  $Q$  of being able to cancel a generator  $\sigma_i$  with its inverse by simple exchange movements over the length  $j = 0, 1, \dots$ , we must sum these probabilities in order weighted by the probability that their predecessors did not happen. Thus

$$Q = Q_0 + (1 - Q_0)Q_1 + \dots + \prod_{k=0}^{j-1} (1 - Q_k)Q_j + \dots \quad (48)$$

Note that since the exchange move is not allowed for  $n = 3$ ,  $Q = Q_0$  for  $n = 3$ . The reduction ratio  $R$  which occurs as a consequence of this probability is  $R = 1 - 2Q$  since each time that the event happens two generators may be cancelled. Note that in this calculation we have considered the probability that a generator can be moved next to its inverse in the word using only the far commutation relation that  $\sigma_i \sigma_j = \sigma_j \sigma_i$  for  $|i - j| > 1$  in a long braid. The heuristic algorithm however uses both braid group moves to attempt to move generators next to their inverses. Thus  $R$  is an upper bound for the reduction ratio achieved by the heuristic algorithm as the braid becomes long.

In §6 we present the results of the algebraic reduction of a large number of braids but a few comments about the efficiency of the algorithm are in order. The only exact algorithm to minimize braid is valid only for  $n \leq 3$  [5] and by comparing this heuristic to this exact algorithm, we find that the heuristic finds a braid the length of which is within five percent of the length found by the exact algorithm and that it reaches the actual minimum in 0.005 of all cases. This shows that the heuristic is quite effective for  $n = 3$  (note that reduction for  $n = 1, 2$  is trivial since  $B_1, B_2$  are free groups).

## 6. Some numerical results

Extensive numerical calculations were made in order to compare the above methods of finding the minimum crossing number of a braid. A large selection of random braids were generated as discussed in §2 and then simulated using all four different methods described above. In §6.1, the comparison is made in terms of the ratio  $\alpha$  of final crossing number to initial crossing number as a function of number of strings and number of initial crossings. When braids were reduced using forces, we chose the final braid by using the translation algorithm described in §2.3 for many angles around the vertical axis of the braid and isolated the braid with minimum crossing number. The reason for this is that the position of the observer affects the crossing number seen from that perspective. In §6.2, we compare the efficiency of our methods, giving an estimate of the algorithmic complexity in terms of the number of strings  $n$  and the other free parameters. Finally in §6.3, we focus on the effect of the three forces on the energy (defined by total length) of the braids, by comparing the final equilibrium state with the initial configuration.

### 6.1. Efficacy Analysis

Table 1 lists the results of our experiments in computing  $\alpha = C_{min}/C(0)$ . It has been found that  $\alpha$  decreases with increasing the initial number of crossings  $C(0)$  but quickly approaches a limiting value. In §5, we have calculated an upper bound for  $\alpha$  using the algebraic method of reduction as the initial crossing number  $C(0)$  gets large. Further investigation shows that if  $C(0) = 10n$  the resultant  $\alpha$  is virtually at the limiting value, so that it is this initial length that was chosen for this simulation since computation time is a very real issue here. Given a value for  $n$  and a minimizing method, we generated a statistical ensemble of 1000 braids, with the same number of crossings  $C(0)$  and number of strings  $n$  but otherwise randomly embedded, and we evolved them in time as long as the equilibrium constraint, described in the previous sections, was satisfied. We then computed a distribution of reduction ratios  $\alpha$ , which turned out to be a Gaussian distribution. In Table 1 are reported the mean values obtained from this analysis, with an error of one standard deviation.

Except for the 3-braid, the average values in Table 1 suggest that the crossing number force is by far the best, among the methods analyzed, in reducing the crossing number. This result was somewhat expected because of the way this force was derived.

**Table 1.** Reduction ratios  $\alpha = C_{min}/C(0)$  as a function of the number of strings  $n$ .

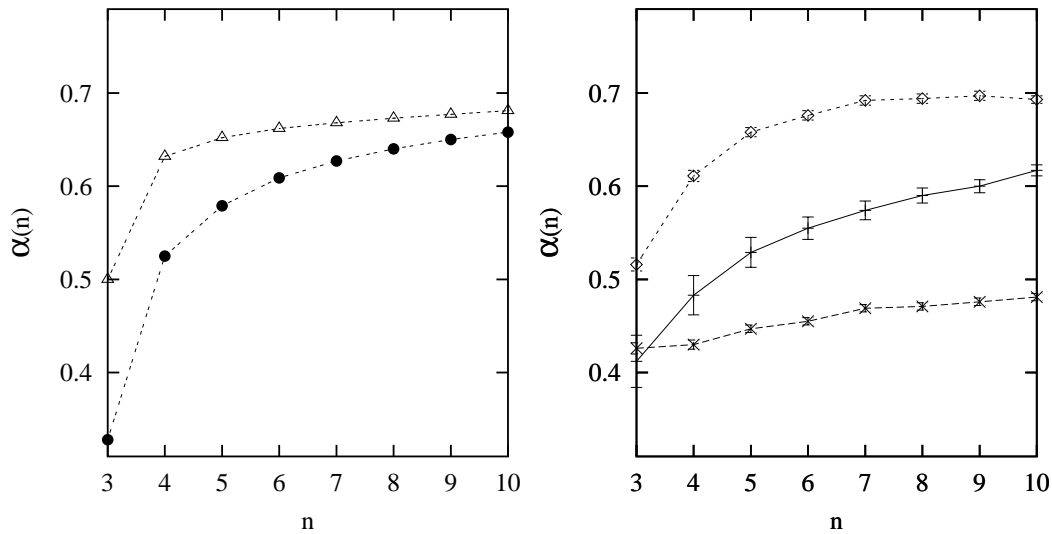
$n$	Heuristic	Heuristic	Constrained	Curvature	Crossing
	Heuristic	Bound	Elastic	Elastic	Force
3	0.328	0.500	$0.412 \pm 0.028$	$0.516 \pm 0.007$	$0.426 \pm 0.006$
4	0.525	0.632	$0.483 \pm 0.021$	$0.611 \pm 0.006$	$0.430 \pm 0.005$
5	0.579	0.652	$0.529 \pm 0.016$	$0.658 \pm 0.005$	$0.447 \pm 0.004$
6	0.609	0.662	$0.555 \pm 0.012$	$0.676 \pm 0.005$	$0.455 \pm 0.004$
7	0.627	0.668	$0.574 \pm 0.010$	$0.692 \pm 0.005$	$0.469 \pm 0.004$
8	0.640	0.673	$0.590 \pm 0.008$	$0.694 \pm 0.005$	$0.471 \pm 0.004$
9	0.650	0.677	$0.600 \pm 0.007$	$0.697 \pm 0.005$	$0.476 \pm 0.004$
10	0.658	0.681	$0.617 \pm 0.006$	$0.693 \pm 0.004$	$0.481 \pm 0.004$

However, it is still worth noticing that it produces reduction ratios at least 15% smaller than the other methods and even 30% smaller than the curvature elastic force. It is interesting that the heuristic algebraic method lies roughly between the two elastic approaches with the constrained elastic being the clear winner.

In Fig. 1, for a better comparison, we show the average reduction ratios  $\alpha$  as a function of the number of string  $n$ . On the left, the results obtained by the heuristic algebraic algorithm are plotted with their correspondent bounds (column 2 and 3 in Table 1). On the right, ratios from constrained and curvature elastic relaxation are displayed with ratios from crossing number force relaxation (column 4, 5 and 6 in Table 1), all with error bars. All the curves exhibit a steep growth followed by a slowly increasing phase, thus suggesting an overall logarithmic behaviour. In one case, namely the curvature elastic relaxation (diamond in the right panel of Fig. 1), we observe a saturation of the reduction ratio to a limiting value  $\alpha_c \sim 0.69$ , even if we cannot conclude this is an asymptotic value due to the relatively small maximum number of strings ( $n = 10$ ) we have achieved in this simulation.

## 6.2. Efficiency Analysis

Having compared by how much we may shorten an average braid  $A$ , we ask how long this will take for the various methods. We will answer this by giving the complexities of all the methods and comparing them by this and their actual relative running times. The algebraic method, as stated before, has complexity  $O(L(A)^2)$  independent of  $n$ . For each of the forces, we must compute and apply the force for each point on the braid. For the repulsive force we need only compute it for the points on the same level for all other strings. If we use  $b$  points per crossing and string for the simulation ( $nbL(A)$  points in total), the complexity per timestep is clearly  $O(n^2bL(A))$ . The number of timesteps required depends upon our equilibrium condition. As described above we compute the maximum distance moved by any point on the braid and we terminate the simulation if



**Figure 1.** Reduction ratios  $\alpha = C_{min}/C(0)$  as a function of the number of strings  $n$ . On the left, we display ratios obtained by using the algebraic algorithm ( $\bullet$ ) and their correspondent bounds ( $\triangle$ ); on the right, ratios are from numerical experiments with global elastic force ( $\diamond$ ), local elastic force ( $+$ ) and crossing number force ( $\times$ ). For the data, refer to Table 1.

this is less than the equilibrium parameter  $\eta$  (for practical purposes a maximum number of timesteps must, in general, also be imposed for certain awkward cases). It would seem intuitive that if  $\eta$  is chosen optimally, the number of steps required would be of order  $n$ . Thus giving the optimal model a complexity of  $O(n^3bL(A))$ .

In spite of this, there seems to be no general method to estimate an optimal  $\eta$  and so we are not able to obtain the optimal complexity in practice. The constrained elastic force and the repulsive force vary linearly in the coordinates of the points and the difference at any timestep between the coordinates is exactly the force (see our choices of parameters in equations (32) and (33)). Thus the number of timesteps increases linearly with  $1/\eta$  giving it a complexity of  $O(n^2bL(A)\eta^{-1})$ .

In the case of the curvature elastic relaxation, the force acting on any point of a certain string depends on all the points belonging to the same string. For what concerns the stopping parameter  $\eta$ , dimensional analysis suggests a dependence as before, namely on  $\eta^{-1}$ . Thus, the complexity for the global elastic force is  $O(nb^2L(A)^2\eta^{-1})$ . Since this force is always implemented together with the repulsive force, whose complexity scales with  $n^2$ , the total complexity is identical to that of the constrained elastic energy.

The crossing force is calculated as a sum over all other strings, that is that the complexity of each timestep is  $O(n^2b^2L(A)^2)$ . The crossing force has two additional parameters to  $\eta$ , namely  $\epsilon$ , the infinitesimal parameter introduced in (16) to avoid singularities, and  $R$ , the maximum square distance that the sum of the points on any

horizontal plane are allowed to have. From the form of the force in equation (25) we see that it is of order  $\lambda r^{-1}\epsilon^{-1}$ . The results presented in this paper have been found by using  $\lambda \sim \epsilon^0$  and  $\epsilon = 0.05$ . Clearly  $\epsilon$  too close to zero is not acceptable because of the force blowup at  $\epsilon = 0$ . Too large  $\epsilon$  is also unacceptable since the force becomes too strong and the points move too far at each timestep to preserve continuity of the braid string; this transition seems to occur when  $\epsilon$  becomes greater than 0.5. As far as we have investigated the choice of free parameters, these values for  $\lambda$  and  $\epsilon$  can be assumed as optimal values. Therefore, acceptable final states are reachable in  $\sim \eta^{-1}\epsilon^{-1}$  timesteps giving the algorithm a total time complexity of  $O(n^2b^2L(A)^2\epsilon^{-1}\eta^{-1})$ . The complexity seems to be independent of  $R$ .

We note in passing that both for the curvature elastic force and the crossing number force we actually used a grid of  $N = 200$  evenly spaced points along each string: in this case, the factor  $bL(A)$  simply must be read as  $N$  in the complexity estimate.

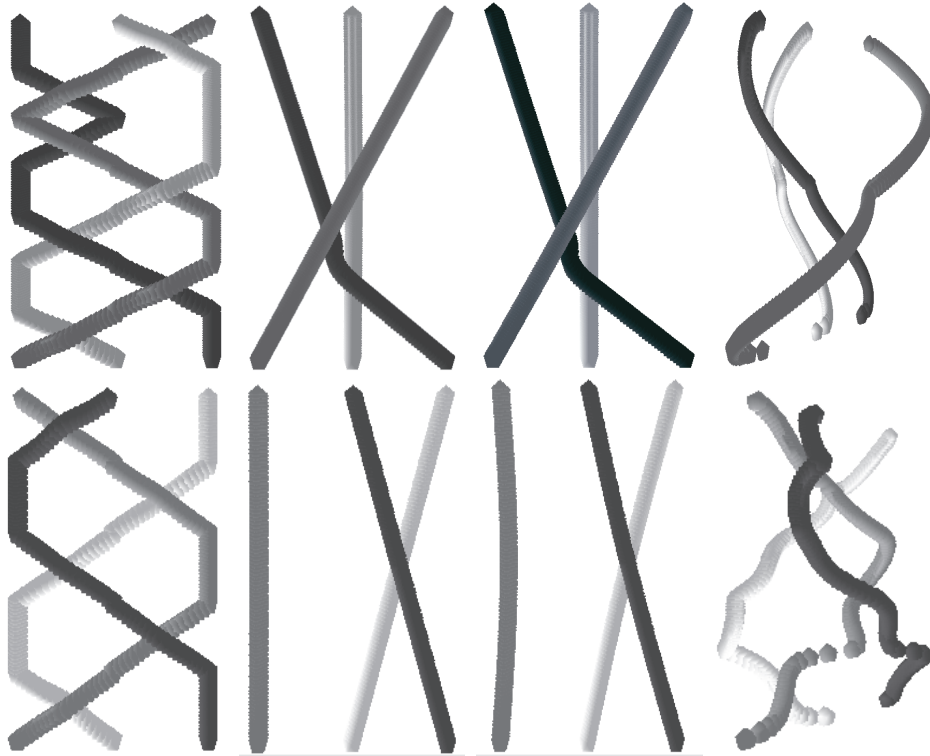
It's worth stressing that the actual amount of computation time required for the minimum crossing force is the largest. The algebraic algorithm is much faster than the elastic energy simulations in practice even though the parameter  $b$  can essentially be regarded as constant. The reason for this seems to be that the average case complexity for the heuristic is very close to linear.

### 6.3. Energy Analysis

As a final step in our comparison, we present results concerning the energy of the final braid. We limit ourselves to the three relaxing methods, since any energy estimate depends on the actual configuration of the braid in the embedding space. In fact, we took the total length of the braid to be its energy. This choice, besides being the simplest and most natural, has the advantage to give us a qualitative idea of the physical configuration of the final braid. Consider the braid  $\sigma_1\sigma_2\sigma_1^{-1}\sigma_2\sigma_1^{-1}\sigma_1\sigma_2^{-1}$ . In Fig. 2, we display the initial embedding and the final configuration of this braid after it has been relaxed by our forces. We note great similarity between the elastic energy approaches and a marked difference between the elastic and crossing number forces. The crossing number force, while driving the strings outward (to greater total braid energy) achieves a more balanced braid. There is a curious feature in the final configuration of a braid relaxed under the crossing number force which can be seen in the figure. The parts of the braid which are close (vertically) to a crossing are closer to the vertical centre of the braid than the rest of the string. The elastic forces, by construction, draw the braid in on itself and thus create a braid of lower energy which sometimes results in trapping crossings; this is the main reason why the elastic approach will not, in general, actually reach the minimal length of the braid. Fig. 2 displays the same four pictures for the braid  $\sigma_1\sigma_2^{-1}\sigma_1^{-1}\sigma_2^{-1}\sigma_1$  also in order to make more apparent the features of the forces.

Table 2 gives the mean values of the final energy for the constrained and curvature elastic force as well as the minimum crossing force, obtained from the same set of data above. For the sake of comparison, the mean initial energy of each ensemble of randomly





**Figure 2.** This figure gives the initial embedding and the final configuration after the local, global and crossing number forces have been applied for the two braids  $\sigma_1\sigma_2\sigma_1^{-1}\sigma_2\sigma_1^{-1}\sigma_1\sigma_2^{-1}$  and  $\sigma_1\sigma_2^{-1}\sigma_1^{-1}\sigma_2^{-1}\sigma_1$  respectively. We see great similarity between the elastic approaches but substantial differences between them and the crossing number force. Note that the diagrams for the crossing number force have been rotated by  $\pi/4$  to make more apparent the curious deformations of the strings. (The images were generated using BraidLink, a software program written by the first author.)

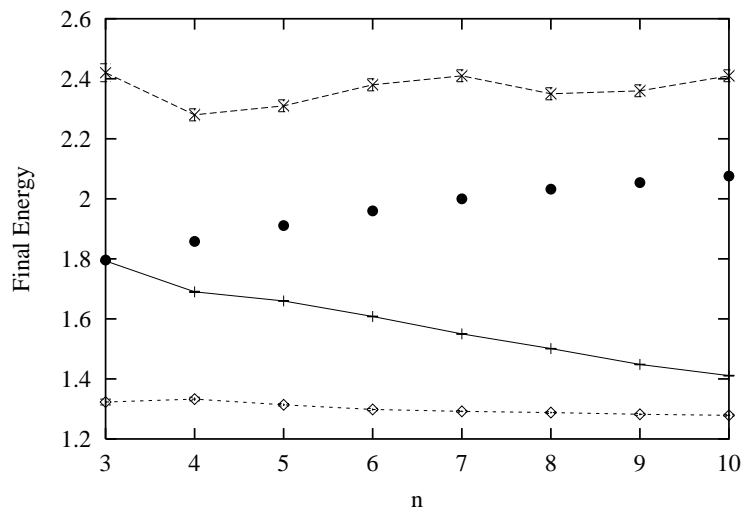
generated braids is given in the second column. Since the total length depends upon the number of strings, we have divided the final energy by the number of strings. Note that we have defined a geometrical braid to lie between the planes  $z = 0$  and  $z = 1$  so that this is already normalised. Thus the minimum possible energy of any  $n$ -braid is 1.

As expected, the energy is systematically increased by the crossing number force (see in Fig. 3 crosses versus bullets). Besides, the fact that we confine the physical braid in a cylinder in order to prevent the occurrence of singularities, imposes a limit on the final energy, which more or less oscillates about a fixed value. On the contrary, the constrained and curvature elastic forces reduce the energetic content of the braid. While the curvature force reduces the energy more effectively than the local, the descent of energy as a function of  $n$  is steeper for the local energy (see Fig. 3) and so we may expect an intersection of these methods at about  $n = 13$ . Note that the mean initial energy shows a slight dependence on  $n$ , due to the embedding procedure we use.

Once a minimal configuration has been reached, one may wish to know whether it is a local or a global minimum. This is a very difficult question to answer and we

**Table 2.** Total length per string.

$n$	Initial Energy	Local Elastic	Global Elastic	Crossing Force
3	$1.796 \pm 0.001$	$1.793 \pm 0.003$	$1.323 \pm 0.010$	$2.42 \pm 0.03$
4	$1.858 \pm 0.001$	$1.690 \pm 0.002$	$1.333 \pm 0.006$	$2.28 \pm 0.02$
5	$1.911 \pm 0.001$	$1.660 \pm 0.001$	$1.314 \pm 0.004$	$2.31 \pm 0.02$
6	$1.960 \pm 0.001$	$1.608 \pm 0.001$	$1.298 \pm 0.004$	$2.38 \pm 0.02$
7	$2.000 \pm 0.001$	$1.550 \pm 0.001$	$1.292 \pm 0.003$	$2.41 \pm 0.02$
8	$2.032 \pm 0.001$	$1.501 \pm 0.001$	$1.288 \pm 0.003$	$2.35 \pm 0.02$
9	$2.054 \pm 0.001$	$1.448 \pm 0.001$	$1.282 \pm 0.003$	$2.36 \pm 0.02$
10	$2.076 \pm 0.001$	$1.411 \pm 0.001$	$1.279 \pm 0.003$	$2.41 \pm 0.02$



**Figure 3.** The total length per string is displayed here as a function of the number of strings for the global (×) and local (+) elastic energies and the crossing number force (×) as well as the initial energy before relaxation (●).

have not endeavored to do so. However, because of the constraint that the endpoints of the braid may not move, we may safely say that the number of distinct local minima is finite and low.

## 7. Conclusions

We have investigated, by means of computer simulation, different methods to reduce the crossing number of a braid over its equivalence class. As a group theoretical question, this problem is difficult (if the minimum is to be found [22]) but can be profitably approached using a heuristic algorithm presented above. A braid can also be regarded as a topological object divested of this algebraic approach. Here the strings may move

(except the endpoints) in the embedding manifold without crossing each other. For algorithmic purposes a systematic way to move the strings must be found based on certain principles. Two of our approaches centre on a physical model of the strings as elastic strings made of flexible material. Elasticity may be modelled using a nearest neighbour or curvature approach, both of which were investigated. Another way to systematically move the strings is to construct a force not based on a physical idea but by using the crossing number (as an integral) as a potential in a Lagrangian. This last approach has proved to be the most successful in terms of finding the shortest braid, on average. It is however the most time consuming method. The algebraic approach, while only third (out of the four methods) in reduction efficacy, is the fastest by far.

In many applications, the braid is already an embedded topological object and not an element of the braid group. Here the two energy methods find their application as they are the only physically relevant methods. In solar physics, for example, the magnetic field lines may be modelled as braids. These seem to behave as elastic configurations over time. It must be mentioned that the endpoints of these braids do move but in a random fashion. Research about this added complication is in progress. In physical applications, we are most concerned about the energy of a braided configuration and the elastic model seems to be the most realistic for a variety of applications. While the constrained approach is more successful in terms of crossing number, the curvature fares better in an energetic sense.

What has clearly emerged from the discussion above is that minimum energy and minimum crossing number for braids are different things. While reducing energy does also reduce crossing number, reducing crossing number does not necessarily reduce energy and crossing number may be reduced much further after the minimum energy configuration has been reached. Thus, it is clear that the elastic approaches terminate in a *local* minimum as far as the equivalence class of the initial braid is concerned. From the point of view of ideal knot theory, this result is significant because it has often been suggested that by reducing some form of knot energy, one may find a knot which is particularly simple over its equivalence class. Whether this measure of simplicity coincides with minimum crossing number over all possible projections (the traditional measure of simplicity used by knot tabulators such as Tait) has given rise to some debate for which our result provides additional fuel.

We conclude our investigation by saying that the algebraic method provides a useful minimisation approach for purely group theoretical work, the crossing force is the best approach when one wishes to find an especially short braid (and is not bound to a purely group theoretical framework) and the curvature elastic energy is best scheme to minimise elastic braid energy, i.e. total string length.

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