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RIGID AND NON-RIGID ACHIRALITY

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In order to completely characterize a molecule it is useful to understand the symmetries of its molecular bond graph in 3-space. For many purposes the most important type of symmetry that a molecule can exhibit is mirror image symmetry. However, the question of whether a molecular graph is equivalent to its mirror image has different interpretations depending on what assumptions are made about the rigidity of the molecular structure. If there is a deformation of 3-space taking a molecular bond graph to its mirror image then the molecule is said to be *topologically achiral*. If a molecular graph can be embedded in 3-space in such a way that it can be rotated to its mirror image, then the molecule is said to be rigidly achiral. We use knot theory in $\mathbf{R}^3$ to produce hypothetical knotted molecular graphs which are topologically achiral but not rigidly achiral, this answers a question which was originally raised by a chemist.

A *molecular bond graph* is a graph in $\mathbf{R}^3$ which is a geometric model of the structure of a molecule, see [**Walb**] and [**Was**]. We will be working primarily with molecular bond graphs which consist only of a simple closed curve K in $\mathbf{R}^3$. Since we are addressing a question raised by chemists and are working in $\mathbf{R}^3$, we choose to use the term "achiral" from the chemical literature rather than using the corresponding mathematical term "amphicheiral" which is generally used for knots in S^3. It is not hard to show that K is topologically achiral if and only if there is an orientation reversing diffeomorphism of $\mathbf{R}^3$ leaving K setwise invariant. If K is rigidly achiral then there is some embedding of K in 3-space which can be rotated to its mirror image. This embedding is said to be a *symmetry presentation* for K. Let h be this rotation composed with a reflection so that $h(K) = K$. Since K is only supposed to be a model of reality we shall make the assumption that this rotation is through a rational angle. Hence h must be of finite order. On the other hand, any finite order diffeomorphism of $(\mathbf{R}^3, K)$ is conjugate to a rotation composed with a reflection. Thus K is rigidly achiral if and only if there is a finite order orientation reversing diffeomorphism of $(\mathbf{R}^3, K)$.

By giving K an orientation we can distinguish further between two types of topological achirality. If there is a diffeomorphism of $(\mathbf{R}^3, K)$ which reverses the orientations of both R^3 and K, then K is said to be *negative achiral*. Whereas, if there is a diffeomorphism of $\mathbf{R}^3$ and K which reverses the orientation of $\mathbf{R}^3$ but preserves the orientation of K, then K is *positive achiral*. We shall show that no prime knot is rigidly negative achiral in $\mathbf{R}^3$, although many prime knots are topologically negative achiral in $\mathbf{R}^3$. Since there are examples of prime knots which are negative achiral in $\mathbf{R}^3$ but not positive achiral in $\mathbf{R}^3$, we can obtain examples of negative achiral knots which have no symmetry presentation. This is in contrast to Hartley's more difficult construction in S^3 of a knot which is negative achiral in S^3 but has no orientation reversing diffeomorphism of order two [**Ha**]. In addition, by using the recent results of [**MS**] we will show that Hartley's techniques can be used to construct positive achiral knots in $\mathbf{R}^3$ which have no symmetry presentation.

We observe, as follows, that there is actually no diffeomorphism of S^3 of any finite order which respects Hartley's knot but reverses its orientation. Suppose h is a finite order diffeomorphism of S^3 respecting a non-trivial knot K, but reversing the orientation of K. Then $h|K$ (i.e. h restricted to K) is a finite order orientation reversing diffeomorphism of a circle. So by Smith Theory [**Sm**] h must fix two points of K. Also h^2 must preserve the orientation of K and fix at least those two points of K. Hence, in fact, h^2 must fix every point of K. Now since K is non-trivial, by the Smith Conjecture [**MB**] h^2 is the identity map. Thus, if such a map h is of any finite order then it must be of order two.

We begin by explaining the effect of considering knots in $\mathbf{R}^3$ rather than S^3. Let h be an orientation reversing diffeomorphism of (S^3, K). By the Lefschetz fixed point theorem, h fixes some point p of S^3. If necessary, change h in a neighborhood of p so that h will fix some point which is not on K. By picking this point to be the point at infinity, h will restrict to a diffeomorphism of $(\mathbf{R}^3, K)$. On the other hand, any diffeomorphism of $(\mathbf{R}^3, K)$ extends to a diffeomorphism of (S^3, K). Hence K is topologically achiral in $\mathbf{R}^3$ if and only if K is topologically achiral in S^3.

If K is rigidly achiral in $\mathbf{R}^3$, then K is rigidly achiral in S^3, again by extending the diffeomorphism of $\mathbf{R}^3$ to S^3. But the converse is not always true. Let h be an orientation reversing finite order diffeomorphism of (S^3, K). By Smith Theory [**Sm**] the fixed point set of h is either two points or a 2-sphere. Suppose the fixed point set is a 2-sphere F. Let the components of $S^3 - F$ be the balls B and C. Then $h(B) = C$, and the intersection of K and F is non-empty. Now by Smith Theory for a circle, either h reverses the orientation of K and fixes two points on K, or h preserves the orientation of K and fixes no point of K. Thus since K intersects F, in fact K must intersect F in two points. Hence K is precisely the connected sum of a knot and its mirror image. In this case, we can pick the point at infinity to be any point on $F - K$. Thus h

restricts to $(\mathbf{R}^3, K)$. For emphasis we restate this result, together with its converse, as follows.

PROPOSITION. *A knot is rigidly negative achiral in* $\mathbf{R}^3$ *if and only if it is the connected sum of a knot and its mirror image.*

Suppose now that K is prime. Then the fixed point set of h could not have been a 2-sphere. Thus the fixed point set is two points. As mentioned above, either both fixed points are on K or neither fixed point is on K. If both fixed points are on K then h will not restrict to a diffeomorphism of $(\mathbf{R}^3, K)$. But if both points are off K then h preserves the orientation of K. Hence no prime knot is rigidly negative achiral in $\mathbf{R}^3$. On the other hand, a knot is rigidly positive achiral in $\mathbf{R}^3$ if and only if it is rigidly positive achiral in S^3.

It was observed by **[Ka]** that the knots numbered 8_{17}, 10_{79}, 10_{81}, 10_{88}, 10_{109}, 10_{115}, and 10_{118} are all prime knots which are negative achiral in S^3 but not positive achiral in S^3, since they are all non-invertible. Thus any of these is an example of a knot which is negative achiral in $\mathbf{R}^3$, but not rigidly achiral in $\mathbf{R}^3$, and hence has no symmetry presentation in $\mathbf{R}^3$. Figure 1 illustrates a symmetry presentation for 8_{17} in S^3 which cannot be restricted to a symmetry presentation for 8_{17} in $\mathbf{R}^3$.

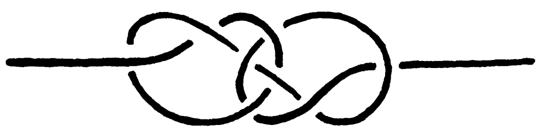

FIGURE 1

A symmetry presentation for 8_{17} in S^3.

Now we want to construct a positive achiral knot in $\mathbf{R}^3$ which has no symmetry presentation. As explained above, in this case it is equivalent to consider the problem in S^3. We choose to work in S^3 so that we will have more mathematical machinery at our disposal. We will call a knot *hyperbolic* if the exterior $E(K)$ of K in S^3 has a complete hyperbolic structure of finite volume. Suppose $E(K)$ contains no essential torus, then by Thurston's Hyperbolization Theorem **[Th]**, K is either hyperbolic or a torus knot. A torus knot cannot be topologically achiral in S^3. Suppose K is a hyperbolic knot which is topologically achiral in S^3; then there is an orientation reversing diffeomorphism h of (S^3, K). By Mostow's Rigidity Theorem **[Mo]**, $h \mid E(K)$ is homotopic to an isometry g. It follows from **[Wald]** that $h \mid E(K)$ is actually isotopic to g. Now g is of finite order and

g extends to a finite order diffeomorphism of (S^3, K). Since g is orientation reversing, K must be rigidly achiral in S^3. So in order to find an example of a positive achiral knot which is not rigidly achiral we will need a knot whose exterior contains an essential torus. We begin our construction with two lemmas.

LEMMA 1. *Let K be a hyperbolic knot which is rigidly positive achiral in S^3. There is a unique integer $n > 0$ such that there is a diffeomorphism of (S^3, K) of order 2^n, which reverses the orientation of S^3 and preserves the orientation of K.*

Proof. Since K is rigidly positive achiral in S^3, there is a diffeomorphism f of (S^3, K) which reverses the orientation of S^3 and preserves the orientation of K. Since f is orientation reversing the order of f is $p2^n$, where p is an odd number and n is a positive integer. Let $g = f^p$; then g is orientation reversing and the order of g is 2^n. Suppose h is a diffeomorphism of (S^3, K) which reverses the orientation of S^3 and preserves the orientation of K, and the order of h is 2^r with $r > 0$ and $r \neq n$. The exterior $E(K)$ has a complete hyperbolic structure of finite volume. So by Mostow's Rigidity Theorem [**Mo**] together with [**Wald**], $g|E(K)$ and $h|E(K)$ are isotopic to isometries g' and h' respectively. Also the finite action generated by g' and h' on $E(K)$ extends to a finite action of (S^3, K).

Since K is hyperbolic, $E(K)$ is not Seifert fibered. Hence $\pi_1(E(K))$ has trivial center. Thus by [**Gi**], no finite order diffeomorphism of (S^3, K) is isotopic to the identity. Since g and g' are isotopic and are both of finite order, in fact, they must be of the same order. Thus the order of g' is 2^n, and similarly the order of h' is 2^r.

Without loss of generality $r > n$. The orientation of K is preserved by both g' and h'. Let $q = 2^{r-n}$. Now g' and $(h')^q$ induce the same action on K. Since the action generated by g' and h' on $E(K)$ is finite, it follows from the Smith Conjecture [**MB**] that g' and $(h')^q$ induce the same action on $E(K)$. But g' is orientation reversing and $(h')^q$ is orientation preserving. This contradiction implies that $r = n$. □

LEMMA 2. *Let K be a knot in S^3; and let f be an orientation reversing diffeomorphism of (S^3, K) which is of order $n \neq 2$. Then there is an unknotted simple closed curve A which is disjoint from K, which contains the fixed points of f, and which is setwise invariant under f.*

Proof. Since the order of f is not two, f^2 is a non-trivial orientation preserving diffeomorphism of finite order. By Smith Theory [**Sm**], the fixed point set of f is either two points or a 2-sphere, and the fixed point set of f^2 is either the empty set or a circle. Since the fixed point set of f is contained in the fixed point set of f^2, the fixed point set of f must, in fact, be two points and the fixed point set of f^2 must be a circle. Let A be this circle. Then A contains the fixed points of f. By the Smith conjecture [**MB**], since A is the fixed point set of f^2, A is not knotted. Thus $A \neq K$. Also since f^2 preserves the orientation of K, no point of K is fixed by f^2. So A is disjoint from K. Let x be any point on A. Since $f^2(x) = x$, we have $f^2(f(x)) = f(f^2(x)) = f(x)$. Thus $f(x)$ is a fixed point of f^2. Hence $f(x)$ is also a point on A. Therefore $f(A) = A$. $\square$

Let K'' be a knot whose exterior $E(K'')$ contains an incompressible non-boundary parallel torus T. By [**Sch**], T separates S^3 into a knot complement Q and a solid torus V. A knot K' whose complement is Q is said to be a *companion* of K''. Let Ψ be a homeomorphism from V to an unknotted solid torus W, which is standardly embedded in S^3, such that h takes a longitude to a longitude and a meridian to a meridian, preserving the orientation of each. Let $K = \Psi(K'')$. Then K is said to be a *cocompanion* of K''.

THEOREM. *Suppose K and K' are hyperbolic knots, and there exist orientation reversing diffeomorphisms h and h' of (S^3, K) and (S^3, K') respectively, which preserve the orientations of the knots. Suppose further that the orders of h and h' are 2^q and 2^r, respectively with $q \neq r$ and $q > 1$. Then there exist a prime knot K'' with companion K' and cocompanion K, such that K'' is positive achiral but not rigidly positive achiral in S^3.*

Proof. Since the order of h is not two, by Lemma 2, there is an unknotted axis A disjoint from K such that $h(A) = A$. Let N be a tubular neighborhood of A which is also disjoint from K and $h(N) = N$. Let W be the complement in S^3 of N. Then W is an unknotted solid torus and h restricts to (W, K). It also follows from Lemma 2 that A contains the fixed points of h. Hence $h|W$ is fixed point free. Since $h(K) = K$, it follows from a covering space argument that K is not homologically trivial in W. Let μ be a meridian of W, and let $w = \mathrm{Lk}(K, \mu)$, the algebraic linking number of K and μ. Then $w \neq 0$.

Let V be a tubular neighborhood of K' which is invariant under h'. Let Ψ be a homeomorphism from V to W which takes a longitude to a longitude and a meridian to a meridian preserving the orientation of each. Let $K'' = \Psi^{-1}(K)$.

First we show that K'' is prime. Suppose not. Then it follows from **[Sch]** that there is a meridional disk of W which meets K in precisely one point. By Lemma 2, $h|W$ is fixed point free. So by lifting an appropriate disk in the orbit space $W/\langle h\rangle$ we can find an equivariant collection δ of meridional disks which each meet K in precisely one point. Let B be one component of $W - \delta$. Since $h|W$ is fixed point free, $h(B) \neq B$, by the Brouwer fixed point theorem. Now either there exists more than one i such that K meets $h^i(B)$ in a knotted arc, or K meets every $h^i(B)$ in an unknotted arc. Thus either K is trivial or K is composite. But both possibilities are impossible since by hypothesis K is hyperbolic. Hence K'' is prime.

It follows from **[Ha]** that K'' is positive achiral in S^3, since K' is positive achiral in S^3 and K is positive achiral in W. We shall show that K'' is not rigidly positive achiral in S^3. Suppose there exists a finite order diffeomorphism f of (S^3, K'') which reverses the orientation of S^3 but preserves the orientation of K. By taking f to a power, if necessary, we can assume that the order of f is a power of two. Since K and K' are both hyperbolic and K'' is prime, up to homotopy there is a unique essential torus T in $E(K'')$. By **[MS]**, we can assume that T is chosen in such a way that $f(T) = T$. Let the components of $S^3 - T$ be the knot complement Q and the solid torus V. Then $f(V) = V$ and $f(Q) = Q$. Since Q is the complement of K', we can actually pick K' to be a core of V, such that $f(K') = K'$.

Recall that $\mathrm{Lk}(K, \mu) = w \neq 0$. Let m be a meridian of V, then also $w = \mathrm{Lk}(K, m)$. Since $f(V) = V$, the image of m under f will also be a meridian m'; and since $f(K'') = K''$, it follows that $\mathrm{Lk}(K'', m') = w$. But f reverses the orientation of V and preserves the orientation of K and $w \neq 0$, so in fact, $f(m) = -m'$. Now K' is a core of V so f must also preserve the orientation of K'. Thus f is actually an orientation reversing diffeomorphism of (S^3, K') which preserves the orientation of K', and has order a power of two. Since K' is hyperbolic, we can apply Lemma 1 to conclude that the order of f is actually 2^r.

Now f restricts to a diffeomorphism of (V, K''). By construction there is a diffeomorphism Ψ from V to the unknotted solid torus W, such that $K = \Psi(K'')$, and Ψ takes a longitude to a longitude and a meridian to a meridian preserving the orientation of each. Let $g = \Psi f \Psi^{-1}$; then g is an order 2^r diffeomorphism of (W, K) which reverses the orientation of W but preserves the orientation of K. Since $f(Q) = Q$, for homological reasons f takes a longitude of V to a longitude of V. Thus g takes a longitude of W to a longitude of W. So, because W is unknotted, g extends to S^3. Now g is an order 2^r diffeomorphism of (S^3, K) which reverses the orientation of S^3 but preserves the orientation of K. But by hypothesis there is an orientation reversing diffeomorphism h of (S^3, K) which preserves the orientation of K and is of order 2^q. Since K is hyperbolic, it follows from Lemma 1 that $q = r$. But this contradicts the hypothesis that $q \neq r$. Hence f does not exist. So K'' is not rigidly positive achiral in S^3. $\square$

If K is any achiral two bridge knot, then K is hyperbolic. Also, it follows from **[HK]** that for any achiral two bridge knot K, there is an orientation reversing diffeomorphism h of (S^3, K) which preserves the orientation of K and is of order 2^q where $q > 1$. So it is not hard to construct knots as in our theorem.

COROLLARY. *Suppose K'' is the knot obtained by the theorem. Then K'' is positive achiral in $\mathbf{R}^3$, but has no symmetry presentation.*

Proof. Since K'' is prime it is not rigidly negative achiral in $\mathbf{R}^3$. However, by the equivalence of positive achirality in $\mathbf{R}^3$ and S^3, the knot K'' is positive achiral but not rigidly positive achiral in $\mathbf{R}^3$. Hence K'' has no symmetry presentation. $\square$

Now we have the machinery to obtain the desired example. Let K be the figure eight knot. It can be seen in Figure 2 that (W, K) has an orientation reversing diffeomorphism h of order four, which preserves the orientation of K. In addition, the solid torus W is the complement of the simple closed curve which is the fixed point set of h^2.

Let K' be the knot numbered 10_{99} in th Rolfsen-Bailey tables **[Ro]**. Since the knot 10_{99} is topologically achiral in S^3 and is a 3-bridge knot, it follows from **[Sch]** that it is hyperbolic. It can be seen from Figure 3 that (S^3, K') has an orientation reversing diffeomorphism of order two, which preserves the orientation of K'.

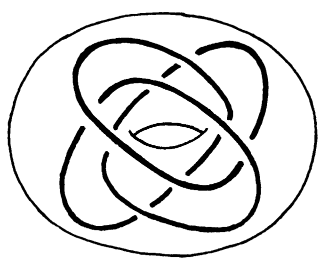

FIGURE 2

A symmetry presentation for the figure eight knot in a solid torus

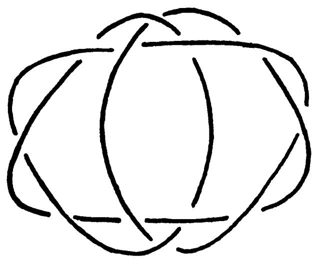

FIGURE 3
A symmetry presentation for 10_{99}

Let V be a tubular neighborhood of K'. Let Ψ be a diffeomorphism from W to V which takes a longitude to a longitude and a meridian to a meridian, preserving the orientation of each. Let $K'' = \Psi(K)$. Then K'' is constructed as in our theorem. So K'' is positive achiral in $\mathbf{R}^3$ but has no symmetry presentation.

In contrast to the situation for knots, it is easy to find graphs which are topologically achiral but not rigidly achiral in $\mathbf{R}^3$. Let K be any prime achiral knot, for example the figure eight knot, and let C be an unknotted simple closed curve which meets K at one point (see Figure 4). Since K can be deformed to its mirror image, and C can be slid back in place at the end of the isotopy, the graph will be topologically achiral. However, any finite order orientation reversing diffeomorphism leaving the graph invariant would take K to itself, fixing the point of intersection. Thus the diffeomorphism would actually fix two points on K and reverse the orientation of K. As we have shown, this is not possible since K is prime.

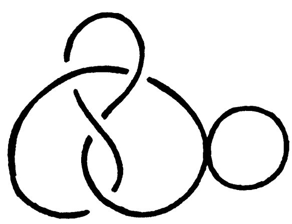

FIGURE 4
A topologically achiral graph which is not rigid achiral in $\mathbf{R}^3$

Applications. The field of chemical topology was born in 1962, when E. Wasserman **[Was]** synthesized the first molecule containing linked rings. This led to speculation about how to synthesize a knotted molecule. However synthesis did not seem likely until 1983, when D. Walba **[Walb]**

synthesized the first molecular mobius strip. Now, if he can clip the bonds of a strip containing three half twists he will obtain a trefoil knot. Recently J. Simon **[Si]** used topological techniques to analyze the symmetries of Walba's molecular mobius strip. In this paper we have considered knots and graphs in 3-space (denoted by $\mathbf{R}^3$) as models of hypothetical molecules in the real world. This is in contrast with the usual knot theory which considers the embeddings of knots in S^3 (i.e. 3-space together with a point at infinity). It is important to make this distinction since the real world is modelled by $\mathbf{R}^3$ and not by S^3.

The history of the particular problem that we have analyzed here began with Mislow **[Mi]**, who gave examples of disubstituted biphenyls that are rigidly achiral yet have no chemically accessible symmetry presentations. This led Walba **[Walb]** to ask whether such a phenomenon can occur if we allow complete freedom of movement of the molecular graph, that is if we replace chemically accessible by topologically accessible. In order to address this question, we made the assumption that a molecular bond graph which is rigidly achiral is one which can actually be rotated through a rational angle to obtain the mirror image graph. Since a molecular bond graph is only a model of reality, this assumption does not seem unreasonable. With this assumption we then produced examples of positive achiral knots, negative achiral knots and achiral graphs, all of which have no symmetry presentations. Thus we have illustrated in several different ways that it is not the case that every hypothetical molecular bond graph which is topologically achiral is actually rigidly achiral. On the other hand, it is unknown whether any of our examples could, in fact, be synthesized as molecules. Given the difficulty of synthesizing even the trefoil knot, perhaps a knot or graph which is topologically achiral in $\mathbf{R}^3$ but has no symmetry presentation will never be synthesized.

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