CROATICA CHEMICA ACTA CCACAA 59 (3) 669—684 (1986)

CCA-1678

YU ISSN 0011 1643
UDC 541
Original Scientific Paper

Configuration Census. Topological Chirality and the New Combinatorial Invariants

*Kenneth C. Millett**

Department of Mathematics, University of California, Santa Barbara, Santa Barbara 93106, California, U.S.A.

Received September 3, 1985

In this paper we describe new mathematical methods which can be used to distinguish between configurations of knotted and/or linked chains in space and to determine their topological chirality. These new methods are primarily algebraic and combinatorial and are easily understood in a calculational context. The methods are presented and discussed through the study of several fundamental examples. The polynomial invariants are compared and the development of other sensitive algebraic-combinatorial invariants which may have important applications in chemistry is discussed. A table of the polynomials associated to the basic examples is given.

1. INTRODUCTION

Chemists have long been interested in studying the idea that certain chemical properties may be identified as being related to the spacial configuration of the associated molecular graphs[13]. In particular, if one assumes perfect flexibility of the graph, one is lead to consider the topological properties of the placement, specifically, the topological equivalence of potentially distinct configurations and the topological chirality of the placement[2,3,11]. The identification of an effective means to distinguish between topologically knotted and/or linked molecular graphs and, especially, between enantiomers of a specific topologically chirally knotted or linked molecular graph has been an important goal of mathematically oriented chemists. In this paper we shall limit our consideration to the rather special case of placement of a collection of oriented (or directed) circles in space. Although this should only be understood as a first step in a much more elaborate consideration of the placement or molecular graphs in space it is a special case of interest in its own right (for example, with respect to the study of long polymer chains where examples of such objects have been synthesized since the 1960's) and since they may provide an insight into the relative usefulness of various theoretical approaches to census problems and to the study of chirality. For a brief survey of those concepts and many of the results of classical knot theory which may have relevance for the description of knot-like molecules and a discussion of census and topological chirality in the setting of the

* Partially supported by National Science Foundation Grant No DMS-8503733.

mathematical knowledge of that period, the reader is refered to the paper of Boeckmann and Schill.[3]

The classical mathematical methods which apply to these situations such as the linking number between the oriented constituents are useful in some contexts but, for the case of a family of oriented circles, the traditional algebraic-topological method of the Alexander polynomial[1,10] is extraordinarily successful for many census problems for the simpler knots and links but is completely inappropriate for questions of chirality. This has meant that for many years the search for mathematical methods to identify and classify various configurations and, especially, to detect the chirality of a specific placement in space took on the form of rather more elaborate geometric and algebraic considerations. In the spring of 1984 there was a very suprising discovery which has had a profound impact upon the classical knot theory. V. F. R. Jones[7], using considerations from the mathematical theories of representations of braids, braid groups, and certain von Neumann algebras, discovered a trace on a class of Hecke algebras that he employed to define a new algebraic invariant which was able, for example, to distinguish between the two enantiomers of the simplest knotted configuration, the trefoil knot. Stimulated by the desire to discover a more direct and combinatorial mathematical context in which these new invariants could be computed and understood, W. B. R. Lickorish and I[8], and, independently, others[6] and, several months later, two researchers in Warsaw[9], discovered that there was an essentially combinatorial vision that allowed one to define an even richer invariant to study these oriented knotted configurations and which was more effective than previous elementary methods. Subsequently, in the spring of 1985, Robert Brandt, Lickorish and I[4] and, independently, Ho, discovered still another, completely independent, algebraic invariant that could be used to distinguish between even more knots and links if one was willing to discard the (rather fundamental) distinction between the various possible orientations.

In this paper we shall limit our consideration to the informal mathematical aspects of these developments and shall describe the fundamental combinatorial, algebraic, and computational aspects of these new polynomials from the perspective of the combinatorics of the planar presentations of the (oriented) knots or links. Furthermore we shall describe the way in which most topological stereoisomers can be easily distinguished by virtue of these methods. These considerations are illustrated by complete discussion of a family of representative examples. Finally we shall conclude with a discussion of the advantages and limitations of these methods as well as a discussion of the recent developments. A small table of the two-variable and the one-variable polynomials associated to some knots and links of low crossing number will be presented in an appendix. M. B. Thistlethwaite will publish a much more grandiose tabulation on microfiche[12].

2. THE ALGEBRAIC AND COMBINATORIAL FORMALISM

We wish to study the spacial properties of the placements of oriented families of chains in space. An excellent mathematical discussion of these concepts of found in Rolfsen[10]. The informal mathematical description that we shall use of these concepts is a follows: by a chain we shall mean any topological object, for example a graph, which is topologically the same as the circle, i. e. simple closed curve; by an orientation we shall mean the choice of a direction on each of the circles of the family, by a spacial property we shall mean anything which is not changed by a distortion of the ambient space which does not change a chosen orientation of the space, i. e. does not take us from a »right-handed« orientation of space to a »left-handed« orientation of space. An example of a spacial configuration is shown in Figure 1.

The effective consideration of such examples is made possible by the study of the combinatorial properties of particularly well behaved projections of the specific example under consideration onto a plane. These projections, as illustrated in Figure 1, have the property that all projections of segments cross each other in separated places, i. e. there are no »tangential« or »triple, . . .-point« intersections, and, in order to understand the placement in space, the projection are broken so as to show how one strand passes over or under the other. (This approach appears to have been first utilized by K. F. Gauss in his study of electrodynamics in 1833 and was further developed by the Reverend Kirkman in his consideration of Kelvin's theory of vortex atoms in 1885.)

Figure 1.

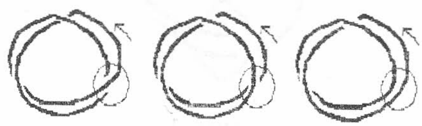
In order to take into consideration the choice of orientation on each of the chains we shall place an arrow on each strand to indicate the specific choice of orientation. One of the earliest goals of researchers in this field was the tabulation of all possible »prime« placements and the combinatorics of these projected images provided one of the fundamental tools for the generation of the placements which were then tabulated according to the number of crossings necessary in a simplest realization. To give an appreciation for the magnitude of this census problem one only need note that, ignoring all questions of orientation, there are, according to Thistlethwaite[1], 12,965 prime knots (the simplest »atoms« of knotting) having planar presentations with fewer than 14 crossings. Adding orientation and combinations, there are about 20,000 distinct knots in this range! In practice, their census has only become effectively possible with the use of contemporary computers. Historically, one attempted to find numerical or algebraic invariants associated to the combinatorics of these realizations which measured or, at least, reflected the spacial properties of the object under consideration. It was in this spirit that Alexander[1], in 1928, defined a polynomial involving a single variable, t, and having integer coefficients, by taking the determinant associated to a matrix which was constructed from information describing certain aspects of the combinatorics of the projected representation. A certain combinatorial aspect of this approach remained largely unrecognized and unappreciated until it was exploited by J. Conway[5] in his normalization of the Alexander polynomial and his calculational approach. Since this aspect provides the key combinatorial insight for the new polynomials we shall first describe how this method of calculation works.

We shall consider the situation where we have three planar pictures of oriented links in each of which we have identified a small circular region of the picture which contains either a single crossing or, in the last case, no crossing at all and such that outside these small circular regions the planar pictures are exactly the same. We shall label these cases by K^{+}, K^{-}, and K_0, respectively, when the motifs inside the circular regions are those given in Figure 2.

\+ − 0

Figure 2.

A specific occurance of the type is illustrated in Figure 3. This is one of several situations that will serve to describe the nature of the invariants that we shall want to study.



\+ − 0

Figure 3.

The (Conway normalized) Alexander polynomial, $\Delta_L(t)$, of an oriented knot or link, L, is a polynomial consisting of a sum of finitely many terms each of which is the product of an integer and some power (either positive, zero, or negative!) of the variable »t« and which satisfies the following fundamental formulae:

(i) if U denotes the standard unknotted circle in the plane, then $\Delta_U(t) = l$, and

(ii) if K^{+}, K^{-}, and K_0 are planar pictures of oriented links in each of which we have identified a small circular region of the picture containing either a single crossing or, in the last case, no crossing at all, according to the convention shown in Figure 2, and such that outside these small circular regions the planar pictures are exactly the same, then the normalized Alexander polynomial satisfies the formula $\Delta_{K+}(t) - \Delta_{K-}(t) + (t^{1/2} - t^{-1/2})\, \Delta_0(t) = 0$.

Furthermore, a fundamental property of the polynomial is that any two topologically equivalent placements have exactly the same polynomial. Thus the polynomial can be used as a tool to distinguish between knots or to identify knots in a tabulation. Indeed, it is a remarkably effective tool for such matters when it is applied to simple knots or links.

The aspect that we wish to exploit is the idea that the above formulae provide a way to calculate the Alexander polynomial for any oriented link: By changing the appropriate crossings, in some sequence, any link can be changed to an unlink whose polynomial can be given by a simple formula. (The concept of an »unlink« requires a bit of care. The formal definition is any placement of closed strands that is topologically equivalent, i. e. »can be spacially moved to«, the distant union of some number of standard unknotted circles. Examples are shown in Figure 3, case »—«; Figure 4, cases »+« and »0«; and in Figure 5, all cases.) Assuming that the polynomial is already known for all instances of fewer crossings, we may then calculate the required polynomial. We shall give specific detailed examples of this sort of calculation for the new invariants. The critical issue at this point is the observation that any calculation of this sort involves many arbitrary choices and appears to refer only to the specific planar picture of the spacial configuration under consideration. It was not until 1981 that an attempt to show that the Alexander polynomial could be defined in this way and also be shown to be topological invariant of the spacial configuration was published by Ball and Mehta[7]. From a purely »mathematical« perspective their methods were not completely convincing but essentially the same approach was finally carried out to a completely satisfactory mathematical conclusion during the recent combinatorial development of the new invariants.

In 1984 a completely new polynomial invariant, now referred to as the Jones polynomial, $V_K(t)$, was defined for any oriented link in space by V. F. R. Jones[7]. This new polynomial has very many properties similar to those of the Alexander polynomial, e. g. it depends only upon the topological type of the spacial placement, and is yet significantly more sensitive to various aspects of the spacial placement. When studying the basic properties of the polynomial, Jones and, independently, Lickorish and the author noticed that a formula analogous to that for the Alexander polynomial also occured. Specifically, if one had the three oriented links K^+, K^-, and K_0, related as in the previous paragraph, then

$$t^{-1} V_{K^+}(t) - t\, V_{K^-}(t) - (t^{1/2} - t^{-1/2})\, V_{K_0}(t) = 0.$$

It is also true that $V_U(t) = l$ where U denotes the unknot, as above. (The reader should be warned that there is as yet no universal agreement in the mathematical literature on the choice of exponents and signs of the terms in the recursive formula. Therefore caution should be used in making comparisons between tables to be sure that the same convention is employed. Here I have chosen to use that given by Jones). Thus, as before, this formula could be used to calculate the actual polynomials by a recursive method just as in the case of the Alexander polynomial. Moreover, one notices that there is a fundamental asymmetry in the roles played by the variables »t« and »t^{-1}« in the basic formula and the configurations K^+ and K^-. It is this fact that indicates that this sort of polynomial may be able to provide information about the topological chirality of the spacial placement since a configuration is topologically chiral, i. e. not equivalent to its mirror reflection (take the mirror to be the plane of projection to note that a reflection means simply »change all crossings in the projection«), if the associated Jones polynomial is changed when one changes the signs of all the exponents of the variable »t«.

To better understand what this means we shall want to completely study a specific example, i. e. the right-handed trefoil knot, $T = K^+$, shown in Figure 3. In this case the second configuration, K^-, is the unknot, U, so that by our normalization assumption we must have that $V_{K^-}(t) = 1$. Thus, in order to complete the calculation of V_T we need to have computed the polynomial associated to the K_0 case. As before this is accomplished by studying the effect of changing and removing a crossing as shown in Figure 4.

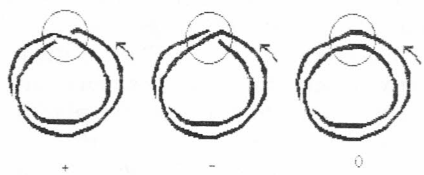


Figure 4.

Here we find »K_0« as the first situation which we shall denote K_0^+. The third case »K_0«$_0$, is clearly another version of the unknot so that its polynomial is required to be »1« by our normalization. Thus, to complete the calculation we see that we must know what polynomial is to be associated to two topologically unlinked unknotted circles. This, of course, is to be computed by considering still another diagram of situations. For example, we may employ the ones shown in Figure 5. Here we find the unknot in both the »+« and »—« configurations so that we may solve for the polynomial of K_0- as follows:

$$t^{-1} \cdot 1 - t \cdot 1 - (t^{1/2} - t^{-1/2})\, V_{K_{0^-}}(t) = 0,$$

so that

$$V_{K_{0^-}}(t) = (t^{-1} - t)/(t^{1/2} - t^{-1/2}) = -(t^{1/2} + t^{-1/2}) \equiv \breve{\mu}$$

which we define to be the algebraic quantity $\breve{\mu}$ because the expression appears very often in calculations.

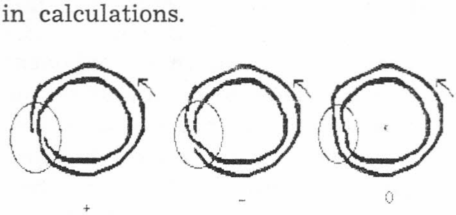


Figure 5.

Returning to our calculation of $V_{K_{0+}}(t)$ using the equation associated to Figure 4 we calculate as follows:

$$t^{-1}\, V_{K_{0+}}(t) - t \cdot V_{K_{0^-}}(t) - (t^{1/2} - t^{-1/2}) \cdot 1 = 0,$$

so that

$$V_{K_{0+}}(t) = -t^2(t^{1/2} + t^{-1/2}) + t(t^{1/2} - t^{-1/2})$$
$$= -t^{5/2} - t^{3/2} + t^{3/2} - t^{1/2}$$
$$= -t^{5/2} - t^{1/2}.$$

Finally we have the information required to complete the calculation of the polynomial associated to the right-handed trefoil knot, T, illustrated in Figure 3 as K^+. Thus we calculate as follows:

$$t^{-1} V_T(t) - t \cdot 1 - (t^{1/2} - t^{-1/2} V)_{K_0}(t) = 0,$$

and since $K_0 = K_{0+}$,

$$V_T(t) = t^2 + t^1 \cdot (t^{1/2} - t^{-1/2})(-t^{5/2} - t^{1/2}) = t^1 + t^3 - t^4.$$

It is a this point that a key observation comes into play and shows us why this new polynomial is likely to bring powerful new calculational tools into the study of the chirality of such objects.

Key Observation: If we let K denote an oriented link and let $\overline{K}$ denote its mirror image, then $V_{\overline{K}}(t) = V_K(t^{-1})$.

Suppose that we want to know if T is topologically chiral, that is, inequivalent to its mirror image. By the above observation, we can be sure that $\overline{T}$ is topologically chiral if $V_{\overline{T}}(t) \neq V_T(t^{-1})$. This is clearly the case since $V_{\overline{T}}(t) = -t^{-4} + t^{-3} + t^{-1} \neq t + t^3 - t^4 = V_T(t)$. This is how Jones first discovered that his polynomial was completely different form the classical Alexander polynomial which could not distinguish between the right-handed and left-handed trefoils and how one is lead to employ this new polynomial to test the chirality of a given configuration. Although the Jones polynomial is a remarkably effective tool for distinguishing between topological configurations and, especially, for testing topological chirality this is not the end of the development since there are extensions of these ideas to create still more powerful and mysterious polynomial invariants that can be associated to such configurations in space. Fortunately these new polynomials do not require the development of algebraic or combinatorial tools significantly beyond those which we already have available in the previous calculational method.

The two-variable polynomial, $P_L(l, m)$, of an oriented knot or link, L, is a polynomial consisting of a sum of finitely many terms each of which is the product of an integer and some powers (either positive, zero, or negative) of the variables, »l« and »m«, and which satisfies the following fundamental formulae:

(i) if U denotes the standard unknotted circle in the plane, then $P_U(l, m) = 1$, and

(ii) if K^+, K^-, and K_0 are planar pictures of oriented links in each of which we have identifed a small circular region of the picture containing either a single crossing or, in the last case, no crossing at all, according to the convention shown in Figure 2, and such that outside these small circular regions the planar pictures are exactly the same, then the two-variable polynomial satisfies the formula

$$l \cdot P_{K^+}(l, m) + l^{-1} P_{K^-}(l, m) + m P_{K_0}(l, m) = 0.$$

Furthermore, a fundamental property of the polynomial is that any two topologically equivalent placements have exactly the same polynomial.

To illustrate the use of this polynomial invariant one may repeat the above calculation of the polynomial associated to the right-handed trefoil as follows: From Figure 5 we find:

$$l \cdot 1 + l^{-1} \cdot 1 + m\, P_{K_{0-}} (1, m) = 0,$$

giving

$$P_{K_{0-}} (lm) = -(l + l^{-1})\, m^{-1} \equiv \mu,$$

which we define to be the algebraic quantity μ because it appears very often as a unit. Continuing, with the calculation from Figure 4, we have

$$l \cdot P_{K_{0+}} (l, m) + l^{-1} \cdot P_{K_{0-}} (l, m) + m \cdot 1 = 0,$$

giving

$$\begin{aligned} P_{K_{0+}} (1, m) &= -l^{-2} (-(l + l^{-1})\, m^{-1})\, m l^{-1} \\ &= (l^{-1} + l^{-3})\, m^{-1} - m\, l^{-1}. \end{aligned}$$

Thus we are, once again, in the position to calculate the polynomial for the right-handed trefoil from Figure 3 as follows (using the fact that $K_0 = K_{0+}$):

$$l \cdot P_T (l, m) + l^{-1} \cdot 1 + m\, P_{K_0} (l, m) = 0,$$

giving

$$\begin{aligned} P_T (l, m) &= -l^{-2} - m\, l^{-1} ((l^{-1} + l^{-3})\, m^{-1} - m\, l^{-1}) \\ &= -l^{-4} - 2\, l^{-2} + l^{-2} m^2. \end{aligned}$$

The question of the effect upon the polynomial of the reflection of the knot or link in a mirror is answered in a manner analogous to the response given for the Jones polynomial since in this case as well the role of the variable is reversed by the change of orientation. Thus we have the following:

Key Observation: If we let K donote denote an oriented link and let $\overline{K}$ denote its mirror image, then $P_{\overline{K}} (l, m) = P_K (l^{-1}, m)$.

As a consequence, one calculates $P_{\overline{T}} (l, m) = -2\, l^2 - l^4 + l^2 m^2$ and thereby proves again that the left-handed trefoil and the right-handed trefoil are distinct and therefore the trefoil is topologically chiral.

Because of a desire to study unoriented configurations Brandt, Lickorish and I were lead to consider the most general form of a functional relationship that could hold between algebraic invariants associated to the possible combinatorial operations that one could apply to a planar presentation of an unoriented knot or link. Because of the requirement of spacial invariance one quickly discovers that most such possibilities lead to previously known invariants or to a trivial one. There is, however, one possibility that does lead to a new algebraic invariant. In Figure 6 we depict the four possible operations that could be applied to a crossing in a generic planar presentation of a spacial configuration. The lack of any orientation makes it unclear which diagram in the figure should be labeled »+« and which should be labeled »—«, with a similar problem arising between the diagrams labeled »0« and »∞«. However the symmetry in the roles played by the associated polynomials in the defining formula neutralises this ambiguity.

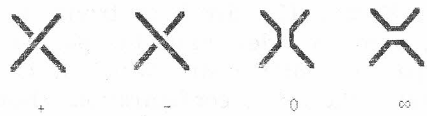


Figure 6.

The *one-variable polynomial,* $Q_L(x)$, of an oriented knot or link, L, is a polynomial consisting of a sum of finitely many terms each of which is the product of an integer and some powers (either positive, zero, or negative!) of the variable, »x«, and which satisfies the following fundamental formulae:

(i) if U denotes the standard unknotted circle in the plane, then $Q_U(x) = l$, and

(ii) if K^+, K^-, K_0, and K_∞ are planar pictures of oriented links in each of which we have identified a small circular region of the picture containing either a single crossing or, in the last cases, no crossing at all, according to the convention shown in Figure 6, and such that outside these small circular regions the planar pictures are *exactly* the same, then the *one-variable polynomial* statisfies the formula

$$Q_{K^+}(x) + Q_{K^-}(x) = x\,\{Q_{K_0}(x) + Q_{K_\infty}(x)\}.$$

Furthermore, a fundamental property of the polynomial is that any two topologically equivalent placements have exactly the same polynomial.

To illustrate the use of this polynomial invariant one may repeat the above calculation of the polynomial associated to the right-handed trefoil. However, in this case there are three polynomials to be calculated in order to determine the fourth. Consider the configurations, shown in Figure 7,

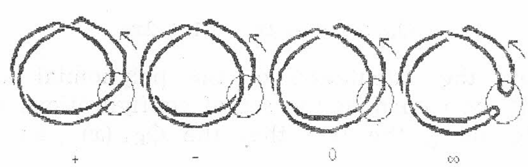


Figure 7.

analogous to those shown in Figure 3. Here we find that $T = K_+$ and that both K_- and K_∞ are trivial knots so that, by definition, their polynomials are identically l. Thus, as above, we must compute the polynomial associated to K_0. This is, of course, accomplished by using the set of configurations shown in Figure 8 which are analogous to those depicted in Figure 4.

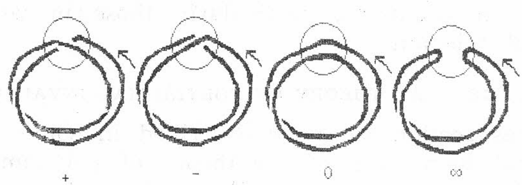


Figure 8.

Here we discover that K_0 and K_∞ are both trivial knots. Thus, just as in the previous cases, we need only determine the polynomial associated to the trivial link of two separated components, which it is convenient to denote by U^2. For this we employ the set of configurations shown in Figure 9 which is the analogue of Figure 5.

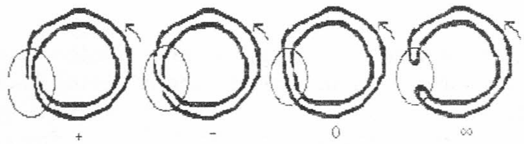


Figure 9.

Here we find that $K_0 = U^2$ is the configuration whose associated polynomial we wish to calculate and that all the other configurations are equivalent to the trivial knot. As a consequence of the fundamental formula we have:

$$Q_U(x) + Q_U(x) = x\{Q_{U^2}(x) + Q_U(x)\}$$

so that

$$1 + 1 = x\{Q_{U^2}(x) + 1\}$$

and, therefore,

$$Q_{U^2}(x) = 2x^{-1} - l \equiv \hat{\mu}.$$

Thus, to compute the polynomial associated to the K_+ depicted in Figure 8 we have;

$$Q_{K^+}(x) + Q_{U^2}(x) = x\{Q_U(x) + Q_U(x)\}$$

so that

$$Q_{K^+}(x) = -2x^{-1} + 1 + 2x.$$

Finally to complete the calculation of the polynomial associated to the right-handed trefoil we return to the set of configurations in Figure 7 from which we compute, using the fact that the $Q_{K+}(x)$ just computed is the $Q_{K_0}(x)$;

$$Q_T(x) + Q_U(x) = x\{Q_{K_0}(x) + Q_U(x)\}$$

so that

$$Q_T(x) = -1 + x\{-2x^{-1} + 1 + 2x + 1\} = -3 + 2x + 2x^2.$$

Thus we see that although there is some formal similarity between abstract structure of this last polynomial and the previous ones, the resulting polynomials seem to have little in common. This, we shall see, proves to be an advantage in certain situations, particularly those in which questions of orientation are not relevant.

3. THE GENERAL THEORY OF POLYNOMIAL INVARIANTS

In the previous section we have described in some detail the fundamental calculational foundation of the theory of polynomials associated to oriented and unoriented knotted and/or linked chains in space. In this section we shall outline the broader aspects of the various theories, the fundamental properties they all enjoy, and try to delineate the various strengths and weaknesses of the theories.

The first thing to note is that the *Alexander polynomial* and the *Jones polynomial* are both special cases of the *two-variable polynomial* in that they are gotten by specific choices of variables:

Alexander polynomial $l = i$ $m = i\,(t^{1/2} — t^{-1/2})$

Jones polynomial $l = it$ $m = i\,(t^{1/2} — t^{-1/2})$

where $i^2 = —1$. Thus one might expect that the two-variable polynomial is a more powerful discriminator in the study of oriented knots and links. Indeed this is the case, even for questions of chirality, since there is an eleven crossing knot which is chiral but its chirality is not detected by the Jones polynomial but is detected by the two-variable polynomial. Unfortunately, there are also knots which are chiral but which have polynomials which do not exhibit the hoped for asymmetry with respect at the change of sign of exponents. Nevertheless the Jones and two-variable polynomials are extraordinarily successful in their ability to detect chirality when one considers the entire population that has been tabulated to this point.

With respect to the census problem the Jones and two-variable polynomials are rather more successful than the already extremely successful Alexander polynomial, especially if one is confronted with identifying or distinguishing knots of more than 10 crossings. They are not perfect as there are famlies of examples for which none of the polynomials will have distinct values. These arise by the operation of mutation of Conway[5] which only becomes important at 11 crossings where the first such examples occur. Unfortunately there are other very small families of examples which the two-variable polynomial fails to distinguish. The new *one-variable polynomial* seems strikingly more successful in these census problems if one is willing to neglect the questions of orientation. It is important to understand that this polynomial is completely insensitive to questions of orientation of space and its constituent chains. Nevertheless, by direct calculation, one discovers that the one-varibale polynomial distinguishes all the prime knots through 9 crossings and all the prime links through 8 crossings and it is able to distinguish families of knots where the previous polynomials fail. Also, it too fails to distinguish between mutants. Furthermore, there are additional cases where all the presently known polynomial invariants fail to successfully distinguish between knotted configurations which are known to be distinct by virtue of other algebraic-topological invariants.

For knots, configurations consisting of a single chain, the polynomials are insensitive to the specific orientation of the chain. This is, however, not the case for links of more than one component except for the one-variable polynomial which was defined so as to be insensitive to the relative choices of chain orientation. For the Jones polynomial, changing the orientation of one of the constituent chain changes the polynomial only by the multiplication of the polynomial by a power of the variable t, the precise power being determined by the algebraic linking information between the chain whose orientation is changed and the other constituent chains. No such relationship between the associated polynomials is known for the two-variable polynomial at this time!

There are two natural operations which form new links form a pair of links. The first of these is the »distant union« where one simply considers the two separated links as one whole link. In this case, in each of the polynomial theories, the resulting polynomial is simply the product of the two separate polynomials with $\tilde{\mu}$, μ, or $\hat{\mu}$, as appropriate for the desired polynomial. The second of these operations is a »connected union« where one considers the above distant union, selects a small segment from a chain in each, removes it, and joins their ends together in a parallel fashion. The resulting polynomial is even simpler than the distant union. It is the product of the polynomials associated to its constituents.

There are, at present, two major problems with this theory as it relates to possible chemical applications. The first is that the relationship between the algebraic structure of the polynomial invariants and the specific topological or spacial nature of the configurations to which they are associated is not yet understood well enough to even guess if there might be some deep connection that could be exploited in a chemical theory. There is, however, the very striking and provocative nature of the way in which the polynomials are developed from those associated to other states in which one has broken the bonding pattern in relevant family of possible ways. To the novice it would appear that there may be something going on here that could provide some new insights in chemistry. However such matters are, for the present, only a matter of conjecture.

The second difficulty with this polynomial theory arises in problems where one wants to take a census of a large collection of spacial configurations or wishes to study a single extremely complex configuration. The problem is the complexity of the current calculational algorithms in terms of the running time on even the very rapid contemporary computers. Recall that to employ the defining functional formula to calculate the polynomial of, for example, the Jones polynomial one must calculate the Jones polynomials associated to two simpler configurations. Thus, if one begins each calculation afresh, one is confronted with a potentially exponentially growing tree of calculations as a function of the number of crossings in a planar presentation of the configuration. Even with a reasonably efficient means of making the calculation at each stage the number of such calculations makes a simple-minded approach unfeasible for relatively complicated examples, i. e. having projections of, say, 50 crossings. Thus a basic question arises. *Does there exist an algorithm for the calculation of the polynomial invariants which is of polynomial growth as a function of the number of crossings in a planar presentation of the knot or link?*

If one is only interested in determining whether a given configuration is knotted or not it is quite possible that the entire calculation can be reduced to the calculation of a certain special value of the associated polynomials or of certain terms of the polynomials. At this time, however, there does not yet appear to be a truely effective and simple method which determines very rapidly the knottedness of a sufficiently large proportion of knotted configurations so as to provide an effective filter.

Such questions are of considerable interest since a positive resolution would provide new rapid and powerful techniques in the study of randomly generated knots and links. Furthermore, one can easily imagine future applications to computer assisted studies of electron microscope pictures of large molecular chains, e. g. DNA.

4. CONCLUSION

In this article, we have described a new family of algebraic and combinatorial invariants associated to knotted and/or linked oriented or unoriented chains in space. These new invariants were introduced through a formalism proposed for the *Alexander polynomial* by the work of Conway and made more attractive by the discovery that the recently discovered *Jones polynomial* also satisfied an analogous formal structure. Thus, the *two-variable polynomial* and the most recent of this new trend, the *one-variable polynomial,* were presented by way of the vehicle of a sample calculation which, at once, indicates the most elementary algorithm to implement a computer assisted calculation of these invariants, indicates the elementary properties of these invariants, and indicates the strengths and current weaknesses of these invariants as a research tool.

We have shown how the Jones polynomial and the two-variable polynomial are rather effective in the determination of the chirality of most knotted or linked configurations despite the fact that there are a very small number of exceptional cases among the configurations having realisations as planar projections of up to 14 crossings. Similarly, the Jones, the two-variable, and especially the recently discovered, one-variable polynomials are remarkably effective tools in distinguishing and classifying knotted configurations despite the existence of a relatively small number of exceptional cases.

In addition, however, one sees the fundamental simplicity of the proposed mathematical relationships and the analogy of these relationships with the most elementary considerations of chemical models. As a consequence they appear to be attractive areas for further research, both from the purely mathematical point of view and from the perspective of one who is interested in using geometrical and topological models for chemical and physical phenomena.

APPENDIX: POLYNOMIALS OF SIMPLE KNOTS AND LINKS

Interpretation of the tables is as follows: Knots are listed with the classical Alexander-Briggs notation (see Rolfsen [*R*] for a convenient table of their pictures) 3_1, 4_1, 5_1, $5_2, \ldots, 8_{21}$, and 'coded' forms of the polynomials will be given. The one-variable polynomial $Q_L(x) = \Sigma^s_{-r}\, a_j\, x^i$ will be written $a_{-r}\, x^{-r} + a_{-r+1} + a_{-r+2} + \ldots + a_s$, with $a_0\, x^0$ written a_0.

TABLE

Values of the One-Variable Polynomial

3_1	— 3 + 2 + 2
4_1	— 3 — 2 + 4 + 2
5_1	5— 2 — 6 + 2 + 2
5_2	1 — 4 — 2 + 4 + 2
6_1	1 + 4 — 6 — 4 + 4 + 2
6_2	5 — 2 — 10 + 0 + 6 + 2
6_3	5 — 6 — 12 + 4, + 8 + 2
7_1	— 7 + 4 + 16 — 6 — 10 + 2 + 2
7_2	— 3 + 6 + 8 — 10 — 6 + 4 + 2
7_3	— 3 + 2 + 6 — 6 — 4 + 4 + 2
7_4	1 + 8 — 4 — 12 + 0 + 6 + 2
7_5	1 + 0 — 4 — 6 + 2 + 6 + 2
7_6	5 + 2 — 12 — 10 + 6 + 8 + 2
7_7	5 + 6 — 18 — 14 + 10 + 10 + 2
8_1	— 3 — 6 + 14 + 12 — 14 — 8 + 4 + 2
8_2	— 7 + 0 + 22 + 2 — 20 — 4 + 6 + 2
8_3	1 — 8 + 4 + 12 — 8 — 6 + 4 + 2
8_4	— 3 + 2 + 14 — 2 — 16 — 2 + 6 + 2
8_5	— 11 + 14 + 26 — 16 — 24 + 2 + 8 + 2
8_6	1 — 4 + 2 + 2 — 8 + 0 + 6 + 2
8_7	— 7 + 4 + 20 — 8 — 20 + 2 + 8 + 2
8_8	1 + 4 + 6 — 10 — 14 + 4 + 8 + 2
8_9	— 7 + 4 + 16 — 10 — 16 + 4 + 8 + 2
8_{10}	— 11 + 14 + 22 — 22 + 8 + 10 + 2
8_{11}	— 3 + 6 + 4 —12 — 10 + 6 + 8 + 2
8_{12}	5 + 2 — 8 — 12 — 4 + 8 + 8 + 2
8_{13}	— 3 + 10 + 10 — 22 — 16 + 10 + 10 + 2
8_{14}	1 + 8 + 0 — 22 — 10 + 12 + 10 + 2
8_{15}	— 7 + 16 + 10 — 32 — 16 + 16 + 12 + 2
8_{16}	— 3 + 10 + 18 — 22 — 30 + 8 + 16 + 4
8_{17}	— 3 + 6 + 12 — 20 — 24 + 10 + 16 + 4
8_{18}	5 + 2 + 12 — 26 — 36 + 14 + 24 + 6
8_{19}	— 11 + 10 + 20 — 10 — 12 + 2 + 2
8_{20}	— 7 + 12 + 12 — 14 — 8 + 4 + 2
8_{21}	— 7 + 8 + 6 — 12 — 2 + 6 + 2
$2^2{}_1$	— $2x^{-1}$ + 1 + 2
$4^2{}_1$	$2x^{-1}$ — 1 — 4 + 2 + 2
$5^2{}_1$	$2x^{-1}$ — 1 — 8 + 0 + 6 + 2
$6^3{}_2$	$4x^{-1}$ — 4 + 1 + 1 + 0 — 16 + 0 + 12 + 4

The *two-variable polynomial* of a knot is of the form $P_L(l, m)\ \Sigma_{i=0}\, p_i(l)\, m$ where $p_i(l) \equiv 0$ if i is odd and is a polynomial in even powers of l otherwise. The numbers in the i^{th} rounded bracket of the coded form of the polynomial give the coefficients in $p_{2(i-1)}$, the number in square brackets being the coefficient of l^0, and as $p_i(l)$ contains only even powers of l, no entry occurs for the coefficient of an odd power. Thus, for example, the polynomial associated to the left-handed trefoil which we computed above to be $-2\,l^2 - l^4 + l^2\ m^2$, will be found listed in the table as 3_1 with the associated coded form of the polynomial given as ([0]) — 2 — 1) ([0] 1).

TABLE

Values of the Two -Variable Polynomial

3_1	([0] —2 —1) ([0] 1)
4_1	(—1 [—1] —1) ([1])
5_1	([0] 0 3 2) ([0] 0 —4 —1) ([0] 0 1)
5_2	([0] — 1 1 1) ([0] 1 —1)
6_1	(—1 [0] 1 1) ([1] —1)
6_2	([2] 2 1) ([—1] —3 —1) ([0] 1)
6_3	(1 [3] 1) (—1 [3] —1) ([1])
7_1	([0] 0 0 —4 —3) ([0] 0 0 10 4) ([0] 0 0 —6 —1) ([0] 0 0 1)
7_2	([0] —1 0 —1 —1) ([0] 1 —1 1)
7_3	(—2 —2 1 0 [0]) (1 3 —3 0 [0]) (—1 1 0 [0])
7_4	(—1 0 2 0 [0]) (1 —2 1 [0])
7_5	([0] 0 2 0 —1) ([0] 0 —3 2 1) ([0] 0 1 —1)
7_6	([1] 1 2 1) ([—1] —2 —2) ([0] 1)
7_7	(1 2 [2]) (—2 [—2] —1) ([1])
8_1	(—1 [0] 0 —1 —1) ([1] —1 1)
8_2	([0] —3 —3 —1) ([0] 4 7 3) ([0] —1 —5 — 1) ([0] 0 1)
8_3	(1 0 [—1] 0 1) (—1 [2] —1)
8_4	(—2 [—2] 0 1) (1 [3] —2 —1) ([—1] 1)
8_5	(—2 —5 —4 [0]) (3 8 4 [0]) (—1 —5 —1 [0]) (1 0 [0])
8_6	([2] 1 —1 —1) ([—1] —2 2 1) ([0] 1 —1)
8_7	(—2 —4 [—1]) (3 8 [3]) (—1 —5 [—1]) (1 [0])
8_8	(—1 —1 [2] 1) (1 2 [—2] —1) (—1 [1])
8_9	(—2 [—3] —2) (3 [8] 3) (—1 [—5] —1) ([1])
8_{10}	(—3 —6 [—2]) (3 9 [3]) (—1 —5 [—1]) (1 [0])
8_{11}	([1] —1 —2 —1) ([—1] —1 2 1) ([0] 1 —1)
8_{12}	(1 1 [1] 1 1) (—2 [—1] —2) ([1])
8_{13}	([0] —2 —1) (—1 [—1] 2 1) ([1] —1)
8_{14}	([1]) ([1] —1 1 1) ([0] 1 —1)
8_{15}	([0] 0 1 —3 —4 —1) ([0] 0—2 5 3) ([0] 0 1 —2)
8_{16}	([0] —2 —1) ([2] 5 2) ([—1] —4 —1) ([0] 1)
8_{17}	(—1 [—1] —1) (2 [5] 2) (—1 [—4] —1) ([1])
8_{18}	(1 [3] 1) (1 [1] 1) (—1 [—3] —1) ([1])
8_{19}	(—1 —5 —5 0 0 [0]) (5 10 0 0 [0]) (—1 —6 0 0 [0]) (1 0 0 [0])
8_{20}	([—1] —4 —2) ([1] 4 1) ([0] —1)
8_{21}	([0] —3 —3 —1) ([0] 2 3 1) ([0] 0 —1)

Because the coding of the polynomials associated to links is rather more complicated, we shall give their complete algebraic expressions. Furthermore, since the two-variable polynomial takes the relative orientations of the constituent chains into consideration (changing *all* directions leaves the polynomial unchanged!) there are two polynomials associated to most two component links. We shall give both in those cases. Which one you have can be easily determined from the coefficient of the term in m^{-1}. In these simple cases this term will be $-(-l^2)^{-\lambda}(l + l^{-1})$ where λ is the linking number of the two oriented constituent components. Where one polynomial is given, all polynomials are equal independent of the relative choices of orientations.

2_1^2	$(l + l^3)\, m^{-1} - lm$
	$(l^{-3} + l^{-1})\, m^{-1} - l^{-1} m$
4_1^2	$(-l^3 - l^5)\, m^{-1} + (3\, l^3 + l^5)\, m - l^3 m^3$
	$(-l^{-5} - l^{-3})\, m^{-1} + (l^{-3} - l^{-1})\, m$
5_1^2	$(-l^{-1} - l)\, m^{-1} + (l^{-1} + 2l + l^3)\, m - l^3 m^3$
6^3_2	$(l^{-2} + 2 + l^2)\, m^{-2} + (-l^{-2} - 2 - l^2)\, m^2 + m^4$

REFERENCES

1. J. W. Alexander, *Trans. Amer. Math. Soc.* **30** (1928) 275.
2. R. Ball and M. L. Mehta, *J. Physique* **42** (1981) 1193.
3. J. Boeckman and G. Schill, *Tetrahedron* **30** (1974) 1945.
4. R. D. Brandt, W. B. R. Lickorish, and K. C. Millett, *A polynomial invariant for unoriented knots and links,* 1985 preprint.
5. J. H. Conway, *An enumeration of knots and links, and some of their algebraic properties, Computational Problems in Abstract Algebra,* Pergamon Press, New York (1970), 329—358.
6. P. Freyd, D. Yetter, J. Hoste, W. B. R. Lickorish, K. Millett, and A. Ocneanu, *Bull. Amer. Math. Soc.* **12** (2) (1985) 239.
7. V. F. R. Jones, *Bull. Amer. Math. Soc.* **12** (1) (1985) 103.
8. W. B. R. Lickorish and K. C. Millett, *A polynomial invariant of oriented links,* MSRI preprint 04212-85.
9. J. Przytycki and P. Traczyk, *Invariants of links of Conway type,* 1985 preprint.
10. D. Rolfsen, *Knots and links,* Publish or Perish Inc., Berkeley, Ca., 1976.
11. J. Simon, *Topological chirality of certain molecules,* 1985 preprint.
12. M. B. Thistlethwaite, *Knots to 13-crossings,* Math. Comp., to appear.
13. E. Wassermann, *Scientific American* **207** (5), (1962) 294—302.

SAŽETAK

Konfiguracijski popis, topologijska hiralnost i nove kombinatorijske invarijante

K. C. Millett

Opisane su nove matematičke metode koje se mogu upotrijebiti za razlikovanje konfiguracija čvorova u prostoru i za određivanje njihove topologijske kiralnosti.