A New Algorithm for Numerical Calculation of Link Invariants

Tetsuo Deguchi and Kyoichi Tsurusaki

Department of Physics, Faculty of Science,
University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113, Japan

Abstract

We introduce an algorithm for numerical calculation of derivatives of the Jones polynomial. This method gives a new tool for determining topology of knotted closed loops in three dimensions using computers.
1 Introduction

In chemistry and biology, knotted macromolecules such as DNA knots can be synthesized in experiments. In statistical mechanics of macromolecules, topological classification of configurations of polymer chains is an interesting and unsolved problem. Topological constraints could severely restrict available degrees of freedom in the configuration space, and would have important effects on thermodynamic quantities such as the entropy of the system. This problem was first formulated by Delbrück in '60s. Since then, several numerical works have been done. In these works unknotting probabilities of closed loops are evaluated in different systems such as the closed self-avoiding random walks and the rod-bead model.

In all these numerical researches, the special values ($\Delta_K(-1)$ or $\Delta_K(2)$) of the Alexander polynomial $\Delta_K(t)$ have been used as tools for classifying knots. In the algorithms, a closed loop is considered as trivial if the special value of the Alexander polynomial is found to be one. However, it is known that the Alexander polynomial does not distinguish some knots from the trivial knot (see also [13]). Consequently, the special values of the Alexander polynomial are not complete invariants for classification.

Recently various new link invariants, such as the Jones, the HOM-
FLY, and the Kauffman polynomials are introduced. \cite{14, 15, 16, 17}

If we could apply these new invariants to computer calculations, we would have a systematic method of determining topology of closed loops in 3 dimensions. However, it is not easy to calculate directly any special value of the new link polynomials for long closed loops with large number of steps. If we calculate the link polynomials through the Markov trace, the number of processes in computer calculation grows exponentially with respect to the step number \( N \) of the loops. Furthermore, in numerical calculation of link polynomials, we have to assign a proper number to the variable \( t \) so that the polynomials do not become numerically too large (overflow). Thus it seems that we could not directly calculate the Jones polynomial for large closed loops using computers.

The purpose of this paper is to show that if we devise new diagrammatic method using oriented link diagrams, then derivatives of link polynomials can be easily calculated using computers. This approach has the following two advantages.

1. We can evaluate derivatives of link polynomials in a calculation time proportional to some power of \( N \) (the length of loops).

2. We can avoid the overflow which could occur in evaluation of polynomials.

The outline of this paper consists of the following. In \S 2 we in-
roduce a state model for the Jones polynomials using oriented link diagrams, and construct an algorithm for calculating the derivatives. In §3 we show by examples that the derivatives of the Jones polynomial have enough information to distinguish knots from the trivial knot. In §4 applying the algorithm we estimate unknotting probability of closed self-avoiding random walks.

2 Algorithm of calculating the derivatives

2.1 Oriented state model

Let us consider diagrammatic methods for calculation of link polynomials. We call the methods state models. We have two types of state models of the Jones polynomial, that of unoriented link diagrams, and that of oriented link diagrams. We call a state model using oriented (unoriented) link diagrams oriented (unoriented) state model. L.H. Kauffman introduced an unoriented diagrammatic method called bracket polynomial for the Jones polynomial. [20] It seems, however, that the bracket polynomial is not suitable for calculation of derivatives of the Jones polynomial using computers.

We formulate an oriented state model of the Jones polynomial. [18, 19] Any oriented link diagram can be decomposed into the tangle diagrams given in Fig. 2.1.
For the tangle diagrams we define diagram weights. The nonzero diagram weights are given by the following.

\[
U_{12} = t^2, U_{21} = 1, U^{12} = 1, U^{21} = t^{-2},
\]

\[
G(\pm; 1)_{11}^{11} = G(\pm; 1)_{22}^{22} = 1, \quad G(\pm; 1)_{21}^{12} = G(\pm; 1)_{12}^{21} = t^2,
\]

\[
G(\pm; 2)_{21}^{12} = G(\pm; 2)_{22}^{21} = 1, \quad G(\pm; 2)_{21}^{21} = t^{-2} - t^2,
\]

The other nonzero diagram weights are given by the following relations.

\[
U_{ab} = \tilde{U}_{ab}, \quad U^{ab} = \tilde{U}^{ab},
\]

\[
G(\pm; 1) = G(\pm; 3), \quad G(\pm; 2) = G(\pm; 4).
\]

We introduce matrix notation \( X = X^{ab}_{cd}E^a_c \otimes E^b_d \), where \((E^a_c)_{ij} = \delta_{ai}\delta_{cj}\). For example we have

\[
U_{ab} = \tilde{U}_{ab} = \begin{pmatrix} 0 & t^2 \\ 1 & 0 \end{pmatrix},
\]
\[ G(+; 1) = G(+; 3) = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 - t^4 & t^2 & 0 \\
0 & t^2 & 0 & 0 \\
0 & 0 & 0 & 1 
\end{pmatrix}. \] (5)

We now consider state sum of the oriented state model. We can represent any given link \( L \) by a link diagram. We decompose the link diagram into pieces of the oriented tangle diagrams given in Fig. 2.1. We put variables on the edges of the tangle diagrams (see Fig. 2.2).

The variables can take two values, 1 and 2. Let each one of the variables take either 1 or 2, then we have a configuration (of variables) on the link diagram. We now assign the diagram weights in eqs. (4) and (2) to the oriented tangle diagrams and take multiplication of the diagram weights. Then we take summation over all the possible configurations on the link diagram. Let the symbol \( \phi(L) \) denote the sum. We call the sum \( \phi(L) \) oriented state sum. For example, we give the oriented state sum for the knot 3\_1 (see Fig. 2.2).

\[ \phi(L) = G_{ef}^{ab}(-; 1) \cdot G_{gh}^{cd}(-; 3) \cdot G_{ij}^{fg}(-; 4) \cdot U_{ad} \cdot U_{ac} \cdot \tilde{U}_{ei} \cdot \tilde{U}_{jh}. \] (6)

Here we have assumed the Einstein notation for sums over repeated indices. Another quantity necessary for calculation of the link poly-
nominal is the writhing number. The writhing number is defined as follows. The oriented crossings have two types \( G(+) \) and \( G(-) \). Each of these crossing types has been labeled with +1 or -1. The writhe of a link is defined by the sum of the labels for all the crossings in the link diagram. We thus define the Jones polynomial \( \alpha_J(L) \) using \( \phi(L) \) and writhe by

\[
\alpha_J(L) = \frac{\phi(L)}{t^2 + t^{-2}} \cdot (t^2)^{\text{writhe}}.
\]  

(7)

By checking the Reidemeister moves of the tangle diagrams[18] we can show that the definition (7) gives an isotopy invariant of knots and links. It is the Jones polynomial.

The oriented state model has the advantage that all the nonzero entries of the diagram weights of \( U \) and \( \tilde{U} \) do not involve the \( \pm \) sign although the nonzero entries are off-diagonal. If we take the limit \( t \to 1 \), then the oriented state model satisfies the following properties.

\[
\lim_{t \to 1} U = \lim_{t \to 1} \tilde{U} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},
\]

\[
\lim_{t \to 1} G_{cd}^{ab} (k; \pm) = \delta_d^a \delta_c^b \quad \text{(for} \quad k = 1, 2, 3, 4). \quad \text{(8)}
\]

where \( \delta_d^a \) and \( \delta_c^b \) denote the Kronecker delta.

Let us compare the oriented state model with the unoriented one. If we use the unoriented state model (bracket polynomial), in the
limit $t \to 1$, the nonzero entries of the matrices $U$ have $\pm$ factors. Therefore we have to count how many times the signs $\pm$ occur in a given configuration, and thus calculation time will grow as fast as $2^N$ with respect to the system size $N$.

### 2.2 Expansion of the state sum

Let us discuss calculation of derivatives of the Jones polynomial. We set

$$t^2 = 1 + \varepsilon,$$

and consider expansion of the Jones polynomial with respect to $\varepsilon$. Because the Jones polynomial is link invariant, the coefficients are also link invariants. The oriented state model in the last section directly leads to an algorithm for calculation of the coefficients. We expand the matrices $G$ and $U$ in terms of the parameter $\varepsilon$. We calculate the oriented state sum using the expanded matrices. For an illustration we consider the matrices $G(+; 1)$ and $U_{ab}$

$$G_{cd}^{ab}(+; 1) = \delta_d^a \delta_c^b + \varepsilon \cdot G_{cd}^{ab}(+; 1) {\ }^{(1)} + \varepsilon^2 \cdot G_{cd}^{ab}(+; 1) {\ }^{(2)}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} + \varepsilon \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -2 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \varepsilon^2 \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} ,$$

$$U_{ab} = U_{ab}^{(0)} + \varepsilon \cdot U_{ab}^{(1)}$$
\[
= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \varepsilon \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.
\] (10)

We call the matrices of 0-th, 1-st, 2-nd orders \ldots in the \varepsilon expansion matrices of 0-th order, 1-st order, 2-nd order, \ldots, respectively.

Let us show how to evaluate the second order contributions in the oriented state sum for the knot \(3_1\) (Fig 2.2). We first expand \(\phi(L)\) in eq. (6) by \(\varepsilon\).

\[
\phi(L) = 2 + \varepsilon \left\{G_{ef}^{ab}(-; 1)^{(1)} \delta^c_h \delta^d_g \delta^f_j \delta^g_i U_{ad}^{(0)} U_{bc}^{(0)} \bar{U}^{e_i(0)} \bar{U}^{j_h(0)} + \ldots \right\}
+ \varepsilon^2 \left\{G_{ef}^{ab}(-; 1)^{(1)} G_{gh}^{cd}(-; 3)^{(1)} \delta^f_j \delta^g_i U_{ad}^{(0)} U_{bc}^{(0)} \bar{U}^{e_i(0)} \bar{U}^{j_h(0)}
+ G_{ef}^{ab}(-; 1)^{(1)} \delta^c_h \delta^d_g G_{ij}^{fd}(-; 4)^{(1)} U_{ad}^{(0)} U_{bc}^{(0)} \bar{U}^{e_i(0)} \bar{U}^{j_h(0)} + \ldots \right\}
+ o(\varepsilon^2).
\] (11)

We now consider the first term of the 2-nd order \(G_{ef}^{ab}(-; 1)^{(1)}\), \(G_{gh}^{cd}(-; 3)^{(1)}\) \ldots in the expansion (11). This term is equivalent to the configuration of Fig 2.3 where the two matrices enclosed with circles are 1-st order and all the other are 0-th order.

We can readily evaluate the term without directly calculating the oriented state sum with respect to all the variables on the diagram. We identify the two variables on those edges of the braiding diagrams that are connected by the dotted lines each other, and then take the sum for the remaining independent variables. For any link diagram
we can thus reduce the number of independent variables into at most 4 in calculation of the second order contributions. Thus we have the following

\[
\sum_{a,b,c,d,e,f,g,h} \delta_{i}^{g} \delta_{j}^{f} \cdot G_{ab}^{cd}(1) \cdot G_{gh}^{ef}(3) \cdot \delta_{j}^{g} \cdot \delta_{i}^{f} \cdot U_{ad}(0) \cdot U_{bc}(0) \cdot \tilde{U}_{ei}^{(0)} \cdot \tilde{U}_{jh}^{(0)} = \sum_{a,b,g,h}' G_{ab}^{cd}(1) \cdot G_{gh}^{ef}(3) = -4. \tag{12}
\]

Here the symbol \(\sum'\) means that we take the summation for the independent variables \(a, b, g, h\) where \(c, d, e\) and \(f\) are assumed to be conjugate of \(b, a, g\) and \(h\), respectively; when \(a = 1\), then \(d = 2\). It is important to note that in calculation of the term in (12) we can eliminate the parts of the Kronecker deltas and the matrices \(U^{(0)}\) because of the property (8).

To finish this section, we make a comment. We can apply the method in this section to other link polynomials. We can calculate derivatives of the HOMFLY polynomial, in particular, of the Alexander polynomial. For an illustration, the oriented state model for the Alexander polynomial is given in Appendix A.

3 On derivatives of the Jones polynomial
3.1 Tools of classifying knots

We give a table of the derivatives of the Jones polynomial and the special value of the Alexander polynomial ($\Delta_K(-1)$) for knots.

Table 3.1

It is easy to see from the table that derivatives of the Jones polynomial are useful in classifying knot types. Since link polynomials are Laurent polynomials of a variable $t$, we can recover link polynomials from their derivatives (if we previously know something about the links such as upper bound of the crossing number etc.).

You may think that the second derivative of the Jones polynomial is not sufficient to distinguish a non-trivial knot from different knots. However, if we calculate the third order, then we may have much more precise distinction of knots (at least as far as prime knots are concerned). Further, if we calculate the fourth order we can distinguish even such knots that cannot be distinguished by the Alexander polynomial.

Let us consider a composite knot $(3_1)(3_1)(3_1)$ and a prime knot $8_{10}$ that share the same Alexander polynomial (see e.g., Ref. [10]). From Table 3.1 we see that the fourth derivative of the Jones polynomial distinguishes the two knots while for the Alexander polynomial at $t = -1$ ($\Delta_K(-1)$) the values for knots $(3_1)(3_1)(3_1)$ and $8_{10}$ coincide.
When we calculate the Alexander and the Jones polynomials for composite knots (links) it is useful that the link polynomial for the composite link $L_1 \# L_2$ is given by $\alpha(L_1 \# L_2) = \alpha(L_1)\alpha(L_2)$.

We think that the algorithm can make up for possible faults of the Alexander polynomial and thus we can determine knot types of closed loops much more exactly.

### 3.2 Remarks on derivatives of the Jones polynomial

It is noteworthy that derivatives of the Jones polynomial have many applications in knot theory. The following formulas have been given. [21]

\[
\frac{d}{dt} V_K(t = 1) = 0, \quad (13)
\]

\[
\frac{d^2}{dt^2} V_K(t = 1) = \text{const.} \times a_2(K). \quad (14)
\]

Here $a_2(K)$ is the second coefficient of the Conway polynomial (the Alexander polynomial) [12], which is related to Arf invariant. [10, 21]

We may discuss derivatives of the Jones polynomial from the viewpoint of perturbation theory of the Chern-Simons field theory. The coefficients for the terms in the perturbational expansion of the Wilson lines are expressed in terms of the Feynman integrals. [22] The numerical calculation of derivatives of the Jones polynomial corre-
sponds to evaluation of the Feynman integrals.

4 Numerical results and concluding remarks

We can apply the algorithm introduced in the present paper to any system of closed loops. For an illustration using the second derivative of the Jones polynomial we analyzed the system of rings [8] generated by closed Gaussian random walks.

Graph 4.1

The probability of occurrence of the trivial knot is plotted in the logarithmic scale as a function of the number of steps \( N \) of generated closed loops. We call the probability of the trivial knot unknotting probability. With the number of steps \( N \) fixed we evaluate the unknotting probability \( P_0 = N_t/M \) by counting the number \( N_t \) of trivial knots when we generate \( M = 1000 \) closed random walks.

From Graph 4.1 we see that the unknotting probability has an exponentially decaying behavior \( P_0(N) \sim \exp(-N/N_0) \), where we call \( N_0 \) characteristic length. We may consider \( N_0 \) necessary steps to form a nontrivial knot. From Graph 4.1. we have an estimation of characteristic length \( N_0; 300 < N_0 < 370 \).

Let us consider efficiency of our algorithm. We plot the time necessary for calculation of the second coefficients as a function of
the number of steps \((N)\) of given closed loops.

Graph 4.2

We see from Graph 4.2 that the calculation time for the second derivative of the Jones polynomial behaves asymptotically as \(N^2\) with respect to \(N\). From the result we may expect that the time for calculation of the \(r\)-th derivative grows as \(N^r\), or at least non-exponentially with respect to \(N\).

This result makes a clear difference from the other approaches to the Jones polynomial. We can calculate the Jones polynomial through explicit evaluation of the Markov trace or diagrammatic calculation using the skein relation. If these methods are applied to computer calculations, then they yield exponentially growing calculation time with respect to \(N\). We thus conclude that derivatives of link polynomials give a simple and systematic computer-orientated method of determining topology of given closed loops in 3 dimensions and that the algorithm in the paper can be applied to various problems related to knotted configurations in statistical physics and many body problem.

Acknowledgements
We would like to thank Prof. M. Wadati for his keen interest in this work.
References

[1] F.B. Dean, A. Stasiak, T. Koller and N.R. Cozzarelli, J. Biol. Chem. 260 (1985) 4795;
S.A. Wasserman, J.M. Duncan and N.R. Cozzarelli, Science 229 (1985) 171; Science 232 (1986) 951.

[2] D.W. Sumners, Geometry and Topology, ed. C. McCrory and T. Shifrin, (Marcel Dekker Inc., New York and Basel, 1987) 297.

[3] S.F. Edwards, J. Phys. A1 (1968) 15.

[4] N. Saito and Y. Chen, J. Chem. Phys. 59 (1973) 3701.

[5] F.W. Wiegel, Phase transitions and critical phenomena eds. C. Dom and J.L. Lebowitz, (Academic Press, London, 1983) p. 100;
J.P.J. Michels and F.W. Wiegel, Proc. R. Soc. London A403 (1986) 269.

[6] M. Delbrück, in Mathematical Problems in the Biological Sciences, ed. R.E. Bellman, Proc. Symp. Appl. Math. 14 (1962) 55.

[7] A.V. Vologodskii, A.V. Lukashin, M.D. Frank-Kamenetskii, and V.V. Anshelevich, Sov. Phys. JETP 39 (1974) 1059.
[8] J. des Cloizeaux and M. L. Mehta, J. Phys. (Paris) 40 (1979) 665.

[9] J.P.J. Michels and F. W. Wiegel, Phys. Lett. 90A (1982) 381.

[10] K. Koniaris and M. Muthukumar, Phys. Rev. Lett. 66 (1991) 2211.

[11] S. Kinoshita and H. Terasaka, Osaka J. Math. 9 (1957) 131.

[12] J.H. Conway, in Computational Problems in Abstract Algebra, (Pergamon Press, Oxford and New York, 1969) p. 329.

[13] D. Rolfsen, Knots and Links (Publish or Perish, Berkeley, 1976); G. Burde and H. Zieschang, Knots, Walter de Gruyter, Berlin and New York, 1985).

[14] V.F.R. Jones, Bull. Amer. Math. Soc. 12 (1985) 103; Ann. Math. 126 (1987) 335.

[15] P. Freyd, D. Yetter, J. Hoste, W.B.R. Lickorish, K.C. Millett, and A. Ocneanu, Bull. Amer. Math. Soc. 12 (1985) 103; J.H. Przytycki and P. Traczyk, Kobe. J. Math. 4 (1987) 115.

[16] L.H. Kauffman, On Knots, Annals of Mathematics Studies 115, Princeton University Press, (1987).
[17] M. Wadati, T. Deguchi and Y. Akutsu, Phys. Report 180 (1989) p.247.

[18] V.G. Turaev, Math. USSR Izvestiya 35 (1990) 411.

[19] Y. Akutsu, T. Deguchi and T. Ohtsuki, J. Knot Theory and Its Ramifications 1 (1992) 161.

[20] L.H. Kauffman, in the Proceedings of Santa Cruz Conference on the Artin’s Braid Group, Contemp. Math. 78 (1988) 263 (Amer. Math. Soc., Providence, R.I.);
L’Enseignement Mathematique, t.36 (1990) 1.

[21] H. Murakami, Kobe J. Math. 3 (1986) 61.

[22] E. Guadagnini, M. Martellini and M. Mintchev, Nucl. Phys. B330 (1990) 575.

[23] T. Deguchi, J. Phys. Soc. Jpn. 58 (1989) 3441.
A Appendix

We introduce an oriented state model of the Alexander polynomial. The diagram weights $U_{ab} \cdots$ and $G(\pm; k)_{ab}^{cd}$ are defined for the tangle diagrams in Fig. 2.1. The nonzero diagram weights are given by the following.

\begin{align}
U_{11} &= U_{11}^{11} = \tilde{U}_{11} = \tilde{U}_{22} = \tilde{U}_{22}^{22} = 1, U_{22} = U_{22}^{22} = -1, \quad (A.1) \\
G(+; 1)_{11}^{11} &= 1, G(+; 1)_{12}^{12} = G(+; 1)_{21}^{21} = t^{-2}, G(+; 1)_{21}^{21} = 1 - t^{-4}, \\
G(+; 2)_{22}^{22} &= -t^{-4}, G(+; 2)_{11}^{11} = 1, G(+; 2)_{12}^{12} = G(+; 2)_{21}^{21} = t^{-2}, \\
G(+; 2)_{11}^{11} &= t^{-4} - 1, G(+; 2)_{22}^{22} = -t^{-4}, G(+; 3)_{11}^{11} = 1, \\
G(+; 3)_{21}^{21} &= G(+; 3)_{12}^{12} = t^{-2}, G(+; 3)_{12}^{12} = 1 - t^{-4}, \\
G(+; 3)_{22}^{22} &= -t^{-4}, G(+; 4)_{11}^{11} = 1, G(+; 4)_{12}^{12} = G(+; 4)_{21}^{21} = t^{-2}, \\
G(+; 4)_{12}^{12} &= 1 - t^{-4}, G(+; 4)_{22}^{22} = -t^{-4}, G(-; 1)_{11}^{11} = 1, \\
G(-; 1)_{21}^{21} &= G(-; 1)_{12}^{12} = t^2, G(-; 1)_{12}^{12} = 1 - t^4, \\
G(-; 1)_{22}^{22} &= -t^4, G(-; 2)_{11}^{11} = 1, G(-; 2)_{12}^{12} = G(-; 2)_{21}^{21} = t^2, \\
G(-; 2)_{21}^{21} &= t^4 - 1, G(-; 2)_{22}^{22} = -t^4, G(-; 3)_{11}^{11} = 1, \\
G(-; 3)_{21}^{21} &= G(-; 3)_{12}^{12} = t^2, G(-; 3)_{21}^{21} = 1 - t^4, G(-; 3)_{22}^{22} = -t^4, \\
G(-; 4)_{11}^{11} &= 1, G(-; 4)_{12}^{12} = G(-; 4)_{21}^{21} = t^2, G(-; 4)_{11}^{11} = 1 - t^4, \\
G(-; 4)_{22}^{22} &= -t^4. \quad (A.2)
\end{align}

By the oriented state model we can calculate derivatives of the
Alexander polynomial. We give two remarks. (1) $U^{ab} \cdots$, are diagonal matrices, although there are $-1$ in some of the nonzero entries. (2) The nonzero off-diagonal elements of the matrices $G(\pm : j)$ become 1 when $t \to 1$ (cf. eq. (8)).
Figure Captions

Fig. 2.1 Oriented tangle diagrams.

Fig. 2.2 Link diagram of knot $3_1$ and variables $a, b, c, d, e, f, g, h, i, j$.

Fig. 2.3 Configuration for the term

$$
\sum_{a,b,c,d,e,f,g,h} G_{ef}^{ab}(+; 1) \cdot G_{gh}^{cd}(+; 3) \cdot \delta_f^g \delta_i^j \cdot U_{ad}^{(0)} \cdot U_{bc}^{(0)} \cdot \tilde{U}_{ei}^{(0)} \cdot \tilde{U}_{jh}^{(0)}
$$

Table 3.1 The symbol $\Delta_K(-1)$ denotes the Alexander polynomial. Remark that the first derivative of the Jones polynomial for a knot vanishes (see the formula (13)).

Graph 4.1 Unknotting probability $P_0(N)$ as a function of length $N$.

Graph 4.2 Calculation time versus length $N$. 