NMR Quantum Calculations of the Jones Polynomial
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Abstract

The repertoire of problems theoretically solvable by a quantum computer recently expanded to include the approximate evaluation of knot invariants, specifically the Jones polynomial. The experimental implementation of this evaluation, however, involves many known experimental challenges. Here we present experimental results for a small-scale approximate evaluation of the Jones Polynomial by nuclear-magnetic resonance (NMR), in addition we show how to escape from the limitations of NMR approaches that employ pseudo pure states.

Specifically, we use two spin 1/2 nuclei of natural abundance chloroform and apply a sequence of unitary transforms representing the Trefoil Knot, the Figure Eight Knot and the Borromean Rings. After measuring the state of the molecule in each case, we are able to estimate the value of the Jones Polynomial for each of the knots.

INTRODUCTION

The Jones polynomial [1], a great discovery in knot theory, has recently become an interesting topic for quantum computing. In particular, the use of quantum computing has been discussed for approximately evaluating the Jones polynomial by nuclear-magnetic resonance (NMR), in addition we show how to escape from the limitations of NMR approaches that employ pseudo pure states.

Specifically, we use two spin 1/2 nuclei of natural abundance chloroform and apply a sequence of unitary transforms representing the Trefoil Knot, the Figure Eight Knot and the Borromean Rings. After measuring the state of the molecule in each case, we are able to estimate the value of the Jones Polynomial for each of the knots.

THE JONES POLYNOMIAL AND UNITARY MATRICES

The Jones polynomial [1] was a great discovery in knot theory. It marked the beginning of a significant relationship between knot theory and statistical mechanics, particularly through the relationship of the polynomial with the Temperley-Lieb algebra, and through the explicit bracket state sum model [7, 8, 9, 10, 11]. From the topological side the Jones polynomial is striking because it can detect the difference between many knots and their mirror images.

The general algorithm to find the Jones polynomial is in the 2P complexity class, and so this is an algorithm worth understanding in the context of quantum computation.

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The key idea behind the present quantum algorithms to compute the Jones polynomial is to use unitary representations of the braid group derived from Temperley-Lieb algebra representations that take the form

$$\rho(\sigma_i) = AI + A^{-1}U_i$$

where $\sigma_i$ is a standard generator of the Artin braid group, $A$ is a complex number of unit length, and $U_i$ is a symmetric real matrix that is part of a representation of the Temperley-Lieb algebra. For more details about this strategy and the background information about the Jones polynomial, the bracket model for the Jones polynomial will be unitary whenever $U_i$ is a real symmetric matrix. Thus we will obtain a unitary representation of the three-strand braid group.

Quite specifically if we let $A = (a, b)$ and $|A\rangle = (a, b)^T$ the transpose of this row vector, then

$$e = |A\rangle\langle A| = \begin{bmatrix} a^2 & ab \\ ab & b^2 \end{bmatrix}$$

is a standard projector matrix when $a^2 + b^2 = 1$. To obtain a specific representation,

let $e_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ and $e_2 = \begin{bmatrix} a^2 \\ ab \\ b^2 \end{bmatrix}$. It is easy to check that $e_1e_2e_1 = a^2 e_1$ and that $e_2e_1e_2 = a^2 e_2$.

Note also that $e_1e_2 = \begin{bmatrix} a^2 & ab \\ 0 & 0 \end{bmatrix}$ and $e_2e_1 = \begin{bmatrix} a^2 & 0 \\ ab & 0 \end{bmatrix}$.

We define

$$U_i = \delta e_i$$

for $i = 1, 2$ with $a^2 = \delta^{-2}$. Then we have, for $i = 1, 2$

$$U_i^2 = \delta U_i, U_1U_2U_1 = U_1, U_2U_1U_2 = U_2.$$ 

Thus we have a representation of the Temperley-Lieb algebra on three strands. See [1] for a discussion of the properties of the Temperley-Lieb algebra.

Note also that we have

$$trace(U_1) = trace(U_2) = \delta,$$

while

$$trace(U_1U_2) = trace(U_2U_1) = 1$$

where trace denotes the usual matrix trace. We will use these results on the traces of these matrices in Section 3.

Now we return to the matrix parameters: Since $a^2 + b^2 = 1$ this means that $\delta^{-2} + b^2 = 1$ whence $b^2 = 1 - \delta^{-2}$. Therefore $b$ is real when $\delta^2$ is greater than or equal to 1.

We are interested in the case where $\delta = -A^2 - A^{-2}$ and $A$ is a unit complex number. Under these circumstances the braid group representation

$$\rho(\sigma_i) = AI + A^{-1}U_i$$

will be unitary whenever $U_i$ is a real symmetric matrix. Thus we will obtain a unitary representation of the three-strand braid group $B_3$ when $\delta^2 > 1$.

For any $A$ with $d = -A^2 - A^{-2}$ these formulas define a representation of the braid group. With $A = exp(i\theta)$, we have $d = -2\cos(2\theta)$. We find a specific range of angles $\theta$ in the following disjoint union of angular intervals

$$\theta \in [0, \pi/6] \cup [\pi/3, 2\pi/3] \cup [5\pi/6, 7\pi/6] \cup [4\pi/3, 5\pi/3] \cup [11\pi/6, 2\pi]$$

that give unitary representations of the three-strand braid group. Thus a specialization of a more general representation of the braid group gives rise to a continuous family of unitary representations of the braid group.

A Quantum Algorithm for the Jones Polynomial on Three Strand Braids

We gave above an example of a unitary representation of the three-strand braid group. In fact, we can use this representation to compute the Jones polynomial for closures of 3-braids, and therefore this representation provides a test case for the corresponding quantum computation. We now analyse this case by first making explicit...
how the bracket polynomial is computed from this representation. This unitary representation and its application to a quantum algorithm first appeared in [3]. When coupled with the Hadamard test, this algorithm gets values for the Jones polynomial in polynomial time in the same way as the AJL algorithm [2]. It remains to be seen how fast these algorithms are in principle when asked to compute the polynomial itself rather than certain specializations of it.

First recall that the representation depends on two matrices $U_1$ and $U_2$ with

$$U_1 = \begin{bmatrix} \delta & 0 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad U_2 = \begin{bmatrix} \delta^{-1} & \sqrt{1-\delta^{-2}} \\ \sqrt{1-\delta^{-2}} & \delta^{-1} \end{bmatrix}.$$ 

The representation is given on the two braid generators by

$$\rho(\sigma_1) = AI + A^{-1}U_1$$

and

$$\rho(\sigma_2) = AI + A^{-1}U_2$$

for any $A$ with $\delta = -A^2 - A^{-2}$, and with $A = \exp(i\theta)$, then $\delta = -2\cos(2\theta)$. We get the specific range of angles $\theta \in [0, \pi/6] \cup [\pi/3, 2\pi/3] \cup [5\pi/6, 7\pi/6] \cup [4\pi/3, 5\pi/3] \cup [11\pi/6, 2\pi]$ that give unitary representations of the three-strand braid group.

Note that $tr(U_1) = tr(U_2) = \delta$ while $tr(U_1U_2) = tr(U_2U_1) = 1$. If $b$ is any braid, let $I(b)$ denote the sum of the exponents in the braid word that expresses $b$. For $b$ a three-strand braid, it follows that

$$\rho(b) = A^{I(b)}I + \tau(b)$$

where $I$ is the $2 \times 2$ identity matrix and $\tau(b)$ is a sum of products in the Temperley Lieb algebra involving $U_1$ and $U_2$. Since the Temperley Lieb algebra in this dimension is generated by $I, U_1, U_2, U_1U_2$ and $U_2U_1$, it follows that

$$\langle \overline{b} \rangle = A^{I(b)}\delta^2 + tr(\tau(b))$$

where $\overline{b}$ denotes the standard braid closure of $b$, and the sharp brackets denote the bracket polynomial as described in previous sections. From this we see at once that

$$\langle \overline{b} \rangle = tr(\rho(b)) + A^{I(b)}(\delta^2 - 2).$$

It follows from this calculation that the question of computing the bracket polynomial for the closure of the three-strand braid $b$ is mathematically equivalent to the problem of computing the trace of the matrix $\rho(b)$.

The matrix in question is a product of unitary matrices, the quantum gates that we have associated with the braids $\sigma_1$ and $\sigma_2$. The entries of the matrix $\rho(b)$ are the results of preparation and detection for the two dimensional basis of qubits for our machine:

$$\langle i| \rho(b) |j \rangle.$$

Given that the computer is prepared in $|j\rangle$, the probability of observing it in state $|i\rangle$ is equal to $\langle i| \rho(b) |j \rangle^2$.

Thus we can, by running the quantum computation repeatedly, estimate the absolute squares of the entries of the matrix $\rho(b)$. This will not yield the complex phase information that is needed for either the trace of the matrix or the absolute value of that trace.

However, we do know how to write a quantum algorithm to compute the trace of a unitary matrix (via the Hadamard test). Since $\rho(b)$ is unitary, we can use this approach to approximate the trace of $\rho(b)$. This yields a quantum algorithm for the Jones polynomial for three-strand braids (evaluated at points $A$ such that the representation is unitary). Knowing $tr(\rho(b))$ from the quantum computation, we then have the formula for the bracket, as above,

$$\langle \overline{b} \rangle = \text{trace}(\rho(b)) + A^{I(b)}(\delta^2 - 2).$$

Then the normalized polynomial, invariant under all three Reidemeister moves is given by

$$f(\overline{b}) = (-A^2)^{-I(b)}\langle \overline{b} \rangle.$$

Finally the Jones polynomial in its usual form is given by the formula

$$V(\overline{b})(t) = f(\overline{b})(t^{-1/4}).$$

Thus we conclude that our quantum computer can approximate values of the Jones polynomial.

**ON THE RELATIONSHIP WITH THE AJL ALGORITHM**

Here is how the KL (Kauffman-Lomonaco) algorithm described in the previous section becomes a special case of a generalization of the AJL algorithm: Here we use notation from the AJL paper. In that paper, the generators $U_i$ (in our previous notation) for the Temperley-Lieb algebra, are denoted by $E_i$.

Let $L_k = \lambda_k = \sin(k\theta)$. For the time being $\theta$ is an arbitrary angle. Let $A = i\exp(i\theta/2)$ so that $-A^2 - A^{-2} = 2\cos(\theta)$.

We need to choose $\theta$ so that $\sin(k\theta)$ is non-negative for the range of $k$’s we use (these depend on the choice of line graph as in AJL). And we insist that $\sin(k\theta)$ is non-zero except for $k = 0$. Then it follows from trigonometry that $(L_{k-1} + L_{k+1})/L_k = d$ for all $k$.

Recall that the representation of the Temperley-Lieb algebra in AJL is given in terms of $E_i$ such that $E_i^2 = dE_i$ and the $E_i$ satisfy the Temperley-Lieb relations. Each $E_i$ acts non-trivially at the $i$ and $i + 1$ places in the
bit-string basis for the space and each $E_i$ is based upon $L_{a-1}, L_a, L_{a+1}$ where $a = z(i)$ is the endpoint of a walk described by the bitstring using only first $(i - 1)$ bits. Bitstrings represent walks on a line graph. Thus 1011 represents the walk Right, Left, Right, Right ending at node number 3 in

$$1 - - - - - 2 - - - - - 3 - - - - - 4.$$ 

For $p = 1011$, $z(1) = 1, z(2) = 2, z(3) = 1, z(4) = 1, z(5) = 3$.

More precisely, if we let $|v(a)⟩ = [\sqrt{L_{a-1}}/L_a, \sqrt{L_{a+1}}/L_a]^T$ (i.e. this is a column vector. $T$ denotes transpose.) Then

$$E_i = |v(z(i))⟩⟨v(z(i))|.$$ 

Here it is understood that this refers to the action on the bitstrings

$$- - - - - - - - - - 0 1 - - - - - -$$

and

$$- - - - - - - - - - 1 0 - - - - - -$$

obtained from the given bitstring by modifying the $i$ and $i+1$ places. The basis order is 01 before 10. Conceptually, this is a useful description, but it also helps to have the specific formulas laid out.

Now look at the special case of a line graph with three nodes and two edges:

$$1 - - - - - 2 - - - - - 3.$$ 

The only admissible binary sequences are $|110⟩$ and $|101⟩$, so the space corresponding to this graph is two dimensional, and it is acted on by $E_1$ with $z(1) = 1$ in both cases (the empty walk terminates in the first node) and $E_2$ with $z(2) = 2$ for $|110⟩$ and $z(2) = 2$ for $|101⟩$. Then we have

$$E_1|110⟩ = 0, E_1|101⟩ = d|101⟩,$$

$$E_2|xyz⟩ = |v⟩⟨v|xyz⟩$$

where $v = (\sqrt{1/d}, \sqrt{d-1}/d)^T$.

If one compares this two dimensional representation of the three strand Temperley - Lieb algebra and the corresponding braid group representation, with the representation Kauffman and Lomonaco use in their paper, it is clear that it is the same (up to the convenient replacement of $A = exp(i\theta)$ by $A = iexp(i\theta/2)$). The trace formula of AJL is a variation of the trace formula that Kauffman and Lomonaco use. Note that the AJL algorithm as formulated in \cite{2} does not use the continuous range of angles that are available to the KL algorithm. In the sequel to this paper and in a separate paper on the mathematics, we shall show how the entire AJL algorithm generalizes to continuous angular ranges.

**THEORY OF AN NMR SPECTROMETER USED AS A QUANTUM COMPUTER**

By convention, a quantum computer as conceived in theory is assumed to yield an outcome associated with a quantum measurement of some (possibly mixed) quantum state. In contrast, NMR machines implement a restricted version of an Expectation-Value Quantum Computer (EVQC), which in place of an outcome yields, to some finite precision, the expectation value for a measurement of a (again, possibly mixed) quantum state \cite{9}. Reflecting facts of NMR spectrometers, an NMR Quantum Computer (NMRQC) implements only the special measurement operators discussed in \cite{14}, and these measurement operators all have zero trace.

Here are the details. For a Hermitian measurement operator $M$ applied to a density matrix $\rho$, the EVQC of precision $\epsilon$ yields a value $x$ such that

$$|x - Tr(M\rho)| \leq \epsilon \Lambda(M),$$

where $\Lambda(M)$ is the difference between the minimum and the maximum eigenvalue of the measurement operator $M$, which is just the possible range to the trace as $\rho$ varies over all possible density matrices. (The factor $\Lambda(M)$ makes limitations of resolution immune to the mere analytic trick of multiplying the measurement operator by a constant.)

The measurement operators of main interest for the algorithm by which we estimate the trace of a unitary operator are $I_{1z}$ and $I_{1x}$, shortly to be defined.

**Thermal Equilibrium and initial state preparation**

To first order, the initial thermal state density operator of an ensemble (very large number) of quantum systems with $n + 1$ qubits each \cite{15} is given by

$$\rho_{th} \approx \frac{1}{N} (1 - \sum_{l=1}^{n+1} \alpha_l I_{1z}),$$

with $\alpha_l = \frac{\hbar \omega_l}{kT}$,

$$I_{1z} = \frac{1}{2} 1 \otimes \ldots \otimes 1 \otimes \sigma_z \otimes 1 \otimes \ldots \otimes 1,$$

(where the Pauli matrix $\sigma_z$ appears as the $l^{th}$ term in the product), $\omega_l$ is the resonance frequency of qubit $l$, $k$ is Boltzmann’s constant, $T$ is temperature and $N = 2^{n+1}$. The initial density operator required for our algorithm is given by

$$\rho_0 = \frac{1}{N} (1 - \alpha_1 I_{1z})$$

which can be prepared from $\rho_{th}$ by a variety of methods \cite{19}.\n
Algorithm to estimate the trace of $U$

The method presented here is based on the algorithm that first appeared in [17]. As mentioned above we assume that $U$ is given in the form of local operations on $n$ qubits. Given a program for $U$, Barenco et al. [18] describe a procedure to construct a program or local operations for the operator controlled-$U$, $cU$. $cU$ operates on $n + 1$ qubits, does not affect the first qubit, applies $U$ on the remaining $n$ qubits if the first qubit is $|1\rangle$ and does nothing otherwise:

$$cU|1\rangle|\psi\rangle = (1 \otimes U)|1\rangle|\psi\rangle = |1\rangle_U|\psi\rangle$$

$$cU|0\rangle|\psi\rangle = |0\rangle|\psi\rangle.$$

In block matrix form, $cU$ is given by:

$$cU = \begin{pmatrix} 1 & 0 \\ 0 & U \end{pmatrix}$$

We now describe our algorithm:

**Step 1:** Prepare the density operator:

$$\rho_1 = \frac{1}{N} (1 - \alpha_1 I_{1x}) = \frac{1}{N} (1 - \alpha_1 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}) = \frac{1}{N} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

where

$$I_{1x} = \frac{1}{2} \sigma_x \otimes 1$$

and

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

**Step 2:** Apply $cU$ to $\rho_1$:

$$\rho_2 = cU \rho_1 cU^\dagger = \frac{1}{N} (1 - \alpha_2 \begin{pmatrix} 0 & U^\dagger \\ U & 0 \end{pmatrix}).$$

**Step 3:** Measure $\langle I_{1x} + iI_{1y} \rangle$ to estimate

$$\text{trace}((I_{1x} + iI_{1y}) \rho_2) = \frac{\alpha_1}{N} \text{trace}(U),$$

where

$$I_{1y} = \frac{1}{2} \sigma_y \otimes 1$$

and

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

By Eq. (6) the result of this measurement is a complex number, $z$, such that

$$|\text{Re}(z) - \frac{\alpha_1}{N} \text{Re}[\text{trace}(U)]| \leq \epsilon$$

$$|\text{Im}(z) - \frac{\alpha_1}{N} \text{Im}[\text{trace}(U)]| \leq \epsilon.$$

It follows that the measurement result satisfies

$$|z - \text{trace}(U)| \leq \sqrt{2} \epsilon \alpha_1.$$

**EXAMPLE KNOTS AND EXPERIMENTAL RESULTS**

Experimental results for 3 knots on three strands were obtained using the methods outlined above. Specifically, we present results for the Trefoil Knot, the Figure Eight Knot, the Borromean Rings. A 2-spin system (details of the molecule and pulse sequences are given later) was used, the initial state given by the density operator proportional to $I_{1x}$ was prepared and a reference spectrum was then collected. This was followed by application of a controlled-unitary operator corresponding to and representing each knot separately found from the representation

$$s_1 = \rho(\sigma_1) \quad \text{and} \quad s_2 = \rho(\sigma_2).$$

Measurement of the expectation value of $I_{1x} + iI_{1y}$ after applying the controlled-unitary operator yields the trace of the unitary operator representing the knot and thus the estimate of the Jones Polynomial for each knot.

For each of the three knots, the Jones Polynomial was estimated at the complex numbers $e^{i\theta}$ for all $\theta$ in the range $0 \leq \theta \leq \pi/6$ at single degree increments (31 values). Comparison to the theoretical values shows excellent correspondence with experimental observations. Furthermore, the Jones Polynomial itself for each of these knots can be constructed from the experimental results.

**Experimental setup and molecule**

All experiments were performed on a Bruker Avance DMX 750 NMR spectrometer, equipped with a TXI 5 mm probe head with XYZ gradients. The sample was a 9:1 mixture of chloroform and deuterated acetone. It naturally contained about 1% of $^{13}$C-$^1$H chloroform which was the active compound that represented the hardware of our NMR quantum computer. The spin systems Larmor frequencies were 188.6349005 MHz for $^{13}$C and 750.1354275 MHz for $^1$H. The corresponding chemical shifts are 77.2 ppm and 7.235 ppm, respectively. The two spin-$1/2$ nuclei of $^{13}$C-$^1$H chloroform interact through scalar coupling. The corresponding coupling constant is J=209.5 Hz. The longitudinal relaxation times ($T_1$) and transversal relaxation times ($T_2$) of both spin-$1/2$ nuclei are: $^{13}$C $T_1$: 21.8 sec, $^{13}$C $T_2$: 0.19 sec, $^1$H $T_1$: 6.1 sec, $^1$H $T_2$: 0.48 sec. In order to suppress the signal of 99% $^{12}$C-$^1$H chloroform and to prepare the initial operator $I_x$, where $I$ corresponds to $^{13}$C ($^1$H will be referred to as $S$), the following preparation sequence was used in all experiments: the $^1$H spins were saturated by cw irradiation. Subsequently they were dephased by applying a 9.9 $\mu$s 90°($^1$H) pulse followed by a B_0 gradient. This sequence of 90° pulse and gradient was repeated twice with orthogonal gradients. Subsequently the $^{13}$C spin...
was excited using a 19.45 \( \mu \)s 90\( ^\circ \)(\(^{13}\)C) pulse. This preparation sequence was followed by the pulse sequence of the individual experiments (see Figure 7). Finally the \(^{13}\)C signal was detected by measuring 512 points during 452 ms. In order to improve the sensitivity, we decoupled all \(^1\)H spins during the detection period by applying the DIPSI-2 [19] decoupling sequence.

CONCLUSION

In this paper, we showed how the KL algorithm is a special case of a generalized AJL algorithm. Using the KL algorithm, we obtained a unitary representation of the three-strand braid group and discussed a method for computing the Jones polynomial using this representation over a range of complex numbers. Next, the theory of an idealized NMR quantum computer was presented and we showed how the trace of a unitary matrix can be experimentally determined. Experimental realization for three different knots where performed where the experimental data agreed with theoretical calculations. Future work includes generalizing the AJL algorithm for any number of strands, as was done for the three-strand braid group in this work, and their experimental implementations.

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FIG. 2: Experimental results for the Trefoil Knot

FIG. 3: The Figure Eight Knot generated by the sequence $\sigma_1 \sigma_2^{-1} \sigma_1 \sigma_2^{-1}$

FIG. 4: Experimental results for the Figure Eight Knot

FIG. 5: The Borromean Rings generated by the sequence $\sigma_1 \sigma_2^{-1} \sigma_1 \sigma_2^{-1} \sigma_1 \sigma_2^{-1}$
FIG. 6: Experimental results for the Borromean Rings

FIG. 7: Pulse sequence to implement a controlled-$s_{1,2}$ operation (left) and its inverse (right). For $s_1$ set $\gamma$ to 0. (To obtain a propagator of $1 \otimes s_{1,2}$ respectively its inverse, we have to apply a global phase factor of $e^{\mp i\pi \beta/2}$. The propagator of a pulse on the second spin-1/2 is defined as $U_{\text{pulse}} := e^{-i\epsilon S_{\nu}}$, with $S_{\nu} := (1 \otimes \sigma_{\nu}/2), \epsilon \in \{\alpha, \beta, \gamma\}$ and $\nu \in \{y, z\}$ where $\alpha = 0.5\pi - 2\theta$, $\beta = 0.5\pi + \theta$ and $\gamma = \tan^{-1}[\cos 4\theta/\sqrt{4\cos^2 2\theta - 1}] + \pi/2$ and $0 \leq \theta \leq \pi/6$. For the free evolution $U_{\text{evolution}} := e^{-i\pi tJ_{2I_z}S_z}$ with $2I_zS_z := 2(\sigma_z/2 \otimes \sigma_z/2)$. The pulse sequence is applied to the initial density operator $I_{1x}$.