Topological quantum information, virtual Jones polynomials and Khovanov homology

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Abstract. In this paper, we give a quantum statistical interpretation of the bracket polynomial state sum \( \langle K \rangle \), the Jones polynomial \( V_K(t) \) and virtual knot theory versions of the Jones polynomial, including the arrow polynomial. We use these quantum mechanical interpretations to give new quantum algorithms for these Jones polynomials. In those cases where the Khovanov homology is defined, the Hilbert space \( C(K) \) of our model is isomorphic with the chain complex for Khovanov homology with coefficients in the complex numbers. There is a natural unitary transformation \( U: C(K) \rightarrow C(K) \) such that \( \langle K \rangle = \text{Trace}(U) \), where \( \langle K \rangle \) denotes the evaluation of the state sum model for the corresponding polynomial. We show that for the Khovanov boundary operator \( \partial: C(K) \rightarrow C(K) \), we have the relationship \( \partial U + U \partial = 0 \). Consequently, the operator \( U \) acts on the Khovanov homology, and we obtain a direct relationship between the Khovanov homology and this quantum algorithm for the Jones polynomial.
1. Introduction

In this paper, we give a quantum statistical interpretation of the bracket polynomial state sum \( \langle K \rangle \), the Jones polynomial \( V_K(t) \) and generalizations of the Jones polynomial to virtual knot theory. We use this quantum mechanical interpretation to give a new quantum algorithm for computing the original Jones polynomial and these generalizations. In the case of the generalizations, the quantum algorithms in this paper are the first quantum algorithms known for computing these virtual knot and link invariants. The algorithms discussed here are useful for their conceptual simplicity and apply to all values of the polynomial variable that lie in the unit circle in the complex plane. Letting \( C(K) \) denote the Hilbert space for the algorithm (defined in section 3), there is a natural unitary transformation

\[
U: C(K) \rightarrow C(K)
\]

such that

\[
\langle K \rangle = \text{Trace}(U).
\]

The quantum algorithm comes directly from this formula via the Hadamard test (defined in appendix A of this paper). We then show that the framework for our quantum model for the bracket polynomial is a natural setting for the Khovanov homology. The Hilbert space \( C(K) \) of our model has a basis that is in one-to-one correspondence with the enhanced states of the bracket state summation. In fact, \( C(K) \) is isomorphic with the chain complex for the Khovanov homology with coefficients in complex numbers. We show that for the Khovanov boundary operator \( \partial: C(K) \rightarrow C(K) \), we have the relationship \( \partial U + U \partial = 0 \). Consequently, the operator \( U \) acts on the Khovanov homology, and we obtain a direct relationship between the Khovanov homology and this quantum algorithm for the Jones polynomial. The quantum algorithm given here is inefficient and so it remains an open problem to determine better quantum algorithms that involve both the Jones polynomial and the Khovanov homology.
The paper is organized as follows. Section 2 reviews the structure of the bracket polynomial, its state summation, the use of enhanced states and the relationship with the Jones polynomial. Section 3 describes the quantum statistical model for the bracket polynomial and refers to section 7 (appendix A) for details of the Hadamard test and the structure of the quantum algorithm. Section 4 describes virtual knot theory and generalizations to it of the Jones polynomial and an oriented and more powerful version that we call the arrow polynomial. We then explain how the methods of the previous section give quantum algorithms for these polynomial invariants of virtual knots and links. In the case of the original Jones polynomial for classical knots and links, there are other quantum algorithms [1, 16, 19, 33] using unitary representations of the braid group. For virtual knots and links we do not yet know appropriate unitary representations of the virtual braid group and so the algorithms presented here are the only currently known quantum algorithms for the virtual Jones polynomial and the arrow polynomial. Section 5 describes the relationship of the quantum model with the Khovanov homology axiomatically, without using the specific details of the Khovanov chain complex that give these axioms. In section 6, we construct the Khovanov chain complex in detail and show how some of its properties follow uniquely from the axioms of the previous section. In section 7, we discuss how the framework of this paper can be generalized to other situations where the Hilbert space of a quantum information system is also a chain complex. We give an example using the De Rham cohomology. In section 8 (appendix A), we detail the Hadamard test. In section 9 (appendix B), we discuss the efficiency (the lack thereof) of the algorithms presented in this paper and frame this deficiency as a problem for further research.

The results in this paper are new, and the paper itself is partly expository in that we give quick reviews of the bracket polynomial state sum model, the notion of quantum algorithms, virtual knot theory and the properties and definition of the Khovanov homology. Needless to say, a full exposition of these topics would be quite lengthy. Nevertheless, we hope that the reader who is new to some of them will find his or her interest sparked by the relationships that are described here.

2. The bracket polynomial and the Jones polynomial

The bracket polynomial [13] model for the Jones polynomial [9–11, 39] is usually described by the expansion

\[
\langle \langle \rangle \rangle = A \langle \langle \rangle \rangle + A^{-1} \langle \rangle \langle \rangle.
\]

Here the small diagrams indicate parts of otherwise identical larger knot or link diagrams. The two types of smoothing (local diagram with no crossing) in this formula are said to be of type A (A above) and type B (A−1 above).

\[
\langle \bigcirc \rangle = -A^2 - A^{-2},
\]

\[
\langle K \bigcirc \rangle = (-A^2 - A^{-2}) \langle K \rangle,
\]

\[
\langle' \rangle = (-A^3) \langle \bigcirc \rangle,
\]

\[
\langle' \rangle = (-A^{-3}) \langle \bigcirc \rangle.
\]
One uses these equations to normalize the invariant and make a model of the Jones polynomial. In the normalized version, we define

\[ f_K(A) = (-A^3)^{-\text{wr}(K)} \langle K \rangle / \langle \bigcirc \rangle, \]

where the writhe \( \text{wr}(K) \) is the sum of the oriented crossing signs for a choice of orientation of the link \( K \). Since we shall not use oriented links in this paper, see [13] for details of the writhe. One then has that \( f_K(A) \) is invariant under the Reidemeister moves (again see [13]) and the original Jones polynomial \( V_K(t) \) is given by the formula

\[ V_K(t) = f_K(t^{-1/4}). \]

The Jones polynomial has been of much interest since its discovery in 1983 due to its relationship with statistical mechanics, due to its ability to often detect the difference between a knot and its mirror image and due to the many open problems and relationships of this invariant with other aspects of low-dimensional topology.

**The state summation.** In order to obtain a closed formula for the bracket, we now describe it as a state summation. Let \( K \) be any unoriented link diagram. Define a state, \( S \), of \( K \) to be the collection of planar loops resulting from a choice of smoothing for each crossing of \( K \). There are two choices (\( A \) and \( B \)) for smoothing a given crossing, and thus there are \( 2^{c(K)} \) states of a diagram with \( c(K) \) crossings. In a state, we label each smoothing with \( A \) or \( A^{-1} \) according to the convention indicated by the expansion formula for the bracket. These labels are the vertex weights of the state. There are two evaluations related to a state. The first is the product of the vertex weights, denoted by \( \langle K | S \rangle \). The second is the number of loops in the state \( S \), denoted by \( \| S \| \). See [14] for relations of this state summation with the statistical mechanics of the Potts model.

Define the state summation, \( \langle K \rangle \), by the formula

\[ \langle K \rangle = \sum_S \langle K | S \rangle \delta^{\| S \|}, \]

where \( \delta = -A^2 - A^{-2} \). This is the state expansion of the bracket. It is possible to rewrite this expansion in other ways. For our purposes in this paper it is more convenient to think of the loop evaluation as a sum of two loop evaluations, one giving \(-A^2\) and the other giving \(-A^{-2}\). This can be accomplished by letting each state curve carry an extra label of +1 or −1. We describe these enhanced states below.

**Changing variables.** Letting \( c(K) \) denote the number of crossings in the diagram \( K \), if we replace \( \langle K \rangle \) by \( A^{-c(K)} \langle K \rangle \) and then replace \( A^2 \) by \( -q^{-1} \), the bracket is then rewritten in the following form:

\[ \langle \bigcirc \rangle = \langle \bigcirc \rangle - q \langle \bigcirc \rangle \]

with \( \langle \bigcirc \rangle = (q + q^{-1}) \). It is useful to use this form of the bracket state sum for the sake of the grading in the Khovanov homology (to be described below). We shall continue to refer to the smoothings labeled \( q \) (or \( A^{-1} \) in the original bracket formulation) as \( B \)-smoothings.

**Using enhanced states.** We now use the convention of enhanced states where an enhanced state has a label of 1 or \(-1\) on each of its component loops. We then regard the value of the loop \( q + q^{-1} \) as the sum of the value of a circle labeled with a 1 (the value is \( q \)) added to the value of
a circle labeled with an $-1$ (the value is $q^{-1}$). We could have chosen the less neutral labels of $+1$ and $X$ so that

$$q^1 \iff +1 \iff 1$$

and

$$q^{-1} \iff -1 \iff X,$$

since an algebra involving 1 and $X$ naturally appears later in relation to the Khovanov homology. It does no harm to take this form of labeling from the beginning.

Consider the form of the expansion of this version of the bracket polynomial in enhanced states. We have the formula as a sum over enhanced states $s$:

$$\langle K \rangle = \sum_s (-1)^{i(s)} q^{j(s)},$$

where $i(s)$ is the number of $B$-type smoothings in $s$ and $j(s) = i(s) + \lambda(s)$, with $\lambda(s)$ equal to the number of loops labeled 1 minus the number of loops labeled $-1$ in the enhanced state $s$.

One advantage of the expression for the bracket polynomial via enhanced states is that it is now a sum of monomials. We shall make use of this property throughout the remainder of the paper.

### 3. Quantum statistics and the Jones polynomial

We now use the enhanced state summation for the bracket polynomial with variable $q$ to give a quantum formulation of the state sum. Let $q$ be on the unit circle in the complex plane. (This is equivalent to letting the original bracket variable $A$ be on the unit circle and is equivalent to letting the Jones polynomial variable $t$ be on the unit circle.) As the reader will see below, we restrict $q$ to be on the unit circle so that a crucial transformation $U$ is unitary. The transformation $U$ will correspond to a physical process in the model. In quantum mechanical models physical processes are separated into unitary transformations and measurements. Measurements act as projections to a subspace of the Hilbert space, and processes that evolve without measurement are unitary.

Let $C(K)$ denote the complex vector space with orthonormal basis $\{|s\rangle\}$ where $s$ runs over the enhanced states of the diagram $K$. The Dirac notation $|X\rangle$ is a convenient way to designate an element of a vector space. The $X$ in $|X\rangle$ is a label that can be taken from some set of labels or objects. In this case we use $|s\rangle$, taking labels in one-to-one correspondence with the enhanced states of $K$.

The vector space $C(K)$ is the (finite-dimensional) Hilbert space for our quantum formulation of the Jones polynomial. A finite-dimensional Hilbert space is equipped with a positive definite inner product, and in this (Dirac) notation we write

$$|\psi\rangle = \sum_s z_s |s\rangle$$

to denote an arbitrary vector in the Hilbert space. If

$$|\phi\rangle = \sum_s w_s |s\rangle$$
is another vector in \( C(K) \), then the inner product of the two vectors is denoted by

\[
\langle \phi | \psi \rangle = \sum_s \bar{w}_s z_s,
\]

where \( \bar{w} \) denotes the complex conjugate of \( w \). In Dirac notation it is customary to think of the bra

\[
\langle \phi | = \sum s \bar{w}_s \langle s |,
\]

as an element of the dual space with the bra \( \langle s | \) the dual of the ket \( | s \rangle \) so that the bra–ket

\[
\langle s | s' \rangle = \delta(s, s')
\]

is a Kronecker delta (equal to 1 when \( s = s' \) and equal to 0 when \( s \neq s' \)). This expresses the fact that \( \{|s\rangle\} \) is an orthonormal basis for \( C(K) \).

In the quantum model, it is assumed that \( \{|s\rangle\} \) is a measurement basis so that when a state \( |\psi\rangle = \sum_s z_s |s\rangle \) with \( \sum_s |z_s|^2 = 1 \) undergoes measurement, it is projected to one of the basis vectors \( |s\rangle \) with probability \( |z_s|^2 \). A quantum process is a unitary transformation on the Hilbert space. The reader should note that the total probability \( \sum_s |z_s|^2 = 1 \) is preserved (by definition) under such processes. Quantum mechanics may be described succinctly as a theory in which physical states correspond to vectors in a Hilbert space, measurements and their frequencies are described as above, and physical processes that do not involve measurement correspond to unitary transformations of the Hilbert space. In practice, these unitary evolutions are described via the Schrödinger or Dirac equations and involve knowing the Hamiltonian for the system, an operator corresponding to the energy of the interactions. For the purpose of the mathematical design of quantum algorithms, it is sufficient to specify a composition of unitary operators to describe a process. More detailed design of the algorithm will specify Hamiltonians for specific forms of implementation.

**Remark.** While it is customary for a Hilbert space to be written with the letter \( H \), we do not follow that convention here, due to the fact that we shall soon regard \( C(K) \) as a chain complex and take its homology. One can hardly avoid using \( H \) for homology.

A unitary transformation for the bracket model. With \( q \) on the unit circle, we define a transformation

\[
U: C(K) \longrightarrow C(K)
\]

by the formula

\[
U |s\rangle = (-1)^{i(s)} q^{j(s)} |s\rangle
\]

for each enhanced state \( s \). Here \( i(s) \) and \( j(s) \) are as defined in the previous section of this paper. It follows immediately from our definition of the Hilbert space \( C(K) \) that \( U \) is a unitary transformation. That is, the inner product in \( C(K) \) is preserved by \( U \).

Let

\[
|\psi\rangle = \sum_s |s\rangle.
\]

The state vector \( |\psi\rangle \) is the sum over the basis states of our Hilbert space \( C(K) \). For convenience, we do not normalize \( |\psi\rangle \) to length one in the Hilbert space \( C(K) \). We then have

\[\text{New Journal of Physics 13 (2011) 125007 (http://www.njp.org/)}\]
Lemma. The evaluation of the bracket polynomial is given by the following formula:
\[ \langle K \rangle = \langle \psi | U | \psi \rangle. \]

Proof.

\[
\langle \psi | U | \psi \rangle = \sum_{s'} \sum_s \langle s' | (-1)^{i(s)} q^{j(s)} | s \rangle
\]

\[
= \sum_s \sum_{s'} (-1)^{i(s)} q^{j(s)} \langle s' | s \rangle = \sum_{s} (-1)^{i(s)} q^{j(s)} = \langle K \rangle,
\]

since
\[ \langle s' | s \rangle = \delta(s, s'), \]
where \( \delta(s, s') \) is the Kronecker delta, equal to 1 when \( s = s' \) and equal to 0 otherwise. \( \square \)

Quantum algorithms. A few words about quantum algorithms are appropriate at this point. In general, one begins with an initial state \( | \psi \rangle \) and a unitary transformation \( U \). Quantum processes are modeled by unitary transformations, and it is in principle possible to create a physical process corresponding to any given unitary transformation. In practice, one is limited by the dimensions of the spaces involved and by the fact that physical quantum states are very delicate and subject to decoherence. Nevertheless, one designs quantum algorithms at first by finding unitary operators that represent the information in the problem one wishes to calculate. Then the quantum part of the quantum computation is the physical process that produces the state \( U | \psi \rangle \) from the initial state \( | \psi \rangle \). At this point, \( U | \psi \rangle \) is available for measurement. Interaction with the environment is effectively a measurement, and will happen in any case, but one intends a controlled circumstance in which the measurement can occur. If \( \{|e_1\}, \ldots, |e_n\rangle \} \) is a basis for the Hilbert space (denoted here by \( C(K) \)), then we would have
\[ U | \psi \rangle = \sum_k z_k | e_k \rangle, \]
a linear combination of the basis elements. On measuring with respect to this basis, each \( |e_k\rangle \) corresponds to an observable outcome and this outcome will occur with frequency \( |z_k|^2/(\sum_i |z_i|^2) \).

A quantum algorithm for the Jones polynomial. The bracket polynomial evaluation is a quantum amplitude for the measurement of the state \( U | \psi \rangle \) in the \( \langle \psi \rangle \) direction. Since \( \langle \psi | U | \psi \rangle \) can be regarded as a diagonal element of the transformation \( U \) with respect to a basis containing \( | \psi \rangle \), this formula can be used in conjunction with a quantum algorithm that computes diagonal elements of a unitary matrix. The Hadamard test, discussed in appendix A of this paper, is just such an algorithm. Our formula \( \langle K \rangle = \langle \psi | U | \psi \rangle \), coupled with the Hadamard test, gives a new quantum algorithm for computing evaluations of the Jones polynomial. There is much more to be said about quantum algorithms in general and about quantum algorithms for the Jones polynomial in particular. See \([1, 16, 19, 20, 33]\) for more information.

It is useful to formalize the bracket evaluation as a quantum amplitude. This is a direct way to give a physical interpretation of the bracket state sum and the Jones polynomial. Just how this process can be implemented physically depends upon the interpretation of the Hilbert space \( C(K) \). It is common practice in theorizing about quantum computing and quantum
information to define a Hilbert space in terms of some mathematically convenient basis (such as the enhanced states of the knot or link diagram $K$) and leave open the possibility of realization of the space and the quantum evolution operators that have been defined upon it. In principle, any finite-dimensional unitary operator can be realized by some physical system. In practice, this is the problem of constructing quantum computers and quantum information devices. It is not so easy to construct what can be done in principle, and the quantum states that are produced may be all too short-lived to produce reliable computation. Nevertheless, one has the freedom to create spaces and operators on the mathematical level and to conceptualize these in a quantum mechanical framework. The resulting structures may be realized in nature and in present or future technology. In the case of our Hilbert space associated with the bracket state sum and its corresponding unitary transformation $U$, there is a rich extra structure related to the Khovanov homology that we discuss in the next section. One hopes that in a (future) realization of these spaces and operators, the Khovanov homology will play a key role in quantum information related to the knot or link $K$.

There are a number of conclusions that we can draw from the formula $\langle K \rangle = \langle \psi | U | \psi \rangle$. First of all, this formulation constitutes a quantum algorithm for the computation of the bracket polynomial (and hence the Jones polynomial) at any specialization where the variable is on the unit circle. We have defined a unitary transformation $U$ and then shown that the bracket is an evaluation in the form $\langle \psi | U | \psi \rangle$. This evaluation can be computed via the Hadamard test [32] and this gives the desired quantum algorithm. Once the unitary transformation is given as a physical construction, the algorithm will be as efficient as any application of the Hadamard test. The present algorithm requires an exponentially increasing complexity of construction for the associated unitary transformation, since the dimension of the Hilbert space is equal to the $2^{e(K)}$, where $e(K)$ is the number of enhanced states of the diagram $K$. (Note that $e(K) = \sum_S 2^{\|S\|}$, where $S$ runs over the $2^{c(K)}$ standard bracket states, $c(K)$ is the number of crossings in the diagram and $\|S\|$ is the number of loops in the state $S$.) Nevertheless, it is significant that the Jones polynomial can be formulated in such a direct way in terms of a quantum algorithm. By the same token, we can take the basic result of the Khovanov homology that says that the bracket is a graded Euler characteristic of the Khovanov homology as telling us that we are taking a step in the direction of a quantum algorithm for the Khovanov homology itself. This will be discussed below.

4. Quantum algorithms for Jones polynomials for virtual knots and links

In this section, we will extend our quantum algorithm for the Jones polynomial for classical knots to extensions of the Jones polynomial for virtual knots. Classical knot theory studies the embeddings of circles in the three-dimensional (3D) sphere $S^3$. By removing two points from $S^3$, we see that the classical knot theory can be regarded as the study of embeddings of circles in $S^2 \times I$, where $I = [0, 1]$ is a unit interval. In other words, classical knot theory studies the embeddings of knots in a thickened two-sphere. Virtual knot theory is a natural extension of classical knot theory to the study of knots in thickened surfaces of arbitrary genus. When we make this extension, it is natural to ask of a given knot what is the least genus surface that supports it. Thus we take embeddings of circles in thickened surfaces up to doing surgery on the thickened surfaces in the complement of the knot. This will be explained below. The result is a theory of virtual knots that is expressed in terms of diagrams similar to ordinary knot diagrams but containing virtual crossings that are neither over nor under but represent...
artifacts of drawing the virtual knot in the plane rather than on its appropriate surface. There are
generalized Reidemeister moves for the virtual knots, and one sees that the Jones polynomial
generalizes directly and acquires new properties in the virtual domain. For example, there
are infinitely many non-trivial virtual knots with the unit Jones polynomial. We also study a
more powerful generalization of the Jones polynomial that we call the arrow polynomial for
virtual knots. The arrow polynomial takes into account oriented structure in the diagrams that
occurs only on surfaces of higher genus. Both the generalized Jones polynomial and the arrow
polynomial acquire quantum algorithms by using Hilbert spaces spanned by enhanced states.
These quantum algorithms are new, and at the time of writing this, we do not know any other
quantum algorithms for these polynomial invariants of virtual knots.

4.1. Virtual knot theory

Knot theory studies the embeddings of curves in 3D space. Virtual knot theory studies the
embeddings of curves on thickened surfaces of arbitrary genus, up to the addition and removal
of empty handles from the surface. Virtual knots have a special diagrammatic theory, described
below, that makes handling them very similar to handling classical knot diagrams. Many
structures in classical knot theory generalize to the virtual domain.

In the diagrammatic theory of virtual knots, one adds a virtual crossing (see figure 1) that
is non-classical. A virtual crossing is represented by two crossing segments with a small circle
placed around the crossing point.

Moves on virtual diagrams generalize the Reidemeister moves for classical knot and link
diagrams. See figure 1. One can summarize the moves on virtual diagrams by saying that
the classical crossings interact with one another according to the usual Reidemeister moves,
while virtual crossings are artifacts of the attempt to draw the virtual structure in the plane.
A segment of diagram consisting of a sequence of consecutive virtual crossings can be excised
and a new connection made between the resulting free ends. If the new connecting segment
intersects the remaining diagram (transversally), then each new intersection is taken to be
virtual. Such an excision and reconnection is called a detour move. Adding the global detour move to the Reidemeister moves completes the description of moves on virtual diagrams. In figure 1 we illustrate a set of local moves involving virtual crossings. The global detour move is a consequence of moves (B) and (C) in figure 1. The detour move is illustrated in figure 2. Virtual knot and link diagrams that can be connected by a finite sequence of these moves are said to be equivalent or virtually isotopic.

Another way of understanding virtual diagrams is to regard them as representative of oriented Gauss codes [8, 35, 36] (Gauss diagrams). Such codes do not always have planar realizations. An attempt to embed such a code in the plane leads to the production of virtual crossings. The detour move makes the particular choice of virtual crossings irrelevant. Virtual isotopy is the same as the equivalence relation generated on the collection of oriented Gauss codes by abstract Reidemeister moves on these codes.

Figure 3 illustrates the two forbidden moves. Neither of these follows from Reidemeister moves plus detour move, and indeed it is not hard to construct examples of virtual knots that are non-trivial, but will become unknotted on the application of one or both of the forbidden moves. The forbidden moves change the structure of the Gauss code and, if desired, must be considered separately from the virtual knot theory proper.

4.2. Interpretation of virtual links as stable classes of links in thickened surfaces

There is a useful topological interpretation [35, 37] for this virtual theory in terms of embeddings of links in thickened surfaces. Regard each virtual crossing as a shorthand for a detour of one of the arcs in the crossing through a one-handle that has been attached to the two-sphere of the original diagram. By interpreting each virtual crossing in this way, we obtain an embedding of a collection of circles into a thickened surface $S_g \times R$, where $g$ is the number of virtual crossings in the original diagram $L$, $S_g$ is a compact oriented surface of genus $g$ and $R$ denotes the real line. We say that two such surface embeddings are stably equivalent if one can be obtained from another by isotopy in the thickened surfaces, homeomorphisms of the surfaces and the addition or subtraction of empty handles (i.e. the knot does not go through the handle).
We have

**Theorem 1** [4, 6, 35, 37]. Two virtual link diagrams are isotopic if and only if their corresponding surface embeddings are stably equivalent.

In figure 4, we illustrate some points about this association of virtual diagrams and knot and link diagrams on surfaces. Note that the projection of the knot diagram on the torus to a diagram in the plane (in the center of the figure) has a virtual crossing in the planar diagram where two arcs that do not form a crossing in the thickened surface project to the same point in the plane. In this way, virtual crossings can be regarded as artifacts of projection. The same figure shows a virtual diagram on the left and an ‘abstract knot diagram’ [4, 12] on the right. The abstract knot diagram is a realization of the knot on the left in a thickened surface with boundary and it is obtained by making a neighborhood of the virtual diagram that resolves the virtual crossing into arcs that travel on separate bands. The virtual crossing appears as an artifact of the projection of this surface to the plane. For more information about this correspondence [6, 35], see my other papers and the literature on virtual knot theory.
4.3. Review of the bracket polynomial for virtual knots

In this section, we recall how the bracket state summation model [13] for the Jones polynomial [9, 39] is defined for virtual knots and links. In the next section, we give an extension of this model using orientation structures on the states of the bracket expansion. The extension is also an invariant of flat virtual links.

We call a diagram in the plane purely virtual if the only crossings in the diagram are virtual crossings. Each purely virtual diagram is equivalent by the virtual moves to a disjoint collection of circles in the plane.

A state $S$ of a link diagram $K$ is obtained by choosing a smoothing for each crossing in the diagram and labelling that smoothing with either $A$ or $A^{-1}$ according to the convention that a counterclockwise rotation of the overcrossing line sweeps two regions labeled $A$ and that a smoothing that connects the $A$ regions is labeled by the letter $A$. Then, given a state $S$, one has the evaluation $\langle K | S \rangle$ equal to the product of the labels at the smoothings, and one has the evaluation $\|S\|$ equal to the number of loops in the state (the smoothings produce purely virtual diagrams). One then has the formula

$$\langle K \rangle = \sum_S \langle K | S \rangle d^{\|S\| - 1},$$

where the summation runs over the states $S$ of the diagram $K$, and $d = -A^2 - A^{-2}$. This state summation is invariant under all classical and virtual moves except the first Reidemeister move. The bracket polynomial is normalized to an invariant $f_K(A)$ of all the moves by the formula

$$f_K(A) = (-A^3)^{-w(K)} \langle K \rangle,$$

where $w(K)$ is the writhe of the (now) oriented diagram $K$. The writhe is the sum of the orientation signs ($\pm 1$) of the crossings of the diagram. The Jones polynomial, $V_K(t)$, is given in terms of this model by the formula

$$V_K(t) = f_K(t^{-1/4}).$$

This definition is a direct generalization to the virtual category of the state sum model for the original Jones polynomial. It is straightforward to verify the invariances stated above. In this way, one has the Jones polynomial for virtual knots and links.

We have [37]

**Theorem 3.** To each non-trivial classical knot diagram of one component $K$, there is a corresponding non-trivial virtual knot diagram $\text{Virt}(K)$ with the unit Jones polynomial.

**Proof sketch.** This theorem is a key ingredient in the problems involving virtual knots. Here is a sketch of its proof. The proof uses two invariants of classical knots and links that generalize to arbitrary virtual knots and links. These invariants are the Jones polynomial and the involutory quandle denoted by the notation $IQ(K)$ for a knot or link $K$.

Given a crossing $i$ in a link diagram, we define $s(i)$ to be the result of switching that crossing so that the undercrossing arc becomes an overcrossing arc and vice versa. We define the virtualization $v(i)$ of the crossing by the local replacement indicated in figure 6. In this figure we illustrate how, in virtualization, the original crossing is replaced by a crossing that is flanked by two virtual crossings. When we smooth the two virtual crossings in the virtualization we obtain the original knot or link diagram with the crossing switched.

Suppose that $K$ is a (virtual or classical) diagram with a classical crossing labeled $i$. Let $K_{v(i)}$ be the diagram obtained from $K$ by virtualizing the crossing $i$ while leaving the rest of the diagram just as before. Let $K_{s(i)}$ be the diagram obtained from $K$ by switching the crossing $i$
while leaving the rest of the diagram just as before. Then, it follows directly from the expansion formula for the bracket polynomial that
\[ V_{K^{s(i)}}(t) = V_{K^{s(i)}}(t). \]

As far as the Jones polynomial is concerned, switching a crossing and virtualizing a crossing look the same. We can start with a classical knot diagram \( K \) and choose a subset \( S \) of crossings such that the diagram is unknotted when these crossings are switched. Letting \( \text{Virt}(K) \) denote the virtual knot diagram obtained by virtualizing each crossing in \( S \), it follows that the Jones polynomial of \( \text{Virt}(K) \) is equal to unity, the Jones polynomial of the unknot. Nevertheless, if the original knot \( K \) is knotted, then the virtual knot \( \text{Virt}(K) \) will be non-trivial. We outline a proof of this fact below.

The involutory quandle [15] is an algebraic invariant equivalent to the fundamental group of the double-branched cover of a knot or link in the classical case. In this algebraic system, one associates a generator of the algebra \( I\mathcal{Q}(K) \) with each arc of the diagram \( K \) and there is a relation of the form \( c = ab \) at each crossing, where \( ab \) denotes the (non-associative) algebra product of \( a \) and \( b \) in \( I\mathcal{Q}(K) \). See figure 7. In this figure we have illustrated the fact that
\[ I\mathcal{Q}(K^{v(i)}) = I\mathcal{Q}(K). \]

As far as the involutory quandle is concerned, the original crossing and the virtualized crossing look the same.

If a classical knot is knotted, then its involutory quandle is non-trivial [38]. Hence if we start with a non-trivial classical knot and virtualize any subset of its crossings, we obtain a virtual knot that is still non-trivial. There is a subset \( A \) of the crossings of a classical knot \( K \) such that the knot \( SK \) obtained by switching these crossings is an unknot. Let \( \text{Virt}(K) \) denote...
the virtual diagram obtained from $A$ by virtualizing the crossings in the subset $A$. By the above discussion, the Jones polynomial of $\text{Virt}(K)$ is the same as the Jones polynomial of $SK$, and this is 1 since $SK$ is unknotted. On the other hand, the $IQ$ of $\text{Virt}(K)$ is the same as the $IQ$ of $K$, and hence if $K$ is knotted, then so is $\text{Virt}(K)$. We have shown that $\text{Virt}(K)$ is a non-trivial virtual knot with unit Jones polynomial. This completes the proof of the theorem.

It is an open problem whether there are knotted classical knots having unit Jones polynomial. (There are linked links whose linkedness is unseen [7, 31] by the Jones polynomial.) If there exists a classical knot with unit Jones polynomial, then one of the knots $\text{Virt}(K)$ produced by this theorem may be isotopic to a classical knot. Such examples are guaranteed to be non-trivial, but they are usually also non-classical. We do not know at the time of writing whether all such virtualizations of non-trivial classical knots, yielding virtual knots with unit Jones polynomial, are non-classical. It is an intricate task to verify that specific examples of $\text{Virt}(K)$ are non-classical. This has led to an investigation of new invariants for virtual knots. In this way, the search for classical knots with unit Jones polynomial expands to exploration of the structure of the infinite collection of virtual knots with unit Jones polynomial.

In figure 8, we show the Kishino diagram $K$. This diagram has unit Jones polynomial and its fundamental group is infinite cyclic. The Kishino diagram was discovered by Kishino in [25]. Many other invariants of virtual knots fail to detect the Kishino knot. Thus it has been a test case for examining new invariants. Dye and the present author [22] have used the bracket polynomial defined for knots and links in a thickened surface (the state curves are taken as isotopy classes of curves in the surface) to prove the non-triviality and non-classicality of the Kishino diagram. In fact, we have used this technique to show that knots with unit Jones polynomial obtained by a single virtualization are non-classical. See the problem list by Kauffman et al [24] for other
Figure 9. Oriented bracket expansion.

problems and proofs related to the Kishino diagram. In the next section, we describe the arrow polynomial, an extension of the bracket polynomial that can be used to discriminate the Kishino diagram and, in fact, shows that its corresponding flat virtual knot is non-trivial.

A quantum algorithm. We are now in a position to describe a quantum algorithm for the bracket polynomial extended to virtual knots and links. We repeat the construction as described in the beginning of the paper, rewriting the polynomial as a function of $q$ and specializing $q$ to be on the unit circle in the complex plane. We use enhanced states in exactly the same way and obtain a Hilbert space of enhanced states and a unitary transformation on this Hilbert space just as before. The difference here is that we do not know any other way of making a quantum algorithm for this extension of the Jones polynomial to virtual knots and links. In the next section, we extend this Hilbert space further to include the arrow polynomial.

4.4. A quantum algorithm for the arrow polynomial for virtual and flat virtual knots and links

This section describes an invariant for oriented virtual knots and links and for flat oriented virtual knots and links that we call the arrow polynomial [17, 23]. This invariant is considerably stronger than the Jones polynomial for virtual knots and links, and it is a very natural extension of the Jones polynomial, using the oriented diagram structure of the state summation. The construction of the arrow polynomial invariant begins with the oriented state summation of the bracket polynomial. This means that each local smoothing is either an oriented smoothing or a disoriented smoothing as illustrated in figure 9. In [23] we show how the arrow polynomial can be used to estimate virtual crossing numbers. In [17] we discuss the arrow polynomial and also a generalization, the extended bracket polynomial. The extended bracket polynomial is harder to compute than the arrow polynomial, and we shall not discuss its properties in this introduction. See our paper [17] for more on this subject. We will describe a new extension of the arrow polynomial to long virtual knots at the end of the present section.

In figure 9 we illustrate the oriented bracket expansion for both positive and negative crossings in a link diagram. An oriented crossing can be smoothed in the oriented fashion or the disoriented fashion as shown in figure 9. We refer to these smoothings as oriented and disoriented smoothings. To each smoothing we make an associated configuration that will be part of the arrow polynomial state summation. The configuration associated with a state with oriented and disoriented smoothings is obtained by applying the reduction rules described...
Figure 10. Reduction relation for the arrow polynomial.

below. See figure 10. The arrow polynomial state summation is defined by the formula

$$\langle \langle K \rangle \rangle = \Sigma_S \langle K | S \rangle d_1^{\| S \| - 1} [S],$$

where $S$ runs over the oriented bracket states of the diagram, $\langle K | S \rangle$ is the usual product of vertex weights as in the standard bracket polynomial and $[S]$ is a product of extra variables $K_1, K_2, \ldots$ associated with the state $S$. These variables are explained below. Note that we use the notation $\langle \langle K \rangle \rangle$ to indicate the arrow polynomial in this paper and in the figures in this paper. In [17] we have used this notation to refer to the extended bracket generalization of the arrow polynomial. Since we do not use the extended bracket in this paper, it is convenient to use the double-bracket notation here for the arrow polynomial.

Due to the oriented state expansion, the loops in the resulting states have extra combinatorial structure in the form of paired cusps as shown in figure 10. Each disoriented smoothing gives rise to a cusp pair where each cusp has either two oriented lines going into the cusp or two oriented lines leaving the cusp. We reduce this structure according to a set of rules that yields invariance of the state summation under the Reidemeister moves. The basic convention for this simplification is shown in figure 10. Each cusp is denoted by an angle with arrows either both entering the vertex or both leaving the vertex. Furthermore, the angle locally divides the plane into two parts: one part is the span of an acute angle; the other part is the span of an obtuse angle. We refer to the span of the acute angle as the inside of the cusp.

Remark on state reduction. View figure 10. The basic reduction move in this figure corresponds to the elimination of two consecutive cusps on a single loop. Note that we allow cancelation of consecutive cusps along a loop where the cusps both point to the same local region of the two local regions delineated by the loop. We do not allow cancelation of a ‘zigzag’ where two
consecutive cusps point to opposite (local) sides of the loop. In a classical knot or link diagram, all state loops reduce to loops that are free from cusps.

Figure 10 illustrates the basic reduction rule for the arrow polynomial. The reduction rule allows the cancelation of two adjacent cusps when they have insides on the same side of the segment that connects them. When the insides of the cusps are on opposite sides of the connecting segment, no cancelation is allowed. Each state circle is seen as a circle graph with extra nodes corresponding to the cusps. Figure 10 illustrates the simplification of two circle graphs. In one case, the graph reduces to a circle with no vertices. In the other case, there is no further cancelation, but the graph is equivalent to the one without a virtual crossing. The state expansion for $\langle \langle K \rangle \rangle$ is exactly as shown in figure 9, and we use the reduction rule of figure 10 so that each state is a disjoint union of reduced circle graphs. Since such graphs are planar, each is equivalent to an embedded graph (no virtual crossings) via the detour move, and the reduced forms of such graphs have $2n$ vertices that alternate in type around the circle so that $n$ are pointing inward and $n$ are pointing outward. The circle with no vertices is evaluated as $d = -A^2 - A^{-2}$ as is usual for these expansions, and the circle is removed from the graphical expansion. We let $K_n$ denote the circle graph with $2n$ alternating vertex types as shown in figure 10 for $n = 1$ and $n = 2$. Each circle graph contributes $d = -A^2 - A^{-2}$ to the state sum and the graphs $K_n$ for $n \geq 1$ remain in the graphical expansion. Each $K_n$ is an extra variable in the polynomial. Thus a product of the $K_n$s corresponds to a state that is a disjoint union of reduced circle graphs. By evaluating each circle graph as $d = -A^2 - A^{-2}$ (as well as taking its arrow variable $K_n$), we guarantee that the resulting polynomial will reduce to the original bracket polynomial when each of the new variables $K_n$ is set equal to unity. Note that we continue to use the caveat that an isolated circle or circle graph (i.e. a state consisting of a single circle or single circle graph) is assigned a loop value of unity in the state sum. This ensures that $\langle \langle K \rangle \rangle$ is normalized so that the unknot receives the value one.

We have the following proposition, showing that the phenomenon of cusped states and extra variables $K_n$ only occurs for virtual knots and links.

**Proposition 2.** In a classical knot or link diagram, all state loops reduce to loops that are free from cusps.

**Proof.** See [18].

We now have the following state summation for the arrow polynomial

$$\langle \langle K \rangle \rangle = \Sigma_S \langle K | S \rangle d^{\|S\|-1} [S],$$

where $S$ runs over the oriented bracket states of the diagram, $\langle K | S \rangle$ is the usual product of vertex weights as in the standard bracket polynomial, $\|S\|$ is the number of circle graphs in the state $S$, and $[S]$ is a product of the variables $K_n$ associated with the non-trivial circle graphs in the state $S$. Note that each circle graph (trivial or not) contributes to the power of $d$ in the state summation, but only non-trivial circle graphs contribute to $[S]$.

**Theorem 6.** With the above conventions, the arrow polynomial $\langle \langle K \rangle \rangle$ is a polynomial in $A$, $A^{-1}$ and the graphical variables $K_n$ (of which finitely many will appear for any given virtual knot or link). $\langle \langle K \rangle \rangle$ is a regular isotopy invariant of virtual knots and links. The normalized version

$$W[K] = (-A^3)^{-\text{wr}(K)} \langle \langle K \rangle \rangle$$

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is an invariant virtual isotopy. If we set \( A = 1 \) and \( d = -A^2 - A^{-2} = -2 \), then the resulting specialization
\[ F[K] = \langle \langle K \rangle \rangle (A = 1) \]
is an invariant of flat virtual knots and links.

**Proof.** See [18]. \( \square \)

The quantum algorithm. We can now describe the Hilbert space for the arrow polynomial. Just as in the case of the bracket polynomial, we set \( q = -A^{-2} \) and replace the arrow polynomial expansion with an expansion over enhanced states so that
\[ \langle \langle K \rangle \rangle = \sum_i q^{j_i} (-1)^{i_i} [s], \]
where \( q \) is on the unit circle and an enhanced state is a state \( S \) of the arrow polynomial that has an extra label of \( \pm 1 \) attached to each of its loops. The enhanced state \( s \) then contributes \(-q^{\text{sign}(s)}\) to the power of \( q \) and sign for the monomial \( q^{j_i} (-1)^{i_i} [s] \). It remains to define \([s]\) as a unit complex number. For this, we choose one unit complex number for each of the infinitely many variables \( K_n \) for \( n \) a natural number. The algorithm we choose depends on this choice. Then \([s]\) denotes the product of the values \( K_i \) for the loops in the enhanced state that have non-zero arrow numbers. With this numerical specialization of the arrow polynomial, we can define a unitary transformation \( U: \text{Hilb}(K) \rightarrow \text{Hilb}(K) \) by
\[ U[s] = q^{j(s)} (-1)^{i(s)} [s] [s]. \]
Here \( \text{Hilb}(K) \) is the Hilbert space with orthonormal basis the set of \([s]\) where \( s \) is a reduced enhanced state of the arrow polynomial. Each such state has a collection of arrow numbers for its loops and a sign attached to each of its loops for enhancement. We then have that
\[ \text{Trace}(U) = \langle \langle K \rangle \rangle. \]
By the Hadamard test this gives a quantum algorithm for the Arrow polynomial for virtual knots and links.

5. Khovanov homology and a quantum model for the Jones polynomial

In this section we outline how the Khovanov homology is related to our quantum model. This can be done essentially axiomatically, without giving the details of the Khovanov construction. We give the details in the next section. The material on Khovanov homology in this paper can be generalized to encompass the quantum algorithms we have discussed for virtual knot polynomials. This will be the subject of a separate paper. In the present paper, the sections on the Khovanov homology refer to the Khovanov homology for classical knots and links.

The outline for Khovanov homology is as follows:

1. There is a boundary operator \( \partial \) defined on the Hilbert space of enhanced states of a link diagram \( K \)
\[ \partial: C(K) \rightarrow C(K) \]
such that \( \partial \partial = 0 \) and so that if \( C^{i,j} = C^{i,j}(K) \) denotes the subspace of \( C(K) \) spanned by enhanced states \([s]\) with \( i = i(s) \) and \( j = j(s) \), then
\[ \partial: C^{i,j} \rightarrow C^{i+1,j}. \]
That is, we have the formulae
\[ i(\partial |s\rangle) = i(|s\rangle) + 1 \]
and
\[ j(\partial |s\rangle) = j(|s\rangle) \]
for each enhanced state \( s \). In the next section, we shall explain how the boundary operator is constructed.

2. **Lemma.** By defining \( U : C(K) \rightarrow C(K) \) as in the previous section, via
\[ U |s\rangle = (-1)^{i(s)} q^{j(s)} |s\rangle, \]
we have the following basic relationship between \( U \) and the boundary operator \( \partial \):
\[ U \partial + \partial U = 0. \]

**Proof.** This follows at once from the definition of \( U \) and the fact that \( \partial \) preserves \( j \) and increases \( i \) to \( i + 1 \).

3. From this lemma we conclude that the operator \( U \) acts on the homology of \( C(K) \). We can regard \( H(C(K)) = \text{Ker}(\partial) / \text{Image}(\partial) \) as a new Hilbert space on which the unitary operator \( U \) acts. In this way, the Khovanov homology and its relationship with the Jones polynomial have a natural quantum context.

4. For a fixed value of \( j \),
\[ C^{*, j} = \bigoplus_i C^{i, j} \]
is a subcomplex of \( C(K) \) with the boundary operator \( \partial \). Consequently, we can speak of the homology \( (H(C)^{*, j}) \). Note that the dimension of \( C^{ij} \) is equal to the number of enhanced states \( |s\rangle \) with \( i = i(s) \) and \( j = j(s) \). Consequently, we have
\[ \langle K \rangle = \sum_s q^{j(s)} (-1)^{i(s)} = \sum_j q^j \sum_i (-1)^i \dim(C^{ij}) \]
\[ = \sum_j q^j \chi(C^{*, j}) = \sum_j q^j \chi(H(C^{*, j})). \]

Here we use the definition of the **Euler characteristic of a chain complex**
\[ \chi(C^{*, j}) = \sum_i (-1)^i \dim(C^{ij}) \]
and the fact that the Euler characteristic of the complex is equal to the Euler characteristic of its homology. The quantum amplitude associated with the operator \( U \) is given in terms of the Euler characteristics of the Khovanov homology of the link \( K \).
\[ \langle K \rangle = \langle \psi | U | \psi \rangle = \sum_j q^j \chi(H(C^{*, j}(K))). \]

Our reformulation of the bracket polynomial in terms of the unitary operator \( U \) leads to a new viewpoint on the Khovanov homology as a representation space for the action of \( U \). The bracket polynomial is then a quantum amplitude that expresses the Euler characteristics of the homology associated with this action. The decomposition of the chain complex into the
parts $C^{i,j}(K)$ corresponds to the eigenspace decomposition of the operator $U$. The reader will note that in this case the operator $U$ is already diagonal in the basis of enhanced states for the chain complex $C(K)$. We regard this reformulation as a guide to further questions about the relationship of the Khovanov homology with quantum information associated with the link $K$.

As we shall see in the next section, the internal combinatorial structure of the set of enhanced states for the bracket summation leads to the Khovanov homology theory, whose graded Euler characteristic yields the bracket state sum. Thus we have a quantum statistical interpretation of the Euler characteristics of the Khovanov homology theory and a conceptual puzzle about the nature of this relationship with the Hilbert space of that quantum theory. It is this relationship that is the subject of this paper. The unusual point about the Hilbert space is that each of its basis elements has a specific combinatorial structure that is related to the topology of the knot $K$. Thus this Hilbert space is, from the point of view of its basis elements, a form of ‘taking apart’ of the topological structure of the knot that we are interested in studying.

Homological structure of the unitary transformation. We now prove a general result about the structure of a chain complex that is also a finite-dimensional Hilbert space. Let $C$ be a chain complex over the complex numbers with the boundary operator

$$
\partial: C^i \rightarrow C^{i+1},
$$

with $C$ denoting the direct sum of all the $C^i$, $i = 0, 1, 2, \ldots, n$ (for some $n$). Let

$$
U: C \rightarrow C
$$

be a unitary operator that satisfies the equation $U \partial + \partial U = 0$. We do not assume a second grading $j$ as occurs in the Khovanov homology. However, since $U$ is unitary, it follows [29] that there is a basis for $C$ in which $U$ is diagonal. Let $B = \{|s\rangle\}$ denote this basis. Let $\lambda_s$ denote the eigenvalue of $U$ corresponding to $|s\rangle$ so that $U|s\rangle = \lambda_s |s\rangle$. Let $\alpha_{s,s'}$ be the matrix element for $\partial$ so that

$$
\partial|s\rangle = \sum_{s'} \alpha_{s,s'} |s'\rangle,
$$

where $s'$ runs over a set of basis elements so that $i(s') = i(s) + 1$.

Lemma. With the above conventions, we have that for $|s'\rangle$ a basis element such that $\alpha_{s,s'}, \neq 0$ then $\lambda_{s'} = -\lambda_s$.

Proof. Note that

$$
U \partial |s\rangle = U \left( \sum_{s'} \alpha_{s,s'} |s'\rangle \right) = \sum_{s'} \alpha_{s,s'} \lambda_s |s'\rangle,
$$

while

$$
\partial U |s\rangle = \partial \lambda_s |s\rangle = \sum_{s'} \alpha_{s,s'} \lambda_s |s'\rangle.
$$

Since $U \partial + \partial U = 0$, the conclusion of the lemma follows from the independence of the elements in the basis for the Hilbert space. 

In this way we see that eigenvalues will propagate forward from $C^0$ with alternating signs according to the appearance of successive basis elements in the boundary formulae for the
chain complex. Various states of affairs are possible in general, with new eigenvalues starting at some $C^k$ for $k > 0$. The simplest state of affairs would be if all the possible eigenvalues (up to multiplication by $-1$) for $U$ occurred in $C^0$ so that

$$C^0 = \bigoplus \lambda C^0_{\lambda},$$

where $\lambda$ runs over all the distinct eigenvalues of $U$ restricted to $C^0$, and $C^0_{\lambda}$ is spanned by all $|s\rangle$ in $C^0$ with $U|s\rangle = \lambda|s\rangle$. Let us take the further assumption that for each $\lambda$ as above, the subcomplexes

$$C^k_{\lambda} : C^k_{\lambda} \rightarrow C^{k-1}_{\lambda} \rightarrow C^{k-2}_{\lambda} \rightarrow \cdots C^0_{(-1)^k\lambda}$$

have $C = \bigoplus \lambda C^k_{\lambda}$ as their direct sum. With this assumption about the chain complex, define $|\psi\rangle = \sum_s |s\rangle$ as before, with $|s\rangle$ running over the whole basis for $C$. Then it follows just as in the beginning of this section that

$$\langle \psi | U | \psi \rangle = \sum_{\lambda} \lambda \chi(H(C^k_{\lambda})).$$

Here $\chi$ denotes the Euler characteristic of the homology. The point is that this formula for $\langle \psi | U | \psi \rangle$ takes exactly the form we had for the special case of Khovanov homology (with eigenvalues $(-1)^q\lambda$), but here the formula occurs just in terms of the eigenspace decomposition of the unitary transformation $U$ in relation to the chain complex. Clearly there is more work to be done here and we will return to it in a subsequent paper.

*Remark on the density matrix.* Given the state $|\psi\rangle$, we can define the density matrix

$$\rho = |\psi\rangle \langle \psi|.$$ 

With this definition it is immediate that

$$\text{Tr}(U \rho) = \langle \psi | U | \psi \rangle,$$

where $\text{Tr}(M)$ denotes the trace of a matrix $M$. Thus we can restate the form of our result about Euler characteristics as

$$\text{Tr}(U \rho) = \sum_{\lambda} \lambda \chi(H(C^k_{\lambda})).$$

In searching for an interpretation of the Khovanov complex in this quantum context, it is useful to use this reformulation. For the bracket we have

$$\langle K \rangle = \langle \psi | U | \psi \rangle = \text{Tr}(U \rho).$$

*Remark on physics.* We are taking the whole Hilbert space as the state space of a physical system. If the system were a classical system, then the energetic states of the classical system would correspond to the basis we have chosen for the Hilbert space. This is in line with the concepts of quantum mechanics, since the classical states are then in correspondence to a basis for measurement. In the quantum context we think of the elements in the Hilbert space as corresponding to superpositions of possible measurements. All this is then transposed to topological configurations for the knot or link. But the new ingredient is the one from topology that will turn the states of the knot into a chain complex and lead to homological computations. Since we are using enhanced states, each state is a generator for the chain complex. Thus we can regard $C(K)$ itself as the chain complex (over the complex numbers) and add in extra grading structure to boot. There is also the fine structure of the underlying state circles, but this is not
seen by the Hilbert space itself and the chain complex structure can certainly be written just in terms of the basis of the Hilbert space. We want to know what the relationship is between the unitary transformation and the homological structure. This relation is given by the way the grading works in relation to \((-1)^iq^j\) for each state: the constancy of the quantum grading \(j\) under the action of the differential. It is this that makes \(\langle \psi | U | \psi \rangle\) a graded Euler characteristic for the homology. In this way the unitary transformation is linked with the structure of state transitions that govern the homology. At the end of this section we indicate a more general approach to this pattern.

The key conceptual issue is the construction of a Hilbert space whose basis is the set of observable states of a physical system. We can always do this for a statistical mechanical system. Let \(s\) denote such states and \(E(s)\) denote the energy of a state \(s\) (observable and real). Let \(t\) denote time and \(\hbar\) denote Planck’s constant. Define a unitary transformation \(U(t)\) by

\[
U(t)|s\rangle = e^{(i/t)E(s)}|s\rangle.
\]

Define the amplitude

\[
A(t) = \sum_s e^{(i/t)E(s)}.
\]

Note that we have the formula

\[
A(t) = \langle \psi | U(t) | \psi \rangle,
\]

where \(|\psi\rangle = \sum_s |s\rangle\) just as before. Now \(U(t)\) can be regarded as the quantum evolution of the state of the system and we have written this amplitude in analogy with a partition function for the statistical mechanics model.

In this point of view, the Hilbert space for expressing the bracket polynomial as a quantum statistical amplitude is quite naturally the chain complex for the Khovanov homology with complex coefficients, and the unitary transformation that is the structure of the bracket polynomial acts on the homology of this chain complex. This means that the homology classes contain information preserved by the quantum process that underlies the bracket polynomial. We would like to exploit this direct relationship between the quantum model and the Khovanov homology to obtain deeper information about the relationship of topology and quantum information theory, and we would like to use this relationship to probe the properties of these topological invariants.

6. Background on Khovanov homology

In this section, we describe the Khovanov homology along the lines of [2, 26], and we tell the story so that the gradings and the structure of the differential emerge in a natural way. This approach to motivating the Khovanov homology uses elements of Khovanov’s original approach, Viro’s use of enhanced states for the bracket polynomial [34] and Bar–Natan’s emphasis on tangle cobordisms [3]. We use similar considerations in our paper [21].

Two key motivating ideas are involved in finding the Khovanov invariant. First of all, one would like to categorify a link polynomial such as \(\langle K \rangle\). There are many meanings to the term categorify, but here the quest is to find a way of expressing the link polynomial as a graded Euler characteristic \(\langle K \rangle = \chi_q(H(K))\) for some homology theory associated with \(\langle K \rangle\).

We will use the bracket polynomial and its enhanced states as described in the previous sections of this paper. To see how the Khovanov grading arises, consider the form of the
expansion of this version of the bracket polynomial in enhanced states. We have the formula as a sum over enhanced states $s$:

$$\langle K \rangle = \sum_s (-1)^{i(s)} q^{j(s)},$$

where $i(s)$ is the number of $B$-type smoothings in $s$, $\lambda(s)$ is the number of loops in $s$ labeled 1 minus the number of loops labeled $X$, and $j(s) = i(s) + \lambda(s)$. This can be rewritten in the following form:

$$\langle K \rangle = \sum_{i,j} (-1)^i q^j \dim(C_{ij}),$$

where we define $C_{ij}$ to be the linear span (over the complex numbers for the purpose of this paper, but over the integers or the integers modulo two for other contexts) of the set of enhanced states with $i(s) = i$ and $j(s) = j$. Then the number of such states is the dimension $\dim(C_{ij})$.

We would like to have a bigraded complex composed of the $C_{ij}$ with a differential

$$\partial: C_{ij} \rightarrow C_{i+1,j}.$$  

The differential should increase the homological grading $i$ by 1 and preserve the quantum grading $j$. Then we could write

$$\langle K \rangle = \sum_j q^j \sum_i (-1)^i \dim(C_{ij}) = \sum_j q^j \chi(C_{*j}),$$

where $\chi(C_{*j})$ is the Euler characteristic of the subcomplex $C_{*j}$ for a fixed value of $j$.

This formula would constitute a categorification of the bracket polynomial. Below, we shall see how the original Khovanov differential $\partial$ is uniquely determined by the restriction that $j(\partial s) = j(s)$ for each enhanced state $s$. Since $j$ is preserved by the differential, these subcomplexes $C_{*j}$ have their own Euler characteristics and homology. We have

$$\chi(H(C_{*j})) = \chi(C_{*j}),$$

where $H(C_{*j})$ denotes the homology of the complex $C_{*j}$. We can write

$$\langle K \rangle = \sum_j q^j \chi(H(C_{*j})).$$

The last formula expresses the bracket polynomial as a graded Euler characteristic of a homology theory associated with the enhanced states of the bracket state summation. This is the categorification of the bracket polynomial. Khovanov proves that this homology theory is an invariant of knots and links (via the Reidemeister moves of figure 11), creating a new and stronger invariant than the original Jones polynomial.

We will construct the differential in this complex first for mod-2 coefficients. The differential is based on regarding two states as adjacent if one differs from the other by a single smoothing at some site. Thus if $(s, \tau)$ denotes a pair consisting of an enhanced state $s$ and site $\tau$ of that state with $\tau$ of type $A$, then we consider all enhanced states $s'$ obtained from $s$ by smoothing at $\tau$ and relabeling only those loops that are affected by the resmoothing. Call this set of enhanced states $S'[s, \tau]$. Then we shall define the partial differential $\partial_\tau(s)$ as a sum over certain elements in $S'[s, \tau]$, and the differential by the formula

$$\partial(s) = \sum_\tau \partial_\tau(s),$$
with the sum over all type \( A \) sites \( \tau \) in \( s \). It then remains to see what the possibilities are for \( \partial_{\tau}(s) \) so that \( j(s) \) is preserved.

Note that if \( s' \in S'[s, \tau] \), then \( i(s') = i(s) + 1 \). Thus
\[
j(s') = i(s') + \lambda(s') = 1 + i(s) + \lambda(s').
\]
From this we conclude that \( j(s) = j(s') \) if and only if \( \lambda(s') = \lambda(s) - 1 \). Recall that
\[
\lambda(s) = [s : +] - [s : -],
\]
where \([s : +]\) is the number of loops in \( s \) labeled +1, \([s : -]\) is the number of loops labeled −1 (the same as labeled with \( X \)) and \( j(s) = i(s) + \lambda(s) \).

**Proposition.** The partial differentials \( \partial_{\tau}(s) \) are uniquely determined by the condition that \( j(s') = j(s) \) for all \( s' \) involved in the action of the partial differential on the enhanced state \( s \). This unique form of the partial differential can be described by the following structures of multiplication and comultiplication on the algebra \( k[X]/(X^2) \), where \( k = \mathbb{Z}/2\mathbb{Z} \) for mod-2 coefficients, or \( k = \mathbb{Z} \) for integral coefficients:

1. The element 1 is a multiplicative unit and \( X^2 = 0 \).
2. \( \Delta(1) = 1 \otimes X + X \otimes 1 \) and \( \Delta(X) = X \otimes X \).

These rules describe the local relabeling process for loops in a state. Multiplication corresponds to the case when two loops merge to a single loop, while comultiplication corresponds to the case when one loop bifurcates into two loops.

**Proof.** Using the above description of the differential, suppose that there are two loops at \( \tau \) that merge in the smoothing. If both loops are labeled 1 in \( s \), then the local contribution to \( \lambda(s) \) is 2. Let \( s' \) denote a smoothing in \( S'[s, \tau] \). In order for the local \( \lambda \) contribution to become 1, we see that the merged loop must be labeled 1. Similarly, if the two loops are labeled 1 and \( X \), then the merged loop must be labeled \( X \) so that the local contribution for \( \lambda \) goes from 0 to −1. Finally, if the two loops are labeled \( X \) and \( X \), then there is no label available for a single loop that will give −3, so we define \( \partial \) to be zero in this case. We can summarize the result by saying that there is a multiplicative structure \( m \) such that \( m(1, 1) = 1, m(1, X) = m(X, 1) = x, m(X, X) = 0 \), and this multiplication describes the structure of the partial differential when two loops merge.
Since this is the multiplicative structure of the algebra $k[X]/(X^2)$, we take this algebra as summarizing the differential.

Now consider the case when $s$ has a single loop at the site $\tau$. Smoothing produces two loops. If the single loop is labeled $X$, then we must label each of the two loops by $X$ in order to make $\lambda$ decrease by 1. If the single loop is labeled 1, then we can label the two loops by $X$ and 1 in either order. In this second case we take the partial differential of $s$ to be the sum of these two labeled states. This structure can be described by taking a coproduct structure with $\Delta(X) = X \otimes X$ and $\Delta(1) = 1 \otimes X + X \otimes 1$. We now have the algebra $A = k[X]/(X^2)$ with product $m: A \otimes A \to A$ and coproduct $\Delta: A \to A \otimes A$, describing the differential completely. This completes the proof.

Partial differentials are defined on each enhanced state $s$ and a site $\tau$ of type $A$ in that state. We consider states obtained from the given state by smoothing the given site $\tau$. The result of smoothing $\tau$ is to produce a new state $s'$ with one more site of type $B$ than $s$. Forming $s'$ from $s$ we either amalgamate two loops to a single loop at $\tau$ or we divide a loop at $\tau$ into two distinct loops. In the case of amalgamation, the new state $s$ acquires the label on the amalgamated circle that is the product of the labels on the two circles that are its ancestors in $s$. This case of the partial differential is described by the multiplication in the algebra. If one circle becomes two circles, then we apply the coproduct. Thus if the circle is labeled $X$, then the resultant two circles are each labeled $X$ corresponding to $\Delta(X) = X \otimes X$. If the original circle is labeled 1, then we take the partial boundary to be a sum of two enhanced states with labels 1 and $X$ in one case, and labels $X$ and 1 in the other case, on the respective circles. This corresponds to $\Delta(1) = 1 \otimes X + X \otimes 1$. Modulo two, the boundary of an enhanced state is the sum, over all sites of type $A$ in the state, of the partial boundaries at these sites. It is not hard to verify directly that the square of the boundary mapping is zero (this is the identity of mixed partials!) and that it behaves as advertised, keeping $j(s)$ constant. There is more to say about the nature of this construction with respect to Frobenius algebras and tangle cobordisms. In figures 12–14 we illustrate how the partial boundaries can be conceptualized in terms of surface cobordisms. The equality of mixed partials corresponds to topological equivalence of the corresponding surface cobordisms, and to the relationships between Frobenius algebras and the surface cobordism category. In particular, in figure 14 we show how in a key case of two sites (labeled 1 and 2 in that figure) the two orders of partial boundary are

$$\partial_2 \partial_1 = (1 \otimes m) \circ (\Delta \otimes 1)$$

and

$$\partial_1 \partial_2 = \Delta \circ m.$$ 

In the Frobenius algebra $A = k[X]/(X^2)$, we have the identity

$$(1 \otimes m) \circ (\Delta \otimes 1) = \Delta \circ m.$$ 

Thus the Frobenius algebra implies the identity of the mixed partials. Furthermore, in figure 13 we see that this identity corresponds to the topological equivalence of cobordisms under an exchange of saddle points. There is more to say about all of this, but we will stop here. The proof of invariance of the Khovanov homology with respect to the Reidemeister moves (respecting grading changes) will not be given here. See [2, 3, 26]. It is remarkable that this version of the Khovanov homology is uniquely specified by natural ideas about adjacency of states in the bracket polynomial.
Remark on integral differentials. Choose an ordering for the crossings in the link diagram $K$ and denote them by $1, 2, \ldots, n$. Let $s$ be any enhanced state of $K$ and let $\partial_i(s)$ denote the chain obtained from $s$ by applying a partial boundary at the $i$th site of $s$. If the $i$th site is a smoothing of type $A^{-1}$, then $\partial_i(s) = 0$. If the $i$th site is a smoothing of type $A$, then $\partial_i(s)$ is given by the rules discussed above (with the same signs). The compatibility conditions that we have discussed show that partials commute in the sense that $\partial_i(\partial_j(s)) = \partial_j(\partial_i(s))$ for all $i$ and $j$. One then defines signed boundary formulae in the usual way of algebraic topology. One way to think of this regards the complex as the analogue of a complex in de Rham cohomology. Let $\{dx_1, dx_2, \ldots, dx_n\}$ be a formal basis for a Grassmann algebra so that $dx_i \wedge dx_j = -dx_j \wedge dx_i$.

Starting with enhanced states $s$ in $C^0(K)$ (that is, a state with all $A$-type smoothings) define formally $d_i(s) = \partial_i(s)dx_i$ and regard $d_i(s)$ as identical with $\partial_i(s)$ as we have previously regarded it in $C^1(K)$. In general, given an enhanced state $s$ in $C^k(K)$ with $B$-smoothings at locations $i_1 < i_2 < \cdots < i_k$, we represent this chain as $s \, dx_{i_1} \wedge \cdots \wedge dx_{i_k}$ and define

$$\partial(s \, dx_{i_1} \wedge \cdots \wedge dx_{i_k}) = \sum_{j=1}^{n} \partial_j(s) \, dx_j \wedge dx_{i_1} \wedge \cdots \wedge dx_{i_k}.$$
just as in a de Rham complex. The Grassmann algebra automatically computes the correct signs in the chain complex, and this boundary formula gives the original boundary formula when we take coefficients modulo two. Note that in this formalism, partial differentials $\partial_i$ of enhanced states with a $B$-smoothing at site $i$ are zero due to the fact that $dx_i \wedge dx_i = 0$ in the Grassmann algebra. There is more to discuss about the use of Grassmann algebra in this context. For example, this approach clarifies parts of the construction in [27].

It is of interest to examine this analogy between the Khovanov (co)homology and de Rham cohomology. In that analogy the enhanced states correspond to the differentiable functions on a manifold. The Khovanov complex $C^k(K)$ is generated by elements of the form $s \ dx_{i_1} \wedge \cdots \wedge r \ dx_{i_k}$ where the enhanced state $s$ has $B$-smoothings at exactly the sites $i_1, \ldots, i_k$. If we were to follow the analogy with de Rham cohomology literally, we would define a new complex $DR(K)$ where $DR^k(K)$ is generated by elements $s \ dx_{i_1} \wedge \cdots \wedge dx_{i_k}$, where $s$ is any enhanced state of the link $K$. The partial boundaries are defined in the same way as before and the global boundary formula is just as we have written it above. This gives a new chain complex associated with the link $K$. Whether its homology contains new topological information about the link $K$ will be the subject of a subsequent paper.

A further remark on de Rham cohomology. There is another deep relation with the de Rham complex: in [28] it was observed that the Khovanov homology is related to the Hochschild homology and the Hochschild homology is thought to be an algebraic version of the de Rham chain complex (cyclic cohomology corresponds to de Rham cohomology); compare [30].

7. Other homological states

The formalism that we have pursued in this paper to relate the Khovanov homology and the Jones and virtual Jones polynomials with quantum statistics can be generalized to apply to other situations. It is possible to associate a finite dimensional Hilbert space that is also a chain complex (or cochain complex) with topological structures other than knots and links.
To formulate this, let $X$ denote the topological structure and $C(X)$ denote the associated linear space endowed with a boundary operator $\partial: C(X) \rightarrow C(X)$, with $\partial \partial = 0$. We want to consider situations where there is a unitary operator $U: C(X) \rightarrow C(X)$ such that $U \partial + \partial U = 0$ so that $U$ induces a unitary action on $H(X)$, the homology of $C(X)$ with respect to $\partial$.

For example, let $M$ be a differentiable manifold and $C(M)$ denote the de Rham complex of $M$ over the complex numbers. Then for a differential form of the type $f(x)\omega$ in local coordinates $x_1, \ldots, x_n$ and $\omega$ a wedge product of a subset of $x_1 \cdots d x_n$, we have

$$d(f \omega) = \sum_{i=1}^{n} \left( \partial f / \partial x_i \right) d x_i \wedge \omega.$$  

Here $d$ is the differential for the de Rham complex. Then $C(M)$ has the basis set of $| f(x) \omega \rangle$ where $\omega = dx_{i_1} \wedge \cdots \wedge dx_{i_k}$ with $i_1 < \cdots < i_k$. We could achieve $Ud + dU = 0$ if $U$ is a very simple unitary operator (e.g. multiplication by phases that do not depend on the coordinates $x_i$) but in general it will be an interesting problem to determine all unitary operators $U$ with this property.

Even in the case of the Khovanov homology, we could keep the homology theory fixed and ask for other unitary operators $U$ that satisfy $U\partial + \partial U = 0$. Knowing other examples of such operators would shed light on the nature of the Khovanov homology from the point of view of quantum statistics. A problem for further research is to relate the points of view in this paper with the recent work of Edward Witten [40] on the Khovanov homology.

Appendix A. The Hadamard test

In this section, we use a Hilbert space $W$ of dimension two with orthonormal basis $\{|0\rangle, |1\rangle\}$. With a given unitary transformation $U: C(K) \rightarrow C(K)$, we associate a new unitary transformation defined on $W \otimes C(K)$ from which we can define a quantum algorithm to compute diagonal elements of the original transformation $U$. In this algorithm, the Hadamard test, we will be able to describe a quantum computation for $\langle \psi | U | \psi \rangle$ for any $| \psi \rangle$ in $C(K)$. Note that one can be given the transformation $U$ in any orthonormal basis for $C(K)$ to perform this test.

In order to make a quantum computation of the trace of a unitary matrix $U$, one can use the Hadamard test to obtain the diagonal matrix elements $\langle \psi | U | \psi \rangle$ of $U$. The trace is then the sum of these matrix elements as $| \psi \rangle$ runs over an orthonormal basis for the vector space. In the application to the algorithm described here for the Jones polynomial it is only necessary to compute one number of the form $\langle \psi | U | \psi \rangle$. The Hadamard test proceeds as follows.

We define the Hadamard gate $H: W \rightarrow W$ defined by the equations below in the basis $\{|0\rangle, |1\rangle\}$ for $W$.

$$H|0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle),$$

$$H|1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle).$$

We define the controlled $U$ gate as a new unitary operation

$$C_U: W \otimes C(K) \rightarrow W \otimes C(K)$$
The Hadamard test is then based on measuring the composite gate application 
\[(H \otimes 1) \circ C_U \circ (H \otimes 1)(|0\rangle\otimes|\psi\rangle).\]

An appropriate measurement occurs with frequency \(\frac{1}{2} + \frac{1}{2} \text{Re} \langle \psi | U | \psi \rangle\). This yields the real part of the desired \(\langle \psi | U | \psi \rangle\). The imaginary part is obtained by a modification of this process. We describe the details of the operation of the Hadamard gate just below.

**Operating the Hadamard test.** We first obtain
\[\frac{1}{2} + \frac{1}{2} \text{Re} \langle \psi | U | \psi \rangle\]
as an expectation by applying the Hadamard gate to the first qubit of
\[C_U \circ (H \otimes 1)|0\rangle\otimes|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle \otimes |\psi\rangle + |1\rangle \otimes U|\psi\rangle).\]

Here \(C_U\) denotes controlled \(U\), acting as \(U\) when the control bit is \(|1\rangle\), and the identity mapping when the control bit is \(|0\rangle\). We measure the expectation for the first qubit \(|0\rangle\) of the resulting state
\[(H \otimes 1) \circ C_U \circ (H \otimes 1)|0\rangle\otimes|\psi\rangle = \frac{1}{2}(H|0\rangle \otimes |\psi\rangle + H|1\rangle \otimes U|\psi\rangle)\]
\[= \frac{1}{2}((|0\rangle + |1\rangle) \otimes |\psi\rangle + (|0\rangle - |1\rangle) \otimes U|\psi\rangle)\]
\[= \frac{1}{2}(|0\rangle \otimes (|\psi\rangle + U|\psi\rangle) + |1\rangle \otimes (|\psi\rangle - U|\psi\rangle)).\]

This expectation is
\[\frac{1}{2}(\langle \psi | + (\langle \psi | U^\dagger)(|\psi\rangle + U|\psi\rangle) = \frac{1}{2} + \frac{1}{2} \text{Re} \langle \psi | U | \psi \rangle.\]

In figure A.1, we illustrate this computation with a diagram that indicates the structure of the test with parallel lines corresponding to tensor products of the single qubit space (with three lines chosen for illustration as the size of \(U\)). The extra tensor factor is indicated on the top line with the Hadamard matrix \(H\) indicated by a box and the control of \(U\) indicated by a circle with a vertical control line extending down to the \(U\)-box. The half-circle on the top line on the right stands for the measurement of that line that is used for the computation. Thus, figure 5 represents a circuit diagram for the quantum computation of \(\frac{1}{2} + \frac{1}{2} \text{Re} \langle \psi | U | \psi \rangle\) and hence the quantum computation of \(\frac{1}{2} + \frac{1}{2} \text{Re} \langle K \rangle\) when \(U\) is taken to be the unitary transformation corresponding to the bracket polynomial, as discussed in previous sections of this paper.
The imaginary part is obtained by applying the same procedure to
\[ \frac{1}{\sqrt{2}} (|0\rangle \otimes |\psi\rangle - i |1\rangle \otimes U|\psi\rangle). \]

This is the method used in [1, 16, 19], and the reader may wish to contemplate its efficiency in the context of this simple model. Note that the Hadamard test enables this quantum computation to estimate the trace of any unitary matrix \( U \) by repeated trials that estimate individual matrix entries \( \langle \psi | U | \psi \rangle \).

**Appendix B. Comment on the efficiency of the algorithms**

The quantum algorithms given in this paper do not represent a speedup over classical probabilistic computation (as discussed below). It was our intention to show how to reformulate the bracket state sum model for the Jones polynomial in a quantum context and to show how this context is related to the Khovanov homology. In the course of this investigation we obtained new quantum algorithms for the Jones polynomial for classical and virtual knots and for the Poincaré polynomial for the Khovanov homology. It remains to be seen whether these formulations can be further modified to give algorithms that are faster than classical algorithms.

The quantum algorithms in this paper all take the following form. Let \( U \) be some diagonal unitary matrix on an exponentially large Hilbert space. Let \( |\psi\rangle \) be the uniform superposition over the basis states. Then one uses the Hadamard test to estimate \( \langle \psi | U | \psi \rangle \) (which is also expressible as the normalized trace of \( U \)). This quantity is a complex number of magnitude at most one, and by repeated application of the Hadamard test one obtains estimates of the real and imaginary parts to within \( \pm \varepsilon \) using order \( 1/\varepsilon^2 \) trials, as dictated by the usual statistics of binomial distributions.

One may assume, as is usual for quantum algorithms, that the experimenter can implement a standard set of universal quantum gates (e.g. Toffoli and Hadamard); then \( U \) can be implemented using a certain number of gates that scales polynomially with the number of crossings in the knot diagram, as follows. If a classical circuit of \( G \) gates computes a function \( f: \{0, 1\}^n \rightarrow \{0, 1\}^m \), one can use reversible logic elements to obtain a quantum circuit of \( O(G) \) gates implementing the unitary
\[ U_f |x\rangle |y\rangle = |x\rangle |y + f(x) \text{ mod } 2^m\rangle. \]

For details, see chapter 3 of the book by Nielsen and Chuang [32]. Let
\[ |R_m\rangle = \frac{1}{\sqrt{2^m}} \sum_{y=0}^{2^m-1} e^{-i 2\pi y / 2^m} |y\rangle. \]

Then
\[ U_f |x\rangle |R_m\rangle = e^{i 2\pi f(x)/2^m} |x\rangle |R_m\rangle. \]

At the end, one can throw away the ‘ancilla’ qubits in state \( |R_m\rangle \). Note also that the state \( |R_m\rangle \) is producible from a basis state using \( O(m^2 \log m \log \log m) \) gates by a quantum Fourier transform. This method of constructing diagonal unitaries is sometimes called phase-kickback and is described in the paper [5]. The bottom line is that any diagonal unitary is efficiently implementable by quantum gates provided the phases on the diagonal are efficiently computable by classical logic circuits. The phases defining the diagonal unitaries used in the present paper are efficiently computable essentially by counting up the number of crossings of various types.
Although diagonal unitaries are a useful primitive in the design of quantum algorithms and an important ingredient in our formulation of the algorithms in this paper, it is the case that using only this primitive plus a Hadamard test results in a quantum algorithm that can be efficiently simulated by probabilistic classical computation. Specifically, the basis states on \( n \) qubits correspond to the \( 2^n \) bitstrings. We may easily sample uniformly from the set of all \( 2^n \) bitstrings. For each bitstring sampled, we compute the corresponding phase. Then we take the average of our results as an estimate of the normalized trace of \( U \). If \( U \) is diagonal, then each of these diagonal matrix elements has norm one. The standard deviation of the distribution we are sampling from is at most one, and we obtain an estimate with uncertainty \( \epsilon \) after \( \sim 1/\epsilon^2 \) samples, similar to the precision achieved using a Hadamard test. (This argument is specific to phase-kickback-plus-Hadamard-test algorithms. For general quantum algorithms, classical sampling yields poor estimates of outcome probabilities due to exponentially large variance in the relevant random variables.)

This paper is a first step towards a formulation of quantum algorithms for topological invariants like those for virtual knots and links and for Khovanov homology where one must go beyond unitary representations of the Artin braid group. We hope to formulate more efficient algorithms in subsequent papers.

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