Detecting Knottedness with Quantum Computers

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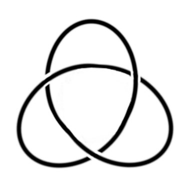
Abstract
We show that computing the Khovanov homology of a knot diagram K in a bigrading (i,j) is in **QMA** if the spectral gap of a certain "Laplacian" operator $\Delta_K^{ij} := (dd^* + d^*d)^{ij}$ can be bounded by an inverse polynomial in the size of K. Motivated by the desire to understand the feasiblity of this, we present data investigating the spectral gap.

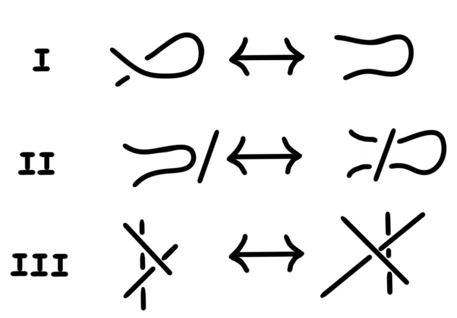
1. Background

1.1 Knots

Definition 1. *A **knot** is an embedding $S^1 \to \mathbb{R}^3$. We represent knots with **knot diagrams** like the one on the right. The number of crossings in a knot diagram is called the **crossing number**.*



Definition 2. *A **Reidemeister move** is any of the three local transformations of a link diagram shown at the right.*



Definition 3. *We say two knot diagrams are **equivalent** if a sequence of Reidemeister moves can transform the first knot diagram into the second knot diagram.*

Definition 4. *A **knot invariant** is a quantity defined on the set of all knots that takes the same value on equivalent knots. Formally, for knots K and K', a function ϕ on knots is an invariant if whenever K and K' are equivalent, $\phi(K) = \phi(K')$.*

1.2 Khovanov Homology

Definition 5. *A **co-chain complex** is a sequence of vector spaces C_i and linear maps $d_i : C_i \to C_{i+1}$, called **differentials**, such that $d_{i-1} \circ d_i = 0$ for all i. We denote a co-chain complex as follows:*

$$\cdots \xrightarrow{d_{i-2}} C_{i-1} \xrightarrow{d_{i-1}} C_i \xrightarrow{d_i} C_{i+1} \xrightarrow{d_{i+1}} \cdots$$

Definition 6. *Each index i of the co-chain complex has an associated **homology**, defined as $H^i = \ker d_i / \operatorname{Im} d_{i-1}$. We call i the **homological grading**.*

Construction 1. *The **Khovanov homology** of a knot diagram K is constructed by creating the cube of resolutions, and taking the homology of an associated co-chain complex.*

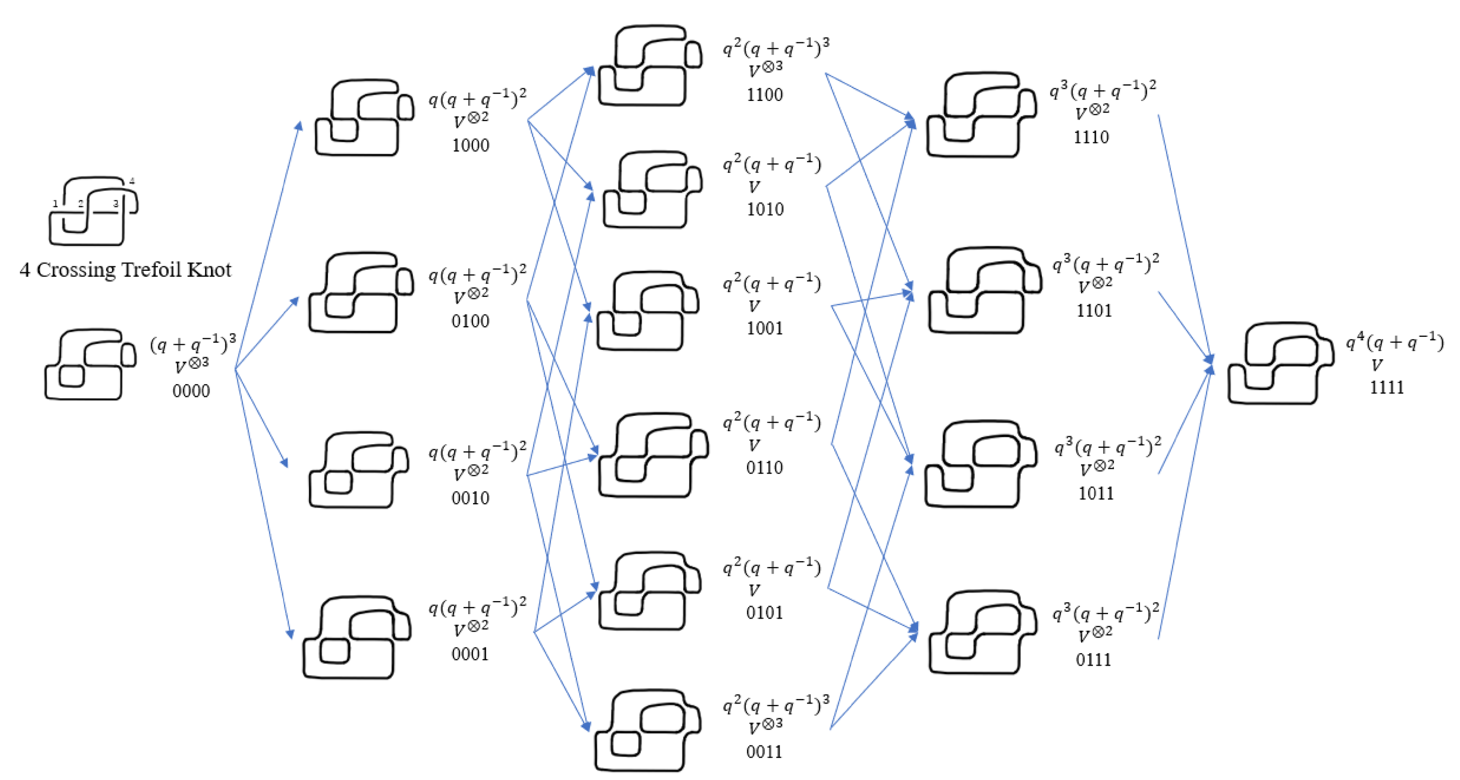


***Figure 1:** Cube of resolutions of a 4-crossing diagram of the trefoil knot.*

Theorem 1 (Khovanov)**.** *Khovanov homology is a knot invariant.*

2. Problem Statement

2.1 Complexity

Definition 7. ***NP** (Non-deterministic Polynomial time) is the class of decision problems whose positive instances have solutions that can be verified in polynomial time.*

Definition 8. ***QMA** (Quantum Merlin-Arthur) is the quantum analog of **NP** consisting of decision problems whose positive instances have* quantum *solutions that can be verified in* quantum *polynomial time.*

2.2 Problem Statement

Problem 1. *What is the complexity of computing the Khovanov homology of a knot diagram as a function of the crossing number?*

We need to make more precise what we mean by "computing the Khovanov homology," as there are different possibilities. We are most interested in the *non-triviality decision problem*.

Khovanov Homology Non-Triviality Problem. Given a diagram K and bigrading $(i,j) \in \mathbb{Z} \times \mathbb{Z}$, output "YES" if and only if $\dim_{\mathbb{C}} \mathrm{Kh}^{ij}(K) > 0$.

From the definition of Khovanov homology, this problem is naively solvable in exponential space. Our goal is to determine if quantum computers can help us to do better.

3. Results

3.1 Preliminaries

Definition 9. *The **quantum phase estimation algorithm** is a quantum algorithm that, given a unitary operator $U : (\mathbb{C}^2)^{\otimes k} \to (\mathbb{C}^2)^{\otimes k}$, an eigenvector $|\psi\rangle$ of U, and a number $N \in \mathbb{N}$ of bits, approximates the eigenvalue of $|\psi\rangle$ by outputting (with high probability) the optimal N-bit approximation of the phase $\theta \in [0,1)$ such that $U|\psi\rangle = e^{2\pi i\theta}$.*

3.2 Non-Triviality of Khovanov Homology

We will sketch an idea for how to use phase estimation to compute Khovanov homology.

Definition 10. *We call $\Delta_K^{i,j} = \Delta^{i,j} = d_{i,j}^* \circ d_{i,j} + d_{i-1,j} \circ d_{i-1,j}^*$ the **Khovanov Laplacian** of the diagram K in bigrading (i,j).*

Definition 11. *For a knot diagram K and bigrading (i,j), the **spectral gap** η_K^{ij} of Δ_K^{ij} is defined as follows:*

$$\eta := \eta_K^{ij} = \frac{\min\left(\operatorname{spec}(\Delta^{ij}) \setminus \{0\}\right)}{\max(\operatorname{spec}(\Delta^{ij}))}$$

where $\operatorname{spec}(\Delta^{ij})$ is the eigenvalue spectrum of Δ^{ij}.

Lemma 1. *For every knot diagram K and bigrading (i,j), $\mathrm{Kh}^{ij}(K) \cong \ker \Delta^{ij}$.*

Thus, deciding non-triviality of Khovanov homology is equivalent to finding some nonzero vector $|\psi\rangle$ such that $\Delta^{ij}|\psi\rangle = 0$. Such a $|\psi\rangle$ serves as a "quantum solution" that can be used to verify $\dim_{\mathbb{C}} \mathrm{Kh}^{ij}(K) > 0$ using phase estimation, as follows.
$\Delta^{ij}|\psi\rangle = 0$ if and only if $e^{it\Delta^{ij}}|\psi\rangle = |\psi\rangle$. Thus, $|\psi\rangle \in \ker \Delta^{ij}$ if and only if it is an eigenvector of $e^{it\Delta^{ij}}$ with eigenvalue $e^{2\pi i 0} = e^0 = 1$ for all t.

Given $|\psi\rangle$, $N \in \mathbb{N}$, and $U := e^{\frac{i\Delta^{ij}}{\sigma_{max}}}$, we can test if $U|\psi\rangle = |\psi\rangle$ using phase estimation: $|\psi\rangle \in \ker \Delta^{ij}$ exactly when $\theta = 0$. For this to work, N should be the index of the first nonzero bit of the binary representation of η. Thus, $N = \lceil -\log_2 \eta \rceil$.
If $|\psi\rangle \in \ker \Delta^{ij}$, then the output θ will be all 0's. If $|\psi\rangle \in (\ker \Delta^{ij})^{\perp}$, then at least one bit of the output θ is guaranteed to be nonzero because of how N was selected. This proves:

Theorem 2. *If $N = O(\log|K|)$, where $|K|$ is the crossing number of a knot diagram K, this procedure is a nondeterministic quantum polynomial time algorithm for the non-triviality of Khovanov homology. That is, deciding non-triviality of Khovanov homology is in **QMA**.*

4. Data

Theorem 2 yields an actual algorithm only if we can find bounds on the spectral gap.

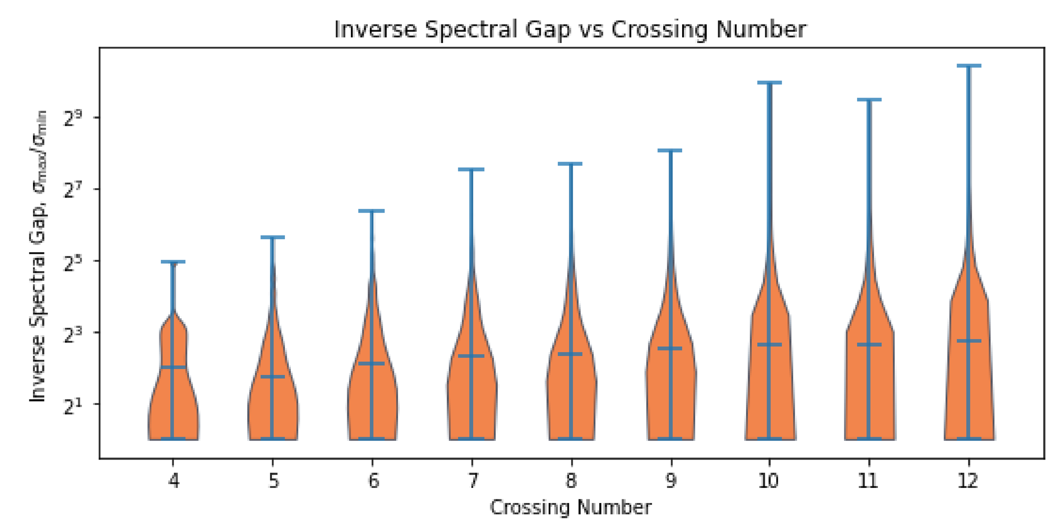


***Figure 2:** Inverse spectral gap vs crossing number for 100 randomly sampled link diagrams for each crossing number 4 through 12. Widths show frequency; extrema and medians are indicated by blue bars. (Diagrams sampled via SnapPy's 4-valent planar graph method.)*

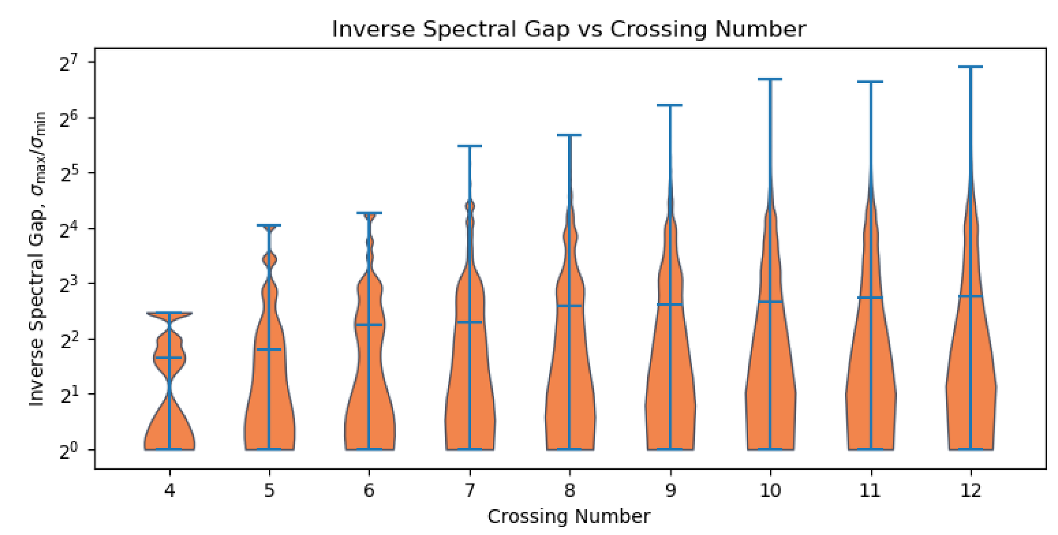


***Figure 3:** Same as previous chart, but only sampling alternating knots.*

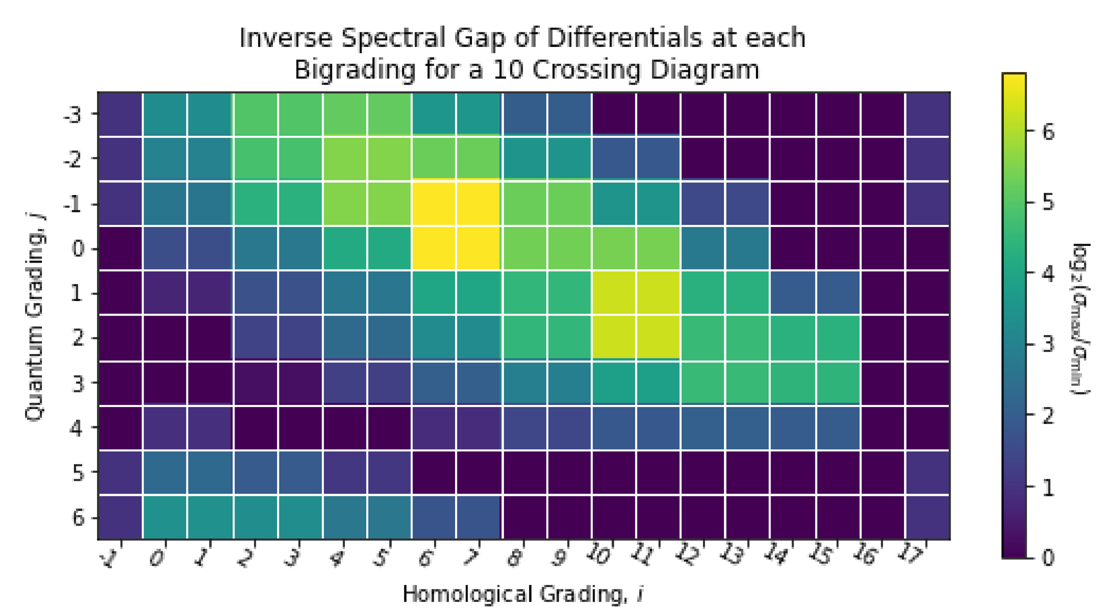


***Figure 4:** Example heat map of the spectral gap at each bigrading for a particular 10-crossing knot diagram. Note the diagonal shape.*

References

[1] M. Culler, N. M. Dunfield, M. Goerner, and J. R. Weeks. SnapPy: a computer program for studying the geometry and topology of 3-manifolds. http://snappy.computop.org

[2] Dror Bar-Natan (2002). On Khovanov's categorification of the Jones polynomial. *Algebraic and Geometric Topology*, 2(1).

[3] Mikhail Khovanov (2000). A Categorification of the Jones Polynomial. *Duke Mathematical Journal*, 101(3).

[4] Alexander Shumakovich (2002). KhoHo: A Program for Computing and Studying Khovanov Homology. GitHub: https://github.com/AShumakovitch/KhoHo.

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