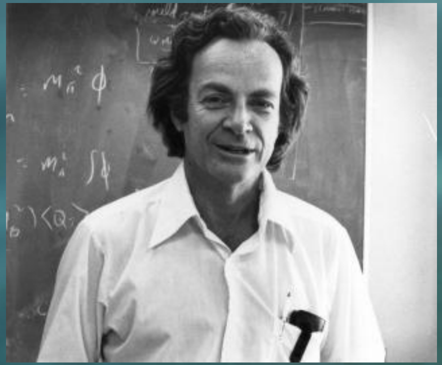
A QUANTUM ALGORITHM FOR KHOVANOV HOMOLOGY

ICERM Workshop on Diagrammatic Categorification

Joint with Alexander Schmidhuber, Michele Reilly, Paolo Zanardi, Seth Lloyd

AARON LAUDA
DEPARTMENT OF MATHEMATICS & PHYSICS
UNIVERSITY OF SOUTHERN CALIFORNIA

October 22nd, 2025



"Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical."

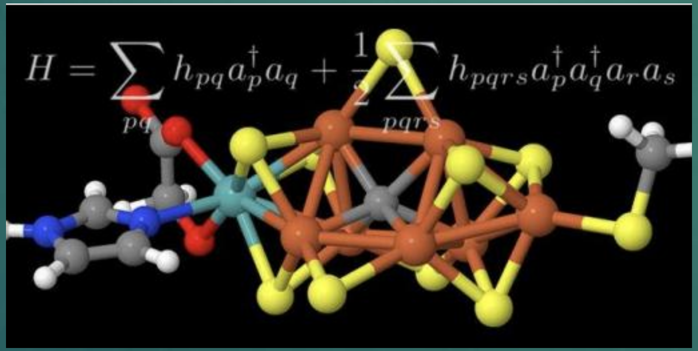
Quantum Advantage

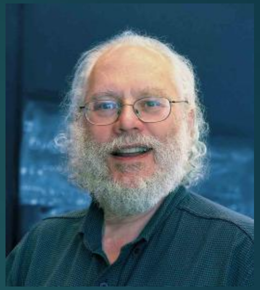
Quantum advantage = exponential speedup over all classical algorithms.

Examples:

- **Shor's algorithm**: integer factorization / Hidden subgroup problem

- **Quantum Chemistry/Materials Science**





Peter Shor

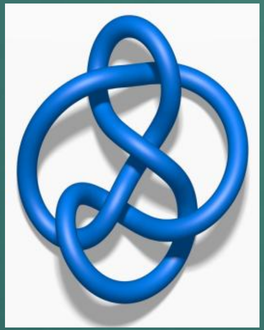
Quantum Advantage

Quantum advantage = exponential speedup over all classical algorithms.

Examples:

- **Jones polynomial**: calculating the Jones polynomial is as hard as any problem that can be computed on a quantum computer

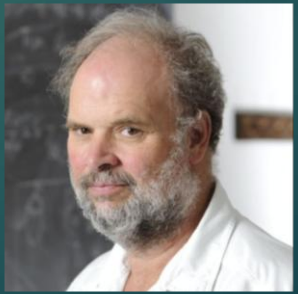
Approximating Jones polynomials



$$-q^3 + 2q^2 - 2q + 3 - 2q^{-1} + 2q^{-2} - q^{-3}$$

Efficient quantum algorithm for approximating the Jones polynomial at roots of unity

Dorit Aharanov



Vaughan Jones

Zeph Landau

Are there problems in categorification that can be naturally computed on a quantum computer?

Crash course in quantum information

Qubits: A qubit is described by a unit vector in $\mathbb{C}^2$:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \quad \alpha, \beta \in \mathbb{C}, \quad |\alpha|^2 + |\beta|^2 = 1$$

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$n \text{ qubits} = \text{vector in } (\mathbb{C}^2)^{\otimes n}$$

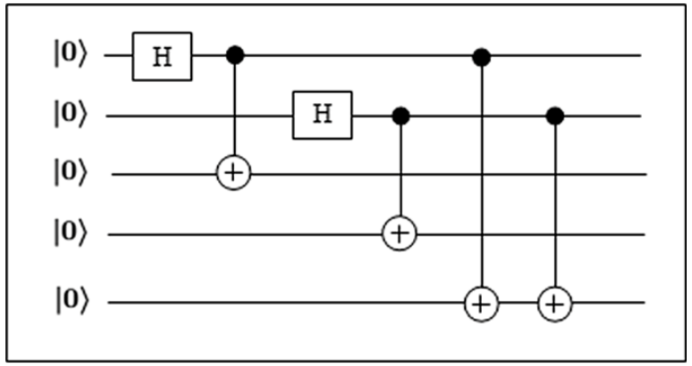
Gates: A quantum gate is a unitary matrix U $\in \mathrm{U}(2^n)$ acting on n qubits :

$$U : (\mathbb{C}^2)^{\otimes n} \to (\mathbb{C}^2)^{\otimes n}, \quad U^\dagger U = I$$

Examples: $H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ $\quad \mathrm{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$

Quantum Circuits: A quantum circuit is a sequence of quantum gates

$$|\psi_{\text{out}}\rangle = U_T \cdots U_2 U_1 |\psi_{\text{in}}\rangle$$



Circuits are efficient if they use few [= poly(n)] gates

Unitarity and Quantum Topology

Jones polynomial works because at q a root of unity, the Temperley–Lieb algebra admits a **unitary path model**.

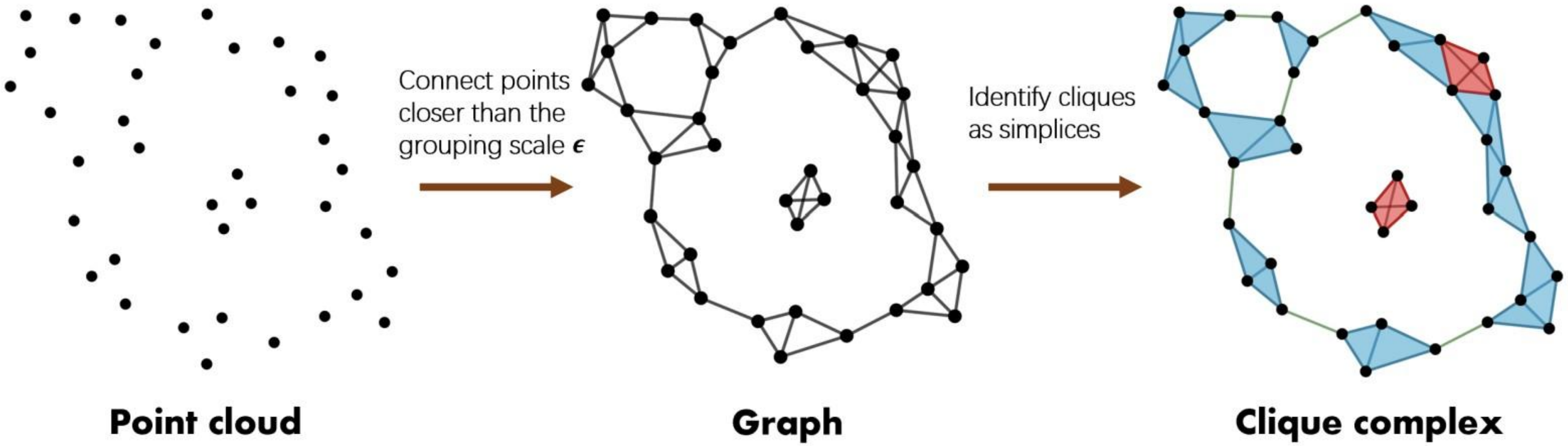
Quantum computation requires **unitary evolution** (Hermitian generators).

For categorification, we must identify Hermitian/unitary analogues of algebraic data.

Quantum Algorithms for Homology

LGZ QUANTUM ALGORITHM FOR TOPOLOGICAL DATA ANALYSIS

Topology of Data



Schmidhuber-Lloyd
arXiv: 2209.14286

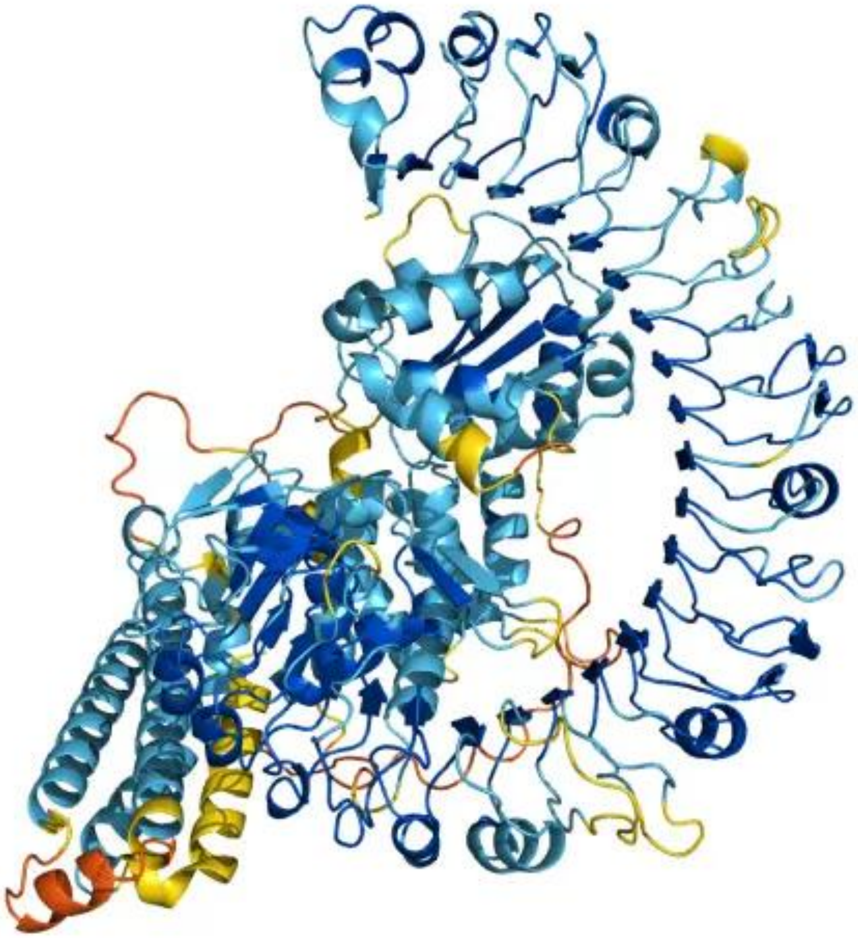
- Topological Data Analysis (TDA) is a way to analyze the structure of data
- Holes that "persist" as the scale varies provide information about the data

EXAMPLE APPLICATION

Protein structure

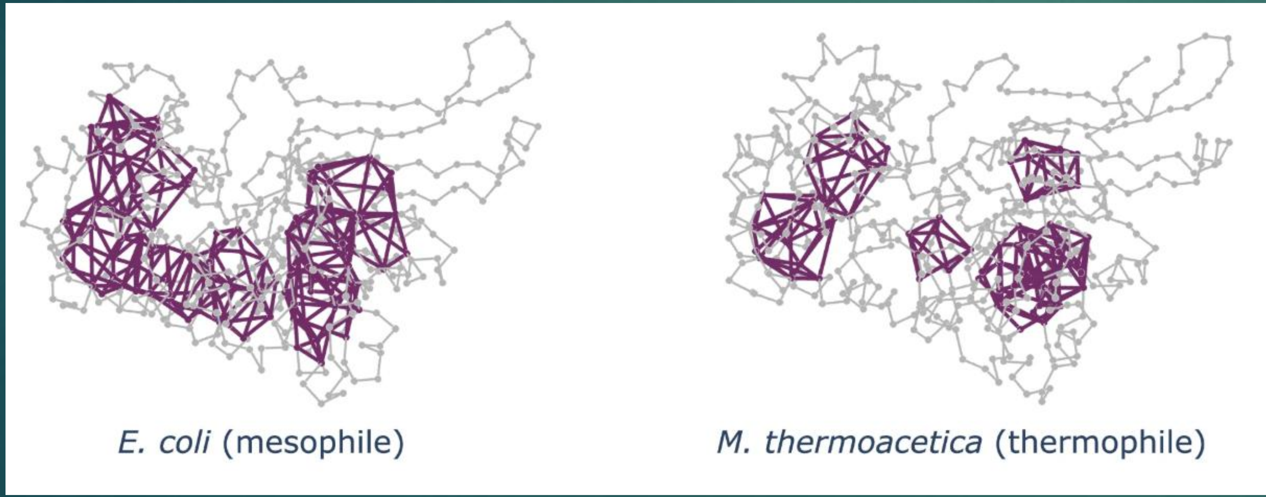
Proteins: shape = function

Predicting protein shape was once one of biology's hardest problems — until **AlphaFold2**, an AI breakthrough that won the 2024 Nobel Prize in Chemistry.



Q8W3K0: A potential plant disease resistance protein.
From Alphafold online bank

Predicting the shape and function of proteins



Madsen *et al.*, *Nature Communications* 16, 7503 (2025).

- Now, with hundreds of millions of predicted structures available, Topological Data Analysis offers a new way to make sense of this protein universe.

- A recent study appearing in *Nature Communications* used TDA to study the protein universe and saw that loops and voids detected by TDA correlated strongly with known protein function.

A quantum algorithm for Topological Data Analysis

- Lloyd, Gamerone, and Zanardi introduced a quantum algorithm for computing Betti numbers of simplicial complexes.
- Relies on combinatorial Hodge theory to compute Betti numbers. Produces a family of Hermitian operators Δ_k
- Uses quantum phase estimation on the unitary operator $U = e^{i\Delta_k t}$

Seth Lloyd

Silvano Garnerone

Paolo Zanardi

Combinatorial Hodge Theory

- Given a chain complex of finite-dimensional vector spaces

$$0 \xrightarrow{\partial_n} C_{n-1} \xrightarrow{\partial_{n-1}} \dots \xrightarrow{\partial_1} C_0 \xrightarrow{\partial_0} 0.$$

- Choose an inner product $(\cdot,\cdot)_d$ on C_d and define an adjoint of the boundary operator $\partial^*: C_{d-1} \to C_d$ by

$$(\partial f, g)_{d-1} = (f, \partial^* g)_d$$

- Define the Hodge Laplacian $\Delta_n = \partial\partial^* + \partial^*\partial : C_n \to C_n$

Theorem (Hodge Theory): $H_k(C) = \ker \Delta_k$

- Gives distinguished "harmonic" representatives of homology

$$\beta_k = \dim H_k = \dim \left(\text{Ker } \partial_k \middle/ \text{Im } \partial_{k+1} \right) = \dim \text{Ker} \left(\partial_k^\dagger \partial_k + \partial_{k+1} \partial_{k+1}^\dagger \right) = \dim \text{Ker} \Delta_k$$

Quantum Phase Estimation

- Given a unitary operator U and an eigenstate $|\Psi\rangle$

$$U|\psi\rangle = e^{i\phi}|\psi\rangle,$$

- Quantum Phase estimation is a circuit with

  INPUT STATE: $|\Psi\rangle|0\rangle$

  OUTPUT STATE: $|\Psi\rangle|\theta\rangle$

- Where $|\theta\rangle$ is given as a binary fraction, e.g.
  - Instead of powers of 10
  - Use powers of 2

$$0.15625 = 1\times10^{-1} + 5\times10^{-2} + 6\times10^{-3} + 2\times10^{-4} + 5\times10^{-5}.$$

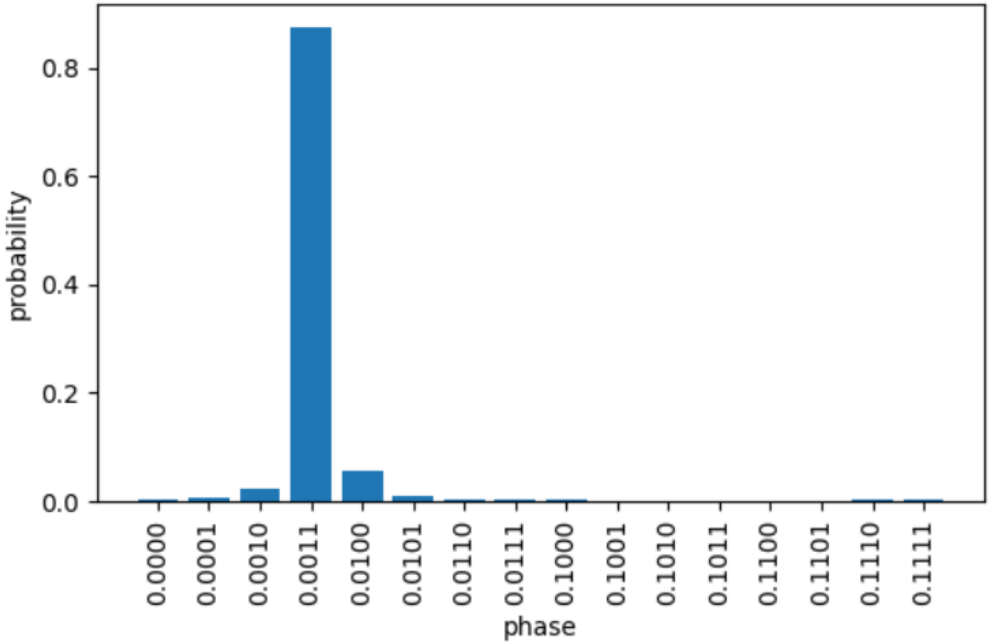
$$0.00101 = 0\times2^{-1} + 0\times2^{-2} + 1\times2^{-3} + 0\times2^{-4} + 1\times2^{-5}.$$

- The precision of approximation determined by the number of bits

Example $U = \begin{pmatrix} 1 & 0 \\ 0 & e^{\frac{2\pi i}{5}} \end{pmatrix}$, eigenstate $|\Psi\rangle = |1\rangle$

$\theta = 0.2$ using a four-bit approximation

- 0.0001 = 0.125
- 0.0011 = 0.1875
- 0.0100 = 0.25
- 0.0101= 0.3125

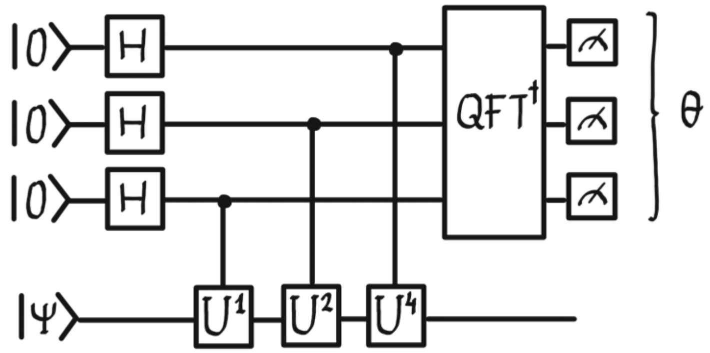


Quantum Phase Estimation

- The key behind phase estimation is the quantum Fourier transform (QFT)

$$\mathrm{QFT}|\theta\rangle = \frac{1}{\sqrt{2^n}} \sum_{k=0} e^{2\pi i\theta k}|k\rangle.$$

$$U^k|\psi\rangle = e^{2\pi i\theta k}|\psi\rangle.$$



$$\frac{1}{\sqrt{2^n}} \sum_{k=0} |\psi\rangle|k\rangle \rightarrow \frac{1}{\sqrt{2^n}} \sum_{k=0} U^k|\psi\rangle|k\rangle = |\psi\rangle \frac{1}{\sqrt{2^n}} \sum_{k=0} e^{2\pi i\theta k}|k\rangle$$

Inverse QFT →

$$|\psi\rangle|\phi\rangle.$$

Conclude by measuring the second register

Key for LGZ algorithm

- Quantum Phase Estimation doesn't need input state to be an eigenstate!
- Input: a superposition of eigenstates $|\Psi\rangle = \sum_i c_i|\psi_i\rangle,$
- Output: eigenphase θ_i with probability $|c_i|^2$
- This allows us to sample the distribution of eigenvalues

LGZ Algorithm

Convergence time governed by the inverse of the spectral gap

$$\left(gap(\Delta_k)\right)^{-1} = \mathcal{O}\left(poly(n)\right)$$

Must be able to efficiently create this state

Input

Uniform mixture over k-simplices:

$\rho_k = \sum_{|s_k|} |s_k\rangle\langle s_k|$

Apply

QPE on Δ_k

Output

histogram of normalized Betti numbers

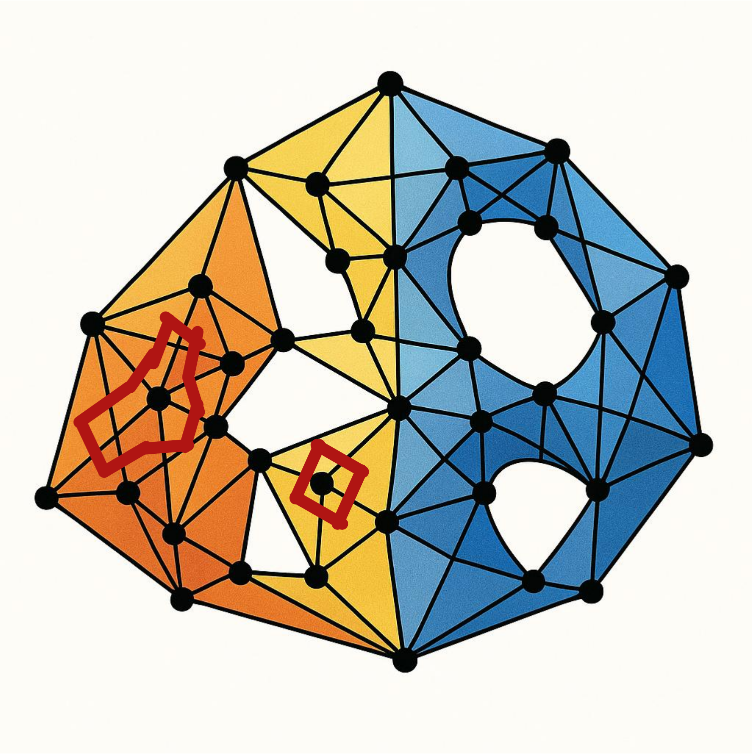
$$\frac{\dim(\ker \Delta_k)}{|S_k|} = \frac{\beta_i}{|S_k|}$$

The Hilbert space C has to have an efficient description, for example, it could be the subspace of a full n−qubit Hilbert space described by a polynomial (in n) number of constraints

The Hodge Laplacian Δ_k has to be efficiently exponentiable $\boldsymbol{U} = \boldsymbol{e}^{i\Delta_k t}$

This is the case if ∂ is local or sparse

Can you hear the shape of data?



- LGZ allows the computation of *all* eigenvalues of the Laplacian (nonzero spectrum depends on inner product)
- Higher eigenvalues provide additional information about the simplicial complex
- First nonzero eigenvalue = spectral gap is a critical quantity that governs random walks along simplices
  - Generalizes Cheeger inequalities from graphs and Riemannian manifolds

Limitations of LGZ algorithm

- Only polynomial speedup in the worst case for simplicial Betti numbers (Schmidhuber, Lloyd)
- Persistence gives an exponential advantage (Gyurik, Schmidhuber, King, Dunjko, Hayakawa)
- Can we find an algorithm with an exponential advantage?

A quantum algorithm for Khovanov homology

HODGE LAPLACIANS IN KHOVANOV HOMOLOGY

Khovanov homology

Khovanov homology is a bigraded homology whose Euler characteristic is the Jones polynomial.

A diagram of a knot or link K is associated to:

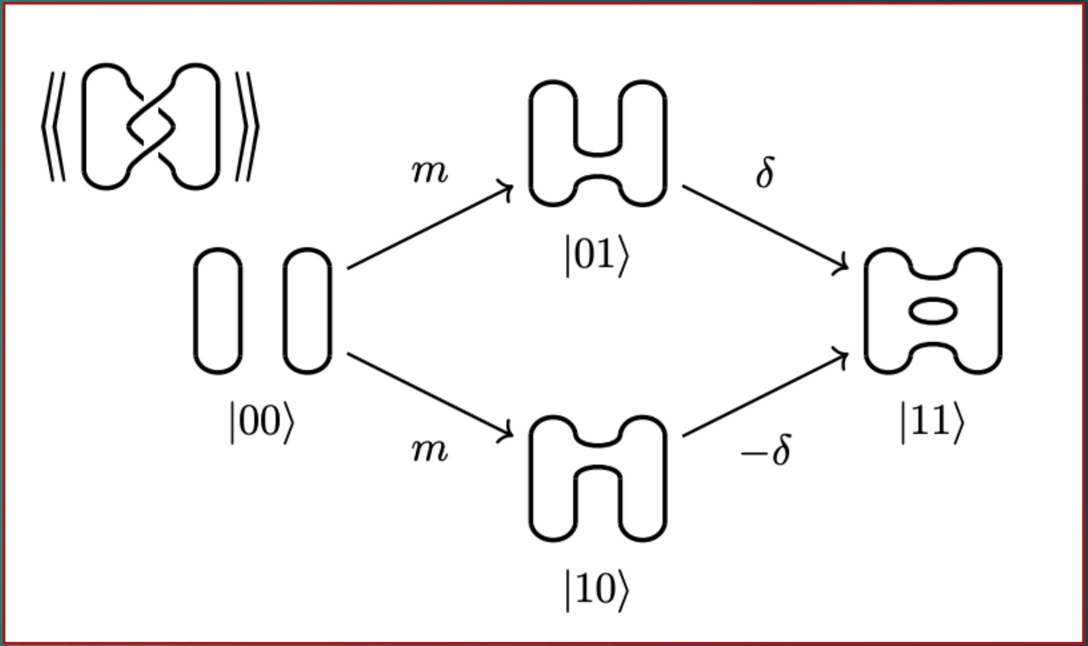
- Chain groups $\mathcal{C}_{i,j}$ indexed by homological grading *i* and quantum grading *j*.
- Define boundary maps $\partial_{i,j} : \mathcal{C}_{i,j} \to \mathcal{C}_{i-1,j}$ using formal rules from a specific Frobenius algebra structure.
- This defines homology groups $Kh^{i,j}(K) := H_{i,j}(K) = \dfrac{\ker \partial_{i,j}}{\operatorname{im} \partial_{i+1,j}}$
- Each $Kh^{i,j}(K)$ is topologically invariant.
- The Jones polynomial is recovered as $\mathrm{J}(K) = \sum_{i,j} (-1)^i q^j \dim(\mathrm{Kh}^{i,j}(K))$

Khovanov homology

- Based on a 2D TQFT defined from the commutative Frobenius algebra

$$V = H^*(S^1) = \mathbb{C}[X]/X^2 = span(\mathbb{1}, X)$$

- Disjoint union of circles for each resolution assigned tensor powers of V
- Differentials come from Frobenius multiplication and comultiplication
- Khovanov homology has no **unitary structure**. No obvious connection to quantum circuits.



Khovanov Hodge Laplacian

- Equip the vector space of the circle $V = span(1, X)$ with a non-degenerate bilinear form $\langle . | . \rangle : V \otimes V \to \mathbb{C}$ where $\mathbb{1}$ and X are orthonormal

- Define adjoints of Frobenius structure

$$m: V \otimes V \to V \qquad |\mathbb{1}\mathbb{1}\rangle \mapsto |\mathbb{1}\rangle, \quad |\mathbb{1}X\rangle \mapsto |X\rangle, \quad |X\mathbb{1}\rangle \mapsto |X\rangle, \quad |XX\rangle \mapsto 0$$

$$\delta: V \to V \otimes V \qquad |\mathbb{1}\rangle \mapsto |\mathbb{1}X\rangle + |X\mathbb{1}\rangle, \quad |X\rangle \mapsto |XX\rangle$$

$$\delta^*: V \otimes V \to V \qquad |\mathbb{1}\mathbb{1}\rangle \mapsto 0, \quad |\mathbb{1}X\rangle \mapsto |\mathbb{1}\rangle, \quad |X\mathbb{1}\rangle \mapsto |\mathbb{1}\rangle, \quad |XX\rangle \mapsto |X\rangle$$

$$m^*: V \to V \otimes V \qquad |\mathbb{1}\rangle \mapsto |\mathbb{1}\mathbb{1}\rangle, \quad |X\rangle \mapsto |\mathbb{1}X\rangle + |X\mathbb{1}\rangle$$

- Gives rise to a Hodge Laplacian $\Delta_{ij}: Kh^{i,j}(K) \to Kh^{i,j}(K)$

Quantum algorithms for Khovanov homology

- Hodge theory allows us to compute Khovanov homology from a Hermitian operator

Hodge theory:

$$\mathrm{Kh}^{i,j}(K) = \frac{\ker \partial_{i,j}}{\operatorname{im} \partial_{i+1,j}} \simeq \ker\left(\partial^*_{i,j}\partial_{i,j} + \partial_{i+1,j}\partial^*_{i+1,j}\right) = \ker \Delta_{i,j}$$

$\Delta_{i,j}$ is:

- Hermitian (a Hamiltonian)
- Positive semi-definite
- Local
- Supersymmetric

→ **Computing Khovanov homology is equivalent to preparing the groundstate of a (supersymmetric) quantum system!**

LGZ for Khovanov homology

Quantum algorithm [LGZ'2007]

Step 1: Construct an equal mixture of the chain space

$$\rho_{i,j} = \frac{1}{|C_{i,j}|} \sum_{c_{i,j} \in C_{i,j}} |c_{i,j}\rangle\langle c_{i,j}|$$

Step 2: Exponentiate $\Delta_{i,j}$ and perform quantum phase estimation on $\rho_{i,j}$

Step 3: Estimate the relative frequency of 0-eigenvalues

$$\frac{\#\text{of zero-eigenvalues}}{\#\text{of samples}} \approx \frac{\dim \operatorname{Ker} \Delta_{i,j}}{\dim \Delta_{i,j}} = \frac{\beta_{i,j}}{|C_{i,j}|}$$

NP-hard in the simplicial case, still open for Khovanov homology

Efficient because of sparsity

Does not work!
We find numerically that the Betti numbers of Khovanov homology are small

Modified LGZ algorithm

- With Alexander Schmidhuber, Michele Reilly, Paolo Zanardi, and Seth Lloyd we modify the LGZ algorithm

Step 1: Construct a low-temperature Gibbs state for $T \approx gap(\Delta_{i,j})$

$$\rho_{i,j}(T) = \frac{e^{-\beta\Delta_{i,j}}}{\mathrm{Tr}[e^{-\beta\Delta_{i,j}}]}$$

Efficiency depends on thermalization time and spectral gap

Step 2: Exponentiate $\Delta_{i,j}$ and perform quantum phase estimation on $\rho_{i,j}$. Measure if zero-eigenvalue was found. This projects onto

$$\sigma_{i,j} = \frac{1}{|\dim \mathrm{Ker}\,\Delta_{i,j}|} \sum_{c_{i,j} \in \mathrm{Ker}\,\Delta_{i,j}} |c_{i,j}\rangle\langle c_{i,j}|$$

Efficient if the temperature is sufficiently low and the spectral gap is inverse-polynomial

Step 3: Perform a SWAP test on copies of $\sigma_{i,j}$, which suceeds with probability

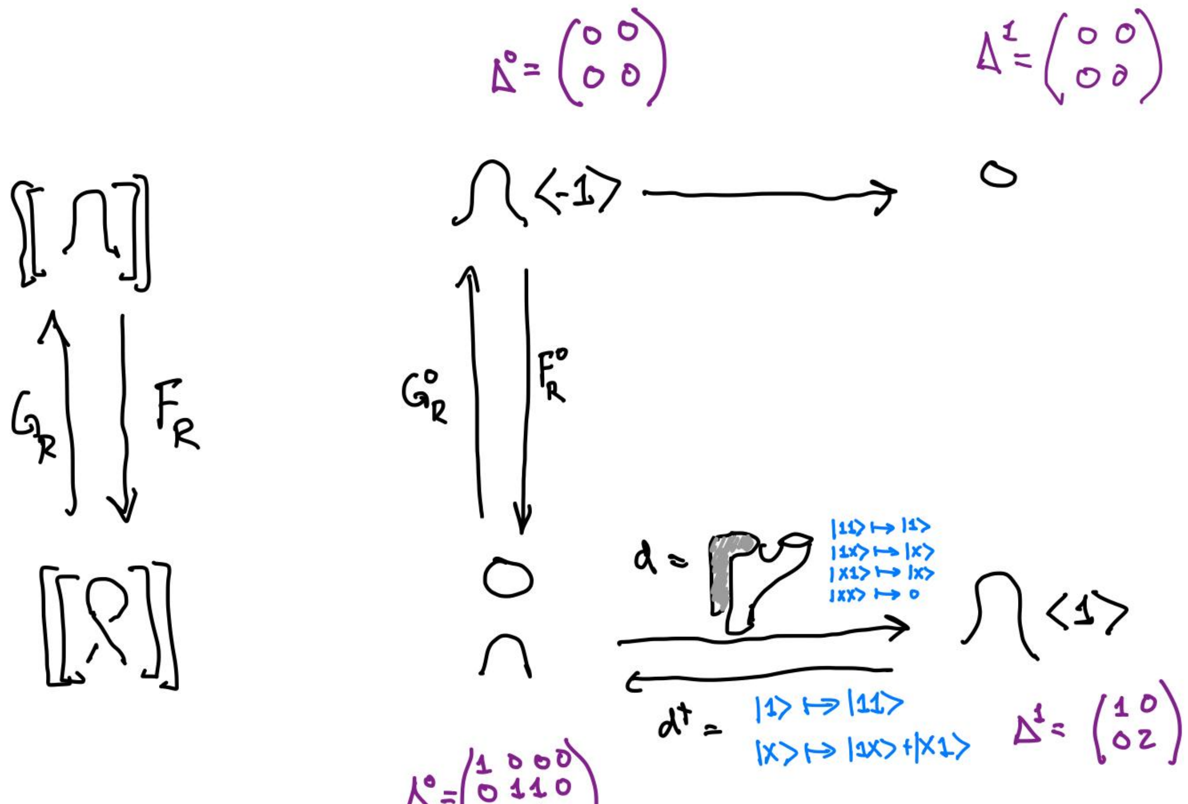
$$p_{\mathrm{succ}} = \frac{1}{2}\left(1 + \frac{1}{\beta_{i,j}}\right)$$

to estimate the Betti number of Khovanov homology

Efficient because the Betti numbers are small!

Laplace spectrum is not a topological invariant

$Spec(\Delta^0) = (0,0)$



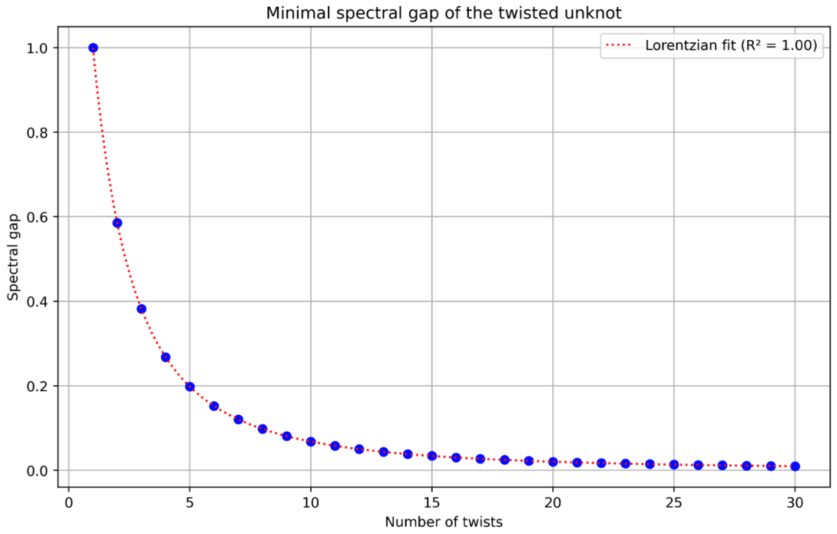
$Spec(\Delta^0) = (0,0,1,2)$

Spectral gap is a quantity associated to a diagram, not a knot

Twisted unknots

Example: Twisted unknot

$TU_n :=$ 



$$\text{gap} = \frac{10.3732}{1 + \frac{(n+1.98306)^2}{0.949381307}}$$

n	Min Gap of TU_n
1	1
2	0.585786
3	0.381966
4	0.267949
5	0.198062
6	0.152241
7	0.120615
8	0.097887
9	0.0810141
10	0.0681483

The spectral gap decreases with n, but rate of decrease is only polynomial in the number of crossings

Open questions

- Sampling the enhanced Khovanov states
- Convergence of Gibbs cooling
- Analytic lower-bounds on the spectral gap of the Khovanov Laplacian?
  - Extensive numerical calculations confirm the gap does not decrease exponentially
- Can the Khovanov Laplacian encode arbitrary quantum Hamiltonians? (QMA-completeness)
- Strong evidence for exponential quantum speedup?
- Quantum algorithms for other homological invariants? (for example, Lee homology)

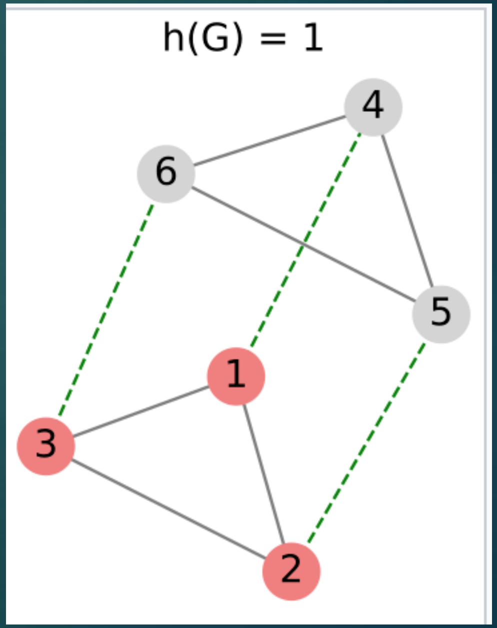
Spectral Gaps in graph theory

Let G be a weighted graph with vertex set V and edge set E

- One can form a graph Laplacian $\Delta = D - A$ where
  - A = adjacency matrix entries = w_{ij}= weights of edges
  - D = degree matrix $d(i) = \sum_{(i,j) \in E} w_{ij}$

- Graph Laplacians have a famous bound on the spectral gap known as Cheeger inequalities

$$2h(G) \geq \lambda \geq \frac{h^2(G)}{2\Delta(G)}$$



Too bad this has nothing to do with Khovanov homology!

Spectral Gaps in Graph Theory

Let G be a weighted graph with vertex set V and edge set E

- Form the *signless* Laplace matrix $Q = D + A$
- Unlike the usual graph Laplacian, Q is positive semidefinite
  - Only zero if the graph G contains a bipartite component
- For a subset $S \subset V$ of vertices let $\boldsymbol{e_{min}(S)}$ be the minimum edges that need to be removed from induced subgraph G_S so that it becomes bipartite
- $\boldsymbol{cut(S)}$ = edges with a boundary in S and $V - S$
- Define the quantity

$$\Psi := \min_{S \subset V} \Psi_S, \qquad \Psi_S := \frac{e_{\min}(S) + |cut(S)|}{|S|}$$

Bounding the spectral gap

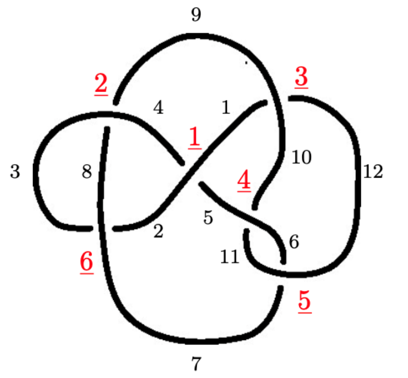
Theorem (Desai, Rao): If $\lambda_{(min)}(Q)$ is the smallest eigenvalue of $Q = D + A$ then

$$\frac{\Psi^2}{4d^*} \leq \lambda_{\min}(Q) \leq 4\Psi$$

where d^* is the largest degree of a vertex in G

Theorem (Schmidhuber, Reilly, Zanardi, Lloyd, L)

One can define a graph $G_q(K)$ associated with the lowest homological degree and arbitrary q-degree in Khovanov homology KH(K) such that $\Delta_{0,q}(K)$ is the signless Laplace matrix of the graph $G_q(K)$

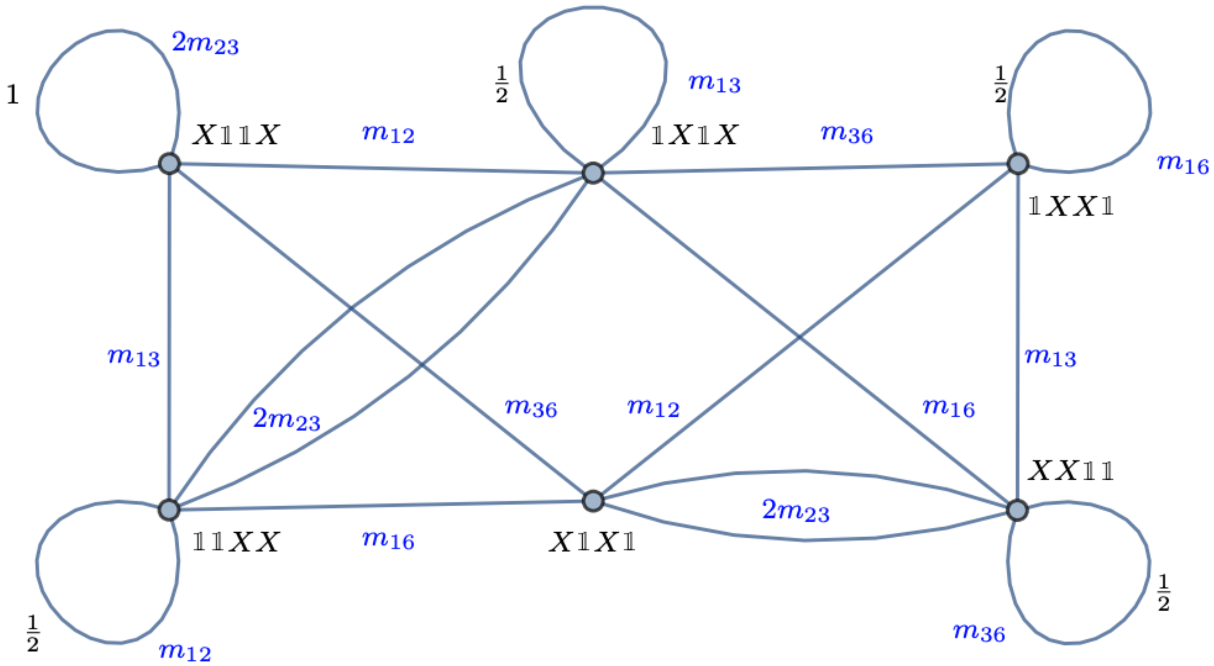


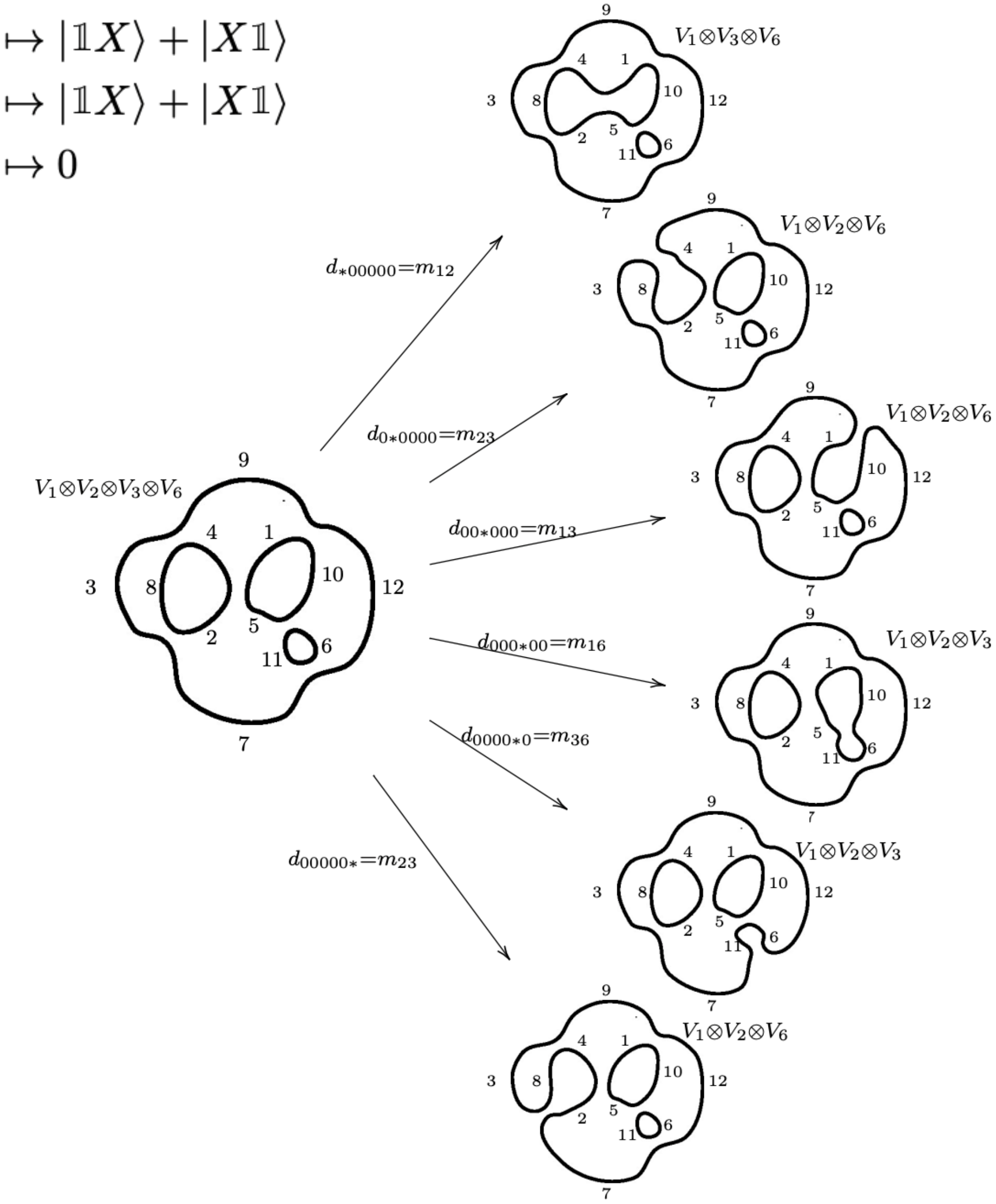
$$\Delta_{(0,0)}(6_3) = \begin{pmatrix} 5 & 2 & 1 & 0 & 1 & 0 \\ 2 & 6 & 1 & 1 & 0 & 1 \\ 1 & 1 & 5 & 0 & 1 & 0 \\ 0 & 1 & 0 & 4 & 1 & 1 \\ 1 & 0 & 1 & 1 & 5 & 2 \\ 0 & 1 & 0 & 1 & 2 & 5 \end{pmatrix}$$

$$\mathfrak{m}_{i,j:=} m_{ij}^{\dagger} m_{ij} : V_i \otimes V_j \to V_i \otimes V_j$$

$$|\mathbb{1}\mathbb{1}\rangle \mapsto |\mathbb{1}\mathbb{1}\rangle$$
$$|\mathbb{1}X\rangle \mapsto |\mathbb{1}X\rangle + |X\mathbb{1}\rangle$$
$$|X\mathbb{1}\rangle \mapsto |\mathbb{1}X\rangle + |X\mathbb{1}\rangle$$
$$|XX\rangle \mapsto 0$$

$$\Delta_0(6_3) = \mathfrak{m}_{12} + 2\mathfrak{m}_{23} + \mathfrak{m}_{13} + \mathfrak{m}_{16} + \mathfrak{m}_{36}.$$





New directions for link homology from quantum algorithms

HODGE LAPLACIANS IN LINK HOMOLOGY

Harmonic Khovanov homology

What is the topological relevance of harmonic Khovanov homology?

- The Khovanov Hodge Laplacian allows us to choose distinguished "harmonic" representatives of homology.
- Harmonic Khovanov homology is functorial
  - Harmonic chains functor is naturally isomorphic to the homology functor
- Spectral gap and higher spectral data are not topological invariants
  - Gives some data associated to a knot diagram not a knot

Jernej Grlj

Can you hear the shape of Khovanov homology?