A new quantum computational set-up for algebraic topology via simplicial sets

(based on arXiv:2309.11304)

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- Computational topology is the study of topological invariants of topological spaces by the methods of algebraic topology and computer science:
  - computational 3–manifold theory;
  - computational knot theory;
  - computational homotopy theory;
  - computational homology theory;
  - topological data analysis.
- Computational topology involves:
  - a wide range of applications;
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- In computational topology, many topological spaces embedded in Euclidean spaces are analyzed by associating abstract simplicial complexes to samplings of them mostly using the techniques of persistent simplicial homology.

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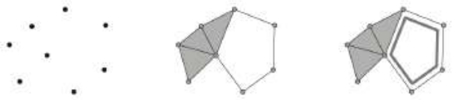
Simplicial approaches



A simplicial complex associated to a sampling (from A. Zomorodian (2010)).

- In spite of their simplicity and intuitiveness, abstract simplicial complexes suffer a number of drawbacks:
  - the product and quotient of two simplicial complexes are defined only under restrictive conditions;
  - face identification is not possible in a simplicial complex;
  - the simplicial complexes usually employed (e.g Čech, Vietoris–Rips, witness, alpha, mapper etc. complexes) are characterized by an explosive growth in the number of simplices as the size of the sampling gets large;
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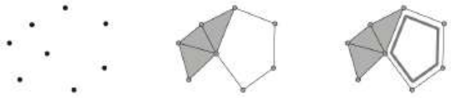

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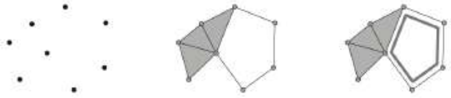

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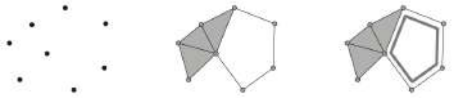

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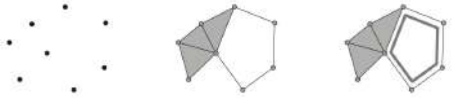

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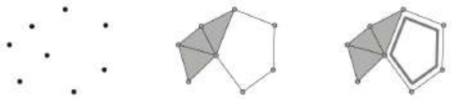

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Simplicial complexes vs. sets

- It is reasonable to search for alternative simplicial approaches to computational topology free of these shortcomings.
- The limitations of abstract simplicial complex theory can be traced back to its regarding as admissible only simplices which are non degenerate and have distinct faces and forbidding distinct simplices to share the same set of faces.
- Simplicial set theory is a generalization of simplicial complex theory which dispenses with this restrictions allowing for a wider range of options:
  - simplicial sets allow for both non degenerate and degenerate simplices and simplices with identified faces;
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The 7 possible 2-simplices in a simplicial set. The triangle abc is the only one allowed in a complex (from A. Zomorodian (2010)).

Two torus triangulations (from D. Bernoulli (2016))

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  - a 2d torus can be represented as a simplicial set with 1 vertex, 3 edges and 2 triangles, while as a simplicial complex with at least 7 vertices and many more edges and triangles;
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- Tidy sets, minimal simplicial sets capturing the topology of simplicial complexes, are available (A. Zomorodian (2010)).
- Incorporation of degenerate simplices, i.e. simplices with an effective dimension smaller than the formal one, is an essential feature of simplicial sets (and also a price to pay for having them):
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- A quantum algorithm with exponential speedup for computing Betti numbers in persistent homology was originally worked out by S. Lloyd *et al.* (2014).
- This opened a new field in quantum computing, quantum topological data analysis, whose development intensified in recent years (S. Gunn and N. Kornerup (2019); C. Gyurik *et al.* (2022); S. Ubaru *et al.* (2021); R. Hayakawa (2022); S. McArdle *et al.* (2022); D. W. Berry *et al.* (2022); M. Black *et al.* (2023))
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- Idea: a given simplicial set is inscribed in a simplicial Hilbert space: simplices turn into simplex vectors forming a distinguished orthonormal basis and the face and degeneracy maps into face and degeneracy operators.
- A foundation of a quantum computational framework for algebraic topology via simplicial set theory is provided.
- Disclaimer: no new quantum algorithms solving specific problems of algebraic topology is presented,
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Simplicial sets

- Simplicial sets generalize simplicial complexes in many ways.
- A simplicial set is a combinatorial blueprint of a topological space, its topological realization.
- Homotopy and homology have a correlate in simplicial set theory.
- A *simplicial set* X consists of a family of n–simplex sets X_n, $n \in \mathbb{N}$, and face and degeneracy maps $d_{ni} : X_n \to X_{n-1}$, $n \geq 1$, $i = 0, \ldots, n$, and $s_{ni} : X_n \to X_{n+1}$, $n \geq 0$, $i = 0, \ldots, n$, obeying the simplicial relations

$$
\begin{aligned}
& d_{n-1i} d_{nj} = d_{n-1j-1} d_{ni} && \text{if } \ 0 \leq i, j \leq n,\ i < j, \\
& d_{n+1i} s_{nj} = s_{n-1j-1} d_{ni} && \text{if } \ 0 \leq i, j \leq n,\ i < j, \\
& d_{n+1i} s_{nj} = \mathrm{id}_n && \text{if } \ 0 \leq j \leq n,\ i = j, j+1, \\
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Simplicial sets

- Simplicial sets generalize simplicial complexes in many ways.
- A simplicial set is a combinatorial blueprint of a topological space, its topological realization.
- Homotopy and homology have a correlate in simplicial set theory.
- A *simplicial set* X consists of a family of n–simplex sets X_n, $n \in \mathbb{N}$, and face and degeneracy maps $d_{ni} : X_n \to X_{n-1}$, $n \geq 1$, $i = 0, \ldots, n$, and $s_{ni} : X_n \to X_{n+1}$, $n \geq 0$, $i = 0, \ldots, n$, obeying the simplicial relations

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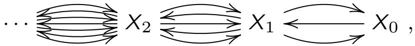

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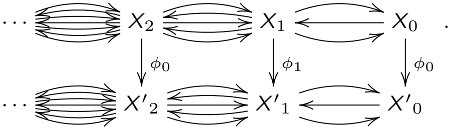

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- The *Cartesian product* $X \times X'$ of X, X' is the simplicial set defined by setting $X \times X'_n = X_n \times X'_n$ and $d \times d'_{ni} = d_{ni} \times d'_{ni}$ and $s \times s'_{ni} = s_{ni} \times s'_{ni}$.
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- With the operations of Cartesian product and disjoint union and the empty and singleton simplicial sets $D*$, $D\emptyset$ as units simplicial sets and morphisms form a bimonoidal category $\underline{\mathrm{sSet}}$.
- The simplicial quantum computational framework involves only parafinite simplicial sets.
- A simplicial set X is called *parafinite* (not to be confused with finite) if the n–simplex set X_n is finite for all n.
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- Example: the simplicial set $K\mathcal{S}$ of an ordered *abstract simplicial complex* $\mathcal{S}$. $K\mathcal{S}$ obtained from $\mathcal{S}$ by allowing simplices with repeated vertices. If $\mathcal{S}$ has finitely many vertices, $K\mathcal{S}$ is parafinite.
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Simplicial objects

- A *simplicial object* X in a general category $\mathcal{C}$ is a simplicial set internal to $\mathcal{C}$.
- A simplicial object X in $\mathcal{C}$ is a family of n–simplex objects X_n, $n \in \mathbb{N}$, and face and degeneracy morphisms $d_{ni} : X_n \to X_{n-1}$, $n \geq 1$, $i = 0, \ldots, n$, and $s_{ni} : X_n \to X_{n+1}$, $n \geq 0$, $i = 0, \ldots, n$, obeying the simplicial relations ssr.
- A morphism $\phi : X \to X'$ of the simplicial objects X, X' of $\mathcal{C}$ is a collection of morphisms $\phi_n : X_n \to X'_n$ with $n \geq 0$ obeying the simplicial morphism relations smr.
- Example: a simplicial set X is just a simplicial object in the category $\underline{\mathrm{Set}}$ of sets and functions.
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Simplicial Hilbert spaces

- The quantum simplicial framework uses *finite dimensional simplicial Hilbert spaces*.
- A finite dimensional simplicial Hilbert space $\mathscr{H}$ is a simplicial set internal to the category $\underline{\mathrm{fdHilb}}$ of finite dimensional Hilbert spaces and linear maps.
- $\mathscr{H}$ has n–simplex spaces $\mathscr{H}_n$ and face and degeneracy operators F_{ni} and S_{ni}.
- The direct product of the simplicial Hilbert spaces $\mathscr{H}$, $\mathscr{H}'$ is the simplicial Hilbert space $\mathscr{H} \otimes \mathscr{H}'$ defined by setting $\mathscr{H} \otimes \mathscr{H}'_n = \mathscr{H}_n \otimes \mathscr{H}'_n$ and $F \otimes F'_{ni} = F_{ni} \otimes F'_{ni}$ and $S \otimes S'_{ni} = S_{ni} \otimes S'_{ni}$.
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Simplicial Hilbert spaces

- The quantum simplicial framework uses *finite dimensional simplicial Hilbert spaces*.
- A finite dimensional simplicial Hilbert space $\mathscr{H}$ is a simplicial set internal to the category $\underline{\mathrm{fdHilb}}$ of finite dimensional Hilbert spaces and linear maps.
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Degenerate simplices of a simplicial set

- A distinguishing feature of a simplicial set X when compared to a simplicial complex is the appearance of infinitely many degenerate simplices, which are topologically invisible.
- An n–simplex $\sigma_n \in X_n$ is *degenerate* if there is some $\tau_{n-1} \in X_{n-1}$ and index i with $0 \leq i \leq n-1$ with $\sigma_n = s_{n-1i}\tau_{n-1}$. 0-simplices are regarded as non degenerate.
- The degenerate simplices of X_n form a subset ${}^sX_n$.
- Example: in the discrete simplicial set DA of a non empty set A all positive degree simplices are degenerate.
- Example: in the simplicial set $K\mathcal{S}$ of an ordered abstract simplicial complex $\mathcal{S}$, all simplices with repeated vertices are degenerate.
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- The practical implementation of algorithms of computational topology involves a finite approximation of a simplicial set containing infinitely many simplices.
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Simplicial homology

- With a simplicial set X and an Abelian group A there are associated a simplicial Abelian group $C(X, \mathsf{A})$ with n–simplex groups

$$C_n(X, \mathsf{A}) = \mathbb{Z}[X_n] \otimes \mathsf{A},$$

along with face and degeneracy morphisms $d_{ni} : C_n(X, \mathsf{A}) \to C_{n-1}(X, \mathsf{A})$, $s_{ni} : C_n(X, \mathsf{A}) \to C_{n+1}(X, \mathsf{A})$ induced by the d_{ni}, s_{ni} of X.

- The boundary morphisms $\partial_n : C_n(X, \mathsf{A}) \to C_{n-1}(X, \mathsf{A})$

$$\partial_n = \sum_{0 \leq i \leq n} (-1)^i d_{ni}$$

obey the homological relations

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- Denote by ${}^s C_n(X, \mathsf{A})$ the subgroup of $C_n(X, \mathsf{A})$ generated by the degenerate simplex set ${}^s X_n$. The group $\overline{C}_n(X, \mathsf{A}) = C_{\mathsf{n}}(X, \mathsf{A}) / {}^{\mathsf{s}}C_{\mathsf{n}}(X, \mathsf{A})$ is the normalized n–chain group.

- The boundary morphisms ∂_n give rise to a normalized boundary morphisms $\overline{\partial}_n : \overline{C}_n(X, \mathsf{A}) \to \overline{C}_{n-1}(X, \mathsf{A})$ obeying

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The simplicial Hilbert space of a simplicial set and the Hilbert simplicial functor

- The *quantum simplicial set framework* is the natural set–up for the analysis and implementation of quantum algorithms of simplicial set theoretic computational topology.
- It allows also in principle the modelling of simplicial quantum computation and circuitry.
- It is an instance of quantum basis coding of classical data, where the latter are simplicial data of a parafinite simplicial set X.
- For $n \in \mathbb{N}$, the n–simplex Hilbert space $\mathscr{H}_n$ is the Hilbert space generated by the n–simplex set X_n.
- $\mathscr{H}_n$ has thus a canonical orthonormal basis $|\sigma_n\rangle$ labelled by the n–simplices $\sigma_n \in X_n$ (n–simplex basis).
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- The face operators $D_{ni} : \mathscr{H}_n \to \mathscr{H}_{n-1}$, $i = 0, \ldots, n$ and $n \geq 1$, and degeneracy operators $S_{ni} : \mathscr{H}_n \to \mathscr{H}_{n+1}$ and $i = 0, \ldots, n$ and $n \geq 0$ are

$$D_{ni} = \sum_{\sigma_n \in X_n} |d_{ni}\sigma_n\rangle\langle\sigma_n|, \tag{3.1}$$

$$S_{ni} = \sum_{\sigma_n \in X_n} |s_{ni}\sigma_n\rangle\langle\sigma_n|. \tag{3.2}$$

- The simplicial relations ssr imply the exchange identities ($1_n \equiv 1_{\mathscr{H}_n}$):

$$D_{n-1i}D_{nj} - D_{n-1j-1}D_{ni} = 0 \qquad \text{for } 0 \leq i, j \leq n, i < j,$$

$$D_{n+1i}S_{nj} - S_{n-1j-1}D_{ni} = 0 \qquad \text{for } 0 \leq i, j \leq n, i < j,$$

$$D_{n+1i}S_{nj} - 1_n = 0 \qquad \text{for } 0 \leq j \leq n, i = j, j+1,$$

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These are the Hilbert simplicial identities.

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- The Hilbert simplicial identities hei entail that the Hilbert data collection $\{\mathscr{H}_n, D_{ni}, S_{ni}\}$ constitutes a finite dimensional simplicial Hilbert space $\mathscr{H}$.
- With any morphism $\phi : X \to X'$ of the parafinite simplicial sets X, X' ssr there is associated a morphism $\Phi : \mathscr{H} \to \mathscr{H}'$ of the simplicial Hilbert spaces $\mathscr{H}$, $\mathscr{H}'$ given by the linear operators $\Phi_n : \mathscr{H}_n \to \mathscr{H}'_n$,

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since indeed

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- **Theorem**: *the map $X \mapsto \mathscr{H}$, $(\phi : X \to X') \mapsto (\Phi : \mathscr{H} \to \mathscr{H}')$ is a functor $\varsigma : \underline{\mathrm{pfsSet}} \to \underline{\mathrm{fdsHilb}}$ of bimonoidal categories (Hilbert simplicial functor).*

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The cosimplicial Hilbert structure

- For a parafinite simplicial set X, the dagger structure of the Hilbert space category $\underline{\mathrm{fdHilb}}$ yields the adjoints ${D_{ni}}^+ : \mathscr{H}_{n-1} \to \mathscr{H}_n$, ${S_{ni}}^+ : \mathscr{H}_{n+1} \to \mathscr{H}_n$,

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where the face and degeneracy star sets $D_{ni}(\sigma_{n-1})$, $S_{ni}(\sigma_{n+1}) \subset X_n$ are

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- One has $|D_{ni}(\sigma_{n-1})| \geq 1$ and $|S_{ni}(\sigma_{n+1})| \leq 1$ (by the surjectivity of the d_{ni} and the injectivity of the s_{ni}).

- Via the $D_{ni}(\sigma_{n-1})$, $S_{ni}(\sigma_{n+1})$, the adjoint operators ${D_{ni}}^+$, ${S_{ni}}^+$ encode special features of X not directly accessible through the operators D_{ni}, S_{ni}.

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- The exchange identities of ${D_{ni}}^+$, ${S_{ni}}^+$ stem from those of D_{ni}, S_{ni} hei. They have the same form except for the reversed order of the factors. They are therefore Hilbert cosimplicial identities.
- These relations entail that the data collection $\{\mathscr{H}_n, {D_{ni}}^+, {S_{ni}}^+\}$ is a finite dimensional cosimplicial Hilbert space $\mathscr{H}^+$.

  NB Unlike fdHilb, the simplicial Hilbert space category fdsHilb is not dagger.
- With any simplicial set morphism $\phi : X \to X'$ of parafinite simplicial sets X, X' there is associated a morphism $\Phi^+ : \mathscr{H}'^+ \to \mathscr{H}^+$ of the cosimplicial Hilbert spaces $\mathscr{H}'^+$, $\mathscr{H}^+$ specified by the adjoint operators ${\Phi_n}^+ : \mathscr{H}'_n \to \mathscr{H}_n$,

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  NB This is a generic feature of simplicial Hilbert spaces.

The cosimplicial Hilbert structure

- The exchange identities of ${D_{ni}}^+$, ${S_{ni}}^+$ stem from those of D_{ni}, S_{ni} hei. They have the same form except for the reversed order of the factors. They are therefore Hilbert cosimplicial identities.
- These relations entail that the data collection $\{\mathscr{H}_n, {D_{ni}}^+, {S_{ni}}^+\}$ is a finite dimensional cosimplicial Hilbert space $\mathscr{H}^+$.

  NB Unlike $\underline{\mathrm{fdHilb}}$, the simplicial Hilbert space category $\underline{\mathrm{fdsHilb}}$ is not dagger.
- With any simplicial set morphism $\phi : X \to X'$ of parafinite simplicial sets X, X' there is associated a morphism $\Phi^+ : \mathscr{H}'^+ \to \mathscr{H}^+$ of the cosimplicial Hilbert spaces $\mathscr{H}'^+$, $\mathscr{H}^+$ specified by the adjoint operators ${\Phi_n}^+ : \mathscr{H}'_n \to \mathscr{H}_n$,

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- A simplicial and a cosimplicial Hilbert structure coexist in this way in the quantum simplicial set–up.

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Defect results

- For a parafinite simplicial set X, the mixed exchange identities involving one of the D_{ni}, S_{ni} and one of the ${D_{ni}}^+$, ${S_{ni}}^+$ have the form

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\begin{aligned}
&{D_{ni}}^+ D_{nj} - D_{n+1j+1} {D_{n+1i}}^+ = {\Delta^{DD}}_{nij} && \text{for } 0 \leq i, j \leq n,\ i \leq j, \\
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Defect results

- $\Delta^{DD}{}_{nij}$, $\Delta^{DS}{}_{nij}$, $\Delta^{SD}{}_{nij}$ detect basic properties of X.
- **Proposition**: *the simplicial set $K\mathcal{S}$ of an ordered finite abstract simplicial complex $\mathcal{S}$ is semi perfect:*

$$\Delta^{DS}{}_{nij} = 0 \qquad \textit{for} \quad 0 \leq i, j \leq n,\ i \leq j,$$

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- The *quantum simplicial register* of a parafinite simplicial set X is a pre-Hilbert space $\mathscr{H}^{(\infty)}$ that stores all the simplicial data of X in the same way as a quantum register is a Hilbert space $\mathbb{C}^{2\otimes n}$ that stores all the configurations of a classical n bit string.
- Mathematically, $\mathscr{H}^{(\infty)}$ is the infinite dimensional pre-Hilbert space

$$\mathscr{H}^{(\infty)} = \bigoplus_{0\leq n<\infty} \mathscr{H}_n \tag{3.3}$$

(algebraic direct sum).
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- A simple simplicial quantum circuit is a unitary simplicial automorphism of $\mathscr{H}$ shm, that is a collection of unitary operators $U_n \in \mathsf{U}(\mathscr{H}_n)$ with $n \geq 0$ such that for $0 \leq i \leq n$

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$$U^{(n)} = U_n \oplus \bigoplus_{0 \leq n' < \infty, n' \neq n} 1_{n'}.$$

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- Simple simplicial quantum circuits can perform only computations at fixed simplicial degree, an important limitation. We need more general circuits for more general computations.
- The simplicial conditions which a general simplicial quantum circuit obeys should be an appropriate generalization of those obeyed by simple circuits.
- For $\emptyset \neq A \subset \mathbb{N}$ a finite subset, the simplicial A–subregister is the finite dimensional Hilbert space

$$\mathscr{H}_A = \bigoplus_{n \in A} \mathscr{H}_n \subset \mathscr{H}^{(\infty)}$$

- Set $\Sigma = \{-1, +1\}$ and $\mathbb{N}_n = \{n' | n' \in \mathbb{N}, 0 \leq n' \leq n\}$. For $\emptyset \neq A \subset \mathbb{N}$ a finite subset, $\alpha \in \Sigma^A$ and $i \in \prod_{n \in A} \mathbb{N}_n$, let $X^{(\alpha)}{}_{Ai} : \mathscr{H}_A \to \mathscr{H}_{\tau_\alpha(A)}$ be

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- Let $p \in \mathbb{N}$, $p > 0$. A p–ary simplicial quantum circuit consists of a collection of unitary operators $U_A \in \mathrm{U}(\mathscr{H}_A)$ with $A \subset \mathbb{N}$ and $|A| = p$ such that for all $\alpha \in \Sigma^A$ and $i \in \prod_{n \in A} \mathbb{N}_n$

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NB Simple simplicial quantum circuits are just 1–ary simplicial quantum circuits ssc.

- A p-ary quantum circuit can be regarded as a family of simplicial quantum gates

$$U^{(A)} = U_A \oplus \bigoplus_{n \notin A} 1_n.$$

Unlike in the simple case, these gates generally do not commute (the subspaces $\mathscr{H}_A$ may have non trivial intersections).

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- Define $\hat{U}_{\phi n} : \mathscr{H} \otimes {\mathscr{H}'}_n \to \mathscr{H} \otimes {\mathscr{H}'}_n$ by

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- **Proposition**: *$\{\hat{U}_{\phi n}\}$ is a simple simplicial quantum circuit.*

Simplicial quantum registers and circuits

- A simple simplicial quantum circuit can be constructed from the following data:
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- Example: For a simplicial group G, the simplex sets G_n are groups, the multiplication and inversion maps $\mu_n : G_n \times G_n \to G_n$ and $\iota_n : G_n \to G_n$ are defined at each degree n and are the components of simplicial morphisms $\mu : G \times G \to G$, and $\iota : G \to G$. With these there are associated simple simplicial quantum circuits $\{\hat{U}_{\mu n}\}$ and $\{\hat{U}_{\iota n}\}$ of $G \times G \times G$ and $G \times G$, respectively.
- If $\{U_n\}$ is a simple simplicial quantum circuit, the operators $U_A = \bigoplus_{n \in A} U_n$, $A \subset \mathbb{N}$ and $|A| = p$, constitute a p–ary simplicial quantum circuit. This example is however trivial.
- One would like to find other more interesting examples simplicial quantum circuits, especially of simplicial quantum circuit data sets.
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Finite simplicial quantum registers and circuits

- To model realistic simplicial quantum registers and circuits with finite storage capabilities, it is necessary to set a cut-off K on the simplicial degree of the relevant parafinite simplicial set X.
- In computational topology, this is tantamount to replacing X by its K–truncation $\mathrm{tr}_K\, X$.
- $\mathrm{tr}_K\, X$, however, belongs to the category of K–truncated simplicial sets, which is related to but distinct from the category of simplicial sets.
- To remain within this latter while essentially keeping the essence of the truncation operation, one uses the K–skeleton $\mathrm{sk}_K\, X$ of X.
- Both the truncation $\mathrm{tr}_K\, X$ and the skeleton $\mathrm{sk}_K\, X$ may be viewed as a finite approximation of X in the appropriate sense.
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- In the quantum simplicial framework, to X there corresponds a simplicial Hilbert space $\mathscr{H}$.
- The Hilbert simplicial encoding map, which defines the simplex basis ssr, is a simplicial set morphism $\varkappa : X \to \mathscr{H}$.
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- Therefore, the operations of K–truncation and K–skeletonization of X turn under Hilbert simplicial encoding into the corresponding operations of the associated simplicial Hilbert space $\mathscr{H}$.

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- In practice, one works with $\mathrm{tr}_K X$ and $\mathrm{tr}_K \mathscr{H}$. In more formal considerations, employing $\mathrm{sk}_K X$ and $\mathrm{sk}_K \mathscr{H}$ allows to use the analysis carried out so far.
- The K–skeletonized quantum simplicial register is the infinite dimensional pre-Hilbert space $(\mathrm{sk}_K \mathscr{H})^{(\infty)}$ hst.
- An K–skeletonized simple simplicial quantum circuit $\{U_n\}_{n\in\mathbb{N}}$ is just a simple simplicial quantum circuit supported on $(\mathrm{sk}_K \mathscr{H})^{(\infty)}$ ssc.
- An K–skeletonized p–ary simplicial quantum circuit $\{U_A\}_{A\subset\mathbb{N},|A|=p}$ is just a p–ary simplicial quantum circuit supported on $(\mathrm{sk}_K \mathscr{H})^{(\infty)}$ sgc.
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Hilbert simplicial homology

- The simplicial homology of a parafinite simplicial set X with coefficients in $\mathbb{C}$ shm has a realization in the associated simplicial Hilbert space $\mathscr{H}$ and cosimplicial Hilbert space $\mathscr{H}^+$.
- The Hilbert simplicial boundary operators $Q_{Dn} : \mathscr{H}_n \to \mathscr{H}_{n-1}$, $n \geq 1$, are

$$Q_{Dn} = \sum_{0 \leq i \leq n} (-1)^i D_{ni}.$$

- By the exchange identities hei, the Q_{Dn} obey the homological relations

$$Q_{Dn-1} Q_{Dn} = 0.$$

- For $n \geq 0$, there are defined the Hilbert simplicial homology spaces

$$\mathrm{H}_{Dn}(\mathscr{H}) = \ker Q_{Dn} / \operatorname{ran} Q_{Dn+1} \qquad (\text{here } \ker Q_{D0} = \mathscr{H}_0).$$

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- The Hilbert cosimplicial coboundary operators are the adjoint operators $Q_{Dn}{}^+$ of Q_{Dn}.

Hilbert simplicial homology

- The simplicial homology of a parafinite simplicial set X with coefficients in $\mathbb{C}$ shm has a realization in the associated simplicial Hilbert space $\mathscr{H}$ and cosimplicial Hilbert space $\mathscr{H}^+$.
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$$ \mathrm{H}_n(X, \mathbb{C}) \simeq \mathrm{H}_{Dn}(\mathscr{H}) \simeq \mathrm{H}_D{}^n(\mathscr{H}^+) \simeq \ker H_{DDn}, $$

where H_{DDn} is the simplicial Hodge Laplacian

$$ H_{DDn} = {Q_{Dn}}^+ Q_{Dn} + Q_{Dn+1} {Q_{Dn+1}}^+. $$

NB This is analogous to Hodge theory of de Rham cohomology.

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Normalized Hilbert simplicial homology

- Such computation may be costly, as it involves also the degenerate simplex subspaces ${}^s\mathscr{H}_n$ of the simplex Hilbert spaces $\mathscr{H}_n$ dsx, which are homologically irrelevant by the normalization theorem nth:

$$ {}^s\mathscr{H}_n = \sum\nolimits_{i=0}^{n-1} \mathrm{ran}\, S_{n-1i}, $$

- The abstract non degenerate n–simplex spaces are

$$ \overline{\mathscr{H}}_n = \mathscr{H}_n / {}^s\mathscr{H}_n. $$

- As $Q_{Dn}{}^s\mathscr{H}_n \subset {}^s\mathscr{H}_{n-1}$, the Q_{Dn} induce an abstract normalized Hilbert simplicial boundary operators $\overline{Q}_{Dn} : \overline{\mathscr{H}}_n \to \overline{\mathscr{H}}_{n-1}$ obeying the homological relations

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- **Abstract Hilbert normalization theorem**: *for every* $n \geq 0$, *one has*

$$\mathrm{H}_n(X, \mathbb{C}) \simeq \mathrm{H}_{Dn}(\overline{\mathscr{H}}).$$

NB This is just the normalization theorem.

- The computation of the abstract homology is not tractable with standard quantum algorithmic techniques.
- In fact, the abstract spaces $\overline{\mathscr{H}}_n$ are non Hilbert complex vector spaces.
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- The orthogonal projector Π_n on ${}^s\mathscr{H}_n$ is

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- The verification proceeds by showing the isomorphism of the abstract and concrete homology spaces (not distinguished henceforth)

$$\mathrm{H}_{Dn}(\overline{\mathscr{H}}) \simeq \mathrm{H}_{Dn}({}^{c}\mathscr{H}).$$

- The proof of the isomorphism is achieved by constructing a chain equivalence of the Hilbert chain complexes $(\overline{\mathscr{H}}, \overline{Q}_D)$, $({}^{c}\mathscr{H}, {}^{c}Q_D)$.
- The chain equivalence is a sequence of chain operators $I_n : \overline{\mathscr{H}}_n \rightarrow {}^{c}\mathscr{H}_n$, $J_n : {}^{c}\mathscr{H}_n \rightarrow \overline{\mathscr{H}}_n$, $n \geq 0$, such that the composite operators $J_n I_n$, $I_n J_n$ are chain homotopic to $\overline{1}_n$, ${}^{c}1_n$, respectively.
- I_n is the operator induced by the orthogonal projector $1_n - \Pi_n$ by virtue of the fact that ${}^{s}\mathscr{H}_n = \ker(1_n - \Pi_n)$. J_n is the canonical projection of ${}^{c}\mathscr{H}_n$ onto $\overline{\mathscr{H}}_n$.
- As a matter of fact, I_n, J_n are reciprocally inverse.

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Simplicial quantum circuits computing normalized simplicial homology

- Homological computations can be performed using simplicial quantum circuits.
- For definiteness, consider a simple simplicial quantum circuit $\{U_n\}_{n\in\mathbb{N}}$ ssc.
- The degenerate n–simplex space ${}^s\mathscr{H}_n$ is invariant under U_n, as Π_n projects on ${}^s\mathscr{H}_n$ dhs and commutes with U_n.
- The orthogonal complement ${}^c\mathscr{H}_n = {}^s\mathscr{H}_n{}^\perp$ is then also invariant under U_n, as U_n is unitary.
- The restriction ${}^cU_n$ of U_n to ${}^c\mathscr{H}_n$ is a unitary operator of ${}^c\mathscr{H}_n$.
- The circuit defines a unitary chain operator of the normalized Hilbert simplicial chain complex:

$$ {}^cU_{n-1}\,{}^cQ_{Dn} - {}^cQ_{Dn}\,{}^cU_n = 0. $$

- As a consequence, each circuit component ${}^cU_n$ yields an automorphism of $\mathrm{H}_{Dn}({}^c\mathscr{H})$, hence of $\mathrm{H}_n(X,\mathbb{C}) \simeq \mathrm{H}_{Dn}({}^c\mathscr{H})$.

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Simplicial quantum circuits computing normalized simplicial homology

- Homological computations can be performed using simplicial quantum circuits.
- For definiteness, consider a simple simplicial quantum circuit $\{U_n\}_{n\in\mathbb{N}}$ ssc.
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- Each component ${}^cU_n$ commute also with the normalized Hilbert simplicial Laplacian ${}^cH_{DDn}$

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Digital encoding a simplicial set

- The *digital encoding* of the simplices of a given parafinite simplicial set X is a precondition for the implementation of simplicial set based algorithms of computational topology in a quantum computer.
- The full simplex set of the K–truncation $\mathrm{tr}_K X$ of X is

$$X^{(K)} = \bigsqcup_{0 \leq n \leq K} X_n.$$

- To encode the simplices of $X^{(K)}$, one needs a k–bit register with

$$k \geq \kappa_{X^K} := \min\{l \,|\, l \in \mathbb{N}, |X^{(K)}| \leq 2^l\}.$$

- A digital encoding of $\mathrm{tr}_K X$ in a k–bit register consists in a bijective mapping $\chi : X^{(K)} \to X_\chi{}^{(K)}$, where $X_\chi{}^{(K)} \subseteq B_2{}^k$ is a k–bit string set such that $|X_\chi{}^{(K)}| = |X^{(K)}|$. ($B_2 = \{0,1\}$ be the digital Boolean domain.) There are altogether $|X^{(K)}|!$ encodings with a given range $X_0 \subseteq B_2{}^k$.
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$$\mathscr{H}^{(K)} = \bigoplus_{0\leq n\leq K} \mathscr{H}_n.$$

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- There is no general prescription for that and χ must be chosen on a case by case basis.
- By contrast, in the simplicial complex framework (S. Lloyd *et al.* (2014)) there is a canonical encoding of the simplices of the relevant simplicial complex in terms of which the boundary maps have a simple form.

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Counting and parametrizing simplices

- Counting simplices is essential for the management of the resources of a simplicial quantum computer.
- For parafinite simplicial set X, let ${}^sX_n$, ${}^cX_n = X_n \setminus {}^sX_n \subseteq X_n$ be the subsets of degenerate and non degenerate n–simplices, respectively.
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- The total number of simplices of an K–truncation of X is

$$|X^{(K)}| = \sum_{0 \le n \le K} |X_n| = \sum_{0 \le m \le K} \binom{K+1}{m+1} |{}^c X_m|.$$

- The content of the non degenerate n–simplex sets ${}^c X_m$ depends on the underlying simplicial set X.
- Example: the simplicial set $K\mathscr{P}_V$ of a finite ordered discrete simplicial complex $\mathscr{P}_V$. For every n, $K_n\mathscr{P}_V$ is the set of all n–element ordered submultiset of an ordered vertex set $V = \{v_0, \ldots, v_d\}$.
  - The non degenerate n–simplices of $K_n\mathscr{P}_V$ are the n–element ordered submultiset of V with no repeats. Their number is

$$|{}^c K_n \mathscr{P}_V| = \binom{d+1}{n+1} \quad \text{for } n \le d,$$
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Counting and parametrizing simplices

- The number of non degenerate n–simplices such that $n \leq K$ with $K \leq d$ is found from here to be given by the expression

$$\sum_{0 \leq n \leq K} |{}^c K_n \mathscr{P}_V| = 2^{d+1} - 1 - \binom{d+1}{K+2} {}_2F_1(1, -d+K+1; K+3; -1).$$

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- For $K \leq d$, the number of simplices of the K–truncation $\mathrm{tr}_K \, K\mathscr{P}_V$ is

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- The encoding of $\mathrm{tr}_K \, K\mathscr{P}_V$ needs $\varkappa_{K\mathscr{P}_V K} = \log_2 |K^{(K)}\mathscr{P}_V|$ bits, where

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&\varkappa_{K\mathscr{P}_V K} \\
&= \log_2 \left[\left(\frac{\mathrm{e}d}{K}\right)^K \frac{d}{(2\pi)^{1/2} K^{3/2}} \right] + O(1/K, K^2/d) \quad \text{for } 1 \ll K \ll d^{1/2}, \\
&= 2d + 2 - \tfrac{1}{2} \log_2(\pi d) + O(d^{-1}, (K-d)\log_2 d) \quad \text{for } 1 \ll K \to d.
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  To encode all the simplex data in degree $n \leq d$ one needs a $2(d+1)$–bit register for the simplicial set $K\mathscr{P}_V$ comparable with the $d+1$–bit register required for the underlying simplicial complex $\mathscr{P}_V$.

- If $\mathcal{S}$ is an ordered finite simplicial complex with vertex set $V = \mathrm{Vert}_{\mathcal{S}}$, $|{}^cK_n\mathscr{P}_V|$, $|K_n\mathscr{P}_V|$ etc. constitute upper bounds for $|{}^cK_n\mathcal{S}|$, $|K_n\mathcal{S}|$ etc, respectively.

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- The simplices of a truncation $\mathrm{tr}_K\, K\mathscr{P}_V$ of $K\mathscr{P}_V$ can be digitally encoded in a $(d+1)r$–bit register with r is an integer such that $r \geq \log_2(K+2)$.
  - A $(d+1)r$–bit string can be represented as $(x_0, \ldots, x_d)$, where the x_a are r–bit strings, which one views as integers in the range 0 to $2^r - 1$.
  - For $0 \leq a \leq d$, let $\varphi_a : \bigsqcup_{0 \leq n} K_n \mathscr{P}_V \to \mathbb{N}$ be the a–th vertex counting map: if $\sigma_n \in K_n \mathscr{P}_V$, then $\varphi_a(\sigma_n)$ is the number of occurrences of the vertex v_a in σ_n.
  - An encoding χ of $\mathrm{tr}_K\, K\mathscr{P}_V$ is a bijection $\chi : K^{(K)}\mathscr{P}_V \to K_\chi{}^{(K)}\mathscr{P}_V$, where

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- This generalizes the bit parametrization of the simplicial complex $\mathscr{P}_V$.
- The face and degeneracy maps $d_{\chi n i}$, $s_{\chi n i}$ of the encoding read as

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for $(x_0, \ldots, x_d) \in K_{\chi n}\mathscr{P}_V$, where for $(x_0, \ldots, x_d) \in \mathbb{N}^{d+1}$,

$$\vartheta_{ai}(x_0, \ldots, x_d) = \begin{cases} 1 & \text{if} \quad \sum_{0 \leq b < a} x_b \leq i < \sum_{0 \leq b \leq a} x_b, \\ 0 & \text{else.} \end{cases}$$

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for $(x_0, \dots, x_d) \in K_{\chi n}\mathscr{P}_V$, where for $(x_0, \dots, x_d) \in \mathbb{N}^{d+1}$,

$$\vartheta_{ai}(x_0, \dots, x_d) = 1 \quad \text{if} \quad \sum_{0 \le b < a} x_b \le i < \sum_{0 \le b \le a} x_b,$$

$$0 \quad \text{else.}$$

Disposing of degenerate simplices

- Disposing of degenerate simplices in a quantum simplicial algorithm reduces to projecting the quantum register $\mathscr{H}^{(K)}$ onto its subspace ${}^c\mathscr{H}^{(K)}$ spanned by the non degenerate n–simplex spaces ${}^c\mathscr{H}_n$ with $0 \leq n \leq K$,

$$ {}^c\mathscr{H}^{(K)} = \bigoplus_{0 \leq n \leq K} {}^c\mathscr{H}_n. $$

- Orthogonal projectors cannot be part of any quantum circuits, as they are not unitary.

- The projection can be achieved nevertheless compatibly with unitarity using Grover's quantum search algorithm (L. K. Grover (1996)) in the variant based on amplitude amplification (G. Brassard and P. Hoyer (1997)).

- The quantum computer is initialized in a state that is a uniform superposition of all n–simp lex states $|\sigma_n\rangle$,

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- The algorithm comprises two stages:
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- In stage i, the state $|\xi_{0n}\rangle$ is yielded by the action of an appropriate unitary operator W_n on some fiducial reference state $|o_n\rangle$, so that

$$|\xi_{0n}\rangle = W_n|o_n\rangle. \tag{4.2}$$

- In stage ii, the state $|^c\xi_{0n}\rangle$ is generated by p_n iteration of the unitary Grover operator G_n

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- The Grover operator $G_n = -W_n D_{0n} {W_n}^+ D_n$, where $D_{0n} = 1_n - 2|o_n\rangle\langle o_n|$ is the conditional sign flip operator of the reference state $|o_n\rangle$ and D_n is the (oracular) conditional sign flip operator of the non degenerate simplex states $|\sigma_n\rangle$.
- The Grover iteration number $p_n = \left[\frac{\pi}{4}{\varrho_{\chi n}}^{1/2}\right]$. If the total to non degenerate n–simplex ratio $\varrho_{\chi n}$ rhr is unknown, it can be determined using a quantum counting algorithm (G. Brassard *et al.* (1998)), which computes the eigenvalues $\mathrm{e}^{\pm i\theta_n}$ of G_n related to $\varrho_{\chi n}$ by $\sin(\theta_n/2) = {\varrho_{\chi n}}^{-1/2}$.
- The two steps contribute additively to the algorithm's complexity.

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Computation of normalized homology

- Computing the simplicial cohomology $\mathrm{H}^n(X, \mathbb{C})$ for $0 \leq n < K$ in the truncation $X^{(K)}$ is equivalent to determining $\ker {}^cH_{DD}{}^{(K)}$, where

$$ {}^cH_{DD}{}^{(K)} = \sum_{0 \leq n \leq K} ({}^cH_{DDn} - \delta_{Kn} {}^cQ_{DK+1} {}^cQ_{DK+1}{}^+) $$

see nsl. (The subtracted term for $n = K$ is due to the the operators ${}^cQ_{DK+1}$, ${}^cQ_{DK+1}{}^+$ being excluded by the truncation.)

- The determination of $\ker {}^cH_{DD}{}^{(K)}$ proceeds by the quantum phase estimation methods (D. S. Abrams and S. Lloyd (1999)).

- This involves the unitary operators $\exp(i\tau {}^cH_{DD}{}^{(K)})$ for varying τ constructed via a Hamiltonian simulation algorithm (R. P. Feynman (1982)). The algorithm's complexity depends inversely on the sparsity of the Hamiltonian (S. Lloyd (1996); D. Aharonov and A. Ta-Shma (2003); D. W. Berry *et al.* (2014)). So, one uses $\exp(i\tau {}^cB^{(K)})$, with ${}^cB^{(K)}$ a Hermitian operator sparser than ${}^cH_{DD}{}^{(K)}$ such that $\ker {}^cB^{(K)} = \ker {}^cH_{DD}{}^{(K)}$.

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- In the quantum phase estimation algorithm, one adjoins next to the 'vector' register ${}^{c}\mathscr{H}^{(K)}$ a large b_t–bit 'clock' register $\mathbb{C}^{2\otimes b_t}$, so that the total Hilbert space is $\mathbb{C}^{2\otimes b_t} \otimes {}^{c}\mathscr{H}^{(K)}$. States are described as density operators.
- The quantum computer is initialized in the mixed state

$$ {}^{tc}\rho_{0n} = |0\rangle_{t\,t}\langle 0| \otimes {}^{c}\rho_{0n}. $$

where ${}^{c}\rho_{0n}$ is the uniform mixture of all non degenerate n–simplex states,

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- The algorithm evolves unitarily the state ${}^{tc}\rho_{0n}$ in an entangled state of the clock and vector registers.
- A measurement of the clock register is carried out. The clock value 0 is found with probability $\dim\ker{}^{c}H_{DDKn}/|{}^{c}X_{n}|$.
- Upon iteration of the algorithm, the clock value 0 is eventually found. The computer is then in the mixed state

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- By the isomorphism $\ker {}^cH_{DDn} \simeq \mathrm{H}_{Dn}({}^c\mathscr{H})$, the final state of the quantum computer encodes the homology space $\mathrm{H}_{Dn}({}^c\mathscr{H})$. Further, the frequency with which the clock value 0 occurs furnishes directly the Betti numbers $\beta_n(X, \mathbb{C}) = \dim\ker {}^cH_{DDKn}$.
- The value of b_t depends on number of bits and the precision desired for the estimation of the eigenvalues of ${}^cB_D{}^{(K)}$. The algorithm involves the use of b_t–bit Welsh–Hadamard and quantum Fourier transforms with combined complexity $O({b_t}^2)$ and one call of an oracular unitary operator U_{DKj} computing $\exp(i2^j\,{}^cB_D{}^{(K)})$ for each j with $0 \leq j \leq b_t - 1$. The complexity of the U_{DKj} depend on the Hamiltonian simulation algorithm employed.

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Conclusions

- Our conclusions are just a wish–to–do item list.
- Understand better the defect structure of the quantum simplicial set–up.
- Refine the notion of simplicial quantum circuits. Find simplicial quantum circuits implementing truly quantum simplicial algorithms.
- Improve the complexity analysis of simplicial quantum algorithms.
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