Quantum LMSR: Accelerating String Rotation

Mark Boady & Gary Pham
College of Computing & Informatics
Drexel University

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Research Motivation

- Many benzenoid hydrocarbons admit multiple boundary-edge codes under different rotations of their outer face.
- These codes depend on the chosen start vertex (commonly the lowest-left) and the traversal direction.
- A single canonical code per isomorphism class enables fast equality checks and compact chemical indexing.

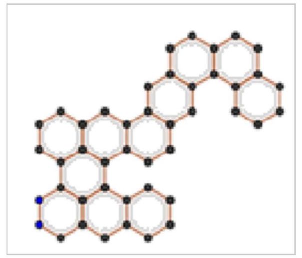

Fig 1: Original Compound

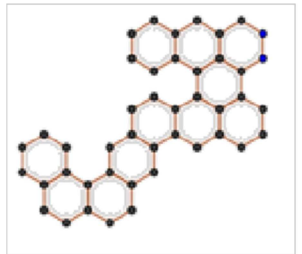

Fig 2: Rotated Compound

Classical Approach

- Traverse the outer face of the molecular graph, recording turn-and-edge types into a sequence.
- Generate all cyclic shifts of this boundary-edge code (string rotations) to capture every possible "view".
- Use a minimal-rotation algorithm (e.g., Booth's or Duval's) to pick the lexicographically smallest string rotation (LMSR).

Computational Problem

- Given a boundary-edge code of length n, find its minimal cyclic rotation (the canonical form).
- Best classical complexity: $O(n)$ or $O(n \log n)$ for minimal-rotation string algorithms.
- Quantum proposal: employ QRAM to load all rotations in superposition and use Grover-style search over indices for a potential speed-up.

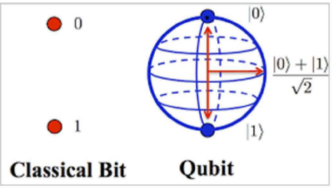

Fig 3: Bit vs Qubit

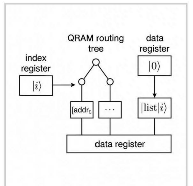

Fig 4: QRAM

Quantum Lists & Superposed Indexing

- **What is a Quantum List?**
  - A mapping between an `index` and a `data` register via QRAM:
  - $\sum_i a_i|i\rangle \otimes |0\rangle \xrightarrow{\text{QRAM}} \sum_i a_i|i\rangle \otimes |\text{list}[i]\rangle$
  - Effectively loads all list entries into superposition at once
- **Key Properties:**
  - *Read-only*: preserves no-cloning (query without destructive overwrite)
  - *Parallel lookup*: one QRAM query accesses every element weighted by its amplitude
  - *Unitary & reversible*: routing and fan-out built entirely from reversible gates
- **Our Proposal:** superpose the index register itself to enable end-to-end quantum parallelism

Quantum Approach

- Use Grover's search to locate minimal rotation index with $O(\sqrt{n})$ queries.
- Encode rotation cost function as quantum oracle:

$$O_f : |i\rangle|0\rangle \to |i\rangle(-1)^{f(i)}|0\rangle.$$

- Amplitude amplification finds marked index faster than classical scan.
- **Key Components:**
  - Phase oracle: Marks minimal rotation indices
  - Diffusion operator: Inverts amplitudes about mean
  - Superposition enables parallel evaluation
  - Quantum parallelism: $O(n) \to O(\sqrt{n})$

Algorithm Steps

- Initialize a loop over rotation indices
- Within each iteration:
  - Step 1: Find the current minimum via the marked-state oracle (Dür & Høyer)
  - Step 2: Prepare the oracle, diffusion operator, and `inc_modM` gate (M = list length)
  - Step 3: Execute Grover search for k iterations
  - Step 4: Measure the quantum register
  - Step 5: Check stopping criteria; if not met, continue
- After exiting the loop, retrieve the minimal-rotation index, undo any modular increments, and return it

Visualization & Results

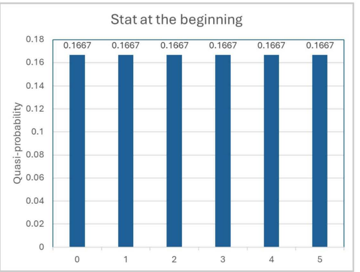

Fig 5: Initial state with uniform superposition

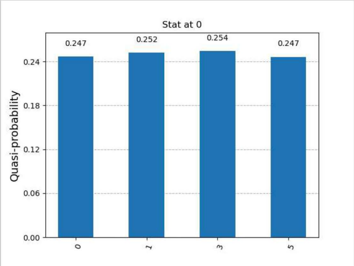

Fig 6: First iteration result

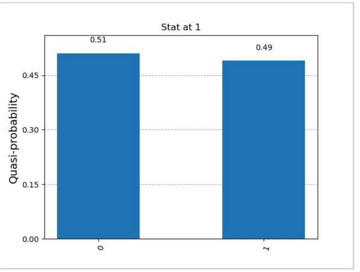

Fig 7: Second iteration result

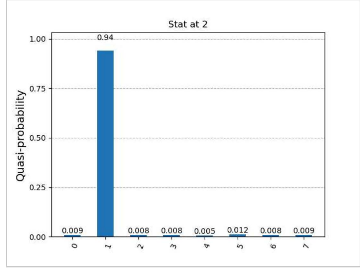

Fig 8: Last iteration result & measurement outcome

Circuit Structure

- Apply Hadamard gates to all index qubits to create superposition
- Perform $\lfloor(\pi/4)\cdot\sqrt{N/M}\rfloor$ Grover iterations per loop:
  - Oracle marks the current minimum rotation index
  - Diffusion operator amplifies marked amplitude
  - `inc_modM` gate increments indices modulo M
- Measure the index register each iteration and check stopping criteria
- Once done, uncompute any modular increments and output the minimal-rotation index

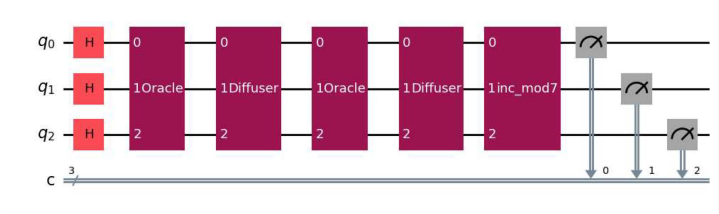

Fig 9: Grover's Algorithm Circuit

Complexity & Resource Analysis

Comparator	Average	Worst	Qubit Usage
Booth's Algorithm	$\Theta(n)$	$\Theta(n)$	n classical bits
Proposed (no QRAM)	$\Theta(n)$	$\Theta(n^2)$	$\Theta(\log n)$
Published LMSR	$\Theta(n^{3/4})$	$\Theta(\sqrt{n}\log n)$	$\Theta((\log n)^2)$
Proposed + QRAM (binary search)	$\Theta(\sqrt{n}\log n)$	$\Theta(\sqrt{n}\log n)$	$n + \Theta(\log n)$
Proposed + QRAM (hashing)	$\Theta(\sqrt{n})$	$\Theta(\sqrt{n}\log n)$	$n + \Theta(\log n)$

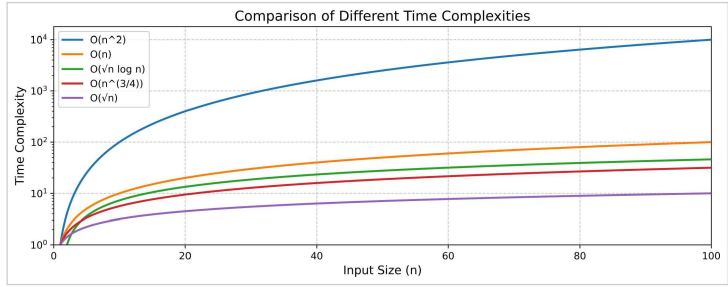

Fig 10: Performance Scaling Analysis

Key Takeaways

- **Rotation as a Unifier:** Across strings, molecules, and quantum data, rotations preserve core structure while offering new "views" for canonicalization.
- **Quantum Enhancement:** QRAM + superposed indexing unlocks massive parallelism, enabling rotation-based searches on quantum hardware.
- **Benzenoid Canonicalization:** Lexicographically minimal rotations of boundary-edge codes yield unique, compact molecular identifiers for chemical databases.

Conclusion

- **Impact & Applications:** Chemical Informatics, Pattern Matching, Foundation for broader quantum data structures.
- **Future Work:** 3D & Dihedral Symmetries, Robust QRAM Architectures, Integration with Quantum Circuits
- **Architecture:** QRAM enables parallel string rotation access with $O(\sqrt{n})$ speedup.