# Linear Combination of Unitaries Decomposition for the Laplace Operator

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## OBJECTIVES

- Construct explicit Linear Combination of Unitaries (LCU) decompositions for the Laplace operator with a variety of boundary conditions
- Provide resource estimates for decompositions
- Investigate performance within the Variational Quantum Linear Solver (VQLS) algorithm and compare results with prior works

## BACKGROUND

### Motivation

- Partial differential equations (PDEs) are central in the physical sciences. Numerical solutions are often highly expensive. E.g. pressure Poisson equations arising in computational fluid dynamics.
- Quantum computing may lead to PDE solvers with exponential improvements over classical algorithms. It is not yet clear which, if any, equations are amenable to quantum methods.
- The Laplace operator is the prototypical elliptic operator and appears in numerous PDEs (Poisson problems, heat equation, wave equation, etc). It provides an ideal test bed for quantum algorithm development.

### LCU Decompositions

- An LCU decomposition for a matrix $A$:
  $A = \sum_{l=1}^{L} c_l A_l$ for $c_l \in \mathbb{C}$ and $A_l$ unitary
- Required in many near-term and fault-tolerant algorithms. E.g. VQLS and LCU based Block Encoding
- Naïve strategies such as Pauli Decomposition often destroy quantum advantage.
- Case-by-case approaches can exploit underlying structure and reduce costs.

### Mathematical Formulation

- We consider Poisson problems with Dirichlet, Neumann, Periodic, or separable mixed BCs.

$$\begin{cases} \Delta u = f & \text{in} \quad \Omega = (0,1)^d \\ \gamma_i \partial_{x_i} u + \beta_i u = a_i(x) & \text{on} \quad \partial\Omega \cap \{x \in R^d \mid x_i = 0,1\} \end{cases}$$

- $\gamma_i = 0$ and $\beta_i = 1$ gives a Dirichlet BC, $\gamma_i = 1$ and $\beta_i = 0$ Neumann, $\gamma_i = 1$ and $\beta_i \neq 0$ Robin. Periodic BCs can also be imposed on $x_i = 0,1$.in the usual way.
- Discrete operators for $d > 1$ can be obtained as a tensor product of $1d$ operators in our setting.
- We use second-order accurate finite difference schemes for Dirichlet, Periodic, and Robin-Neumann problems.

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- Our $1d$ problems take the form
  $L_{n,\alpha_i} U = F + B_{n,i}$
- $i = 1,2,3$ denote Dirichlet, Periodic, and Robin-Neumann, respectively
- $U, F$ are the discretized unknown and forcing function. $B_{n,i}$ is a boundary correction term.

- For $d > 1$, let $\mathbf{n} = (n_1, \dots, n_d)$ and $\alpha = (\alpha_1, \dots, \alpha_d)$. These indicate desired grid size and BC for each spatial direction.
- We can apply $L_{n_i,\alpha_i}$ in the $i^{th}$ dimension, simultaneously for each $i$, with the formula below.
- Analogous unknown, forcing, and boundary corrections terms can be constructed.

$$L^d_{\mathbf{n},\alpha} = \sum_{i=1}^{d} I^{\otimes n_d} \otimes I^{\otimes n_{d-1}} \otimes \cdots \otimes I^{\otimes n_{i+1}} \otimes L_{n_i,\alpha_i} \otimes I^{\otimes n_{i-1}} \otimes \cdots \otimes I^{\otimes n_1}$$

## OUR LCU APPROACH

### Useful Matrices

- $I, X, Z$ → Identity, NOT, and Pauli Z gates
- $X_j$ → $X$ applied to $(j\text{-}1)^{th}$ qubit
- $S_n, S_n^\dagger$ → Increment/Decrement gates
- $CNOT(\mathrm{c}, t)$ → Controlled NOT gate
- $C_{n-1}(Z)$ → Multi-control $Z$ gate
- $\tau_0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ $\tau_1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ $\tau_2 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ $\tau_3 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$ → Non-unitary "tau" matrices

### Basic Relations

- $h_2^2 L_{n,2} = -2I^{\otimes n} + S_n + S_n^\dagger$
- $h_1^2 L_{n,1} = h_2^2 L_{n,2} - \tau_1^{\otimes n} - \tau_2^{\otimes n}$
- $h_3^2 L_{n,3} = h_1^2 L_{n,1} + 2\beta(0) h_3 \tau_0^{\otimes n} - 2\beta(1) h_3 \tau_3^{\otimes n} + X^{\otimes n} \cdot \left(\tau_1^{\otimes n} + \tau_2^{n}\right) \cdot X_n$

### LCU Derivations

- Issue: Tau matrices allow simple and intuitive matrix decompositions for many BCs, but they are not unitary!
- Idea: Find LCU decompositions for tau matrices and combine with the basic relations to obtain final LCUs.
- **Example** (1d Dirichlet Case) The decomposition
  $\tau_1^{\otimes n} + \tau_2^{\otimes n} = \frac{1}{2} X^{\otimes n} - \frac{1}{2} X_1 \cdot B \cdot X_1 \cdot \left(I \otimes C_{n-1}(Z)\right) \cdot B \cdot X_1,$
  where $B = \prod_{t=1}^{n-1} CNOT(0,t),$ is used to give

$$h_1^2 L_{n,1} = h_2^2 L_{n,2} - \frac{1}{2} X^{\otimes n} + \frac{1}{2} X_1 \cdot B \cdot X_1 \cdot \left(I \otimes C_{n-1}(Z)\right) \cdot B \cdot X_1$$

- 1d Robin-Neumann conditions can be treated similarly. Higher-dimensional decompositions are obtained via tensor-products.

## RESULTS

**Summary of LCU decompositions and associated resource requirements**

| | 1d Dirichlet | 1d Robin-Neumann | d-Dimensional Mixed |
|---|---|---|---|
| No. of qubits | $n$ | $n$ | $\sum_{i=1}^{d} n_i$ |
| No. of terms in LCU | 5 | 10 | $10d$ |
| No. of ancilla | 1 | 1 | 0 |
| Gate Cost | $O(n)$ | $O(n)$ | $O(n_m)$ |
| Depth | $O(n)$ | $O(n)$ | $O(n_m)$ |

Worst case gate costs and circuit depths are reported and $n_m = \max\{n_1, \dots, n_d\}$

- The number of LCU terms is independent of spatial discretization in all cases.
- The gate cost, circuit depth, and ancilla requirements depend on increment and Toffoli gate implementation.
- Other approaches can be more efficient in some cases. For example, circuit depth can be reduced if more ancilla are introduced.

### Comparison to Previous Works

- Our $1d$ Dirichlet decomposition ties prior works in number of LCU terms required.
- Under the assumption of a single ancilla qubit and circuit implementations as above, our method enjoys a quadratic reduction in resource requirements in VQLS applications.

### Extensions

- We provide a strategy to treat problems with first-order derivative terms and polynomial coefficients:

$$\frac{d^2}{dx^2} u + p(x) \frac{d}{dx} u = f$$

- For $n$ qubits and $\deg(p) = k < n/2$, there is an associated LCU with $O(n^k)$ terms.
- Future research directions: Treat complex geometries, time dependent problems, and numerical experiments.

## References

Hogancamp, Thomas, Reuben Demirdjian, and Daniel Gunlycke. "Linear-combination-of-unitaries Decomposition for the Laplace Operator." *Physical Review A*, vol. 114, no. 1, 2026, article 012455. American Physical Society. doi:10.1103/vdnz-1lsn