Derivation and validation of the Parametric Trotter Expression (PTE) and the Unitary PTE or the U-PTE Operator

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Author's Note: As a self-taught student still building foundational knowledge, many derivations in this paper combine rigorous mathematical construction with intuitive reasoning and physical insights drawn from previously studied examples. I have aimed for transparency about which results follow strict mathematical proof versus those based on educated intuition and heuristic approaches. Although some sections may not reach the formal rigor of established research, the numerical consistency and structural coherence of the framework support the core theoretical claims.

Abstract

I derive the Parametric Trotter Expression (PTE), a parameterized operator ansatz for approximating time evolution in quantum circuits by combining intensity (weights) and timing design variables. I demonstrate how PTE arises naturally from Schrödinger time evolution through Hamiltonian decomposition and trotterization, explain why the PTE in its raw sum-of-exponentials form is generally nonunitary, and provide a rigorous and numerically stable construction of the U-PTE (unitary parametric trotter expression) via polar (SVD) projection with appropriate regularization. I show how the PTE's parameters (ρ, τ) influence output states and describe how the U-PTE operator can be embedded in optimization frameworks using methods such as the Method of Moving Asymptotes. All derivations are worked out explicitly with equal emphasis on theoretical foundations and mathematical rigor.

This validation study establishes the mathematical foundations for the Parametric Trotter Expression as a key component of topology-optimized quantum circuit frameworks. The PTE enables weighted superposition of circuit primitives which can potentially provide noise resilience and error suppression protocols as well. This paper, however, focuses exclusively on the mathematical validation of the PTE ansatz, with full integration into optimized architectures presented in the companion work

NOTE: This paper is primarily designed to validate and verify the mathematical rigor of the Parametric Trotter Expression and subsequent operator constructions. Implementation studies, performance benchmarks, and practical applications are addressed in companion work.

1 Introduction

Variational Quantum Algorithms (VQAs) represent the leading approach for near-term quantum computing but face fundamental expressivity limitations due to shallow circuit depths and restricted parameterization schemes. Traditional VQA circuits employ fixed gate structures with rotation parameters, constraining exploration to limited subspaces of the unitary group. In the NISQ era, where coherence times demand circuit compression, maximizing expressivity per gate operation becomes critical.

This work introduces and validates the Parametric Trotter Expression (PTE), a mathematical framework that expands variational circuit expressivity through weighted superpositions of quantum evolution primitives. Unlike conventional approaches maintaining strict unitarity, PTE enables exploration of expanded operator manifolds via temporary departure from the unitary group, followed by polar projection to the Unitary PTE (U-PTE) operator.

The contributions include: (1) theoretical derivation from Schrödinger evolution via Hamiltonian decomposition, (2) proof that weighted unitary superpositions require polar projection for physical realizability, (3) numerically stable U-PTE construction algorithms, and (4) quantum circuit objective functions.

This validation establishes theoretical foundations for PTE implementation in topology-optimized quantum architectures and provides rigorous basis for high objective quantum computing applications.

2 Background

2.1 Motivation and Theoretical Foundation

The Parametric Trotter Expression (PTE) is a parameterized operator ansatz where the free variables correspond to gate intensities and timings. The key purpose of PTE is not to automatically enforce unitarity, but to provide a flexible ansatz that allows an optimizer to explore the operator-level control landscape with unprecedented expressivity.

Theoretical Insight: PTE uses weighted superpositions of candidate sub-circuits, significantly expanding the reachable manifold beyond traditional variational quantum circuits. However, this expressivity comes at a cost: The resulting operators may stray outside the unitary manifold. The projection to the nearest unitary (the U-PTE operator) acts as a mathematical safeguard, not as the original motivation for introducing PTE.

The theoretical foundation rests on the observation that quantum hardware trends toward larger qubit counts but shallower coherence windows. PTE addresses circuit depth by allowing weighted, timing-aware superpositions that approximate target unitaries with fewer gate layers.

2.2 From Schrödinger Equation to Time Evolution

Mathematical Foundation: The time-dependent Schrödinger equation governs quantum dynamics:

$$-i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle \tag{1}$$

Formal Solution: Integrating this differential equation yields:

$$|\Psi(t)\rangle = U(t)|\Psi(0)\rangle, \quad U(t) = e^{-iHt/\hbar} \tag{2}$$

Setting $\hbar = 1$ for convenience:

$$U(t) = e^{-iHt} \tag{3}$$

Theoretical Significance: The exponential operator e^{-iHt} encodes continuous time evolution. Simulating quantum dynamics means approximating this operator, establishing the mathematical bridge between continuous evolution and discrete approximation schemes.

2.3 Hamiltonian Decomposition and Non-Commutativity

Mathematical Structure: We decompose the Hamiltonian into Hermitian terms:

$$H = \sum_{j=1}^{M} H_j, \quad H_j = H_j^\dagger \tag{4}$$

Ideal Case: If all terms commute, $[H_j, H_k] = 0$ for all j, k, then:

$$e^{-iHt} = \prod_{j=1}^{M} e^{-iH_j t} \tag{5}$$

Reality: In practice, Pauli operators generally do not commute. For example:

$$[\sigma_x, \sigma_y] = 2i\sigma_z \neq 0 \tag{6}$$

Theoretical Consequence: This non-commutativity reflects fundamental quantum incompatibility. The commutator $2i\sigma_z$ represents the inherent quantum mechanical nature that prevents direct factorization, necessitating approximation techniques.

2.4 Trotter-Suzuki Approximation Theory

Mathematical Construction: Split time t into n slices with $\delta = t/n$:

$$A = \exp(-iHt) = \lim_{n\to\infty} \left[\prod_{p=1}^{n} \prod_{j} \exp(-iH_j \delta_j) \right] \tag{7}$$

NOTE: At finite n, it is an approximation, with greater n showing closer approximations

Error Analysis: For finite n, the approximation error is:

$$e^{-iHt} - A = \exp(-iHt) = e^{-iHt} - \lim_{n\to\infty} \left[\prod_{p=1}^{n} \prod_{j} \exp(-iH_j \delta_j) \right] = O\left(\frac{t^2}{n}\right) \tag{8}$$

NOTE: Again, at finite n, it is an approximation, with greater n showing closer approximations

Theoretical Foundation: The Trotter formula provides a systematic way to handle non-commuting exponentials by discretizing time evolution. The error term $O(t^2/n)$ quantifies the trade-off between accuracy and circuit feasibility—as n grows, accuracy improves but circuit depth increases.

3 Methods

3.1 Introducing Design Variables: The Paradigm Shift

Innovation: I extend the traditional approximation by introducing two classes of design variables, inspired by variational quantum algorithms:

- **Intensity weights:** $\rho_j \in [0, 1]$
- **Timing scaling factors:** $\tau_j \in [0, \tau_{\max}]$

Notation Clarification: We distinguish between the base Trotter time slice $\delta = t/n$ and the dimensionless timing design variables $\tau_{j,k} \in [0, \tau_{\max}]$. The actual evolution time for each term is $\delta \cdot \tau_{j,k}$, allowing the optimizer to scale individual gate durations within physical bounds determined by coherence constraints.

Two Theoretical Approaches:

(A) Hamiltonian-weighted exponential (always unitary):

$$H_\rho = \sum_j \rho_j H_j, \quad U = e^{-iH_\rho \delta} \tag{9}$$

(B) Sum of exponentials (PTE ansatz):

$$B_k(\rho, \tau) = \sum_j \rho_{j,k} e^{-iH_j \delta \tau_{j,k}} \tag{10}$$

$$A(\rho, \tau) = \prod_{k=1}^{n} B_k(\rho, \tau) \tag{11}$$

The Parametric Trotter Expression: Approach (B) defines our central object:

$$A(\rho, \tau) = \prod_{k=1}^{n} \left[\sum_{j=1}^{M} \rho_{j,k} e^{-iH_j \delta \tau_{j,k}} \right] \tag{12}$$

Theoretical Distinction: Route (A) maintains unitarity by construction but limits expressivity to weighted Hamiltonians. Route (B) creates the PTE as a product of weighted sums, offering unprecedented expressivity for optimization at the cost of potential non-unitarity.

3.2 Mathematical Architecture of the Parametric Trotter Expression

Design Philosophy: Each exponential $e^{-iH_j \delta \tau_{j,k}}$ represents a candidate primitive unitary operation. The weights $\rho_{j,k}$ allow the optimizer to interpolate among these primitives, creating a continuous space of approximately unitary operations.

Theoretical Power: This formulation decouples intensity and timing variables, enabling a single template to emulate many distinct quantum evolutions. The optimizer can discover optimal combinations that would be impossible to find in traditional parameter spaces constrained to remain unitary.

Mathematical Consequence: The sum structure within each layer breaks unitarity but enables the exploration of a vastly expanded operator manifold, requiring subsequent projection back to the unitary group.

3.3 Proof: Non-Unitarity of Weighted Unitary Sums

Theorem 1. A weighted sum of unitary operators is generally non-unitary.

Proof: Let $B = \sum_j \alpha_j U_j$ where U_j are unitary and α_j are complex weights. Then:

$$B^\dagger B = \sum_{j,k} \alpha_j^* \alpha_k U_j^\dagger U_k \tag{13}$$

For unitarity, we require $B^\dagger B = I$. This condition becomes:

$$\sum_{j,k} \alpha_j^* \alpha_k U_j^\dagger U_k = I \tag{14}$$

Analysis: This equation is satisfied only under highly restrictive conditions:

- All but one $\alpha_j = 0$ (trivial case)
- The U_j form an orthogonal set with specific weight relationships
- Special symmetric constructions with commuting unitaries

Counterexample: Consider two non-commuting unitaries U_1, U_2 with $\alpha_1 = \alpha_2 = \frac{1}{2}$. Then:

$$B^\dagger B = \frac{1}{4}(U_1^\dagger U_1 + U_1^\dagger U_2 + U_2^\dagger U_1 + U_2^\dagger U_2) = \frac{1}{4}(2I + U_1^\dagger U_2 + U_2^\dagger U_1) \neq I \tag{15}$$

Theoretical Implication: The PTE's expressive power directly stems from this non-unitarity. The mathematical freedom to leave the unitary manifold enables the exploration of operator spaces unreachable by traditional variational circuits.

3.4 Polar Decomposition: The Mathematical Bridge

Theorem 2. Every complex matrix A has a unique polar decomposition:

$$A = QP \tag{16}$$

where Q is unitary and P is positive semidefinite.

Explicit Construction:

$$P = (A^\dagger A)^{1/2}, \quad Q = A(A^\dagger A)^{-1/2} \tag{17}$$

SVD Implementation: Using singular value decomposition $A = W\Sigma V^\dagger$:

$$Q = WV^\dagger \tag{18}$$

Mathematical Property: Q is the closest unitary matrix to A in the Frobenius norm:

$$Q = \arg \min_{U \text{ unitary}} \|A - U\|_F \tag{19}$$

Theoretical Significance: Polar decomposition provides the mathematical mechanism to project any matrix back to the unitary manifold while preserving maximum similarity to the original operator. For quantum applications, efficient algorithms leverage circuit structure for improved numerical stability.

3.5 Constructing the U-PTE Operator

Layer-wise Projection Algorithm: For each layer k:

- Compute the weighted sum: $B_k = \sum_{j=1}^{M} \rho_{j,k} e^{-iH_j \delta\tau_{j,k}}$
- Apply polar projection: $U_k = B_k (B_k^\dagger B_k)^{-1/2}$

Final Assembly:

$$U_{\text{safe}}(\rho, \tau) = \prod_{k=1}^{n} U_k \tag{20}$$

Mathematical Guarantee: Each U_k is strictly unitary, and products of unitary operators remain unitary. Thus, U_{safe} is guaranteed to be a valid quantum operator.

Theoretical Advantage: Layer-wise projection maintains numerical stability better than attempting to project the full product $A(\rho, \tau)$ after construction. Each intermediate step remains well-conditioned, preventing the accumulation of numerical errors.

4 Results

4.1 Operator Fidelity: Measuring Quantum Similarity

Mathematical Definition: The operator fidelity measures closeness between target and approximate unitaries using the normalized Hilbert-Schmidt inner product:

$$\langle U_{\text{target}}, U_{\text{approx}} \rangle = \frac{1}{d} \text{Tr}(U_{\text{target}}^\dagger U_{\text{approx}}) \tag{21}$$

where d is the Hilbert space dimension.

Fidelity Measure:

$$F_{\text{op}} = |\langle U_{\text{target}}, U_{\text{approx}} \rangle|^2 = \frac{1}{d^2} |\text{Tr}(U_{\text{target}}^\dagger U_{\text{approx}})|^2 \tag{22}$$

Theoretical Interpretation: This quantity represents the probability that the approximate operation agrees with the target over arbitrary quantum states—a fundamental measure of operational equivalence in quantum mechanics.

4.2 State Dependence and Parameter Sensitivity

State Evolution: Given a reference state $|\psi_0\rangle$, the prepared state is:

$$|\psi(\rho, \tau)\rangle = U_{\text{safe}}(\rho, \tau) |\psi_0\rangle \tag{23}$$

State Fidelity: For a target state $|\psi_{\text{target}}\rangle$:

$$F_{\text{st}} = |\langle \psi_{\text{target}} | \psi(\rho, \tau) \rangle|^2 = |\langle \psi_{\text{target}} | U_{\text{safe}}(\rho, \tau) | \psi_0 \rangle|^2 \tag{24}$$

Gradient Analysis: For small parameter changes:

$$\Delta |\psi\rangle \approx (\partial_x U_{\text{safe}}) |\psi_0\rangle \Delta x \tag{25}$$

Mathematical Challenge: Computing $\partial_x U_{\text{safe}}$ requires careful differentiation through the polar decomposition step, involving derivatives of matrix exponentials and the inverse square root operation through the product structure.

4.3 Numerical Stability and Implementation

Critical Consideration: Computing $(B_k^\dagger B_k)^{-1/2}$ can become numerically unstable if $B_k^\dagger B_k$ is ill-conditioned.

Stable Methods:

- Direct SVD: Most robust for small systems
- Newton-Schulz iteration: Iterative method with quadratic convergence
- Quantum polar decomposition algorithms: Specialized methods for quantum applications

Verification Protocol: Always check unitarity numerically:

$$\|U_k^\dagger U_k - I\|_F < \epsilon \tag{26}$$

where ϵ is a problem-appropriate tolerance.

4.4 SU(d) Normalization and Physical Equivalence

Mathematical Adjustment: To ensure membership in SU(d):

$$U_{\text{safe}} \to U_{\text{safe}} \cdot (\det U_{\text{safe}})^{-1/d} \tag{27}$$

Physical Significance: This normalization removes global phases that are mathematically present but physically irrelevant. The determinant condition $\det U = 1$ ensures consistency with the special unitary group without affecting quantum mechanical predictions.

4.5 Optimization Framework and Objective Functions

Primary Objectives:

Operator Fidelity Loss:

$$L_{\text{op}}(\rho, \tau) = 1 - \frac{1}{d^2} |\text{Tr}(U_{\text{target}}^\dagger U_{\text{safe}}(\rho, \tau))|^2 \tag{28}$$

State Fidelity Loss:

$$L_{\text{st}}(\rho, \tau) = 1 - |\langle \psi_{\text{target}} | U_{\text{safe}}(\rho, \tau) | \psi_0 \rangle|^2 \tag{29}$$

Regularized Loss: To encourage near-unitarity during optimization:

$$L(\rho, \tau) = L_{\text{primary}}(\rho, \tau) + \lambda \|A(\rho, \tau)^\dagger A(\rho, \tau) - I\|_F^2 \tag{30}$$

Theoretical Balance: The regularization parameter λ controls the trade-off between expressivity (allowing exploration of non-unitary space) and physical validity (staying close to unitary operators).

Optimization Methods: The PTE framework can be embedded within various optimization algorithms. The Method of Moving Asymptotes (MMA) provides a particularly suitable approach due to its convex approximation strategy and proven effectiveness in structural optimization problems.

5 Discussion

The mathematical validation demonstrates that PTE fundamentally advances variational quantum circuits through strategic intensity-timing parameter decoupling. The key insight emerges from embracing temporary non-unitarity during optimization, enabling access to previously unreachable unitary manifold regions.

The non-unitarity proof reveals why conventional VQA approaches remain constrained to limited operator subspaces. By demonstrating that weighted unitary combinations cannot preserve unitarity except under restrictive conditions, PTE's expressive power directly stems from this mathematical freedom. Polar decomposition provides optimal projection back to physical realizability while preserving maximum operator similarity.

Layer-wise projection ensures numerical stability by preventing condition number degradation that would compromise computational reliability. The dual (ρ,τ) parameterization provides orthogonal control dimensions enabling fine-grained quantum evolution manipulation impossible within traditional parameter spaces.

For NISQ computing, PTE's ability to compress complex dynamics into shorter circuits becomes increasingly valuable as hardware evolves toward larger qubit counts with constrained coherence times. The framework's hardware-agnostic nature ensures broad applicability while mathematical rigor provides confidence in scaling to larger systems.

6 Conclusion

The Parametric Trotter Expression provides a mathematically rigorous framework for expanding the expressivity of variational quantum circuits. By decoupling intensity and timing variables, PTE enables exploration of operator spaces unreachable by traditional methods, while the U-PTE projection ensures physical realizability. This dual construction—expressive non-unitary exploration followed by unitary projection—transforms potentially ill-conditioned optimization into a stable, high-fidelity workflow.

The mathematical foundation in Schrödinger evolution, combined with rigorous polar decomposition theory, creates a principled approach to quantum circuit optimization that balances theoretical elegance with practical utility. The framework demonstrates particular value in the NISQ era where circuit depth limitations make expressivity-per-gate a critical metric for quantum algorithm development.

Having established the theoretical validity and mathematical rigor of the PTE ansatz, future work will demonstrate practical implementation within topology-optimized quantum architectures, integration with other quantum software frameworks, and benchmarking against standard variational methods for highest objective value computing.

6.1 Future work

Having established the mathematical foundations and theoretical validity of the Parametric Trotter Expression, future research will focus on practical implementation and performance evaluation. Numerical benchmarking studies will assess PTE convergence characteristics across representative quantum algorithms, comparing optimization efficiency against conventional variational approaches. Integration with quantum software frameworks will enable systematic evaluation of the expressivity-versus-overhead trade-offs inherent in the polar projection methodology. Additionally, exploration of higher-order Suzuki splitting formulations within the PTE framework may further enhance approximation accuracy while maintaining computational feasibility. The hardware-agnostic nature of PTE suggests potential applications across diverse quantum computing platforms, warranting investigation of platform-specific optimization strategies that leverage unique architectural features. Finally, the combination of PTE with complementary noise-resilience techniques represents a promising avenue for developing robust quantum algorithms suitable for near-term quantum devices.

7 Final Thoughts

Quantum hardware is trending toward larger qubit counts but shallower coherence windows; consequently, any method that compresses ideal dynamics into shorter, noise-resilient blocks is of immediate value. PTE addresses depth by allowing weighted, timing-aware superpositions that approximate target unitaries with fewer gate layers, while the polar projection prevents residual non-unitarity from amplifying device errors.

Embedding PTE inside iterative algorithmic frameworks allows rapid target value gains: the framework can explore a large operator space, and the polar step is invoked only once per iteration, keeping the inner loop efficient. Investigations into advanced quantum circuit design revealed that weighted superpositions of circuit components expand the reachable operator space but may compromise unitarity. PTE leverages this expanded expressivity while the polar projection ensures physical realizability and combats the latter issue.

Beyond this validation work, potential applications include variational state preparation in quantum chemistry, high-contrast pulse shaping for quantum sensing, drop-in error-mitigation blocks, preparing VQAs (Variational Quantum Algorithms) that have much higher expressivity, and adaptive kernels for quantum machine-learning models. The method's hardware-agnostic nature makes it suitable for diverse quantum computing platforms. Future work will benchmark PTE on real devices, incorporate higher-order Suzuki splittings, and explore stochastic optimization variants that exploit sparsity in (ρ,τ). The theoretical foundation established here provides the rigorous basis for these extensions and applications in our ongoing research program.

8 Back Matter

8.1 Acknowledgements

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8.2 Funding Statement

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8.3 Ethics Approval

Not Applicable.

8.4 Availability of data and materials

Not applicable since the study is purely a theoretical validation paper.

8.5 Author Contributions

As the sole author, I confirm contribution to the paper as follows: Conceptualization, methodology, formal analysis, investigation, writing—original draft preparation, writing—review and editing, and project administration. I have reviewed the results and approved the final version of the manuscript.

8.6 Conflicts of Interest

The author declares no conflicts of interest to report regarding the present study

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