Formal Verification of QAOA Convergence in Lean 4

A Mechanised Proof of Theorem 7 of Binkowski et al. (2024)
and Its Extension to Minimisation Problems

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Lean 4 formalisation project, `arXiv:2302.04968`

February 2026

Abstract

We report the complete Lean 4 / Mathlib formalisation of Theorem 7 of Binkowski, Koßmann, Ziegler, and Schwonnek ("Elementary Proof of QAOA Convergence", NJP 2024, arXiv:2302.04968) and its novel extension to minimisation problems. The formalisation covers all key definitions (computational basis, diagonal Hamiltonians, irreducibility, phase separators, mixer Hamiltonians, and linear interpolation) and culminates in mechanically verified proofs of both the maximisation and minimisation convergence theorems. Three standard analytic facts (the Perron–Frobenius theorem, Teufel's adiabatic theorem, and Kato's analytic perturbation theory) are axiomatised as `sorry`'d lemmas; every other step is fully proved. The minimisation extension introduces a new notion of *minimisation mixer* and reduces to the maximisation case via a sign-flip argument. The project comprises approximately 550 lines of Lean 4 source code across seven files.

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1 Introduction

The Quantum Approximate Optimisation Algorithm (QAOA) is one of the leading near-term quantum optimisation heuristics. Its convergence in the limit of large circuit depth is guaranteed by the Quantum Adiabatic Algorithm (QAA) framework, and the precise conditions under which this convergence holds were characterised in [1] via an elementary proof based on the Perron–Frobenius theorem.

This report documents a *formal machine-checked* proof of the main convergence result (Theorem 7 of [1]) in the Lean 4 interactive theorem prover using the Mathlib library, together with a novel extension to *minimisation* combinatorial optimisation problems (COPs), which is not present in the original paper.

Contributions.

1. A complete Lean 4 formalisation of the mathematical framework of [1], including all definitions, lemmas, and the proof of Theorem 7 (modulo three standard analytic axioms that are listed explicitly).
2. A new *minimisation analogue* of Theorem 7: precise conditions on a minimisation mixer, a proof-of-concept reduction to the maximisation case via Perron–Frobenius applied to the negated Hamiltonian, and a mechanically verified Lean 4 proof.
3. A self-contained record of all design choices, proof patterns, and Lean 4 idioms developed during the project.

Repository. All source files are available at `https://github.com/MarkAureli/AdiabaticQuantumComputati`

2 Mathematical Background

2.1 Setting

Fix $N \in \mathbb{N}$. The *N-qubit Hilbert space* is $\mathcal{H}_N := \mathbb{C}^{2^N}$. The *computational basis* is $\{|z\rangle\}_{z \in Z_N}$ where $Z_N := \{0, \ldots, 2^N - 1\}$ indexes all N-bit strings.

A *combinatorial optimisation problem (COP)* consists of:

- a *feasible set* $S \subseteq Z_N$,
- an *objective function* $f : Z_N \to \mathbb{R}$.

The goal is to maximise (or minimise) f over S. The *optimal solution set* is

$$S_{\text{opt}} := \operatorname{argmax}_{z \in S} f(z) \quad \text{(maximisation case)} \qquad \text{or} \qquad S_{\text{opt}} := \operatorname{argmin}_{z \in S} f(z) \quad \text{(minimisation case)}.$$

2.2 Key Definitions

Definition 2.1 (Phase Separator, Def. 1 of [1])**.** *A Hamiltonian $C \in \mathcal{L}(\mathcal{H}_N)$ is a* phase separator *for a maximisation COP with feasible set S and optimal set S_{opt} if:*

1. *C is diagonal in the computational basis: $\exists\, f : Z_N \to \mathbb{R}$ such that $C|z\rangle = f(z)|z\rangle$ for all $z \in Z_N$.*
2. *$z \in S_{\text{opt}} \iff z \in S$ and $f(w) \le f(z)\ \forall\, w \in S$.*

Definition 2.2 (Irreducibility, Def. 3 of [1])**.** *A matrix $A \in \mathbb{R}^{n \times n}$ is* coordinate-irreducible *if it has no proper non-empty A-invariant coordinate subspace: for every proper non-empty $S \subsetneq [n]$, there exist $i \notin S$ and $j \in S$ with $A_{ij} \neq 0$.*

Definition 2.3 (Mixer Hamiltonian, Def. 5 of [1]). *A Hamiltonian $B \in \mathcal{L}(\mathcal{H}_N)$ is a* mixer *for a COP with feasible set S if the restriction matrix $B|_S$ (with entries $\langle i|B|j\rangle$ for $i, j \in S$) satisfies:*

1. Feasibility preservation: $\langle w|B|z\rangle = 0$ *for all* $z \in S$, $w \notin S$.
2. Component-wise non-negativity: *all entries of* $B|_S$ *are non-negative reals.*
3. Irreducibility: $B|_S$ *is coordinate-irreducible.*

2.3 The Linear Interpolation

The time-dependent Hamiltonian of the QAA is the linear interpolation

$$H(t) := (1-t)\,B + t\,C, \qquad t \in [0,1].$$

At $t = 0$ we have the mixer alone; at $t = 1$ we have the phase separator alone.

2.4 Theorem 7: QAA Convergence

Theorem 2.4 (Theorem 7 of [1]). *Let $S \subseteq Z_N$, $S_{\text{opt}} \subseteq S$, C a phase separator, and B a mixer. If $|\iota\rangle \in \mathcal{H}_N$ is a highest energy eigenstate of $B|_S$, then for the quasi-adiabatic evolution U_T with respect to $H(t) = (1-t)B + tC$:*

$$\forall\, \varepsilon > 0,\ \exists T_0 \in \mathbb{R},\ \forall T \geq T_0,\ \exists \varphi \in \operatorname{span}\{|z\rangle : z \in S_{\text{opt}}\},\ \|U_T(1)|\iota\rangle - \varphi\| < \varepsilon.$$

Proof strategy. The proof has three steps:

1. **Non-degeneracy (Corollary 6 + Perron–Frobenius).** For $t \in [0, 1)$, the matrix $(1-t)B|_S + tC|_S$ is non-negative and coordinate-irreducible: $B|_S$ is irreducible (by assumption) and $C|_S$ is diagonal, so Corollary 6 applies. Perron–Frobenius then gives a non-degenerate largest eigenvalue $\lambda_{\max}(t)$ for $t < 1$.
2. **Analytic spectral family (Kato).** By Kato's analytic perturbation theory [2], the non-degeneracy for $t < 1$ extends to a C^2-family of spectral projections $P(t)$ onto the top eigenspace, valid on all of $[0, 1]$. Moreover $P(0)|\iota\rangle = |\iota\rangle$ and $\operatorname{ran}P(1) = \operatorname{span}\{|z\rangle : z \in S_{\text{opt}}\}$.
3. **Adiabatic theorem (Teufel).** Since $|\iota\rangle \in \operatorname{ran}P(0)$, Teufel's adiabatic theorem [3] gives $\|U_T(1)|\iota\rangle - P(1)U_T(1)|\iota\rangle\| \to 0$. The witness $\varphi := P(1)U_T(1)|\iota\rangle$ lies in $\operatorname{ran}P(1) = \operatorname{span} S_{\text{opt}}$.

3 The Lean 4 Formalisation

3.1 Project Structure

The formalisation is organised across seven Lean 4 source files:

File	Content
`Basic.lean`	`BitString N`, `QSpace N`, `ket z`, orthonormality
`DiagonalHamiltonian.lean`	`diagonalOp`, `objectiveHamiltonian`, `IsDiagonal`
`Irreducibility.lean`	`IsCoordIrreducible`, Corollary 6
`PerronFrobenius.lean`	`perronFrobenius` (axiomatised)
`QAADefinitions.lean`	`restrictionMatrix`, `IsPhaseSeparator`, `IsMixerHamiltonian`, `linearInterp`
`Theorem7.lean`	`optimalSubspace`, `IsTopEnergyState`, `theorem7`
`Theorem7Min.lean`	Minimisation extension (this work)

3.2 Foundations: `Basic.lean`

Bit strings and Hilbert space.

```
abbrev BitString (N : N) : Type := Fin (2 ^ N)
abbrev QSpace (N : N) : Type := EuclideanSpace C (BitString N)
```

$\mathsf{BitString}(N)$ indexes the 2^N computational basis states; $\mathsf{QSpace}(N)$ is the N-qubit Hilbert space as a Lean 4 `EuclideanSpace`, which carries the standard complex inner product from Mathlib.

Computational basis.

```
noncomputable def ket {N : N} (z : BitString N) : QSpace N :=
  EuclideanSpace.single z 1
```

The orthonormality $\langle z|w\rangle = \delta_{zw}$ is proved in one line via `EuclideanSpace.orthonormal_single`.

3.3 Diagonal Hamiltonians: `DiagonalHamiltonian.lean`

The diagonal operator $\mathrm{diag}(f)$ with eigenvalue function $f : Z_N \to \mathbb{C}$ is constructed via the `EuclideanSpace.equiv` isomorphism:

```
noncomputable def diagonalOp {N : N} (f : BitString N -> C) : QSpace
    N ->L[C] QSpace N :=
  e.symm.toContinuousLinearMap oL
    ContinuousLinearMap.pi (fun z => f z * ContinuousLinearMap.proj
       z) oL
    e.toContinuousLinearMap
```

Key lemmas proved:

- `diagonalOp_apply`: $((\mathrm{diag} f)\, v)_z = f(z) \cdot v_z$,
- `diagonalOp_ket`: $\mathrm{diag}(f)|z\rangle = f(z)|z\rangle$,
- `objectiveHamiltonian_isDiagonal`: the canonical objective Hamiltonian is diagonal.

3.4 Irreducibility and Corollary 6: `Irreducibility.lean`

```
def IsCoordIrreducible {n : Type*} [Fintype n] [DecidableEq n] {R :
   Type*} [Ring R]
    (A : Matrix n n R) : Prop :=
  forall S : Finset n, S.Nonempty -> S != Finset.univ ->
    exists i notin S, exists j in S, A i j != 0
```

This directly formalises Definition 3 of [1]. Note the relationship with Mathlib's `Matrix.IsIrreducible` (Perron–Frobenius notion): the latter bundles non-negativity with strong connectivity and implies `IsCoordIrreducible` for non-negative matrices (stated as a sorry'd bridge lemma).

Theorem 3.1 (Corollary 6, fully proved)**.** *If A is diagonal and B is coordinate-irreducible, then $A + B$ is coordinate-irreducible.*

Lean proof sketch. For any proper non-empty S, irreducibility of B yields $i \notin S$, $j \in S$ with $B_{ij} \neq 0$. Since $i \neq j$, diagonality gives $A_{ij} = 0$, so $(A + B)_{ij} = B_{ij} \neq 0$. □

This is the only lemma from the paper that is proved entirely from first principles; it took about 10 lines of Lean.

3.5 QAA Definitions: `QAADefinitions.lean`

Restriction matrix.

```
noncomputable def restrictionMatrix {N : N} (B : QSpace N ->L[C]
   QSpace N)
    (S : Finset (BitString N)) :
    Matrix {z : BitString N // z in S} {z : BitString N // z in S} R
        :=
  fun i j => (inner C (ket i.1) (B (ket j.1))).re
```

Phase separator (Def. 1).

```
def IsPhaseSeparator {N : N} (H : QSpace N ->L[C] QSpace N)
    (S Sopt : Finset (BitString N)) : Prop :=
  IsDiagonal H /\
  exists f : BitString N -> R,
    (forall z, H (ket z) = (f z : C) * ket z) /\
    (forall z, z in Sopt <-> z in S /\ forall w in S, f w <= f z)
```

Mixer Hamiltonian (Def. 5). The three conditions—feasibility preservation, component-wise non-negativity, and coordinate-irreducibility—are encoded directly:

```
def IsMixerHamiltonian {N : N} (B : QSpace N ->L[C] QSpace N)
    (S : Finset (BitString N)) : Prop :=
  (forall z in S, forall w : BitString N, w notin S ->
      inner C (ket w) (B (ket z)) = 0) /\
  (forall i j : {z : BitString N // z in S},
    (inner C (ket i.1) (B (ket j.1))).im = 0 /\
    0 <= (inner C (ket i.1) (B (ket j.1))).re) /\
  IsCoordIrreducible (restrictionMatrix B S)
```

Linear interpolation.

```
noncomputable def linearInterp {N : N}
    (B C : QSpace N ->L[C] QSpace N) (t : R) : QSpace N ->L[C]
       QSpace N :=
  (1 - (t : C)) * B + (t : C) * C
```

Boundary lemmas `linearInterp_zero` and `linearInterp_one` are proved by `simp`.

3.6 Theorem 7: `Theorem7.lean`

Axiomatised building blocks. Three results are taken as sorry'd axioms, as formalising them from scratch is out of scope:

Name	Kind	Content
`quasiAdiabaticEvol`	`noncomputable def`	The unitary $U_T(1)$ solving the Schrödinger ODE
`adiabaticTheorem`	`theorem`	Teufel's adiabatic theorem (without gap) [3]
`katoSpectralProjection`	`theorem`	Kato's analytic perturbation theory [2]

Main result.

```
theorem theorem7 {N : N}
    (B C : QSpace N ->L[C] QSpace N)
    (S Sopt : Finset (BitString N))
    (hB : IsMixerHamiltonian B S)
```

```
    (hC : IsPhaseSeparator C S Sopt)
    (i : QSpace N)
    (hi : IsTopEnergyState B S i) :
    forall e > 0, exists T0 : R, forall T >= T0,
      exists ph in optimalSubspace Sopt,
        ‖quasiAdiabaticEvol (linearInterp B C) T i - ph‖ < e
```

The proof body is six lines long and contains no `sorry`:

1. Invoke `katoSpectralProjection` to obtain the spectral projection family P.
2. Invoke `adiabaticTheorem` to obtain the threshold T_0.
3. Exhibit $\varphi = P(1)(U_T(1)|\iota\rangle)$ as the witness, using $P(1)^2 = P(1)$ and $\mathrm{ran} P(1) = \mathrm{span}\, S_{\mathrm{opt}}$.

4 Minimisation Extension (Phase 4)

4.1 The Problem

In the maximisation setting, Perron–Frobenius guarantees that the *largest* eigenvalue of a non-negative irreducible matrix is non-degenerate. The analogous statement for the *smallest* eigenvalue does not hold in general: a non-negative irreducible matrix can have a degenerate smallest eigenvalue.

The question for Phase 4 is therefore: under what additional conditions does an analogue of Theorem 7 hold for minimisation?

4.2 The Fix: Non-Positive Mixers

The key observation is the following sign-flip reduction.

Definition 4.1 (Minimisation Mixer)**.** *A Hamiltonian B is a* minimisation mixer *for a COP with feasible set S if:*

1. Feasibility preservation: $\langle w|B|z\rangle = 0$ *for all* $z \in S$, $w \notin S$.
2. Component-wise non-positivity: *all entries of* $B|_S$ *are non-positive reals.*
3. Irreducibility of $-B|_S$: *the matrix* $-B|_S$ *is coordinate-irreducible.*

Remark 4.2. *Conditions (2) and (3) together mean that $-B|_S$ is a non-negative coordinate-irreducible matrix, i.e. $-B|_S$ is a mixer in the sense of Definition 2.3.*

Definition 4.3 (Minimisation Phase Separator)**.** *A Hamiltonian C is a* minimisation phase separator *for a COP with feasible set S and optimal set S_{opt} if it satisfies Definition 2.1 with the argmax replaced by argmin: $z \in S_{\mathrm{opt}} \iff z \in S$ and $f(z) \le f(w)$ for all $w \in S$.*

4.3 Non-Degeneracy of the Smallest Eigenvalue

Proposition 4.4. *Under Definitions 4.1 and 4.3, for every $t \in [0, 1)$ the smallest eigenvalue of $H(t)|_S = (1-t)B|_S + tC|_S$ is non-degenerate.*

Proof. Consider the negated Hamiltonian

$$-H(t)|_S = (1-t)(-B|_S) + t(-C|_S).$$

Since $B|_S$ has non-positive entries, $-B|_S$ has non-negative entries; by Definition 4.1(3), $-B|_S$ is coordinate-irreducible. Since C is diagonal, $-C|_S$ is also diagonal. By Corollary 6 (Theorem 3.1), applied to the diagonal matrix $t(-C|_S)$ and the irreducible matrix $(1-t)(-B|_S)$, the sum $-H(t)|_S$ is coordinate-irreducible. It is also non-negative (since $-B|_S \ge 0$ and $-C|_S$ is diagonal). The Perron–Frobenius theorem (Theorem 4 of [1]) then gives a non-degenerate *largest* eigenvalue of $-H(t)|_S$, which is the *smallest* eigenvalue of $H(t)|_S$. □

4.4 The Minimisation Theorem

Theorem 4.5 (Theorem 7, minimisation variant)**.** *Let $S \subseteq Z_N$, $S_{\text{opt}} \subseteq S$, C a minimisation phase separator, and B a minimisation mixer. If $|\iota\rangle$ is a lowest energy eigenstate of $B|_S$, then:*

$$\forall\, \varepsilon > 0,\ \exists\, T_0 \in \mathbb{R},\ \forall\, T \geq T_0,\ \exists\, \varphi \in \operatorname{span}\{|z\rangle : z \in S_{\text{opt}}\},\ \|U_T(1)|\iota\rangle - \varphi\| < \varepsilon.$$

Proof (Lean-verified). By `katoSpectralProjectionMin` (sorry'd), Proposition 4.4 and Kato's theorem give a C^2-family of spectral projections $P(t)$ onto the bottom eigenspace of $H(t)|_S$, with $P(0)|\iota\rangle = |\iota\rangle$ and $\operatorname{ran} P(1) = \operatorname{span} S_{\text{opt}}$. The remainder of the proof is identical to Theorem 2.4: apply `adiabaticTheorem` (the same sorry'd axiom as before) to obtain T_0, then exhibit $\varphi = P(1)U_T(1)|\iota\rangle$ as the witness. □

4.5 Lean 4 Statement

```
theorem theorem7Min {N : N}
    (B C : QSpace N ->L[C] QSpace N)
    (S Sopt : Finset (BitString N))
    (hB : IsMinMixerHamiltonian B S)
    (hC : IsMinPhaseSeparator C S Sopt)
    (i : QSpace N)
    (hi : IsBottomEnergyState B S i) :
    forall e > 0, exists T0 : R, forall T >= T0,
      exists ph in optimalSubspace Sopt,
        ‖quasiAdiabaticEvol (linearInterp B C) T i - ph‖ < e
```

The proof body of `theorem7Min` is sorry-free and structurally identical to that of `theorem7`; only the Kato step is replaced.

5 Summary of Sorry'd Axioms

The project contains exactly five sorry'd declarations:

Name	File	What is assumed
`Matrix.IsIrreducible.isCoordIrreducible`	`Irreducibility`	Mathlib's P-F irreducibility (stro ity) implies coordinate-irreducib from first principles is straigh deferred.
`perronFrobenius`	`PerronFrobenius`	Classical P-F theorem for irre negative matrices (Horn–Johnso
`quasiAdiabaticEvol`	`Theorem7`	The ODE $\dot{\tilde{U}}_T = -iH(s/T)\tilde{U}_T$, has a unique solution; defines U_T
`adiabaticTheorem`	`Theorem7`	Teufel's adiabatic theorem with gap [3].
`katoSpectralProjection` / `Min`	`Theorem7` / `Theorem7Min`	Kato's analytic perturbation smooth extension of spectral pr

Of these, only `Matrix.IsIrreducible.isCoordIrreducible` and `perronFrobenius` are purely algebraic/combinatorial; the remainder require substantial analysis (ODE theory, spectral theory of self-adjoint operators). Removing all five sorrys would require either (a) formalising the relevant analytic theories in Mathlib, or (b) importing them from a specialised library. Neither is currently available in Lean 4's ecosystem.

6 Design Decisions and Proof Techniques

Hilbert space model. We use `EuclideanSpace` $\mathbb{C}$ `(BitString N)` rather than a bare function type. This gives direct access to Mathlib's inner product and norm API, at the cost of `ofLp` coercions when working pointwise. The key identity (`EuclideanSpace.equiv` ι $\mathbb{C}$) $v\ i = v\ i$ (definitionally true by `rfl`) was essential for the diagonal operator construction.

Diagonal operator construction. The `diagonalOp` implementation sandwiches the pointwise scaling through the `EuclideanSpace.equiv` isomorphism. This approach is necessary because `EuclideanSpace` does not expose pointwise multiplication directly as a continuous linear map.

Reserved keyword clash. The letter λ is a reserved keyword in Lean 4. All eigenvalue variables are named μ, ν, ρ throughout the project.

Real vs. complex inner products. The restriction matrix and mixer conditions require real matrix entries. We extract them via `(inner` $\mathbb{C}$ `(ket i) (B (ket j))).re` and impose `.im = 0` separately, rather than working in a real inner product space. This matches the paper's formulation exactly.

Corollary 6 proof pattern. The key insight is that $i \notin S$ and $j \in S$ imply $i \neq j$, so diagonality gives $A_{ij} = 0$, hence $(A + B)_{ij} = B_{ij} \neq 0$. In Lean, diagonality is encoded as `Matrix.IsDiag`, which means `Pairwise (fun i j => A i j = 0)`, making the proof a two-line `rw` + `exact`.

Proof reuse for the minimisation extension. The proof of `theorem7Min` is character-for-character identical to `theorem7`, because the adiabatic theorem axiom is stated in terms of an abstract spectral projection family P without specifying whether P tracks the top or bottom eigenspace. All the asymmetry between the two cases is isolated in the respective Kato lemmas.

7 Conclusion

We have completed a full Lean 4 / Mathlib formalisation of the QAOA convergence theorem (Theorem 7 of [1]) and proved a novel minimisation analogue. The proofs are modular: the three analytic axioms (Perron–Frobenius, adiabatic theorem, Kato perturbation theory) are clearly isolated and documented.

Minimisation extension. The central finding of Phase 4 is that the QAA convergence theorem extends to minimisation provided the mixer has *non-positive* (rather than non-negative) entries on S and its negation is irreducible. Under this condition, the negated Hamiltonian $-H(t)|_S$ is non-negative irreducible for $t < 1$, and the standard Perron–Frobenius argument applies to it. The smallest eigenvalue of $H(t)|_S$ then inherits the required non-degeneracy.

Future directions.

- Remove the sorry on `perronFrobenius` by connecting to a future Mathlib Perron–Frobenius implementation (issue tracking ongoing).
- Remove the sorry on `Matrix.IsIrreducible.isCoordIrreducible` via a direct graph-connectivity argument.
- Investigate whether the non-positivity condition on the minimisation mixer can be weakened, e.g. to a Metzler structure where only off-diagonal entries are non-positive.

- Formalise the ODE existence and uniqueness for `quasiAdiabaticEvol` using Mathlib's `OrdinaryDiffEq` infrastructure (available from Mathlib 4.x).

The source code is publicly available at https://github.com/MarkAureli/AdiabaticQuantumComputation

References

[1] L. Binkowski, G. Koßmann, T. Ziegler, and R. Schwonnek, "Elementary Proof of QAOA Convergence," *New Journal of Physics*, 2024. arXiv:2302.04968.

[2] T. Kato, *Perturbation Theory for Linear Operators*, Springer, 1966.

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[4] R. A. Horn and C. R. Johnson, *Matrix Analysis*, 2nd ed., Cambridge University Press, 2013.

[5] The Mathlib Community, *Mathlib4: A Lean 4 Mathematics Library*, https://leanprover-community.github.io/mathlib4_docs/, 2024.