

# Quantum Deficiency Theory: Coherence, Complexity, and the Classical Limit

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## Abstract

We develop a structural theory of steady-state degeneracy for finite-dimensional quantum Markov semigroups (Lindblad dynamics). For a quantum network graph  $G$  encoding the support pattern of generators, we define a *structural quantum deficiency*  $\delta_Q^{\text{struct}}(G) := \dim(\mathcal{C}_{\text{struct}}(G)) - 1$  that is parameter-independent and equals the number of strongly connected components of the directed support graph minus one. Our main results are: (1)  $\delta_Q := \dim(\ker \mathcal{L}) - 1$  equals  $\delta_Q^{\text{struct}}(G)$  for Zariski-generic parameters in any fixed support pattern; (2) the non-generic locus where  $\delta_Q > \delta_Q^{\text{struct}}$  is a proper algebraic subvariety characterized by “accidental symmetries”; (3) under  $\sigma$ -GNS quantum detailed balance,  $\delta_Q = 0$  implies exponential convergence to the unique stationary state. The theory connects graph-theoretic properties (strong connectivity) to dynamical properties (ergodicity) via the commutant of the Lindblad algebra. We provide explicit examples where accidental symmetries on measure-zero parameter sets create additional stationary states. The algebraic framework is machine-verified in Lean 4.

## 1 Introduction

The mathematical theory of chemical reaction networks, pioneered by Horn, Jackson, and Feinberg in the 1970s [1, 2, 3], provides a remarkable connection between network topology and dynamical behavior. The centerpiece of this theory is the *Deficiency Zero Theorem*, which guarantees that networks satisfying certain structural conditions—zero deficiency and weak reversibility—admit unique, stable equilibria regardless of rate constants [4]. This topological approach to stability has found widespread applications in systems biology [6], synthetic biology [7],

and beyond.

However, classical CRNT assumes that molecular species can be described by concentrations obeying deterministic mass-action kinetics. At the nanoscale, particularly in biological systems operating near the quantum-classical boundary, this assumption breaks down. Mounting experimental evidence demonstrates that quantum coherence persists in warm, wet biological environments and may play functional roles in photosynthesis [9, 10], enzyme catalysis [11], and magnetoreception [12]. These observations motivate the question: *Can a structural theory of steady-state degeneracy, analogous to CRNT, be developed for quantum systems?*

Here we develop such a theory for open quantum systems governed by Lindblad master equations [13, 14]. Inspired by CRNT’s emphasis on topology over kinetics, we define a *structural quantum deficiency* that depends only on the support pattern of the Lindblad generators, not on their specific values. The Lindblad formalism describes Markovian dynamics of density matrices, encompassing both coherent evolution (via the Hamiltonian) and dissipative processes (via jump operators that model interactions with the environment).

### 1.1 Main Contributions

Our principal contributions are:

1. **Structural Quantum Deficiency.** For a quantum network graph  $G = (V, E_{\text{coh}}, E_{\text{jump}})$  encoding support structure, we define the *structural commutant*  $\mathcal{C}_{\text{struct}}(G)$  and *structural deficiency*  $\delta_Q^{\text{struct}}(G) := \dim(\mathcal{C}_{\text{struct}}(G)) - 1$ . This is computable from  $G$  alone, independent of parameter values.
2. **Graph-Theoretic Formula.** We prove  $\delta_Q^{\text{struct}}(G) = k - 1$  where  $k$  is the number

of strongly connected components of the directed support graph  $D(G)$ . In particular,  $\delta_Q^{\text{struct}}(G) = 0$  iff  $D(G)$  is strongly connected (Theorem 21).

3. **Parameter Robustness.** We prove  $\delta_Q(\theta) = \delta_Q^{\text{struct}}(G)$  for  $\theta$  in a Zariski-open dense subset of the parameter space  $\Theta(G)$ . The exceptional locus where  $\delta_Q > \delta_Q^{\text{struct}}$  corresponds to “accidental symmetries” (Theorem 19).
4. **Convergence under Detailed Balance.** For Lindbladians with  $\delta_Q = 0$  satisfying  $\sigma$ -GNS quantum detailed balance, we prove exponential convergence to the unique stationary state (Theorem 27).
5. **Formal Verification.** The algebraic framework (130 lemmas) is machine-verified in Lean 4; analytic semigroup results (19 axioms) are documented.

## 1.2 Related Work

Classical CRNT is well-established [3, 5]. Stochastic extensions using the chemical master equation have been developed [8], but these remain classical. Baez and collaborators explored connections between quantum mechanics and reaction networks using operator-theoretic methods [23], but their “quantum” formalism describes *classical* stochastic systems. Quantum Petri nets [24] provide an alternative discrete-event model but lack the analytical power of our continuous-time approach. The mathematical theory of quantum Markov semigroups is mature [15, 16, 20]; to our knowledge, no prior work has connected this theory to CRNT’s structural concepts of deficiency and weak reversibility.

## 2 Mathematical Framework

### 2.1 Classical Chemical Reaction Network Theory

A *chemical reaction network* consists of species  $\{X_1, \dots, X_s\}$ , complexes (linear combinations of species), and reactions between complexes. The network defines a directed graph where nodes are complexes and edges are reactions. Under mass-action kinetics, concentrations  $x \in \mathbb{R}_{>0}^s$  evolve as:

$$\frac{dx}{dt} = S \cdot v(x) \quad (1)$$

where  $S$  is the stoichiometric matrix and  $v(x)$  is the vector of reaction rates.

**Definition 1** (Classical Deficiency). *The deficiency of a reaction network is:*

$$\delta = n - \ell - \text{rank}(S) \quad (2)$$

where  $n$  is the number of complexes,  $\ell$  is the number of linkage classes (connected components), and  $S$  is the stoichiometric matrix.

The classical Deficiency Zero Theorem [2] states: *If  $\delta = 0$  and the network is weakly reversible, then for any choice of rate constants, there exists within each stoichiometric compatibility class a unique equilibrium, and this equilibrium is locally asymptotically stable.*

### 2.2 Quantum Dynamics: Lindblad Master Equation

Open quantum systems in contact with Markovian environments evolve according to the Lindblad master equation [13, 14]:

$$\frac{d\rho}{dt} = \mathcal{L}(\rho) = -i[H, \rho] + \sum_k \left( L_k \rho L_k^\dagger - \frac{1}{2} \{L_k^\dagger L_k, \rho\} \right) \quad (3)$$

where  $\rho$  is the density matrix,  $H$  is the system Hamiltonian, and  $\{L_k\}$  are jump (Lindblad) operators describing dissipative processes. The first term generates coherent evolution; the second, called the *dissipator*, describes decoherence and relaxation.

The Lindblad equation preserves the essential properties of density matrices:

- Hermiticity:  $\rho(t)^\dagger = \rho(t)$
- Positivity:  $\rho(t) \geq 0$
- Trace:  $\text{Tr}(\rho(t)) = 1$

**Definition 2** (Lindbladian). *A Lindbladian is a linear superoperator  $\mathcal{L}$  of the form (3). The pair  $(H, \{L_k\})$  specifies the quantum network structure.*

**Definition 3** (Stationary State). *A density matrix  $\rho_*$  is stationary if  $\mathcal{L}(\rho_*) = 0$ .*

**Definition 4** (Faithful State). *A density matrix  $\rho$  is faithful if  $\rho > 0$  (positive definite).*

## 2.3 The Lindblad Algebra and Its Commutant

The structural properties of a Lindbladian are encoded in algebraic objects:

**Definition 5** (Lindblad Algebra). *The Lindblad algebra  $\mathcal{A}$  is the unital  $*$ -subalgebra of  $M_n(\mathbb{C})$  generated by  $\{H, L_1, L_1^\dagger, \dots, L_m, L_m^\dagger\}$ .*

**Definition 6** (Commutant). *The commutant is  $\mathcal{C} = \mathcal{A}' = \{X \in M_n(\mathbb{C}) : [X, A] = 0 \text{ for all } A \in \mathcal{A}\}$ .*

**Lemma 7** (Commutant Characterization).  $\mathcal{C} = \{X \in M_n(\mathbb{C}) : [X, H] = 0, [X, L_k] = 0, [X, L_k^\dagger] = 0 \text{ for all } k\}$ .

*Proof.* If  $X$  commutes with each generator  $H, L_k, L_k^\dagger$ , then  $X$  commutes with all products of these generators, hence with the entire  $*$ -algebra  $\mathcal{A}$ .  $\square$

**Remark.** For Hermitian  $X$ ,  $[X, L_k] = 0$  implies  $[X, L_k^\dagger] = 0$  (take adjoints). But this does *not* hold for general  $X$ : if  $L = E_{12}$  and  $X = E_{12}$ , then  $[X, L] = 0$  but  $[X, L^\dagger] = E_{11} - E_{22} \neq 0$ .

**Definition 8** (Fixed-Point Algebra). *The Heisenberg fixed-point algebra is  $\text{Fix}(\mathcal{L}^*) = \{A : \mathcal{L}^*(A) = 0\}$ .*

**Lemma 9** (Commutant-Fixed Point Relation).  $\mathcal{C} \subseteq \text{Fix}(\mathcal{L}^*)$ , with equality when a faithful stationary state exists.

**Definition 10** (Ergodic Lindbladian). *A Lindbladian is ergodic if  $\text{Fix}(\mathcal{L}^*) = \mathbb{C} \cdot I$ , equivalently  $\mathcal{C} = \mathbb{C} \cdot I$ .*

**Terminology note.** In the QMS literature, “primitive” sometimes requires aperiodicity in addition to irreducibility. We use “ergodic” to mean precisely  $\text{Fix}(\mathcal{L}^*) = \mathbb{C} \cdot I$ , which is equivalent to uniqueness of the stationary state [15].

## 3 Quantum Deficiency Theory

### 3.1 Definition of Quantum Deficiency

**Definition 11** (Quantum Deficiency). *The quantum deficiency of a Lindbladian  $\mathcal{L}$  is:*

$$\delta_Q := \dim(\ker \mathcal{L}) - 1 \quad (4)$$

where  $\ker \mathcal{L} = \{\rho : \mathcal{L}(\rho) = 0\}$  is the space of stationary states.

Equivalently,  $\delta_Q$  counts the number of *independent* stationary states minus one (accounting for normalization). A Lindbladian has  $\delta_Q = 0$  if and only if it has a unique stationary state.

## 3.2 Quantum Network Structure and Parameter Robustness

A key property of classical CRNT deficiency is *rate-constant robustness*:  $\delta = n - \ell - \text{rank}(S)$  depends only on network topology, not kinetic parameters. We develop an analogous structural theory.

**Definition 12** (Quantum Network Graph). *The quantum network graph  $G = (V, E_{\text{coh}}, E_{\text{jump}})$  consists of:*

- Vertices  $V = \{1, \dots, n\}$  (computational basis states)
- Coherent edges: unordered pairs  $\{i, j\}$  with  $i \neq j$  and  $H_{ij} \neq 0$
- Jump edges: ordered pairs  $(i \rightarrow j)$  with  $i \neq j$  and  $(L_k)_{ji} \neq 0$  for some  $k$

Only off-diagonal entries define edges; diagonal entries are unrestricted.

**Definition 13** (Test Operator Set). *For a quantum network graph  $G$ , define the full test set:*

$$\mathcal{S}^*(G) = \{E_{ij}, E_{ji} : \{i, j\} \in E_{\text{coh}}\} \cup \{E_{ji}, E_{ij} : (i \rightarrow j) \in E_{\text{jump}}\}$$

where  $E_{ij} = |i\rangle\langle j|$  is the standard matrix unit. This includes both directions for each edge, matching the Lindblad algebra structure ( $L_k$  and  $L_k^\dagger$ ).

**Definition 14** (Structural Commutant).  $\mathcal{C}_{\text{struct}}(G) = \{X \in M_n(\mathbb{C}) : [X, A] = 0 \text{ for all } A \in \mathcal{S}^*(G)\}$ .

**Definition 15** (Structural Deficiency).  $\delta_Q^{\text{struct}}(G) := \dim(\mathcal{C}_{\text{struct}}(G)) - 1$ .

**Definition 16** (Directed Support Graph). *The directed support graph  $D(G)$  has vertex set  $V$  with arrow  $i \rightarrow j$  iff  $E_{ji} \in \mathcal{S}^*(G)$ .*

**Definition 17** (Structural Primitivity).  *$G$  is structurally ergodic if  $D(G)$  is strongly connected. (Since  $\mathcal{S}^*(G)$  includes both directions, this is equivalent to the undirected support graph being connected.)*

**Remark (Why the test set is symmetric).** Although physical jump operators  $L_k$  may describe directed transitions, the Lindblad  $*$ -algebra necessarily includes  $L_k^\dagger$ , and the commutant conditions require  $[X, L_k] = [X, L_k^\dagger] = 0$ . Hence the structural test set  $\mathcal{S}^*(G)$  must contain both  $E_{ij}$  and  $E_{ji}$  for each edge.

**Definition 18** (Parameter Space). Let  $\text{supp}_{\text{off}}(M) := \{(i, j) : i \neq j, M_{ij} \neq 0\}$  denote the off-diagonal support. Define:

$$\Theta(G) = \{(H, \{L_k\}) : \text{supp}_{\text{off}}(H) \subseteq E_{\text{coh}}, \text{supp}_{\text{off}}(L_k)$$

Diagonal entries of  $H$  and  $L_k$  are unrestricted.

**Remark (Real algebraic structure).** The constraint  $H = H^\dagger$  involves complex conjugation, so  $\Theta(G)$  is naturally a *real* algebraic set. Explicitly, parameterize  $H$  by independent real variables  $(\text{Re } H_{ij}, \text{Im } H_{ij})$  for  $i < j$  (with  $H_{ji} = \overline{H_{ij}}$ ) and real diagonal entries  $H_{ii}$ ; parameterize  $L_k$  by complex entries (real and imaginary parts). The constraint map  $\Phi_\theta$  has entries that are polynomial in these real coordinates. “Zariski-open dense” in Theorem 19(b) means the complement of a proper real algebraic subvariety—equivalently, a set whose complement has Lebesgue measure zero. This is the standard real algebraic geometry setting; see [22] for background.

**Remark (Physical constraints).** Physical constraints—such as particular Lindblad decompositions or positivity requirements on transition rates—may restrict to a proper subset of  $\Theta(G)$ . The genericity statement applies within  $\Theta(G)$ ; for restricted parameter sets, one must verify that the restriction intersects the generic locus.

**Theorem 19** (Parameter Robustness). Let  $G$  be a quantum network graph.

- (a) For any  $\theta \in \Theta(G)$ :  $\delta_Q(\theta) \geq \delta_Q^{\text{struct}}(G)$ .
- (b) There exists a Zariski-open dense  $U \subseteq \Theta(G)$  with  $\delta_Q(\theta) = \delta_Q^{\text{struct}}(G)$  for  $\theta \in U$ .
- (c)  $\delta_Q^{\text{struct}}(G) = 0$  iff  $G$  is structurally ergodic (i.e.,  $D(G)$  is strongly connected).

*Proof.* (a) Let  $S_1, \dots, S_k$  be the strongly connected components of  $D(G)$ . Every generator has block-diagonal form with respect to  $\mathbb{C}^n = \bigoplus_{i=1}^k \mathbb{C}^{S_i}$ , since no matrix unit  $E_{ab}$  with  $a \in S_i$  and  $b \in S_j$

$(i \neq j)$  lies in  $\mathcal{S}^*(G)$ . Hence the Lindbladian splits as  $\mathcal{L} = \bigoplus_{i=1}^k \mathcal{L}_i$  on the corresponding block matrix algebra. Each  $\mathcal{L}_i$  has at least one stationary state, so  $\dim(\ker \mathcal{L}) \geq k$ , hence  $\delta_Q = \dim(\ker \mathcal{L}) - 1 \geq k - 1 = \delta_Q^{\text{struct}}(G)$ .

(b) Define the constraint map  $\Phi_\theta : M_n(\mathbb{C}) \rightarrow M_n(\mathbb{C})^{1+2m}$  by

$$\Phi_\theta(X) = ([X, H], [X, L_1], [X, L_1^\dagger], \dots, [X, L_m], [X, L_m^\dagger]).$$

Then  $\mathcal{C}(\theta) = \ker \Phi_\theta$ . The entries of the matrix representation of  $\Phi_\theta$  are linear in  $\theta$ . Let  $r_G = \underline{\text{rank}}(\Phi_\theta)$ . The set  $\{\theta : \text{rank}(\Phi_\theta) < r_G\}$  is defined by vanishing of all  $r_G \times r_G$  minors, hence is a proper algebraic subvariety. Its complement is Zariski-open dense.

(c) Let  $\mathcal{A}(G)$  denote the unital  $*$ -algebra generated by  $\mathcal{S}^*(G)$ .

( $\Leftarrow$ ) Suppose  $D(G)$  is strongly connected. For any  $a, b \in V$ , choose a directed path  $b = v_0 \rightarrow v_1 \rightarrow \dots \rightarrow v_m = a$ . Each arrow  $v_{t-1} \rightarrow v_t$  means  $E_{v_t, v_{t-1}} \in \mathcal{S}^*(G)$ . Multiplying:  $E_{v_1 v_0} E_{v_2 v_1} \cdots E_{v_m v_{m-1}} = E_{ab}$ . Hence every matrix unit  $E_{ab} \in \mathcal{A}(G)$ , so  $\mathcal{A}(G) = M_n(\mathbb{C})$ . Then  $\mathcal{C}_{\text{struct}}(G) = \mathcal{A}(G)' = M_n(\mathbb{C})' = \mathbb{C} \cdot I$ .

( $\Rightarrow$ ) If  $D(G)$  is not strongly connected, let  $S \subsetneq V$  be a proper SCC. The projection  $P_S = \sum_{i \in S} E_{ii}$  commutes with every element of  $\mathcal{S}^*(G)$  (block-diagonal structure), so  $P_S \in \mathcal{C}_{\text{struct}}(G)$ . Since  $P_S \neq cI$ , we have  $\mathcal{C}_{\text{struct}}(G) \neq \mathbb{C} \cdot I$ .  $\square$

**Corollary 20** (Rate-Robust Uniqueness). If  $G$  is structurally ergodic, any Lindbladian with support  $G$  and Zariski-generic parameters has a unique stationary state.

[Genericity in Action: Accidental Symmetry] Consider  $n = 2$  with quantum network graph  $G$  having  $E_{\text{coh}} = \{\{1, 2\}\}$  and  $E_{\text{jump}} = \{1 \rightarrow 2, 2 \rightarrow 1\}$ . The test set is  $\mathcal{S}^*(G) = \{E_{12}, E_{21}\}$ , the directed support graph  $D(G)$  has both arrows, so  $D(G)$  is strongly connected and  $\delta_Q^{\text{struct}}(G) = 0$ . Explicitly:  $\mathcal{C}_{\text{struct}}(G) = \mathbb{C} \cdot I$ .

**Non-generic aligned family.** Take  $H = \omega \sigma_x$  and  $L = \alpha \sigma_x$  with  $\sigma_x = E_{12} + E_{21}$  and  $\alpha \neq 0$ . Let  $|\pm\rangle = (|1\rangle \pm |2\rangle)/\sqrt{2}$  be the  $\sigma_x$ -eigenstates. The Lindbladian is:

$$\mathcal{L}(\rho) = -i\omega[\sigma_x, \rho] + |\alpha|^2(\sigma_x \rho \sigma_x - \rho)$$

For  $\rho$  diagonal in the  $\{|+\rangle, |-\rangle\}$  basis:  $[\sigma_x, \rho] = 0$  and  $\sigma_x \rho \sigma_x = \rho$  (since  $\sigma_x^2 = I$ ). Thus  $\mathcal{L}(\rho) =$

0. Both  $|+\rangle\langle+|$  and  $|-\rangle\langle-|$  are stationary, giving  $\dim(\ker \mathcal{L}) \geq 2$  and  $\delta_Q \geq 1 > 0 = \delta_Q^{\text{struct}}(G)$ .

This is an *accidental symmetry*: the specific choice  $H \in \langle L, L^\dagger, I \rangle_{*\text{-alg}}$  enlarges the commutant to span  $\{I, \sigma_x\}$ , which is 2-dimensional.

**Restoring genericity.** Perturb  $H' = \omega\sigma_x + \epsilon\sigma_z$  with  $\epsilon \neq 0$  (note  $\sigma_z$  is diagonal and does not change  $E_{\text{coh}}$ ). Now  $[X, H'] = [X, L] = 0$  requires  $[X, \sigma_x] = [X, \sigma_z] = 0$ , which forces  $X \in \mathbb{C} \cdot I$ , and  $\delta_Q = 0$ .

**Theorem 21** (Structural Deficiency Formula). *Let  $G$  be a quantum network graph and let  $k$  be the number of strongly connected components of  $D(G)$ . Then:*

$$\delta_Q^{\text{struct}}(G) = k - 1 \quad (5)$$

*Proof.* Let  $S_1, \dots, S_k$  be the strongly connected components of  $D(G)$ , with  $|S_i| = n_i$ .

*Step 1.* The algebra  $\mathcal{A}(G) = \langle \mathcal{S}^*(G) \rangle$  acts block-diagonally with respect to  $V = S_1 \sqcup \dots \sqcup S_k$ . This follows because no matrix unit  $E_{ij}$  with  $i \in S_a$  and  $j \in S_b$  ( $a \neq b$ ) lies in  $\mathcal{S}^*(G)$ : such an edge would connect different SCCs, contradicting the SCC decomposition.

*Step 2.* Within each SCC  $S_i$ , the restriction of  $\mathcal{A}(G)$  to  $M_{n_i}(\mathbb{C})$  equals  $M_{n_i}(\mathbb{C})$ . This follows from strong connectivity: for any  $a, b \in S_i$ , there is a directed path in  $D(G)$ , so  $E_{ab}$  is in  $\mathcal{A}(G)$  by the matrix-unit multiplication argument (proof of Theorem 19(c)).

*Step 3.* Therefore  $\mathcal{A}(G) \cong M_{n_1}(\mathbb{C}) \oplus \dots \oplus M_{n_k}(\mathbb{C})$ , and the commutant is:

$$\mathcal{C}_{\text{struct}}(G) = \mathcal{A}(G)' \cong \mathbb{C} \oplus \dots \oplus \mathbb{C} = \mathbb{C}^k$$

Thus  $\dim(\mathcal{C}_{\text{struct}}(G)) = k$  and  $\delta_Q^{\text{struct}}(G) = k - 1$ .  $\square$

**Corollary 22** (Extremal Cases). (i)  $\delta_Q^{\text{struct}}(G) = 0$  iff  $D(G)$  is strongly connected ( $k = 1$ ).

(ii)  $\delta_Q^{\text{struct}}(G) = n - 1$  iff  $D(G)$  has no edges ( $k = n$ , each vertex is its own SCC).

**Why the formula  $\delta_Q^{\text{struct}} = k - 1$  is significant.** Classical CRNT deficiency  $\delta = n - \ell - \text{rank}(S)$  involves the stoichiometric matrix rank, not a kernel dimension. Our quantum deficiency  $\delta_Q = \dim(\ker \mathcal{L}) - 1$  is a kernel dimension, yet the structural formula shows that generic kernel degeneracy is *combinatorial*—determined entirely by the SCC count of the support graph. Deviations from the generic value occur only on algebraic subvarieties (Proposition 23). This rigidity is analogous

to, though not identical to, the rate-independence of classical CRNT.

**Proposition 23** (Non-Generic Locus). *Define the deficiency jump locus:*

$$V_G := \{\theta \in \Theta(G) : \delta_Q(\theta) > \delta_Q^{\text{struct}}(G)\}$$

*Then  $V_G$  is a proper algebraic subvariety of  $\Theta(G)$ .*

*Proof.* Fix a linear complement  $W$  of  $\mathcal{C}_{\text{struct}}(G)$  in  $M_n(\mathbb{C})$ , with  $d := \dim W$ . Any  $X \in M_n(\mathbb{C})$  decomposes uniquely as  $X = X_0 + X_1$  with  $X_0 \in \mathcal{C}_{\text{struct}}(G)$  and  $X_1 \in W$ . Since  $\mathcal{C}_{\text{struct}}(G) \subseteq \mathcal{C}(\theta)$  always (elements commuting with all matrix units on the support commute with any matrix of that support, by linearity), we have  $\Phi_\theta(X_0) = 0$ . Thus  $\Phi_\theta(X) = 0$  iff  $\Phi_\theta(X_1) = 0$ . Hence  $\delta_Q(\theta) > \delta_Q^{\text{struct}}(G)$  iff  $\ker(\Phi_\theta|_W) \neq \{0\}$ .

Choose a basis  $\{w_1, \dots, w_d\}$  of  $W$  and represent  $\Phi_\theta|_W : W \rightarrow M_n(\mathbb{C})^{1+2m}$  as a matrix  $M_W(\theta)$  whose entries are polynomial in  $\theta$ . Then:

$$V_G = \{\theta \in \Theta(G) : \ker(\Phi_\theta|_W) \neq \{0\}\} = \{\theta : \text{rank}(M_W(\theta)) < d\}$$

This is defined by the vanishing of all  $d \times d$  minors of  $M_W(\theta)$ , which are polynomials in  $\theta$ . Hence  $V_G$  is an algebraic subvariety. It is proper by Theorem 19(b).  $\square$

### 3.3 Algebraic Characterization

**Theorem 24** (Evans-Frigerio Structure). *For a Lindbladian on  $M_n(\mathbb{C})$  [19, 15]:*

1.  $\text{Fix}(\mathcal{L}^*)$  is a unital  $*$ -subalgebra of  $M_n(\mathbb{C})$
2.  $\dim(\ker \mathcal{L}) = \dim(\ker \mathcal{L}^*)$  (by rank-nullity: both equal  $n^2 - \text{rank}(\mathcal{L})$ )

**Theorem 25** (Deficiency Zero Characterization). *The following are equivalent:*

- (i)  $\delta_Q = 0$  (unique stationary state)
- (ii)  $\mathcal{L}$  is ergodic ( $\mathcal{C} = \mathbb{C} \cdot I$ )
- (iii)  $\text{Fix}(\mathcal{L}^*) = \mathbb{C} \cdot I$
- (iv)  $\mathcal{L}$  is irreducible (no nontrivial invariant projections)

*Proof.* (i)  $\Leftrightarrow$  (iii): If  $\delta_Q = 0$ , then  $\dim(\ker \mathcal{L}) = 1$ . By Theorem 24,  $\dim(\text{Fix}(\mathcal{L}^*)) = \dim(\ker \mathcal{L}^*) = \dim(\ker \mathcal{L}) = 1$ . Since  $I \in \text{Fix}(\mathcal{L}^*)$  (the identity is

always fixed by the dual), we have  $\text{Fix}(\mathcal{L}^*) = \mathbb{C} \cdot I$ . Conversely,  $\text{Fix}(\mathcal{L}^*) = \mathbb{C} \cdot I$  has dimension 1, so  $\dim(\ker \mathcal{L}) = 1$  and  $\delta_Q = 0$ .

(ii)  $\Leftrightarrow$  (iii):  $\mathcal{C} \subseteq \text{Fix}(\mathcal{L}^*)$  always holds. If  $\mathcal{C} = \mathbb{C} \cdot I$ , then  $\text{Fix}(\mathcal{L}^*) \supseteq \mathbb{C} \cdot I$ ; combined with  $\dim(\text{Fix}(\mathcal{L}^*)) = 1$ , this gives  $\text{Fix}(\mathcal{L}^*) = \mathbb{C} \cdot I$ . Conversely,  $\text{Fix}(\mathcal{L}^*) = \mathbb{C} \cdot I$  and  $\mathcal{C} \subseteq \text{Fix}(\mathcal{L}^*)$  give  $\mathcal{C} = \mathbb{C} \cdot I$ .

(iii)  $\Leftrightarrow$  (iv): Standard equivalence [15].  $\square$

### 3.4 Quantum Detailed Balance

**Definition 26** ( $\sigma$ -GNS Quantum Detailed Balance). A Lindbladian  $\mathcal{L}$  satisfies  $\sigma$ -GNS quantum detailed balance with respect to a faithful state  $\sigma > 0$  if:

1.  $\mathcal{L}(\sigma) = 0$ , and
2. the dual generator  $\mathcal{L}^*$  acting on observables is self-adjoint with respect to the  $\sigma$ -GNS inner product

$$\langle A, B \rangle_\sigma := \text{Tr}\left(\sigma A^\dagger B\right),$$

(using the convention linear in the second argument).

Physically, detailed balance expresses thermodynamic reversibility:  $\sigma$  plays the role of an equilibrium state with respect to which the dynamics is reversible. [29, 18, 17]

### 3.5 The Quantum Deficiency Zero Theorem

Our main result is:

**Theorem 27** (Quantum Deficiency Zero Theorem). Let  $\mathcal{L}$  be a Lindbladian on  $M_n(\mathbb{C})$  satisfying:

1.  $\delta_Q = 0$  (i.e.,  $\dim(\ker \mathcal{L}) = 1$ ), and
2.  $\sigma$ -GNS quantum detailed balance with respect to a faithful state  $\sigma > 0$ .

Then  $\sigma$  is the unique stationary state and  $e^{t\mathcal{L}}(\rho_0) \rightarrow \sigma$  exponentially fast in trace norm for any initial  $\rho_0$ .

**Remark.** Structural primitivity ( $\delta_Q^{\text{struct}}(G) = 0$ ) is a sufficient condition for  $\delta_Q = 0$  when parameters are Zariski-generic (Theorem 19(b)), but not equivalent:  $\delta_Q = 0$  can hold for non-generic parameters even when  $\delta_Q^{\text{struct}}(G) > 0$ .

**Proof. Uniqueness.** By  $\delta_Q = 0$ ,  $\dim(\ker \mathcal{L}) = 1$ . By detailed balance,  $\mathcal{L}(\sigma) = 0$ , so  $\sigma \in \ker \mathcal{L}$ . Hence  $\ker \mathcal{L} = \mathbb{C} \cdot \sigma$ , and among density matrices  $\sigma$  is the unique stationary state.

**Exponential convergence.** Let  $\mathcal{L}^*$  denote the dual generator on observables, defined by  $\text{Tr}(A \mathcal{L}(\rho)) = \text{Tr}(\mathcal{L}^*(A) \rho)$ .

*Step 1 (Reversibility).*  $\sigma$ -GNS detailed balance means that  $\mathcal{L}^*$  is self-adjoint with respect to

$$\langle A, B \rangle_\sigma := \text{Tr}\left(\sigma A^\dagger B\right),$$

viewing  $M_n(\mathbb{C})$  as a finite-dimensional Hilbert space with norm  $\|A\|_\sigma := \sqrt{\text{Tr}(\sigma A^\dagger A)}$  [17].

*Step 2 (Spectrum).* Self-adjointness implies that  $\mathcal{L}^*$  is diagonalizable with real eigenvalues. Since  $e^{t\mathcal{L}^*}$  is completely positive and unital,  $\|e^{t\mathcal{L}^*}\|_{\infty \rightarrow \infty} = 1$  for all  $t \geq 0$ , hence the spectral bound satisfies  $\text{Re}(\lambda) \leq 0$  for all eigenvalues  $\lambda$ . Therefore  $\lambda \leq 0$ .

*Step 3 (Spectral gap).* In finite dimension,  $\mathcal{L}$  and  $\mathcal{L}^*$  have the same spectrum, so  $\dim(\ker \mathcal{L}^*) = 1$  as well. Moreover  $\ker \mathcal{L} = \mathbb{C} \cdot \sigma$  while  $\ker \mathcal{L}^* = \mathbb{C} \cdot I$ . Define

$$\gamma := \min\{|\lambda| : \lambda \in \text{spec}(\mathcal{L}^*), \lambda \neq 0\} > 0.$$

*Step 4 (Decay for observables).* Let  $Q_0$  be the  $\sigma$ -GNS orthogonal projection onto  $\ker \mathcal{L}^* = \mathbb{C} \cdot I$ . With the convention linear in the second slot,

$$Q_0(A) = \frac{\langle I, A \rangle_\sigma}{\langle I, I \rangle_\sigma} I = \frac{\text{Tr}(\sigma A)}{\text{Tr}(\sigma)} I = \text{Tr}(\sigma A) I.$$

By the spectral theorem, for all  $A$ ,

$$\|e^{t\mathcal{L}^*}(A) - Q_0(A)\|_\sigma \leq e^{-\gamma t} \|A - Q_0(A)\|_\sigma.$$

*Step 5 (Expectation values).* For  $\rho_t = e^{t\mathcal{L}}(\rho_0)$  and any observable  $A$ ,

$$\text{Tr}(A \rho_t) = \text{Tr}\left(e^{t\mathcal{L}^*}(A) \rho_0\right) \xrightarrow[t \rightarrow \infty]{} \text{Tr}(Q_0(A) \rho_0) = \text{Tr}(\sigma A).$$

*Step 6 (Trace-norm bound).* For any  $A$  with  $\|A\|_\infty \leq 1$ , set  $B_t := e^{t\mathcal{L}^*}(A) - Q_0(A)$ . Then

$$\text{Tr}(A(\rho_t - \sigma)) = \text{Tr}(B_t \rho_0),$$

so  $|\text{Tr}(A(\rho_t - \sigma))| \leq \|B_t\|_\infty$ . Since  $\sigma > 0$  with minimum eigenvalue  $\lambda_{\min}(\sigma) > 0$ ,

$$\|X\|_\infty \leq \lambda_{\min}(\sigma)^{-1/2} \|X\|_\sigma.$$

Also, for  $\|A\|_\infty \leq 1$ ,  $\|A\|_\sigma \leq 1$  and  $|\text{Tr}(\sigma A)| \leq 1$ , hence  $\|A - Q_0(A)\|_\sigma \leq 2$ . Combining with Step 4 gives

$$\|B_t\|_\infty \leq 2 \lambda_{\min}(\sigma)^{-1/2} e^{-\gamma t}.$$

Finally, using the dual characterization  $\|X\|_1 = \sup_{\|A\|_\infty \leq 1} |\text{Tr}(AX)|$ , we obtain

$$\|\rho_t - \sigma\|_1 \leq 2 \lambda_{\min}(\sigma)^{-1/2} e^{-\gamma t},$$

establishing exponential convergence in trace norm with explicit constant.  $\square$

This theorem provides a deficiency-zero stability result in a thermodynamically reversible setting:  $\delta_Q = 0$  fixes uniqueness of the stationary state, while  $\sigma$ -GNS detailed balance supplies faithfulness and a real spectral gap, yielding exponential convergence.

### 3.6 Quantum-Classical Kernel Inequality

We clarify the relationship between quantum and classical steady-state degeneracy.

**Definition 28** (Master Equation Deficiency). *For a classical master equation  $\dot{p} = Rp$  on probability vectors, define  $\delta_{\text{ME}} := \dim(\ker R) - 1$ .*

**Remark.** This is *not* the same as classical CRNT deficiency  $\delta = n - \ell - \text{rank}(S)$ .

**Definition 29** (Diagonal Lindbladian). *A Lindbladian is diagonal if  $H$  and all  $L_k$  are diagonal matrices in some fixed basis.*

For a diagonal Lindbladian, coherences decouple from populations, and the population dynamics reduce to a classical master equation.

**Theorem 30** (Quantum-Classical Kernel Inequality). *Let  $\mathcal{L}$  be a Lindbladian with associated classical rate matrix  $R$ . Then:*

$$\delta_Q \geq \delta_{\text{ME}} \tag{6}$$

with equality when  $\mathcal{L}$  is diagonal.

*Proof.* Classical stationary distributions embed into quantum stationary states as diagonal density matrices. Thus  $\dim(\ker \mathcal{L}) \geq \dim(\ker R)$ . For diagonal Lindbladians, coherences contribute no additional stationary solutions, giving equality.  $\square$

**Open problem.** The relationship between  $\delta_Q^{\text{struct}}$  and classical CRNT deficiency  $\delta = n - \ell - \text{rank}(S)$  remains to be established.

## 4 Key Lemmas

The proof of Theorem 27 relies on several intermediate results of independent interest.

**Lemma 31** (Commutant Closure). *The commutant  $\mathcal{C}$  is closed under:*

1. *Addition and scalar multiplication*
2. *Matrix multiplication*
3. *Conjugate transpose ( $X \in \mathcal{C} \Rightarrow X^\dagger \in \mathcal{C}$ )*
4. *Powers ( $X \in \mathcal{C} \Rightarrow X^n \in \mathcal{C}$  for all  $n \in \mathbb{N}$ )*
5. *Polynomial evaluation ( $X \in \mathcal{C} \Rightarrow p(X) \in \mathcal{C}$  for any polynomial  $p$ )*

**Lemma 32** (Hermitian Commutant is Scalar). *If  $\mathcal{L}$  is ergodic and  $X \in \mathcal{C}$  is Hermitian, then  $X = c \cdot I$  for some  $c \in \mathbb{R}$ .*

*Proof.* Let  $X$  be Hermitian with spectral decomposition  $X = \sum_i \lambda_i P_i$ . By Lemma 31, each spectral projection  $P_i$  lies in  $\mathcal{C}$ . Ergodicity implies the only projections in  $\mathcal{C}$  are 0 and  $I$ . Thus  $X$  has a single eigenvalue, so  $X = \lambda I$ .  $\square$

**Lemma 33** (Ergodic  $\Leftrightarrow$  Irreducible). *A Lindbladian is ergodic if and only if it is irreducible (no nontrivial invariant projections).*

**Lemma 34** (Kernel Invariance). *Let  $\rho$  be a stationary state. The kernel of  $\rho$  is invariant under  $L_k^\dagger$  for all  $k$ :*

$$L_k^\dagger(\ker \rho) \subseteq \ker \rho.$$

This invariance property follows from the positivity structure of the Lindblad equation [15]. Note that this does *not* imply the kernel projection commutes with  $L_k$ ; that stronger statement is false in general (see the amplitude damping counterexample below).

## 5 Applications

### 5.1 Two-Level System: Amplitude Damping Counterexample

Consider a two-level system with Hamiltonian  $H = \omega |1\rangle\langle 1|$  and decay  $L = \sqrt{\gamma}|0\rangle\langle 1|$ . This models spontaneous emission (zero-temperature relaxation).

The Lindblad algebra is generated by  $\{H, L, L^\dagger\}$ . Direct computation shows the only matrices commuting with  $H$ ,  $L$ , and  $L^\dagger$  are scalar multiples of  $I$ . Thus the system is ergodic and  $\delta_Q = 0$ .

The unique stationary state is  $\rho_* = |0\rangle\langle 0|$  (ground state), which is *not faithful* (rank 1).

**Important:** This system does *not* satisfy  $\sigma$ -GNS detailed balance—there is no “backward” jump operator to balance the decay. Therefore Theorem 27 does not apply directly. Convergence still occurs (all initial states decay to the ground state), but this requires a separate argument.

This example illustrates that  $\delta_Q = 0$  alone guarantees *uniqueness* of the stationary state, but *not* faithfulness. Faithfulness requires the additional detailed-balance hypothesis, which physically corresponds to finite-temperature thermalization rather than zero-temperature relaxation.

## 5.2 Fenna–Matthews–Olson Complex

The FMO complex is a pigment-protein structure in green sulfur bacteria that transfers excitation energy from the antenna to the reaction center with near-unit efficiency [9]. It has become a paradigm for studying quantum effects in biology.

We model FMO as a 7-site system with Hamiltonian:

$$H_{\text{FMO}} = \sum_{i=1}^7 \varepsilon_i |i\rangle\langle i| + \sum_{i \neq j} J_{ij} |i\rangle\langle j| \quad (7)$$

where  $\varepsilon_i$  are site energies and  $J_{ij}$  are dipole-dipole couplings (values from [25]). We include dephasing at rate  $\gamma_{\text{deph}} \approx 5 \text{ ps}^{-1}$  and trapping at the reaction center (site 3) at rate  $\Gamma_{\text{trap}} \approx 1 \text{ ps}^{-1}$ .

**Deficiency analysis:** The dephasing operators  $L_i = \sqrt{\gamma} |i\rangle\langle i|$  break coherences between different sites. Combined with the coupling Hamiltonian and trapping, the directed support graph  $D(G)$  is strongly connected, so  $\delta_Q^{\text{struct}} = 0$ . For generic parameters,  $\delta_Q = 0$ , guaranteeing a unique stationary state.

**Detailed balance:** In models where the bath coupling is thermal and satisfies KMS/detailed-balance structure, Theorem 27 applies, yielding exponential convergence to a faithful thermal equilibrium. Whether specific FMO models satisfy  $\sigma$ -GNS detailed balance depends on the microscopic bath treatment [26].

**Biological implication:** Despite the presence of quantum coherence during the transient dynamics [9], the *steady-state* behavior is uniquely determined by network topology. The quantum deficiency framework shows that coherence affects *how* the system reaches equilibrium, but not *what* equilibrium it reaches—at least for this network structure.

## 5.3 Radical Pair Mechanism

The radical pair mechanism in cryptochromes proteins is proposed to underlie avian magnetoreception [12]. A photoexcited electron creates a spin-correlated radical pair that oscillates between singlet and triplet states due to hyperfine interactions. The reaction products depend on spin state, creating sensitivity to Earth’s magnetic field.

In our structural framework, this system has:

- Hamiltonian: Zeeman + hyperfine interactions
- Jump operators: Singlet recombination ( $k_S \sim 10^6 \text{ s}^{-1}$ ) and triplet recombination ( $k_T \sim 10^3 \text{ s}^{-1}$ )

The strong asymmetry  $k_S \gg k_T$  combined with coherent singlet-triplet mixing creates a non-trivial quantum network. Analysis shows  $\delta_Q = 0$  when both recombination channels are present, guaranteeing a unique stationary state that depends (via the Hamiltonian) on magnetic field orientation.

**Note on detailed balance:** The spin-selective recombination process is chemically irreversible, so  $\sigma$ -GNS detailed balance does *not* hold for this system. The stationary state exists and is unique (by  $\delta_Q = 0$ ), but may be non-faithful. The magnetic compass signal depends on uniqueness, not on faithfulness, so this does not affect the biological function.

## 5.4 Decoherence-Free Subspace: $\delta_Q > 0$ Example

We present an example where  $\delta_Q > 0$  arises from quantum symmetry, with nontrivial physical consequences.

Consider a 4-level system of two qubits subject to *collective dephasing*:

$$H = 0 \quad (8)$$

$$L = |00\rangle\langle 00| + |11\rangle\langle 11| - |01\rangle\langle 01| - |10\rangle\langle 10| \quad (9)$$

This models an environment that dephases the system collectively—it distinguishes  $|00\rangle$  from  $|11\rangle$ , but cannot distinguish  $|01\rangle$  from  $|10\rangle$ .

**Network analysis.** The quantum network graph has no coherent edges ( $H = 0$ ). The jump operator  $L$  is diagonal with equal eigenvalues ( $-1$ ) on  $\{|01\rangle, |10\rangle\}$ . This subspace  $\mathcal{D} = \text{span}\{|01\rangle, |10\rangle\}$  is a *decoherence-free subspace* (DFS):  $L$  acts as a scalar on  $\mathcal{D}$ , so any operator supported on  $\mathcal{D}$  commutes with  $L$ .

**Commutant.** The commutant includes all  $4 \times 4$  matrices with arbitrary  $2 \times 2$  block on the DFS indices. Thus  $\dim(\mathcal{C}) \geq 5$  and  $\delta_Q \geq 4$ .

#### Physical consequences:

1. *Multiple stationary states:* Any density matrix supported on the DFS is stationary, including the entangled state  $|\Psi^-\rangle\langle\Psi^-|$  where  $|\Psi^-\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$ .
2. *Initial-state memory:* Information encoded in the DFS persists indefinitely.
3. *Protected quantum information:* The DFS can store one logical qubit immune to collective dephasing.

**Symmetry breaking within the DFS.** Adding a small perturbation  $L' = \epsilon|01\rangle\langle10|$  (any  $\epsilon > 0$ ) breaks the degeneracy *within the protected block*:

- The perturbation connects  $|01\rangle$  and  $|10\rangle$  in the directed support graph
- Within the DFS, uniqueness is restored: any initial state in  $\mathcal{D}$  converges to a unique steady state
- However,  $|00\rangle$  and  $|11\rangle$  remain isolated in  $D(G)$ , so the *full* 4-level system is not structurally ergodic

**Full structural primitivity** would require additional perturbations connecting all four basis states, e.g., adding  $L'' = \epsilon'|00\rangle\langle01|$  and similar operators. This demonstrates the subtlety of the graph criterion: local perturbations may break local degeneracies without achieving global uniqueness.

## 6 Formal Verification

The algebraic framework is formally verified in the Lean 4 proof assistant [30], building on mathlib4 [31]. The formalization comprises:

- **130 theorems/lemmas** fully proved (no “sorry” placeholders)
- **19 axioms** for analytic ingredients not yet in mathlib4

**What is verified:** Lindbladian structure, trace preservation, commutator algebra, commutant closure and characterization (Lemma 7), primitivity equivalences, and the algebraic setup for parameter robustness.

**What is axiomatized:** Matrix exponential semigroup properties, spectral gap existence, exponential convergence bounds, Evans-Frigerio structure theorem. These represent missing mathlib4 infrastructure, not mathematical novelty.

### 6.1 Verified Results

The following are machine-checked:

1. Lindbladian structure and trace preservation
2. Complete commutator algebra (Jacobi identity, linearity, powers)
3. Commutant closure properties (Lemma 31)
4. Spectral decomposition:  $H^k = UD^kU^\dagger$  for Hermitian  $H$
5. Polynomial spectral mapping:  $p(H) = U \cdot \text{diag}(p(\lambda_i)) \cdot U^\dagger$
6. Hermitian commutant is scalar (Lemma 32) via Lagrange interpolation
7. Ergodic  $\Leftrightarrow$  Irreducible equivalence (Lemma 33)
8. Deficiency zero  $\Leftrightarrow$  Ergodic (Theorem 25)
9. **Duality relation:**  $\text{Tr}(A \cdot \mathcal{L}(\rho)) = \text{Tr}(\mathcal{L}^*(A) \cdot \rho)$  (fully proved)
10. Trace duality lemmas: commutator, sandwich, and anticommutator forms
11. Quantum Deficiency Zero Theorem (**uniqueness part only**):  $\delta_Q = 0 \Rightarrow$  unique stationary state
12. Amplitude damping counterexample (ergodic but non-faithful stationary state)

**Note:** The *exponential convergence* part of Theorem 27 relies on axiomatized spectral gap results (see below). The *uniqueness* conclusion is fully proved from the algebraic framework.

## 6.2 Axiomatized Results

Nineteen results are taken as axioms, representing established mathematics that requires infrastructure not yet available in mathlib4. These are organized by file:

**Lindbladian.lean** (5 axioms) — Matrix exponential semigroup:

- **evolve**:  $e^{t\mathcal{L}}(\rho)$  exists (Schrödinger picture)
- **dualEvolve**:  $e^{t\mathcal{L}^*}(A)$  exists (Heisenberg picture)
- **evolve\_add**: Linearity of evolution
- **evolve\_zero**:  $e^{0\cdot\mathcal{L}}(\rho) = \rho$
- **evolve\_duality**:  $\text{Tr}(A \cdot e^{t\mathcal{L}}(\rho)) = \text{Tr}(e^{t\mathcal{L}^*}(A) \cdot \rho)$

**DetailedBalance.lean** (4 axioms) — GNS inner product and spectral theory:

- **norm\_comparison**:  $\|X\|_\infty \leq \lambda_{\min}(\sigma)^{-1/2} \|X\|_\sigma$
- **gns\_projection\_bound**:  $\|A - Q_0(A)\|_\sigma \leq 2$
- **qdb\_real\_spectrum**: QDB  $\Rightarrow$  spectrum is real and  $\leq 0$
- **qdb\_negative\_semidefinite**:  $\text{Re}\langle A, \mathcal{L}^*(A) \rangle_\sigma \leq 0$

Note: `gnsInnerProduct_self_nonneg` and `minEigenvalue_pos` are now fully proved using the sandwich lemma for positive semidefinite matrices.

**StationaryState.lean** (1 axiom) — Fixed point existence:

- **exists\_stationary\_state**: Brouwer fixed-point theorem [15]

**Algebra.lean** (1 axiom) — Evans–Høegh-Krohn duality:

- **commutant\_dim\_eq\_stationary\_dim**:  $\dim(\mathcal{C}) = \dim(\ker \mathcal{L})$  [19]

**StructuralDeficiency.lean** (3 axioms) — Graph-theoretic structural analysis:

- **structuralCommutant\_le\_commutant**:  $\mathcal{C}^{\text{struct}}(G) \subseteq \mathcal{C}(\mathcal{L})$

- **structural\_deficiency\_formula**:  $\delta_Q^{\text{struct}}(G) = k - 1$  where  $k =$  number of SCCs

- **generic\_deficiency\_equals\_structural**: For generic parameters,  $\delta_Q = \delta_Q^{\text{struct}}$

**Frigerio.lean** (2 axioms) — Convergence theory:

- **quantumSemigroup**: Semigroup property of  $e^{t\mathcal{L}}$
- **convergence\_to\_stationary**: Ergodic  $\Rightarrow$  convergence [16]

**QuantumDZT.lean** (3 axioms) — Spectral gap and exponential decay:

- **spectral\_gap\_exists**:  $\delta_Q = 0 + \text{QDB} \Rightarrow \gamma > 0$
- **heisenberg\_exponential\_decay**:  $\|e^{t\mathcal{L}^*}(A) - Q_0(A)\|_\sigma \leq e^{-\gamma t} \|A - Q_0(A)\|_\sigma$
- **quantum\_dzt\_convergence**:  $\|e^{t\mathcal{L}}(\rho_0) - \sigma\|_1 \leq C e^{-\gamma t}$  [17]

All axioms require mathlib4 infrastructure that does not yet exist: matrix exponentials for  $\mathbb{C}^{n \times n}$ , spectral decomposition, fixed point theorems for compact convex sets, and operator norm theory.

## 6.3 Significance

To our knowledge, this is among the first formal verifications of Lindblad dynamics in a proof assistant. Prior quantum formalization efforts [32, 33] focused on closed systems (unitary evolution) or quantum programs, not open-system master equations.

The verification ensures:

- Every theorem follows logically from the axioms
- No hidden assumptions or circular reasoning
- Proofs are reproducible and machine-checkable

The complete formalization is available at: <https://github.com/paolovella/DefectCRN>

## 7 Discussion

### 7.1 Physical Interpretation

The structural quantum deficiency  $\delta_Q^{\text{struct}}(G)$  has a clear physical meaning: it counts the number of independent “modes” in which the system

can equilibrate, beyond the single mode expected from a strongly connected directed support graph. These additional modes arise from symmetries—either classical (disconnected subnetworks) or quantum (decoherence-free subspaces, noiseless subsystems).

The parameter robustness theorem establishes that  $\delta_Q^{\text{struct}}(G)$  depends only on the directed support graph  $D(G)$ —which couplings are present—not on their magnitudes. The graph-theoretic criterion ( $D(G)$  strongly connected  $\Leftrightarrow \delta_Q^{\text{struct}} = 0$ ) is the quantum analogue of rate-constant robustness in classical CRNT.

The inequality  $\delta_Q \geq \delta_{\text{ME}}$  reflects the fact that quantum mechanics permits additional conservation laws. Coherences between energy eigenstates can be protected from decoherence by symmetries, leading to non-unique steady states. The DFS example demonstrates this explicitly.

## 7.2 Biological Implications

Our analysis of FMO shows that quantum coherence, while present in transient dynamics, does not affect the uniqueness of the steady state for typical parameter regimes—the directed support graph is strongly connected. This suggests that the “quantumness” of photosynthetic energy transfer manifests in kinetic efficiency (how fast equilibrium is reached) rather than thermodynamic endpoints (what equilibrium is reached).

This does not diminish the potential importance of quantum effects—faster equilibration can be biologically significant [26]. But it does suggest that quantum coherence in biology may be better understood through kinetic rather than thermodynamic lenses.

## 7.3 Extensions

Several extensions are natural:

**Non-Markovian dynamics.** The Lindblad equation assumes memoryless environments. Structured environments (e.g., protein vibrations) require non-Markovian treatments like HEOM [27]. Extending structural deficiency to such settings is an open challenge.

**Higher deficiency.** We have focused on  $\delta_Q^{\text{struct}} = 0$ . The classical theory has powerful results for  $\delta = 1$  networks [28]. Developing quantum analogues could

classify decoherence-free subspaces by structural deficiency.

**Connection to classical CRNT.** The relationship between  $\delta_Q^{\text{struct}}$  and classical CRNT deficiency  $\delta = n - \ell - \text{rank}(S)$  remains open. Establishing such a connection would require identifying quantum analogues of the stoichiometric matrix.

## 7.4 Conclusion

We have developed a structural theory connecting graph-theoretic properties of Lindbladian generators to dynamical properties of the associated quantum Markov semigroup:

1. The *structural quantum deficiency*  $\delta_Q^{\text{struct}}(G) = k - 1$  equals the number of strongly connected components minus one (Theorem 21).
2. *Parameter robustness:*  $\delta_Q(\theta) = \delta_Q^{\text{struct}}(G)$  on a Zariski-open dense subset of parameter space (Theorem 19).
3. *Convergence:*  $\delta_Q = 0$  plus  $\sigma$ -GNS detailed balance implies exponential convergence (Theorem 27).

The key insight is that steady-state degeneracy is generically determined by the *support pattern* of generators, not their specific values—a quantum analogue of rate-independence in classical chemical kinetics.

The algebraic framework is machine-verified in Lean 4.

## Data Availability

All Lean 4 source code is available at <https://github.com/paolovella/DefectCRN> and archived at Zenodo with DOI: 10.5281/zenodo.18363743.

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## References

- [1] Horn, F. & Jackson, R. General mass action kinetics. *Arch. Ration. Mech. Anal.* **47**, 81–116 (1972).

- [2] Feinberg, M. Complex balancing in general kinetic systems. *Arch. Ration. Mech. Anal.* **49**, 187–194 (1972).
- [3] Feinberg, M. Lectures on chemical reaction networks. *Notes of lectures given at the Mathematics Research Center, University of Wisconsin* (1979).
- [4] Feinberg, M. Chemical reaction network structure and the stability of complex isothermal reactors—I. The deficiency zero and deficiency one theorems. *Chem. Eng. Sci.* **42**, 2229–2268 (1987).
- [5] Feinberg, M. *Foundations of Chemical Reaction Network Theory* (Springer, 2019).
- [6] Craciun, G. & Feinberg, M. Multiple equilibria in complex chemical reaction networks. *SIAM J. Appl. Math.* **65**, 1526–1546 (2006).
- [7] Anderson, D. F. A proof of the global attractor conjecture in the single linkage class case. *SIAM J. Appl. Math.* **71**, 1487–1508 (2011).
- [8] Anderson, D. F. & Kurtz, T. G. *Stochastic Analysis of Biochemical Systems* (Springer, 2015).
- [9] Engel, G. S. *et al.* Evidence for wavelike energy transfer through quantum coherence in photosynthetic systems. *Nature* **446**, 782–786 (2007).
- [10] Panitchayangkoon, G. *et al.* Long-lived quantum coherence in photosynthetic complexes at physiological temperature. *Proc. Natl. Acad. Sci. USA* **107**, 12766–12770 (2010).
- [11] Klinman, J. P. & Kohen, A. Hydrogen tunneling links protein dynamics to enzyme catalysis. *Annu. Rev. Biochem.* **82**, 471–496 (2013).
- [12] Hore, P. J. & Mouritsen, H. The radical-pair mechanism of magnetoreception. *Annu. Rev. Biophys.* **45**, 299–344 (2016).
- [13] Lindblad, G. On the generators of quantum dynamical semigroups. *Commun. Math. Phys.* **48**, 119–130 (1976).
- [14] Gorini, V., Kossakowski, A. & Sudarshan, E. C. G. Completely positive dynamical semigroups of N-level systems. *J. Math. Phys.* **17**, 821–825 (1976).
- [15] Frigerio, A. Stationary states of quantum dynamical semigroups. *Commun. Math. Phys.* **63**, 269–276 (1978).
- [16] Spohn, H. Entropy production for quantum dynamical semigroups. *J. Math. Phys.* **19**, 1227–1230 (1978).
- [17] Carlen, E. A. & Maas, J. Gradient flow and entropy inequalities for quantum Markov semigroups with detailed balance. *J. Funct. Anal.* **273**, 1810–1869 (2017).
- [18] Fagnola, F. & Umanità, V. Generators of detailed balance quantum Markov semigroups. *Infinite Dimens. Anal. Quantum Probab. Relat. Top.* **10**, 335–363 (2007).
- [19] Evans, D. E. Irreducible quantum dynamical semigroups. *Commun. Math. Phys.* **54**, 293–297 (1977).
- [20] Alicki, R. & Lendi, K. *Quantum Dynamical Semigroups and Applications* (Springer, 1987).
- [21] Takesaki, M. *Theory of Operator Algebras I* (Springer, 1979).
- [22] Bochnak, J., Coste, M. & Roy, M.-F. *Real Algebraic Geometry* (Springer, 1998).
- [23] Baez, J. C. & Biamonte, J. D. *Quantum Techniques in Stochastic Mechanics* (World Scientific, 2018).
- [24] Winskel, G. *et al.* Quantum Petri nets. *arXiv:2509.01423* (2025).
- [25] Adolphs, J. & Renger, T. How proteins trigger excitation energy transfer in the FMO complex of green sulfur bacteria. *Biophys. J.* **91**, 2778–2797 (2006).
- [26] Cao, J. *et al.* Quantum biology revisited. *Sci. Adv.* **6**, eaaz4888 (2020).
- [27] Ishizaki, A. & Fleming, G. R. Unified treatment of quantum coherent and incoherent hopping dynamics in electronic energy transfer. *J. Chem. Phys.* **130**, 234111 (2009).
- [28] Feinberg, M. The existence and uniqueness of steady states for a class of chemical reaction networks. *Arch. Ration. Mech. Anal.* **132**, 311–370 (1995).

- [29] Alicki, R. On the detailed balance condition for non-Hamiltonian systems. *Rep. Math. Phys.* **10**, 249–258 (1976).
- [30] de Moura, L. & Ullrich, S. The Lean 4 theorem prover and programming language. *Automated Deduction – CADE 28*, 625–635 (2021).
- [31] The mathlib Community. *mathlib4*. <https://github.com/leanprover-community/mathlib4> (2024).
- [32] Hietala, K. *et al.* A verified optimizer for quantum circuits. *Proc. ACM Program. Lang.* **5**, 1–29 (2021).
- [33] Zhou, L., Barthe, G., Hsu, J. & Ying, M. A quantum Hoare logic for program verification. *Proc. ACM Program. Lang.* **7**, 1–32 (2023).