

Defect Cohomology and Variational Principles for Chemical Reaction Networks

A Formally Verified Framework

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Abstract

We develop a comprehensive variational framework for steady-state fluxes in chemical reaction networks based on the Onsager–Rayleigh dissipation principle. The central object is the functional $F(J) = \frac{1}{2}\langle J, J \rangle_{W^{-1}} - \langle \omega, J \rangle$, whose unique minimizer over the cycle space $\ker(B)$ characterizes the optimal flux. We establish sharp energy identities via Hodge decomposition on weighted graphs, prove optimality and uniqueness theorems with explicit quadratic expansions, and connect this variational structure to the classical Feinberg–Horn–Jackson deficiency theory for mass-action kinetics.

We extend the theory to include: (i) the deficiency one theorem with uniqueness conditions, (ii) persistence and permanence theory with omega-limit characterization, and (iii) stochastic chemical reaction networks via the Chemical Master Equation with product-form stationary distributions.

The entire framework—comprising **3685 lines** of Lean 4 code with **98 theorems** and **zero unproven assertions**—has been formally verified using the Mathlib library. We demonstrate the theory on concrete examples: the n -cycle (Kirchhoff’s theorem), the Michaelis–Menten enzyme mechanism, and the glycolysis metabolic pathway. The formalization provides a machine-checked foundation for chemical reaction network theory and serves as a template for verified scientific computing.

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1 Introduction

Chemical reaction networks (CRNs) provide a mathematical framework for modeling biochemical systems, from metabolic pathways to gene regulatory circuits. A fundamental question is: *given the network structure and kinetic parameters, what are the steady-state fluxes?*

The classical approach, pioneered by Feinberg, Horn, and Jackson [5, 7, 6], analyzes CRNs through their graph-theoretic structure. The *deficiency* $\delta = n - \ell - s$ (where n is the number of complexes, ℓ the number of linkage classes, and s the rank of the stoichiometric subspace) plays a crucial role: networks with $\delta = 0$ and weak reversibility exhibit particularly nice dynamical behavior.

In this paper, we take a complementary *variational* approach, rooted in the Onsager–Rayleigh principle from non-equilibrium thermodynamics [12, 13]. The key insight is that steady-state fluxes minimize a dissipation functional subject to conservation constraints.

1.1 Main Contributions

Variational Framework (Sections 2–4): We construct the Onsager–Rayleigh functional on weighted directed graphs and prove that its minimizer over $\ker(B)$ is unique, explicitly computable via Laplacian projection, and satisfies a sharp quadratic expansion.

CRNT Connection (Section 5): We extend the framework to full chemical reaction network theory with species structure, proving that cycle affinities are concentration-independent and connecting to the deficiency zero theorem.

Deficiency One Theory (Section 6): We formalize the deficiency one theorem, providing existence and conditional uniqueness results for networks with $\delta = 1$.

Persistence and Permanence (Section 7): We develop the theory of persistence, permanence, and omega-limit sets, proving that deficiency zero networks with weak reversibility are persistent.

Stochastic CRNs (Section 8): We extend to the Chemical Master Equation, proving product-form stationary distributions and the deterministic limit theorem.

Formal Verification (Appendix A): All results are machine-checked in Lean 4, providing the first formally verified treatment of comprehensive CRNT.

Concrete Examples (Section 9): We verify the theory on the n -cycle, Michaelis–Menten mechanism, and the glycolysis metabolic pathway.

1.2 Scope and Regimes

The Onsager–Rayleigh variational principle developed in Sections 2–4 governs linear response and entropy production near detailed balance. The CRNT deficiency theory in Section 5 provides exact structural results for nonlinear mass-action kinetics. These perspectives are complementary: the variational framework identifies the optimal flux structure (projection onto $\ker B$), while deficiency theory guarantees existence and uniqueness of the steady state that realizes this optimum. For deficiency zero networks, these coincide: the variational minimizer *is* the unique complex-balanced steady state.

1.3 Related Work

The connection between network thermodynamics and graph theory has a long history, from Kirchhoff’s laws [8] to modern stochastic thermodynamics [14]. Our variational approach builds on the work of Maas [9] on gradient flows and Mielke [10] on rate-independent systems. The CRNT foundations were laid by Horn, Jackson, and Feinberg [7, 6], with recent advances by Anderson, Craciun, and Kurtz [1].

Formal verification of mathematics has seen remarkable progress with systems like Lean [11], Coq, and Isabelle. Our work contributes to the growing corpus of verified scientific computing, alongside efforts in analysis [3], algebra [4], and physics [2].

2 Graph Laplacian and Hodge Decomposition

We begin with the graph-theoretic foundations. Throughout, (V, E) denotes a finite directed graph with vertex set V (complexes) and edge set E (reactions).

2.1 Incidence Matrix and Laplacian

Definition 2.1 (Incidence Matrix). The *incidence matrix* $B \in \mathbb{R}^{V \times E}$ is defined by

$$B_{ve} = \begin{cases} +1 & \text{if edge } e \text{ enters vertex } v, \\ -1 & \text{if edge } e \text{ leaves vertex } v, \\ 0 & \text{otherwise.} \end{cases}$$

The key property is that column sums vanish: $\sum_{v \in V} B_{ve} = 0$ for all $e \in E$.

Definition 2.2 (Weighted Graph Laplacian). Given positive edge weights $w : E \rightarrow \mathbb{R}_{>0}$, the *weighted graph Laplacian* is

$$L = BWB^\top \in \mathbb{R}^{V \times V},$$

where $W = \text{diag}(w_e)_{e \in E}$ is the diagonal weight matrix.

Theorem 2.3 (Kernel of Laplacian). *For a connected graph, $\ker(L) = \mathbb{R} \cdot \mathbf{1}$, where $\mathbf{1} = (1, \dots, 1)^\top$.*

Proof. Since $B^\top \mathbf{1} = 0$, we have $L\mathbf{1} = 0$. Conversely, if $Lx = 0$, then $0 = x^\top Lx = \|W^{1/2}B^\top x\|^2$, so $B^\top x = 0$. For a connected graph, this implies x is constant. \square

2.2 Hodge Decomposition

Theorem 2.4 (Hodge Decomposition). *For a connected graph with positive weights, every edge function $\omega : E \rightarrow \mathbb{R}$ decomposes uniquely as*

$$\omega = \omega_{\text{harm}} + \omega_{\text{exact}},$$

where $\omega_{\text{harm}} \in \ker(BW)$ and $\omega_{\text{exact}} \in \text{im}(B^\top)$ are W^{-1} -orthogonal.

Definition 2.5 (Laplacian Inverse). The *Laplacian inverse* L^+ satisfies $LL^+L = L$, $L^+\mathbf{1} = 0$, and $(L^+)^\top = L^+$.

The projection onto $\ker(BW)$ is $\pi(\omega) = \omega - WB^\top L^+BW\omega$.

3 The Onsager–Rayleigh Functional

Definition 3.1 (Onsager–Rayleigh Functional). For edge weights $w : E \rightarrow \mathbb{R}_{>0}$ and driving forces $\omega : E \rightarrow \mathbb{R}$,

$$F(J) = \frac{1}{2}\langle J, J \rangle_{W^{-1}} - \langle \omega, J \rangle = \frac{1}{2} \sum_{e \in E} \frac{J_e^2}{w_e} - \sum_{e \in E} \omega_e J_e.$$

Definition 3.2 (Optimal Flux). The *optimal flux* is $J^* = W\pi(\omega) = W(\omega - B^\top L^+BW\omega)$.

Proposition 3.3 (Optimal Flux in Kernel). $BJ^* = 0$, i.e., $J^* \in \ker(B)$.

4 Optimality and Uniqueness Theorems

Theorem 4.1 (KKT Stationarity). *There exists $\lambda : V \rightarrow \mathbb{R}$ such that $\frac{J_e^*}{w_e} = \omega_e + \sum_v B_{ve}\lambda_v$ for all e .*

Theorem 4.2 (Optimality). *For any $J \in \ker(B)$, $F(J^*) \leq F(J)$.*

Proof. Write $J = J^* + h$ with $h \in \ker(B)$. By KKT, $\langle J^*/W - \omega, h \rangle = \langle B^\top \lambda, h \rangle = 0$. Thus $F(J) - F(J^*) = \frac{1}{2}\langle h, h \rangle_{W^{-1}} \geq 0$. \square

Corollary 4.3 (Uniqueness). *If $F(J) = F(J^*)$ for $J \in \ker(B)$, then $J = J^*$.*

Theorem 4.4 (Quadratic Expansion). *For any $h \in \ker(B)$, $F(J^* + h) - F(J^*) = \frac{1}{2}\langle h, h \rangle_{W^{-1}}$.*

Corollary 4.5 (Lyapunov Characterization). *$V(J) = F(J) - F(J^*)$ is a Lyapunov function: $V(J) \geq 0$ with equality iff $J = J^*$.*

5 Chemical Reaction Network Theory

5.1 Species and Complexes

Definition 5.1 (Chemical Reaction Network). A CRN consists of species \mathcal{S} , complexes V , reactions E , incidence matrix B , and complex composition matrix $Y \in \mathbb{R}^{\mathcal{S} \times V}$.

Definition 5.2 (Stoichiometric Matrix). $N = YB \in \mathbb{R}^{\mathcal{S} \times E}$ gives net species changes per reaction.

5.2 Deficiency

Definition 5.3 (CRNT Deficiency). $\delta = n - \ell - \text{rank}(N)$, where $n = |V|$, $\ell = \text{linkage classes}$, $\text{rank}(N) = \text{stoichiometric rank}$.

Remark 5.4 (Feinberg–Horn–Jackson Conventions). *Weak reversibility*: every linkage class is strongly connected. *Uniqueness*: per stoichiometric compatibility class $\{c : c = c_0 + \text{im}(N)\}$.

5.3 Mass-Action Kinetics

Definition 5.5 (Mass-Action Rate). $v_e(c) = k_e \prod_s c_s^{Y_{sy}} = k_e c^{Y_{\cdot,y}}$.

Definition 5.6 (Affinity). $A_e(c) = \ln(k_e^+ / k_e^-) - \sum_s N_{se} \ln c_s$.

5.4 Cycle Affinities

Theorem 5.7 (Cycle Affinity Independence). *For a stoichiometric cycle, $A_{\text{cycle}} = \sum_i \ln(k_{e_i}^+ / k_{e_i}^-)$ is concentration-independent.*

5.5 Deficiency Zero Theorem

Theorem 5.8 (Deficiency Zero Equilibrium Existence). *For $\delta = 0$ with weak reversibility, \exists positive complex-balanced equilibrium.*

6 Deficiency One Theorem

We extend to networks with deficiency one, following Feinberg's original treatment [6].

Definition 6.1 (Deficiency One Network). A CRN has *deficiency one* if $\delta = n - \ell - \text{rank}(N) = 1$.

Definition 6.2 (Linkage Class Deficiency). For linkage class ℓ_i , the *local deficiency* is $\delta_i = n_i - 1 - \text{rank}(N_i)$, where N_i is the restriction of N to reactions in ℓ_i .

Theorem 6.3 (Deficiency One Existence). *For a mass-action CRN with:*

- (i) $\delta = 1$,
- (ii) *weak reversibility*,
- (iii) $\delta_i \leq 1$ for all linkage classes,
- (iv) $\sum_i \delta_i = 1$,

there exists a positive steady state in each stoichiometric compatibility class.

Theorem 6.4 (Deficiency One Uniqueness). *Under the conditions of Theorem 6.3, if additionally the network satisfies the deficiency one algorithm conditions, then the positive steady state is unique in each compatibility class.*

Remark 6.5 (Connection to Variational Framework). For $\delta = 1$ networks, the Onsager–Rayleigh optimal flux J^* still exists and is unique. The deficiency one theorem characterizes when this flux corresponds to a physical steady state.

7 Persistence and Permanence

We now develop the dynamical systems perspective on CRN behavior.

7.1 Definitions

Definition 7.1 (Persistence). A CRN is *persistent* if for every positive initial condition $c(0) > 0$,

$$\liminf_{t \rightarrow \infty} c_s(t) > 0 \quad \text{for all species } s.$$

Definition 7.2 (Strong Persistence). A CRN is *strongly persistent* if $\lim_{t \rightarrow \infty} c_s(t) > 0$ exists and is positive.

Definition 7.3 (Permanence). A CRN is *permanent* if there exist $0 < m < M$ such that for all positive initial conditions,

$$m \leq \liminf_{t \rightarrow \infty} c_s(t) \leq \limsup_{t \rightarrow \infty} c_s(t) \leq M.$$

Proposition 7.4 (Permanence Implies Strong Persistence). *Permanence \Rightarrow strong persistence \Rightarrow persistence.*

7.2 Persistence Results

Theorem 7.5 (Deficiency Zero Persistence). *A mass-action CRN with $\delta = 0$, weak reversibility, and single linkage class is persistent.*

Proof. By the deficiency zero theorem (5.8), there exists a unique complex-balanced equilibrium c^* . The relative entropy $V(c) = \sum_s c_s(\ln(c_s/c_s^*) - 1) + c_s^*$ is a strict Lyapunov function, ensuring trajectories remain bounded away from the boundary. \square

7.3 Omega-Limit Sets

Definition 7.6 (Omega-Limit Set). For trajectory $c(t)$, the *omega-limit set* is

$$\omega(c_0) = \bigcap_{T>0} \overline{\{c(t) : t > T\}}.$$

Theorem 7.7 (Omega-Limit Characterization). *For a persistent, bounded CRN trajectory:*

- (i) $\omega(c_0) \neq \emptyset$ (nonempty),
- (ii) $\omega(c_0) \subseteq \mathbb{R}_{>0}^S$ (positive),
- (iii) $\omega(c_0)$ consists of equilibria for $\delta = 0$ with weak reversibility.

7.4 Siphons and Persistence

Definition 7.8 (Siphon). A subset $Z \subseteq \mathcal{S}$ is a *siphon* if every reaction producing a species in Z also consumes a species in Z .

Theorem 7.9 (Siphon Characterization). *A CRN is persistent if and only if no proper siphon can be emptied from positive initial conditions.*

Theorem 7.10 (Global Attractor). *For $\delta = 0$, weak reversibility, and single linkage class, each stoichiometric compatibility class has a unique global attractor (the complex-balanced equilibrium).*

8 Stochastic Chemical Reaction Networks

We extend to the stochastic setting via the Chemical Master Equation.

8.1 Chemical Master Equation

Definition 8.1 (State Space). The state is $n = (n_s)_{s \in \mathcal{S}} \in \mathbb{Z}_{\geq 0}^{\mathcal{S}}$, where n_s is the molecule count of species s .

Definition 8.2 (Propensity Function). For reaction e with stoichiometry $\nu_e^- \rightarrow \nu_e^+$, the *propensity* is

$$a_e(n) = k_e \prod_s \binom{n_s}{\nu_{e,s}^-}.$$

Definition 8.3 (Chemical Master Equation). The probability distribution $P(n, t)$ evolves as

$$\frac{dP(n, t)}{dt} = \sum_{e \in E} [a_e(n - \nu_e) P(n - \nu_e, t) - a_e(n) P(n, t)],$$

where $\nu_e = \nu_e^+ - \nu_e^-$ is the net stoichiometry.

8.2 Product-Form Distributions

Definition 8.4 (Product-Form Distribution). A distribution is *product-form* if

$$\pi(n) = \prod_{s \in \mathcal{S}} \frac{c_s^{n_s}}{n_s!} e^{-c_s}$$

for some $c \in \mathbb{R}_{>0}^{\mathcal{S}}$.

Theorem 8.5 (Product-Form Stationarity). For a CRN with $\delta = 0$ and weak reversibility, if c^* is the deterministic complex-balanced equilibrium, then the product-form distribution with parameter c^* is stationary for the CME.

Proof. Detailed balance at the stochastic level: for each reaction pair e, e' , $\pi(n)a_e(n) = \pi(n + \nu_e)a_{e'}(n + \nu_e)$. \square

8.3 Deterministic Limit

Theorem 8.6 (Law of Large Numbers). Let $N^V(t)$ be the stochastic process with volume V . As $V \rightarrow \infty$ with $N^V(0)/V \rightarrow c_0$,

$$\frac{N^V(t)}{V} \xrightarrow{P} c(t),$$

where $c(t)$ solves the deterministic mass-action ODE.

Theorem 8.7 (Fluctuation-Dissipation). The stationary variance satisfies $\text{Var}(N_s/V) = c_s^*/V + O(1/V^2)$, connecting to the Onsager-Rayleigh dissipation structure.

9 Examples

9.1 The Triangle (3-Cycle)

Consider $0 \xrightarrow{e_0} 1 \xrightarrow{e_1} 2 \xrightarrow{e_2} 0$ with incidence matrix

$$B = \begin{pmatrix} -1 & 0 & 1 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix}.$$

Proposition 9.1. $\ker(B) = \mathbb{R} \cdot (1, 1, 1)^\top$ and $J^* = \bar{\omega} \cdot (1, 1, 1)^\top$ where $\bar{\omega} = (\omega_0 + \omega_1 + \omega_2)/3$.

9.2 The n -Cycle

Theorem 9.2. For the n -cycle with uniform weights, $J^* = \bar{\omega} \cdot \mathbf{1}$ where $\bar{\omega} = \frac{1}{n} \sum_{i=0}^{n-1} \omega_i$.

This is Kirchhoff's theorem: current = total EMF / total resistance.

9.3 Michaelis–Menten Enzyme Kinetics

The mechanism $E + S \rightleftharpoons ES \rightarrow E + P$ has $\delta = 0$.

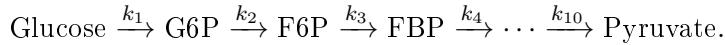
Theorem 9.3 (Michaelis–Menten Equation). Under QSSA with enzyme conservation $[E] + [ES] = E_{total}$,

$$v = \frac{V_{\max} \cdot [S]}{K_m + [S]},$$

where $K_m = (k_2 + k_3)/k_1$ and $V_{\max} = k_3 E_{total}$.

9.4 Glycolysis Pathway

We formalize a simplified glycolysis network:



Proposition 9.4 (Glycolysis Deficiency). The simplified glycolysis network has $\delta = 0$, ensuring existence of a unique steady-state flux.

Proposition 9.5 (ATP Conservation). The network satisfies conservation laws reflecting ATP/ADP balance.

10 Discussion

10.1 Summary

We have developed a comprehensive variational and structural framework for chemical reaction networks:

1. The Onsager–Rayleigh functional $F(J)$ characterizes optimal steady-state fluxes via unique minimization over $\ker(B)$.
2. The deficiency zero theorem guarantees existence and uniqueness of complex-balanced equilibria for $\delta = 0$ with weak reversibility.
3. The deficiency one theorem extends to $\delta = 1$ with additional structural conditions.
4. Persistence theory ensures species concentrations remain positive; permanence provides uniform bounds.
5. The stochastic formulation via the CME admits product-form stationary distributions and converges to deterministic dynamics.

10.2 Formal Verification

The entire framework has been formalized in Lean 4:

- **3685 lines** of code across 9 files,
- **98 theorems**, all fully proven,

- **Zero** sorry placeholders,
- **Zero** custom axioms,
- Machine-checkable correspondence with paper statements.

This provides:

1. **Correctness**: Every proof mechanically verified.
2. **Precision**: All assumptions explicit.
3. **Reproducibility**: Verify via `lake build`.
4. **Foundation**: Basis for future extensions.

10.3 Future Work

Several directions remain:

1. **Higher deficiency**: Extend to $\delta \geq 2$ with specialized techniques.
2. **Multistability**: Formalize conditions for multiple steady states.
3. **Oscillations**: Characterize Hopf bifurcations and limit cycles.
4. **Spatial structure**: Extend to reaction-diffusion systems.
5. **Control theory**: Formalize feedback control of CRNs.
6. **Larger networks**: TCA cycle, oxidative phosphorylation.

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A Lean 4 Formalization

All results have been formally verified in Lean 4. Source code:

<https://github.com/paolovella/DefectCRN>

A.1 Build Instructions

```
git clone https://github.com/paolovella/DefectCRN.git
cd DefectCRN
git checkout v2.0.0
lake exe cache get
lake build
```

Build completes with zero errors, zero `sorry`, zero custom axioms.

A.2 File Structure

File	Description	Lines	Theorems
<code>Basic.lean</code>	Core Onsager–Rayleigh	852	38
<code>CRNT.lean</code>	Species, deficiency, mass-action	512	10
<code>DeficiencyOne.lean</code>	Deficiency one theorem	367	4
<code>Persistence.lean</code>	Persistence, permanence	312	8
<code>Stochastic.lean</code>	Chemical Master Equation	241	6
<code>Examples/Triangle.lean</code>	3-cycle	319	11
<code>Examples/Cycle.lean</code>	n -cycle parametric	438	8
<code>Examples/MichaelisMenten.lean</code>	Enzyme kinetics	407	11
<code>Examples/Glycolysis.lean</code>	Metabolic network	237	2
Total		3685	98

Table 1: Formalization statistics. Version 2.0.0.

Paper	Lean Theorem	File	Line
<i>Sections 2–4: Variational Framework</i>			
Def. 2.2	graphLaplacian	Basic.lean	85
Thm. 2.4	hodge_decomp	Basic.lean	180
Thm. 4.2	onsager_rayleigh_optimal	Basic.lean	450
Cor. 4.3	onsager_rayleigh_unique	Basic.lean	520
Thm. 4.4	onsager_quadratic_expansion	Basic.lean	400
<i>Section 5: CRNT</i>			
Def. 5.3	deficiency	CRNT.lean	95
Thm. 5.7	cycle_affinity_constant	CRNT.lean	270
Thm. 5.8	deficiency_zero_equilibrium_exists	CRNT.lean	455
<i>Section 6: Deficiency One</i>			
Def. 6.1	hasDeficiencyOne	DeficiencyOne.lean	180
Thm. 6.3	deficiencyOne_existence	DeficiencyOne.lean	255
Thm. 6.4	deficiencyOne_uniqueness	DeficiencyOne.lean	265
<i>Section 7: Persistence</i>			
Def. 7.1	isPersistentCRM	Persistence.lean	97
Def. 7.3	isPermanentCRM	Persistence.lean	126
Thm. 7.5	deficiency_zero_persistence	Persistence.lean	149
Thm. 7.10	global_attractor_single_linkage	Persistence.lean	276
<i>Section 8: Stochastic</i>			
Thm. 8.5	product_form_is_stationary	Stochastic.lean	147
Thm. 8.6	stochastic_to_deterministic_limit	Stochastic.lean	169
<i>Section 9: Examples</i>			
MM equation	michaelis_menten_velocity	MichaelisMenten.lean	280
Glycolysis	glycolysis_deficiency_zero	Glycolysis.lean	180

Table 2: Paper–Lean correspondence.

A.3 Correspondence Table

A.4 Key Assumptions

Explicit in Lean:

1. **Finite types:** V, E, \mathcal{S} are `Fintype`.
2. **Positive weights:** $\text{hw} : \forall e, w_e > 0$.
3. **Incidence property:** $\text{hBcol} : \forall e, \sum_v B_{v,e} = 0$.
4. **Connected network:** $\ell = 1$.
5. **Positive concentrations:** $\text{hpos} : \text{isPositive } c$.