Supporting Information for "Reaction Yield Oscillates over Reaction Time in First-Order Chemical Reactions"

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In this supporting information, we mathematically prove that the number of yield oscillations is at most $\lfloor \frac{n}{2} \rfloor$ for a reaction path network with n equilibrium states, and we construct a network that achieves this upper bound.

1 Preliminalies

This section establishes the fundamental concepts of chemical reaction networks and auxiliary lemmas used throughout this supporting information.

We first introduce some basic notation. For a positive integer k, let $[k] = \{1, 2, \ldots, k\}$. For a matrix $A \in \mathbb{R}^{n\times n}$, the matrix exponential is defined as $\mathrm{e}^A = \sum_{d=0}^{\infty} \frac{A^d}{d!}$. For a real number $x \in \mathbb{R}$, the floor function $\lfloor x \rfloor$ denotes the largest integer less than or equal to x.

We consider networks of chemical reactions [5, 6]. For each equilibrium state i, let E_i denote its potential energy. For states i and j that can transition between each other, let $E_{i-j}(= E_{j-i})$ denote the potential energy of their transition state. The rate constant K_{ij} from state j to state i is given by

$$K_{ij} = \Gamma \frac{k_B T}{h} \exp\left(-\frac{E_{i-j} - E_j}{RT}\right),$$

where k_B is the Boltzmann constant, h is the Planck constant, R is the gas constant, T is the temperature, and Γ is the transmission coefficient.

We represent a chemical reaction network with n equilibrium states as a weighted undirected graph $G = (V, E, w_V, w_E)$ with vertex set $V = [n]$ and edge set E. Each vertex $i \in V$ corresponds to an equilibrium state, and each edge $\{i, j\} \in E$ represents a possible transition between states i and j. The weight functions $w_V : V \to \mathbb{R}_{>0}$ and $w_E : E \to \mathbb{R}_{>0}$ are defined by $w_V(i) = \exp(-E_i/RT)$ and $w_E(i, j) = \Gamma \frac{k_B T}{h} \exp(-E_{i-j}/RT)$, respectively. For this weighted graph, the graph Laplacian matrix $L = (L_{ij})_{ij}$ is defined as

$$L_{ij} = \begin{cases} \sum_{k:\{i,k\}\in E} w_E(i,k) & \text{if } i = j; \\ -w_E(i,j) & \text{if } \{i,j\} \in E; \\ 0 & \text{if } i \neq j \text{ and } \{i,j\} \notin E. \end{cases}$$

Let $\pi = (\pi_1, \pi_2, \ldots, \pi_n)$ be the normalized weighted degree vector, where

$$\pi_i = \frac{w_V(i)}{\sum_{j=1}^n w_V(j)}.$$

Let $\Pi = \mathrm{diag}(\pi)$ be the corresponding diagonal matrix. The transition dynamics of the chemical reaction network are described by the rate constant matrix $K = -L\Pi^{-1}$ [6].

For any $i, j \in V$, we define the function $f_{ij}(t)$ to represent the quantity in state i at time t when the system initially occupies state j at time $t = 0$. Then $f_{ij}(t)$ is given by the (i, j) entry of the matrix exponential e^{tK}:

$$f_{ij}(t) = (\mathrm{e}^{tK})_{i,j} = \boldsymbol{e}_i^\top \mathrm{e}^{tK} \boldsymbol{e}_j,$$

where $\boldsymbol{e}_i$ denotes the standard basis vector whose ith entry is 1 and all other entries are 0.

To investigate the oscillatory behavior of $f_{ij}(t)$, we define the following notion of *extremal times.*

Definition 1 (Extremal times)**.** Fix arbitrary $i, j \in V$. A time $t \in [0, \infty]$ is an *extremal maximum* (respectively, *extremal minimum*) of $f_{ij}(t)$ if:

- When $t < \infty$, there exists $\delta > 0$ such that $f_{ij}(s) < f_{ij}(t)$ (respectively, $f_{ij}(s) > f_{ij}(t)$) for all $s \in (t - \delta, t + \delta)$ with $s \neq t$.
- When $t = \infty$, there exists $T \geq 0$ such that f_{ij} is monotonically increasing (respectively, decreasing) on $[T, \infty)$.

1.1 Auxiliary Lemmas

In this section, we establish several lemmas that will be essential to our analysis.

Let $\mathbf{1}$ and $\mathbf{0}$ denote the all-ones and all-zeros vectors of appropriate dimension. For a vector $\boldsymbol{v} = (v_i)_i \in \mathbb{R}^n$, we define the ℓ_1-norm as $\|\boldsymbol{v}\|_1 = \sum_{i=1}^n |v_i|$. For a matrix $A = (A_{i,j})_{i,j} \in \mathbb{R}^{n\times n}$, its ℓ_1-norm is defined as $\|A\|_1 = \max_{1\leq j\leq n} \sum_{i=1}^n |A_{i,j}|$. It is well-known that for any matrix A and vector $\boldsymbol{v}$, the inequality $\|A\boldsymbol{v}\|_1 \leq \|A\|_1 \cdot \|\boldsymbol{v}\|_1$ holds.

We now describe a lemma which bounds the number of zeros of exponential polynomials.

Lemma 1 (Descartes' rule of signs (cf. [7, 8])**.** *For a non-zero exponential polynomial $f(t) = \sum_{i=1}^n a_i \mathrm{e}^{b_i t}$ with arbitrary real coefficients a_i and b_i, the number of finite real zeros (i.e., real numbers t with $|t| < \infty$ satisfying $f(t) = 0$) is at most $n - 1$.*

The following lemma provides an integral representation for the difference of matrix exponentials and will be used throughout this supporting information.

Lemma 2 (Duhamel's formula [2])**.** *For any two matrices $A, B \in \mathbb{R}^{n\times n}$ and all $t \geq 0$,*

$$\mathrm{e}^{tA} - \mathrm{e}^{tB} = \int_0^t \mathrm{e}^{(t-s)B}(A - B)\mathrm{e}^{sA}\mathrm{d}s.$$

For completeness, we provide a proof of this lemma.

Proof. For $s \in [0,t]$, let $F(s) = \mathrm{e}^{(t-s)B}\mathrm{e}^{sA}$. We have $F(0) = \mathrm{e}^{tB}$ and $F(t) = \mathrm{e}^{tA}$. Then, we have $\frac{\mathrm{d}F(s)}{\mathrm{d}s} = -B\mathrm{e}^{(t-s)B}\mathrm{e}^{sA} + \mathrm{e}^{(t-s)B}A\mathrm{e}^{sA} = \mathrm{e}^{(t-s)B}(A-B)\mathrm{e}^{sA}$. By the fundamental theorem of calculus, we obtain $\int_0^t \frac{\mathrm{d}F(s)}{\mathrm{d}s}\mathrm{d}s = \int_0^t \mathrm{e}^{(t-s)B}(A-B)\mathrm{e}^{sA}\mathrm{d}s = F(t) - F(0) = \mathrm{e}^{tA} - \mathrm{e}^{tB}$. This completes the proof. □

We now define Metzler matrices [3] and their nonexpansiveness.

Definition 2 (Nonexpansive Metzler matrices)**.** A matrix $A \in \mathbb{R}^{n\times n}$ is said to be *Metzler* if $A_{i,j} \geq 0$ for all $i \neq j$. A Metzler matrix $A \in \mathbb{R}^{n\times n}$ is called *nonexpansive* if $\mathbf{1}^\top A \leq \mathbf{0}^\top$.

We now bound matrix exponentials of nonexpansive Metzler matrices.

Lemma 3 (Property of nonexpansive Metzler matrices)**.** *Let $A \in \mathbb{R}^{n\times n}$ be a nonexpansive Metzler matrix. Then, for every $t \geq 0$, the matrix exponential e^{tA} satisfies $\|\mathrm{e}^{tA}\|_1 \leq 1$.*

Proof. For a Metzler matrix A with $\mathbf{1}^\top A \leq \mathbf{0}^\top$, we define $y(t) = \mathbf{1}^\top \mathrm{e}^{tA}$. Then $y(t)$ satisfies the differential equation $\frac{\mathrm{d}y(t)}{\mathrm{d}t} = y(t)A$ with initial condition $y(0) = \mathbf{1}^\top$.

We first show that $y(t) \leq \mathbf{1}^\top$ for all $t \geq 0$. Suppose, for contradiction, that $y_i(t) > 1$ for some i and $t > 0$. By continuity, there exists $t_0 > 0$ such that $\max_{j\in[n]} y_j(t_0) = y_i(t_0) = 1$ and $\frac{\mathrm{d}y_i}{\mathrm{d}t}(t_0) > 0$. Now, we have $\frac{\mathrm{d}y_i}{\mathrm{d}t}(t_0) = (y(t_0)A)_i = \sum_{j=1}^n y_j(t_0)A_{j,i}$. Since A is Metzler, $A_{i,j} \geq 0$ for $i \neq j$. Moreover, $y_j(t_0) \leq y_i(t_0) = 1$ for all j. Therefore, $\frac{\mathrm{d}y_i}{\mathrm{d}t}(t_0) \leq \sum_{j=1}^n A_{j,i} = (\mathbf{1}^\top A)_i \leq 0$. This contradicts $\frac{\mathrm{d}y_i}{\mathrm{d}t}(t_0) > 0$. Hence, $y(t) \leq \mathbf{1}^\top$ for all $t \geq 0$.

Since A is Metzler, e^{tA} is nonnegative for all $t \geq 0$. Thus, the ℓ_1-norm equals $\|\mathrm{e}^{tA}\|_1 = \max_j \sum_i (\mathrm{e}^{tA})_{i,j} = \max_{j\in[n]}(y(t))_j \leq 1$. □

Combining Lemmas 2 and 3, we obtain the following bound.

Lemma 4 (Duhamel's bound for nonexpansive Metzler matrices)**.** *For any two nonexpansive Metzler matrices $A, B \in \mathbb{R}^{n\times n}$ and all $t \geq 0$,*

$$\|\mathrm{e}^{tA} - \mathrm{e}^{tB}\|_1 \leq t\,\|A - B\|_1.$$

Proof. By Lemmas 2 and 3, we have

$$\begin{aligned}
\|\mathrm{e}^{tA} - \mathrm{e}^{tB}\|_1 &= \left\| \int_0^t \mathrm{e}^{(t-s)B}(A-B)\mathrm{e}^{sA}\mathrm{d}s \right\|_1 \leq \int_0^t \|\mathrm{e}^{(t-s)B}(A-B)\mathrm{e}^{sA}\|_1\,\mathrm{d}s \\
&\leq \int_0^t \|\mathrm{e}^{(t-s)B}\|_1\,\|A-B\|_1\,\|\mathrm{e}^{sA}\|_1\,\mathrm{d}s \\
&\leq \int_0^t \|A-B\|_1\,\mathrm{d}s = t\,\|A-B\|_1,
\end{aligned}$$

where in the third inequality we used $\|\mathrm{e}^{(t-s)B}\|_1 \leq 1$ and $\|\mathrm{e}^{sA}\|_1 \leq 1$. This completes the proof of the lemma. □

We now analyze the structure of matrix exponentials for block matrices with zero upper-right block.

Lemma 5. *Let $A \in \mathbb{R}^{n\times n}$ be a matrix of the form*

$$A = \begin{pmatrix} a & \mathbf{0}^\top \\ \boldsymbol{b} & B \end{pmatrix},$$

where $a \in \mathbb{R}_{>0}$ is a scalar, $\boldsymbol{b} \in \mathbb{R}^{n-1}$ is a column vector, and $B \in \mathbb{R}^{(n-1)\times(n-1)}$ is a submatrix. Then, for any $t \in \mathbb{R}_{\geq 0}$, the matrix exponential e^{tA} is given by

$$\mathrm{e}^{tA} = \begin{pmatrix} \mathrm{e}^{ta} & \mathbf{0}^\top \\ \boldsymbol{\psi}(t) & \mathrm{e}^{tB} \end{pmatrix}, \tag{1}$$

where $\boldsymbol{\psi}(t) = \int_0^t \mathrm{e}^{sa}\mathrm{e}^{(t-s)B}\boldsymbol{b}\,\mathrm{d}s$. Furthermore, in the special case where $B = O$, we have $\boldsymbol{\psi}(t) = \frac{\mathrm{e}^{ta}-1}{a}\boldsymbol{b}$.

Proof. Given the block structure of A, we can prove by induction that powers of A take the form:

$$A^d = \begin{pmatrix} a^d & \mathbf{0}^\top \\ \boldsymbol{\phi}_d & B^d \end{pmatrix},$$

where $\boldsymbol{\phi}_d$ satisfies that $\boldsymbol{\phi}_1 = \boldsymbol{b}$, and for $d \geq 2$, $\boldsymbol{\phi}_d = a\boldsymbol{\phi}_{d-1} + B\boldsymbol{\phi}_{d-1}$. Thus, we obtain

$$\mathrm{e}^{tA} = \sum_{d=0}^{\infty} \frac{t^d}{d!} \begin{pmatrix} a^d & \mathbf{0}^\top \\ \boldsymbol{\phi}_d & B^d \end{pmatrix} = \begin{pmatrix} \sum_{d=0}^\infty \frac{(ta)^d}{d!} & \mathbf{0}^\top \\ \sum_{d=0}^\infty \frac{t^d}{d!}\boldsymbol{\phi}_d & \sum_{d=0}^\infty \frac{(tB)^d}{d!} \end{pmatrix} = \begin{pmatrix} \mathrm{e}^{ta} & \mathbf{0}^\top \\ \boldsymbol{\psi}(t) & \mathrm{e}^{tB} \end{pmatrix},$$

where $\boldsymbol{\psi}(t) = \sum_{d=0}^\infty \frac{t^d}{d!}\boldsymbol{\phi}_d$.

To determine the explicit expression for $\boldsymbol{\psi}(t)$, we utilize the fundamental property that $\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{tA} = A\mathrm{e}^{tA}$. Applying this to the equation (1) and focusing on the bottom-left block, we get

$$\frac{\mathrm{d}\boldsymbol{\psi}(t)}{\mathrm{d}t} = \mathrm{e}^{ta}\boldsymbol{b} + B\boldsymbol{\psi}(t). \tag{2}$$

Additionally, we have the initial condition $\boldsymbol{\psi}(0) = \mathbf{0}$.

We claim that $\boldsymbol{\psi}(t) = \int_0^t \mathrm{e}^{sa}\mathrm{e}^{(t-s)B}\boldsymbol{b}\,\mathrm{d}s$ satisfies both the differential equation (2) and the initial condition. For the initial condition, this is immediate. For the equation (2), applying Leibniz's integral rule yields the required result as follows.

$$\begin{aligned} \frac{\mathrm{d}\boldsymbol{\psi}(t)}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \mathrm{e}^{sa}\mathrm{e}^{(t-s)B}\boldsymbol{b}\,\mathrm{d}s = \mathrm{e}^{ta}\mathrm{e}^{0B}\boldsymbol{b} + \int_0^t \mathrm{e}^{sa}\frac{\partial}{\partial t}[\mathrm{e}^{(t-s)B}]\boldsymbol{b}\,\mathrm{d}s \\ &= \mathrm{e}^{ta}\boldsymbol{b} + \int_0^t \mathrm{e}^{sa}[B\mathrm{e}^{(t-s)B}]\boldsymbol{b}\,\mathrm{d}s = \mathrm{e}^{ta}\boldsymbol{b} + B\int_0^t \mathrm{e}^{sa}\mathrm{e}^{(t-s)B}\boldsymbol{b}\,\mathrm{d}s \\ &= \mathrm{e}^{ta}\boldsymbol{b} + B\boldsymbol{\psi}(t). \end{aligned}$$

By the uniqueness theorem for linear differential equations, this establishes the explicit form of $\boldsymbol{\psi}(t)$.

For the special case where $B = O$, we have $\mathrm{e}^{(t-s)B} = \mathrm{e}^{O} = I$, which directly leads to $\boldsymbol{\psi}(t) = \int_0^t \mathrm{e}^{sa}\,\mathrm{d}s \cdot \boldsymbol{b} = \frac{\mathrm{e}^{ta}-1}{a}\boldsymbol{b}$. This completes the proof. □

Finally, we present two useful results on spectral properties of symmetric matrices and graph Laplacians.

Lemma 6 (Courant-Fischer theorem (cf. [4]))**.** *Let A be a real symmetric matrix satisfying $A\mathbf{1} = \mathbf{0}$. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of A in non-increasing order. If $\lambda_1 = 0$ (i.e., 0 is the largest eigenvalue of A), then the second largest eigenvalue is given by $\max_{\boldsymbol{x}\neq\mathbf{0},\,\boldsymbol{x}\perp\mathbf{1}} \frac{\boldsymbol{x}^\top A\boldsymbol{x}}{\boldsymbol{x}^\top\boldsymbol{x}}$.*

Lemma 7 (Eigenvalues on a path graph (cf. [1]))**.** *Consider a path graph with n vertices, where all edges have weight 1. Let L be its graph Laplacian matrix. Then, the second smallest eigenvalue λ_2 of L is given by*

$$\lambda_2 = \max_{\boldsymbol{x}\neq\mathbf{0},\,\boldsymbol{x}\perp\mathbf{1}} \frac{-\sum_{i=1}^{n-1}(x_{i+1}-x_i)^2}{\sum_{i=1}^n x_i^2} = 2\cos\left(\frac{\pi}{n}\right) - 2.$$

2 Finiteness of Extremal Maximum Times

In this section, we prove that the number of extremal maximum times is at most $\lfloor \frac{n}{2} \rfloor$.

Theorem 1. *For any $i, j \in [n]$, the number of extremal maximal times of $f_{ij}(t)$ is at most $\lfloor \frac{n}{2} \rfloor$.*

To prove Theorem 1, we show the following lemma.

Lemma 8. *Suppose that for any $i, j \in [n]$, $\frac{\mathrm{d}f_{ij}}{\mathrm{d}t}(t)$ is not identically zero. Then, the equation $\frac{\mathrm{d}f_{ij}}{\mathrm{d}t}(t) = 0$ has at most $n-2$ solutions in the interval $[0, \infty)$, and one additional solution at $t = \infty$.*

Proof. Since K is self-adjoint, all eigenvalues of K are real [6]. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of K. Since $K\pi = \mathbf{0}$, K has an eigenvalue 0. Moreover, it follows from the Gershgorin circle theorem that $0 = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ [6]. Let $\boldsymbol{u}_k$ be an eigenvector corresponding to λ_k for $k \in [n]$. Let $U = (\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_n)$ and $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$. Using the eigendecomposition of K and the properties of the matrix exponential, we can express $f_{ij}(t)$ as

$$\begin{aligned} f_{ij}(t) = \boldsymbol{e}_i^\top \mathrm{e}^{tK} \boldsymbol{e}_j = \boldsymbol{e}_i^\top U \mathrm{e}^{t\Lambda} U^{-1} \boldsymbol{e}_j &= \sum_{k=1}^{n} \boldsymbol{e}_i^\top \boldsymbol{u}_k (U^{-1})_k \boldsymbol{e}_j \cdot \mathrm{e}^{t\lambda_k} \\ &= (\boldsymbol{u}_1)_i (U^{-1})_{1,j} + \sum_{k=2}^{n} (\boldsymbol{u}_k)_i (U^{-1})_{k,j} \cdot \mathrm{e}^{t\lambda_k}, \end{aligned}$$

where $(\boldsymbol{u}_k)_i$ is the ith component of $\boldsymbol{u}_k$, and $(U^{-1})_{k,j}$ is the (k, j) entry of U^{-1}. Therefore, we obtain

$$\frac{\mathrm{d}f_{ij}}{\mathrm{d}t}(t) = \sum_{k=2}^{n} (\boldsymbol{u}_k)_i (U^{-1})_{k,j} \lambda_k \cdot \mathrm{e}^{t\lambda_k}.$$

By Lemma 1, the equation $\frac{\mathrm{d}f_{ij}(t)}{\mathrm{d}t} = 0$ has at most $n-2$ finite real solutions. Moreover, since $\lambda_k \leq 0$ for all k, we have $\lim_{t\to\infty} \frac{\mathrm{d}f_{ij}(t)}{\mathrm{d}t} = 0$. □

Lemma 8 immediately yields Theorem 1 as follows.

Proof of Theorem 1. By the continuity of $f_{ij}(t)$, between any two extremal maximum times, there exists at least one extremal minimum time. Thus, if there are k extremal maximum times, there must be at least $k-1$ extremal minimum time. By Lemma 8, the total number of extremal maximum times in $[0, \infty]$ is at most $n - 1$. Thus, we have $k + (k - 1) \leq n - 1$, which implies $k \leq \lfloor \frac{n}{2} \rfloor$. □

3 Tightness of the Upper Bound

In this section, we present the following result.

Theorem 2. *There exists a reaction path network that possesses exactly $\lfloor \frac{n}{2} \rfloor$ extremal maximum times.*

To establish Theorem 2, we explicitly construct a network and demonstrate that it exhibits precisely the claimed number of extremal maximum times.

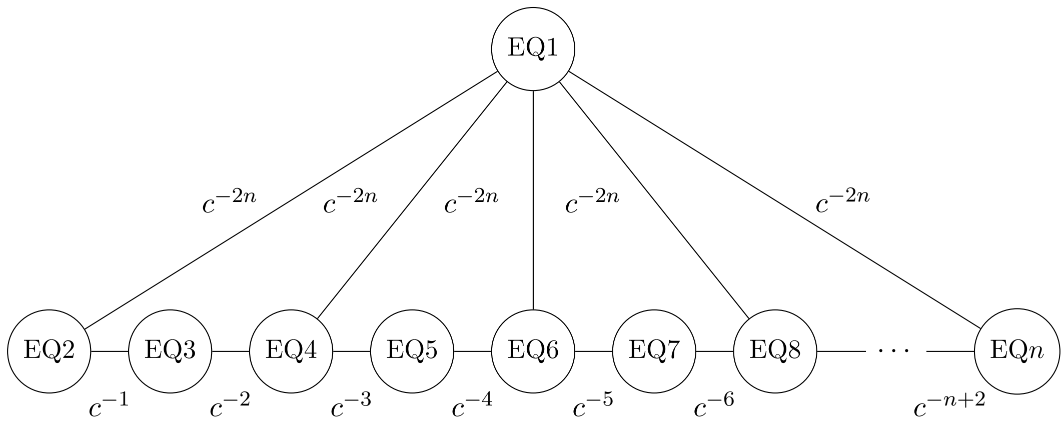

Figure 1: Graph with connections from EQ1 to even-numbered nodes. In the figure, we consider the case where n is even.

3.1 Network Description

We consider a weighted graph $G = (V, E, w_V, w_E)$ with n vertices, where $V = [n]$ and $n \geq 2$. The vertices are labeled as EQ1, EQ2, ..., EQn, illustrated in Figure 1. The edge set E is designed with a specific structure consisting of two types of connections. First, there is a path connecting vertices EQ2, EQ3, ..., EQn in sequence. Second, there are additional edges connecting vertex EQ1 to all vertices EQj where j is even and $2 \leq j \leq n$.

Let $c > 1$ be a positive constant satisfying $c > 2500n^9$. We now define the weight functions w_V and w_E. The vertex weight function $w_V : V \to \mathbb{R}_{>0}$ assigns a very small weight to vertex 1 and the same weight to all other vertices. Specifically,

$$w_V(i) = \begin{cases} \frac{1}{c^{2n}(n-1)+1} & \text{if } i = 1; \\ \frac{c^{2n}}{c^{2n}(n-1)+1} & \text{if } i = 2, 3, \ldots, n. \end{cases}$$

The edge weight function $w_E : E \to \mathbb{R}_{>0}$ is defined according to the connection type:

$$w_E(i, j) = \begin{cases} c^{-2n}, & \text{if } i = 1 \text{ and } j \text{ is even;} \\ c^{-(i-1)}, & \text{if } i, j \in \{2, 3, \ldots, n\} \text{ and } |i - j| = 1, \text{ where } i < j. \end{cases}$$

We first define $K^{\text{path}} \in \mathbb{R}^{(n-1)\times(n-1)}$ as the graph Laplacian matrix for the path connecting vertices $2, 3, \ldots, n$. This matrix has off-diagonal entries $(K^{\text{path}})_{i,i+1} = (K^{\text{path}})_{i+1,i} = c^{-i}$ for consecutive vertices along the path, and diagonal entries chosen to ensure each row sums to zero. Specifically, the diagonal entries are $-c^{-1}$ for the first vertex, $-c^{-n+2}$ for the last vertex, and $-c^{-i+1} - c^{-i}$ for interior vertices, with all other entries being zero. The explicit form of K^{path} is

$$K^{\text{path}} = \begin{pmatrix} -c^{-1} & c^{-1} & 0 & \cdots & 0 & 0 \\ c^{-1} & -c^{-1} - c^{-2} & c^{-2} & \cdots & 0 & 0 \\ 0 & c^{-2} & -c^{-2} - c^{-3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -c^{-n+3} - c^{-n+2} & c^{-n+2} \\ 0 & 0 & 0 & \cdots & c^{-n+2} & -c^{-n+2} \end{pmatrix}.$$

For the weighted graph $G = (V, E, w_V, w_E)$, the graph Laplacian matrix $L \in \mathbb{R}^{n\times n}$ is written as

$$L = \begin{pmatrix} \lfloor \frac{n-1}{2} \rfloor c^{-2n} & -c^{-2n}\,\mathbf{1}_{\mathrm{odd}}^\top \\ -c^{-2n}\,\mathbf{1}_{\mathrm{odd}} & -K^{\mathrm{path}} + c^{-2n}\,\mathrm{diag}(\mathbf{1}_{\mathrm{odd}}) \end{pmatrix},$$

where $\mathbf{1}_{\mathrm{odd}}$ is the $(n-1)$-dimensional vector where ith entry equals 1 if i is odd and 0 if i is even. The vertex weight function w_V defines the equilibrium distribution vector π as

$$\pi = \left(\frac{1}{c^{2n}(n-1)+1}, \frac{c^{2n}}{c^{2n}(n-1)+1}, \frac{c^{2n}}{c^{2n}(n-1)+1}, \ldots, \frac{c^{2n}}{c^{2n}(n-1)+1} \right)^\top.$$

Finally, the rate constant matrix is given by $K = -L\Pi^{-1}$, where $\Pi = \mathrm{diag}(\pi)$.

3.2 Proof of Theorem 2

We define $f(t) = \boldsymbol{e}_2^\top \mathrm{e}^{tK} \boldsymbol{e}_1$, which represents the quantity in equilibrium state EQ2 at time t when the system initially occupies equilibrium state EQ1. To prove Theorem 2, we analyze the oscillatory behavior of $f(t)$.

The following lemma is crucial for our analysis. To state it, we define $\boldsymbol{q} = \frac{1}{\lceil \frac{n-1}{2} \rceil} \boldsymbol{b}_{\mathrm{odd}} \in \mathbb{R}^{n-1}$ and, for each $\ell \in [n-1]$, we define $\mathbf{1}_{[1:\ell]} \in \mathbb{R}^{n-1}$ as the vector whose first ℓ components are 1 and remaining components are 0.

Lemma 9. *For each $\ell \in [n-1]$, let $t_\ell = c^{\ell-1/2}$. Then, for all $\ell \in [n-1]$, we have*

$$\left| f(t_\ell) - \frac{1}{\ell} \mathbf{1}_{[1:\ell]}^\top \boldsymbol{q} \right| \leq 24nc^{-1/2}. \tag{3}$$

We defer the proof of Lemma 9 to Section 3.3. We now proceed to show Theorem 2.

Proof of Theorem 2. We show that $f(t)$ has exactly $\lfloor \frac{n}{2} \rfloor$ extremal maximum times. Our approach is to establish an oscillatory pattern in $f(t)$ by analyzing its values at the time points $t_\ell = c^{\ell-1/2}$ for $\ell \in [n-1]$. Note that $f(0) = \boldsymbol{e}_2^\top \boldsymbol{e}_1 = 0$.

First, when ℓ is even, that is, $\ell = 2k$ for $k = 1, 2, \ldots, \lfloor \frac{n-1}{2} \rfloor$, using Lemma 9, we obtain

$$f(t_{2k}) = \boldsymbol{e}_2^\top \mathrm{e}^{t_{2k}K} \boldsymbol{e}_1 \leq \frac{1}{2k} \mathbf{1}_{[1:2k]}^\top \boldsymbol{q} + 24nc^{-1/2} = \frac{1}{2\lceil \frac{n-1}{2} \rceil} + 24nc^{-1/2}.$$

Next, when ℓ is odd, that is, $\ell = 2k+1$ for $k = 0, 1, \ldots, \lfloor \frac{n-2}{2} \rfloor$, by Lemma 9, we have

$$\begin{aligned} f(t_{2k+1}) = \boldsymbol{e}_2^\top \mathrm{e}^{t_{2k+1}K} \boldsymbol{e}_1 &\geq \frac{1}{2k+1} \mathbf{1}_{[1:2k+1]}^\top \boldsymbol{q} - 24nc^{-1/2} = \frac{k+1}{\lceil \frac{n-1}{2} \rceil (2k+1)} - 24nc^{-1/2} \\ &= \frac{1}{2\lceil \frac{n-1}{2} \rceil} + \frac{1}{2\lceil \frac{n-1}{2} \rceil} \cdot \frac{1}{2k+1} - 24nc^{-1/2}. \end{aligned}$$

Since $c > 2500n^9$ and $n \geq 2$, we have $24nc^{-1/2} < 48nc^{-1/2} < \frac{48n}{50n^{4.5}} < \frac{1}{n^2} < \frac{1}{n}$. Since $f(0) = 0$, we get

$$f(t_1) \geq \frac{1}{\lceil \frac{n-1}{2} \rceil} - 24nc^{-1/2} > \frac{1}{n} - 24nc^{-1/2} > 0 = f(0). \tag{4}$$

Moreover, for each $k = 0, 1, \ldots, \lfloor \frac{n-3}{2} \rfloor$, we have

$$f(t_{2k+1}) - f(t_{2k+2}) \geq \frac{1}{2\lceil \frac{n-1}{2} \rceil} \frac{1}{2k+1} - 48nc^{-1/2} \geq \frac{1}{n^2} - 48nc^{-1/2} > 0. \tag{5}$$

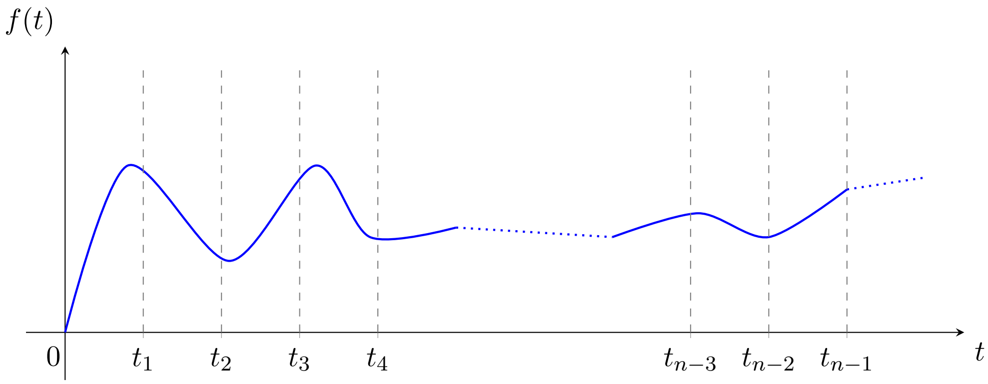

Figure 2: Example of the oscillation pattern of $f(t)$ when n is even.

For each $k = 1, 2, \ldots, \lfloor \frac{n-2}{2} \rfloor$, we obtain

$$f(t_{2k+1}) - f(t_{2k}) \geq \frac{1}{2\lceil \frac{n-1}{2} \rceil} \frac{1}{2k+1} - 48nc^{-1/2} > 0. \tag{6}$$

By continuity of f and the inequalities (5) and (6), there exists at least one extremal maximum time in each interval $[t_{2k}, t_{2k+2}]$ for $k = 1, 2, \ldots, \lfloor \frac{n-3}{2} \rfloor$. Moreover, from the inequalities (4) and (5), there exists at least one extremal maximum time in $[0, t_2]$. These imply that at least $\lfloor \frac{n-3}{2} \rfloor + 1$ extremal maximum times exist in $\left[0, t_{2\lfloor \frac{n-3}{2} \rfloor + 2}\right]$.

Additionally, when n is even, the inequality (6) with $k = \frac{n-2}{2}$ gives $f(t_{n-1}) > f(t_{n-2})$. If f increases monotonically and converges, then $t = \infty$ becomes an extremal maximum time; otherwise, f decreases at some time in (t_{n-1}, ∞) and there exists at least one finite extremal maximum time. Thus, there exists at least one extremal maximum time in $(t_{n-1}, \infty]$. Figure 2 illustrates these arguments for the case when n is even.

Combining these results, when n is odd, the total number of extremal maximum times is at least $\lfloor \frac{n-3}{2} \rfloor + 1 = \lfloor \frac{n}{2} \rfloor$, while when n is even, there are at least $\lfloor \frac{n-3}{2} \rfloor + 1 + 1 = \lfloor \frac{n}{2} \rfloor$ extremal maximum times. Therefore, $f(t)$ has at least $\lfloor \frac{n}{2} \rfloor$ extremal maximum times in $[0, \infty]$.

By Theorem 1, which establishes that the number of extremal maximum times is at most $\lfloor \frac{n}{2} \rfloor$, we conclude that the constructed network achieves exactly $\lfloor \frac{n}{2} \rfloor$ extremal maximum times. □

3.3 Proof of Lemma 9

We prove Lemma 9 by carefully analyzing the structure of the rate matrix K and its spectral properties.

3.3.1 Additional Notations

To analyze the dynamics, we introduce several auxiliary matrices We set $t_0 = c^{1/4}$ as our reference time. Note that for any $\ell \in [n-1]$, we have $t_\ell - t_0 = c^{\ell - 1/2} - c^{1/4} \geq 0$.

We decompose the rate matrix K in two complementary ways to isolate the effects of different network components. In our first decomposition, we write $K = K_1 + (K - K_1)$, where K_1 captures the interaction between the first node and the path component:

$$K_1 = -\begin{pmatrix} \lfloor \frac{n-1}{2} \rfloor c^{-2n} & \mathbf{0}^\top \\ -c^{-2n} \mathbf{1}_{\mathrm{odd}} & O \end{pmatrix} \Pi^{-1} = \frac{c^{2n}(n-1)+1}{c^{2n}} \begin{pmatrix} -\lfloor \frac{n-1}{2} \rfloor & \mathbf{0}^\top \\ \mathbf{1}_{\mathrm{odd}} & O \end{pmatrix}.$$

In our second decomposition, we write $K = K_2 + (K - K_2)$, where K_2 includes the path dynamics:

$$K_2 = \frac{c^{2n}(n-1)+1}{c^{2n}} \begin{pmatrix} -\lfloor \frac{n-1}{2} \rfloor & \mathbf{0}^\top \\ \mathbf{1}_{\mathrm{odd}} & K^{\mathrm{path}} \end{pmatrix}.$$

For each $\ell \in [n]$, let $(K^{\mathrm{path}}_{i,j})_{1\le i,j\le \ell}$ denote the upper-left $\ell \times \ell$ principal submatrix of K^{path}. For $\ell \in [n-2]$, we define the perturbation matrix $E_\ell = \mathrm{diag}(0, 0, \dots, 0, 1) \in \mathbb{R}^{\ell\times\ell}$ and the perturbed path matrix

$$B_\ell = (K^{\mathrm{path}}_{i,j})_{1\le i,j\le \ell} + c^{-\ell} E_\ell.$$

Additionally, we set $B_{n-1} = K^{\mathrm{path}}$. Finally, for each $\ell \in [n-1]$, we define the embedding of B_ℓ into the full $(n-1)\times(n-1)$ spcace as

$$A_\ell = \begin{pmatrix} B_\ell & O \\ O & O \end{pmatrix} \in \mathbb{R}^{(n-1)\times(n-1)}.$$

3.3.2 Proof Sketch of Lemma 9

First, we outline the proof strategy. We will decompose the expression for $f(t_\ell)$ into several components and analyze each one separately. The key approximation steps will be as follows:

$$\begin{aligned} f(t_\ell) &= \boldsymbol{e}_2^\top \mathrm{e}^{t_\ell K} \boldsymbol{e}_1 \\ &= \boldsymbol{e}_2^\top \mathrm{e}^{(t_\ell - t_0)K} \mathrm{e}^{t_0 K} \boldsymbol{e}_1 \\ &\approx \boldsymbol{e}_2^\top \mathrm{e}^{(t_\ell - t_0)K} \mathrm{e}^{t_0 K_1} \boldsymbol{e}_1 && \text{(Step 1)} \\ &\approx \boldsymbol{e}_2^\top \mathrm{e}^{(t_\ell - t_0)K} (0, \boldsymbol{q})^\top && \text{(Step 2)} \\ &\approx \boldsymbol{e}_2^\top \mathrm{e}^{(t_\ell - t_0)K_2} (0, \boldsymbol{q})^\top && \text{(Step 3)} \\ &\approx \boldsymbol{e}_1^\top \mathrm{e}^{(t_\ell - t_0)(n-1)K^{\mathrm{path}}} \boldsymbol{q} && \text{(Step 4)} \\ &\approx \boldsymbol{e}_1^\top \mathrm{e}^{(t_\ell - t_0)(n-1)A_\ell} \boldsymbol{q} && \text{(Step 5)} \\ &\approx \frac{1}{\ell} \mathbf{1}_{[1:\ell]}^\top \boldsymbol{q}, && \text{(Step 6)} \end{aligned}$$

where the symbol $\approx$ indicates that the absolute value of the difference between the terms on either side is bounded by some constant (independent of c) multiplied by $c^{-1/2}$.

We will establish bounds for each approximation step and then combine them to obtain the final result.

Step 1: Approximating $\mathrm{e}^{t_0 K}$ by $\mathrm{e}^{t_0 K_1}$

First, we have

$$\|K - K_1\|_1 = \max_{1\le j\le n} \sum_{i=1}^{n} |(K_1)_{i,j}| \le \frac{c^{2n}(n-1)+1}{c^{2n}} (2c^{-1} + c^{-3n}) \le 4nc^{-1}.$$

By Lemma 4, we get

$$\|\mathrm{e}^{t_0 K} - \mathrm{e}^{t_0 K_1}\|_1 \le t_0 \|K - K_1\|_1 \le 4nc^{1/4} c^{-1} \le 4nc^{-1/2}.$$

Therefore, by Lemma 3, we obtain

$$\begin{aligned} \|\boldsymbol{e}_2^\top \mathrm{e}^{(t_\ell - t_0)K} \mathrm{e}^{t_0 K} \boldsymbol{e}_1 - \boldsymbol{e}_2^\top \mathrm{e}^{(t_\ell - t_0)K} \mathrm{e}^{t_0 K_1} \boldsymbol{e}_1\|_1 &\le \|\boldsymbol{e}_2^\top \mathrm{e}^{(t_\ell - t_0)K}\|_1 \cdot \|\mathrm{e}^{t_0 K} - \mathrm{e}^{t_0 K_1}\|_1 \cdot \|\boldsymbol{e}_1\|_1 \\ &\le 4nc^{-1/2}. \end{aligned} \tag{7}$$

Step 2: Approximating $\mathrm{e}^{t_0 K_1}\boldsymbol{e}_1$ by $(0,\boldsymbol{q})^\top$

By Lemma 5, we obtain

$$\mathrm{e}^{t_0 K_1} = \begin{pmatrix} \mathrm{e}^{-t_0 \frac{c^{2n}(n-1)+1}{c^{2n}} \lfloor \frac{n-1}{2} \rfloor} & \mathbf{0}^\top \\ \frac{\mathrm{e}^{-t_0 \frac{c^{2n}(n-1)+1}{c^{2n}} \lfloor \frac{n-1}{2} \rfloor} - 1}{-\lfloor \frac{n-1}{2} \rfloor} \mathbf{1}_{\mathrm{odd}} & O \end{pmatrix},$$

and

$$\mathrm{e}^{t_0 K_1}\boldsymbol{e}_1 = \left(\mathrm{e}^{-t_0 \frac{c^{2n}(n-1)+1}{c^{2n}} \lfloor \frac{n-1}{2} \rfloor}, \frac{\mathrm{e}^{-t_0 \frac{c^{2n}(n-1)+1}{c^{2n}} \lfloor \frac{n-1}{2} \rfloor} - 1}{-\lfloor \frac{n-1}{2} \rfloor} \mathbf{1}_{\mathrm{odd}}^\top \right)^\top .$$

Therefore, we have

$$\begin{aligned} \left\| \mathrm{e}^{t_0 K_1}\boldsymbol{e}_1 - (0,\boldsymbol{q})^\top \right\|_1 &\leq 2\mathrm{e}^{-t_0 \frac{c^{2n}(n-1)+1}{c^{2n}} \lfloor \frac{n-1}{2} \rfloor} \\ &= 2\mathrm{e}^{-c^{1/4} \frac{c^{2n}(n-1)+1}{c^{2n}} \lfloor \frac{n-1}{2} \rfloor} && (\text{by } t_0 = c^{1/4}) \\ &\leq 2\mathrm{e}^{-c^{1/4}} \\ &\leq 2c^{-1/2}. && (\text{by } c \geq 1) \end{aligned}$$

From this, we get

$$\begin{aligned} \left\| \boldsymbol{e}_2^\top \mathrm{e}^{(t_\ell - t_0)K} \mathrm{e}^{t_0 K_1}\boldsymbol{e}_1 - \boldsymbol{e}_2^\top \mathrm{e}^{(t_\ell - t_0)K} (0,\boldsymbol{q}^\top)^\top \right\|_1 &\leq \left\| \boldsymbol{e}_2^\top \mathrm{e}^{(t_\ell - t_0)K} \right\|_1 \cdot \left\| e^{t_0 K_1}\boldsymbol{e}_1 - (0,\boldsymbol{q}^\top)^\top \right\|_1 \\ &\leq 2c^{-1/2} \\ &\leq 2nc^{-1/2}. \end{aligned} \tag{8}$$

Step 3: Approximating $\mathrm{e}^{(t_\ell - t_0)K}$ by $\mathrm{e}^{(t_\ell - t_0)K_2}$

Since we have

$$K - K_2 = \frac{c^{2n}(n-1)+1}{c^{2n}} \begin{pmatrix} 0 & c^{-2n}\,\mathbf{1}_{\mathrm{odd}}^\top \\ \mathbf{0} & -c^{-2n}\,\mathrm{diag}(\mathbf{1}_{\mathrm{odd}}) \end{pmatrix},$$

we can bound the norm of the difference between K and K_2:

$$\|K - K_2\|_1 \leq 4 \cdot c^{-2n}.$$

By Lemma 4, we obtain

$$\begin{aligned} \left\| \boldsymbol{e}_2^\top \mathrm{e}^{(t_\ell - t_0)K} (0,\boldsymbol{q}^\top)^\top - \boldsymbol{e}_2^\top \mathrm{e}^{(t_\ell - t_0)K_2} (0,\boldsymbol{q}^\top)^\top \right\|_1 &\leq \|\mathrm{e}^{(t_\ell - t_0)K} - \mathrm{e}^{(t_\ell - t_0)K_2}\|_1 \\ &\leq (t_\ell - t_0)\|K - K_2\|_1 \\ &\leq c^{\ell - 1/2} \cdot 4 \cdot c^{-2n} \\ &\leq c^{n} \cdot 4 \cdot c^{-2n} \\ &\leq 4c^{-n} \\ &\leq 4nc^{-1/2}. \end{aligned} \tag{9}$$

Step 4: Approximating $\boldsymbol{e}_2^\top \mathrm{e}^{(t_\ell - t_0)K_2}(0, \boldsymbol{q}^\top)^\top$ by $\boldsymbol{e}_1^\top \mathrm{e}^{(t_\ell - t_0)(n-1)K^{\mathrm{path}}}\boldsymbol{q}$

By Lemma 5, we have

$$\mathrm{e}^{(t_\ell - t_0)K_2} = \begin{pmatrix} \mathrm{e}^{-(t_\ell - t_0)\frac{c^{2n}(n-1)+1}{c^{2n}}\lfloor \frac{n-1}{2} \rfloor} & \mathbf{0}^\top \\ * & \mathrm{e}^{(t_\ell - t_0)\frac{c^{2n}(n-1)+1}{c^{2n}}K^{\mathrm{path}}} \end{pmatrix},$$

where $*$ denotes an appropriate vector. Thus, we get

$$\boldsymbol{e}_2^\top \mathrm{e}^{(t_\ell - t_0)K_2}(0, \boldsymbol{q}^\top)^\top = \boldsymbol{e}_1^\top \mathrm{e}^{(t_\ell - t_0)\frac{c^{2n}(n-1)+1}{c^{2n}}K^{\mathrm{path}}}\boldsymbol{q}.$$

Since $\frac{c^{2n}(n-1)+1}{c^{2n}}K^{\mathrm{path}}$ and $(n-1)K^{\mathrm{path}}$ are both nonexpansive Metzler matrices, we have

$$\|\mathrm{e}^{(t_\ell - t_0)\frac{c^{2n}(n-1)+1}{c^{2n}}K^{\mathrm{path}}} - \mathrm{e}^{(t_\ell - t_0)(n-1)K^{\mathrm{path}}}\|_1 \le (t_\ell - t_0)\|c^{-2n}K^{\mathrm{path}}\|_1 \le 4c^{-n}.$$

Finally, we obtain

$$\left|\boldsymbol{e}_2^\top \mathrm{e}^{(t_\ell - t_0)K_2}(0, \boldsymbol{q}^\top)^\top - \boldsymbol{e}_1^\top \mathrm{e}^{(t_\ell - t_0)(n-1)K^{\mathrm{path}}}\boldsymbol{q}\right| \le 4c^{-n} \le 4nc^{-1/2}. \tag{10}$$

Step 5: Approximating $\mathrm{e}^{(t_\ell - t_0)(n-1)K^{\mathrm{path}}}$ by $\mathrm{e}^{(t_\ell - t_0)(n-1)A_\ell}$

By construction, it is straightforward to verify that for all $\ell \in [n-1]$,

$$\|K^{\mathrm{path}} - A_\ell\|_1 = 2c^{-\ell} + 2c^{-(\ell+1)} \le 4c^{-\ell}.$$

Since K^{path} and A_ℓ are nonexpansive Metzler matrices, by Lemma 4, we obtain

$$\begin{aligned}
\left\|\boldsymbol{e}_1^\top \mathrm{e}^{(t_\ell - t_0)(n-1)K^{\mathrm{path}}}\boldsymbol{q} - \boldsymbol{e}_1^\top \mathrm{e}^{(t_\ell - t_0)(n-1)A_\ell}\boldsymbol{q}\right\|_1 &\le \|\boldsymbol{e}_1^\top\|_1 \cdot \|\mathrm{e}^{(t_\ell - t_0)(n-1)K^{\mathrm{path}}} - \mathrm{e}^{(t_\ell - t_0)(n-1)A_\ell}\|_1 \cdot \|\boldsymbol{q}\|_1 \\
&\le \|\mathrm{e}^{(t_\ell - t_0)K^{\mathrm{path}}} - \mathrm{e}^{(t_\ell - t_0)A_\ell}\|_1 \\
&\le (t_\ell - t_0)(n-1)\|K^{\mathrm{path}} - A_\ell\|_1 \\
&\le 4(t_\ell - t_0)(n-1)c^{-\ell} \\
&\le 4t_\ell nc^{-\ell} \\
&= 4nc^{\ell-1/2}c^{-\ell} \\
&= 4nc^{-1/2}.
\end{aligned} \tag{11}$$

Step 6: Approximating $\boldsymbol{e}_1^\top \mathrm{e}^{(t_\ell - t_0)(n-1)A_\ell}$ by $\frac{1}{\ell}\mathbf{1}_\ell^\top$

We consider the eigenvalues of the matrix B_ℓ. Note that B_ℓ is symmetric. Let $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_\ell$ be eigenvalues, and let $\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_\ell$ be orthonormal eigenvectors. Note that $\lambda_1 = 0$ and $\boldsymbol{v}_1 = \mathbf{1}$. By Lemma 6, we have

$$\begin{aligned}
\lambda_2 &= \max_{\boldsymbol{x} \ne \mathbf{0}, \boldsymbol{x} \perp \mathbf{1}} \frac{\boldsymbol{x}^\top B_\ell \boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}} \\
&= \max_{\boldsymbol{x} \ne \mathbf{0}, \boldsymbol{x} \perp \mathbf{1}} \frac{-\sum_{i=1}^{\ell-1} c^{-i}(x_{i+1} - x_i)^2}{\sum_{i=1}^{\ell} x_i^2}
\end{aligned}$$

$$
\begin{aligned}
&\le c^{-\ell+1} \max_{\boldsymbol{x}\neq \boldsymbol{0},\, \boldsymbol{x}\perp \boldsymbol{1}} \frac{-\sum_{i=1}^{\ell-1}(x_{i+1}-x_i)^2}{\sum_{i=1}^{\ell} x_i^2} \\
&= c^{-\ell+1}\cdot\left(2\cos\left(\frac{\pi}{\ell}\right)-2\right) && \text{(by Lemma 7)} \\
&\le -\frac{\pi^2}{\ell^2}c^{-\ell+1}. && \text{(by the inequality } \cos x \ge 1-\tfrac{x^2}{2} \text{ for any } x\ge 0)
\end{aligned}
$$

By the spectral decomposition $B_\ell = \sum_{k=1}^{\ell} \lambda_k \boldsymbol{v}_k \boldsymbol{v}_k^\top$, we obtain

$$
\mathrm{e}^{(t_\ell - t_0)(n-1)B_\ell}\boldsymbol{e}_1 = \frac{1}{\ell}\boldsymbol{1} + \sum_{k=2}^{\ell} \mathrm{e}^{(t_\ell-t_0)(n-1)\lambda_k} v_k v_k^\top \boldsymbol{e}_1.
$$

This implies that

$$
\begin{aligned}
\left\|\mathrm{e}^{(t_\ell - t_0)(n-1)B_\ell}\boldsymbol{e}_1 - \frac{1}{\ell}\boldsymbol{1}\right\|_1 &\le \sum_{k=2}^{\ell+1} \mathrm{e}^{(t_\ell-t_0)(n-1)\lambda_k}\cdot |v_k^\top \boldsymbol{e}_1|\cdot \|v_k\|_1 \\
&\le \sum_{k=2}^{\ell+1} \mathrm{e}^{(t_\ell-t_0)(n-1)\lambda_k} && \text{(by } |v_k^\top \boldsymbol{e}_1|\le 1 \text{ and } \|v_k\|_1 \le 1) \\
&\le n\exp\left((t_\ell-t_0)(n-1)\lambda_2\right) \\
&\le n\exp\left((t_\ell-t_0)\lambda_2\right) \\
&\le n\exp\left(-(t_\ell-t_0)\frac{\pi^2}{n^2}c^{-\ell+1}\right) \\
&\le n\exp\left(-(c^{\ell-1/2}-c^{1/4})\frac{\pi^2}{n^2}c^{-\ell+1}\right) \\
&\le n\exp\left(-c^{\ell-3/4}\frac{\pi^2}{n^2}c^{-\ell+1}\right) \\
&\le n\mathrm{e}^{-\frac{\pi^2}{n^2}c^{1/4}}.
\end{aligned}
$$

Since $c > n^9$, we obtain

$$
\begin{aligned}
\left|\boldsymbol{e}_1^\top \mathrm{e}^{(t_\ell-t_0)(n-1)A_\ell}\boldsymbol{q} - \frac{1}{\ell}\boldsymbol{1}_{[1:\ell]}^\top \boldsymbol{q}\right| &\le \left\|\boldsymbol{e}_1^\top \mathrm{e}^{(t_\ell-t_0)(n-1)A_\ell} - \frac{1}{\ell}\boldsymbol{1}_{[1:\ell]}^\top\right\|_1 \\
&= \left\|\boldsymbol{e}_1^\top \mathrm{e}^{(t_\ell-t_0)(n-1)B_\ell} - \frac{1}{\ell}\boldsymbol{1}^\top\right\|_1 \\
&\le n\mathrm{e}^{-\frac{\pi^2}{n^2}c^{1/4}} \\
&\le nc^{-1/2}. \qquad (12)
\end{aligned}
$$

Combining the Bounds

Summing up the inequalities (7), (8), (9), (10), (11), and (12) together with the triangle inequality, we obtain the inequality (3), completing the proof of Lemma 9.

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