The Eyring–Kramers law for Markovian jump processes with symmetries

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Abstract

We prove an Eyring–Kramers law for the small eigenvalues and mean first-passage times of a metastable Markovian jump process which is invariant under a group of symmetries. Our results show that the usual Eyring–Kramers law for asymmetric processes has to be corrected by a factor computable in terms of stabilisers of group orbits. Furthermore, the symmetry can produce additional Arrhenius exponents and modify the spectral gap. The results are based on representation theory of finite groups.

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1 Introduction

The Eyring–Kramers law characterises the mean transition times between local minima of a diffusion in a potential landscape. Consider the stochastic differential equation

$$\mathrm{d}x_t = -\nabla V(x_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t\;, \tag{1.1}$$

where $V : \mathbb{R}^d \to \mathbb{R}$ is a confining potential, and W_t is a d-dimensional standard Brownian motion. If V has just two quadratic local minima x^* and y^*, separated by a quadratic saddle z^*, the Eyring–Kramers law states that the expected first-passage time τ from x^* to a small ball around y^* is given by

$$\mathbb{E}^{x^*}[\tau] = \frac{2\pi}{|\lambda_1(z^\star)|}\sqrt{\frac{|\det(\nabla^2 V(z^\star))|}{\det(\nabla^2 V(x^\star))}}\,\mathrm{e}^{[V(z^\star)-V(x^\star)]/\varepsilon}\bigl[1+\mathcal{O}(\varepsilon^{1/2}|\log\varepsilon|^{3/2})\bigr]\;. \tag{1.2}$$

Here $\nabla^2 V(x^\star)$ and $\nabla^2 V(z^\star)$ denote the Hessian matrices of V at $x^\star$ and $z^\star$ respectively, and $\lambda_1(z^\star)$ is the unique negative eigenvalue of $\nabla^2 V(z^\star)$ (hence $z^\star$ is called a saddle of index 1). A critical point is called quadratic if the Hessian matrix is non-singular.

The exponential behaviour in $\mathrm{e}^{[V(z^\star)-V(x^\star)]/\varepsilon}$ of (1.2) was first proposed by van t'Hoff, and justified physically by Arrhenius [1]. The more precise formula with the prefactors depending on Hessians was introduced by Eyring [14] and Kramers [19]. Mathematical proofs for these formulas are much more recent. The Arrhenius law has first been justified by Wentzell and Freidlin, using the theory of large deviations [25, 26]. The first rigorous proof of the full Eyring–Kramers law (1.2) was provided by Bovier, Eckhoff, Gayrard and Klein, using potential-theoretic methods [10, 11]. These methods have also been applied to lattice models [9, 12] and used to extend the Eyring–Kramers law to systems with non-quadratic saddles [7] and to stochastic partial differential equations [8, 2]. Other approaches to proving (1.2) include an analysis of Witten Laplacians acting on p-forms [15, 21]. See for instance [4] for a recent survey.

If the potential V has $N > 2$ local minima, the characterisation of metastable timescales becomes more involved. It has been known for a long time that the diffusion's generator admits N exponentially small eigenvalues, and that they are connected to metastable timescales [22, 23, 18, 17]. In fact, results in [11] show that one can order the local minima $x_1^*, \dots, x_N^*$ of V in such a way that the mean transition time from each x_k^* to the set $\{x_1^*, \dots, x_{k-1}^*\}$ of its predecessors is close to the inverse of the kth small eigenvalue.

The only limitation of these results is that they require a non-degeneracy condition to hold. In short, all relevant saddle heights have to be different (see Section 2.2 for a precise formulation). While this condition holds for generic potentials V, it will fail whenever the potential is invariant under a symmetry group G. Let us mention two examples of such potentials, which will serve as illustrations of the theory throughout this work.

Example 1.1. The papers [5, 6] introduce a model with N particles on the periodic lattice $\Lambda = \mathbb{Z}_N := \mathbb{Z}/N\mathbb{Z}$, which are coupled harmonically to their nearest neighbours, and subjected to a local double-well potential $U(y) = \frac{1}{4}y^4 - \frac{1}{2}y^2$. The associated potential reads

$$V_\gamma(x) = \sum_{i\in\Lambda} U(x_i) + \frac{\gamma}{4} \sum_{i\in\Lambda} (x_{i+1} - x_i)^2 . \tag{1.3}$$

The potential V_γ is invariant under the group G generated by three transformations: the cyclic permutation $r : x \mapsto (x_2, \dots, x_N, x_1)$, the reflection $s : x \mapsto (x_N, \dots, x_1)$ and the sign change $c : x \mapsto -x$. The transformations r and s generate the dihedral group D_N, and since c commutes with r and s, G is the direct product $D_N \times \mathbb{Z}_2$.

It has been shown in [5] that for weak coupling γ, the model behaves like an Ising model with Glauber spin-flip dynamics [12, Section 3], while for large γ the systems synchronizes, meaning that all components x_i tend to be equal.

Example 1.2. Consider a variant of the previous model, obtained by restricting V_γ to the space $\{x \in \mathbb{R}^\Lambda \colon \sum x_i = 0\}$. For weak coupling, this system will mimic a Kawasaki-type dynamics with conserved "particle" number [12, Section 4]. The symmetry group G is the same as in the previous example.

The potential-theoretic approach has been extended to some particular degenerate situations, by computing equivalent capacities for systems of capacitors in series or in parallel [3, Chapter 1.2]. This is close in spirit to the electric-network analogy for random walks on graphs [13]. However, for more complicated symmetric potentials admitting many local minima, the computation of equivalent capacities becomes untractable. This is why we develop in this work a general approach based on Frobenius' representation theory for finite groups. The basic idea is that each irreducible representation of the group G will yield a subset of the generator's eigenvalues. The trivial representation corresponds to initial distributions which are invariant under G, while all other representations are associated with non-invariant distributions.

In the present work, we concentrate on the case where the process itself is a Markovian jump process, with states given by the local minima, and transition probabilities governed by the Eyring–Kramers law between neighbouring minima. We expect that the results can be extended to diffusions of the form (2.1), is a similar way as in the asymmetric case. The main results are Theorems 3.2, 3.5 and 3.9 in Section 3, which provide sharp estimates for the eigenvalues and relate them to mean transition times.

The remainder of the article is organised as follows. In Section 2, we define the main objects, recall results from the asymmetric case, as well as some elements of representation theory of finite groups. Section 3 contains the results on eigenvalues and transition times for symmetric processes. These results are illustrated in Section 4 for two cases of Example 1.2. The remaining sections contain the proofs of these results. Section 5 collects all proofs related to representation theory, Section 6 contains the estimates of eigenvalues, and Section 7 establishes the links with mean transition times. Finally Appendix A gives some information on the computation of the potential landscape of Example 1.2.

Notations: We denote by $a \wedge b$ the minimum of two real numbers a and b, and by $a \vee b$ their maximum. If A is a finite set, $|A|$ denotes its cardinality, and $1_A(x)$ denotes the indicator function of $x \in A$. We write $\mathbb{1}$ for the identity matrix, and $\mathbf{1}$ for the constant vector with all components equal to 1. The results concern Markovian jump processes $\{X_t\}_{t \geqslant 0}$ on finite sets $\mathcal{X}$, defined on a filtered probability space $(\Omega, \mathcal{F}, \mathbb{P}, \{\mathcal{F}_t\}_{t \geqslant 0})$. We denote their generator by L, that is, L is a matrix with non-negative off-diagonal elements, and zero row sums. The law of X_t starting with an initial distribution μ is denoted $\mathbb{P}^\mu\{\cdot\}$, and $\mathbb{E}^\mu[\cdot]$ stands for associated expectations. If $\mu = \delta_i$ is concentrated in a single point, we write $\mathbb{P}^i\{\cdot\}$ and $\mathbb{E}^i[\cdot]$.

2 Setting

2.1 Metastable markovian jump processes

Let $\mathcal{X}$ be a finite set, and let L be the generator of a Markovian jump process on $\mathcal{X}$. We assume that the elements of L can be written in the form

$$L_{ij} = \frac{c_{ij}}{m_i} \, \mathrm{e}^{-h_{ij}/\varepsilon} \;, \qquad i, j \in \mathcal{X} \;, i \neq j \;, \tag{2.1}$$

where $\varepsilon > 0$, $c_{ij} = c_{ji} > 0$, $m_i > 0$ and $0 \leqslant h_{ij} \leqslant +\infty$ (it will be convenient to write $h_{ij} = +\infty$ to indicate that $L_{ij} = 0$). In addition, we assume that there exists a function $V : \mathcal{X} \to \mathbb{R}_+$ such that L is reversible with respect to the measure $m \, \mathrm{e}^{-V/\varepsilon}$:

$$m_i \, \mathrm{e}^{-V_i/\varepsilon} \, L_{ij} = m_j \, \mathrm{e}^{-V_j/\varepsilon} \, L_{ji} \qquad \forall i, j \in \mathcal{X} \;. \tag{2.2}$$

Since we assume $c_{ij} = c_{ji}$, this is equivalent to

$$V_i + h_{ij} = V_j + h_{ji} \qquad \forall i, j \in \mathcal{X} \;. \tag{2.3}$$

Our aim is to understand the behaviour as $\varepsilon \to 0$ of the Markov process X_t of generator L, when L is invariant under a group G of bijections of $\mathcal{X}$.

Let $\mathcal{G} = (\mathcal{X}, E)$ be the undirected graph with set of edges $E = \{(i,j) \in \mathcal{X}^2 \colon L_{ij} > 0\}$. It will be convenient to associate with an edge $e = (i,j) \in E$ the *height of the saddle between i and j* defined by $V_e = V_i + h_{ij} = V_j + h_{ji}$, and to write $c_e = c_{ij} = c_{ji}$.

2.2 The asymmetric case

We now explain how the small-ε asymptotics of the eigenvalues of the generator L can be determined from the graph $\mathcal{G}$ and the notions of communication height and metastable hierarchy, following [10, 11].

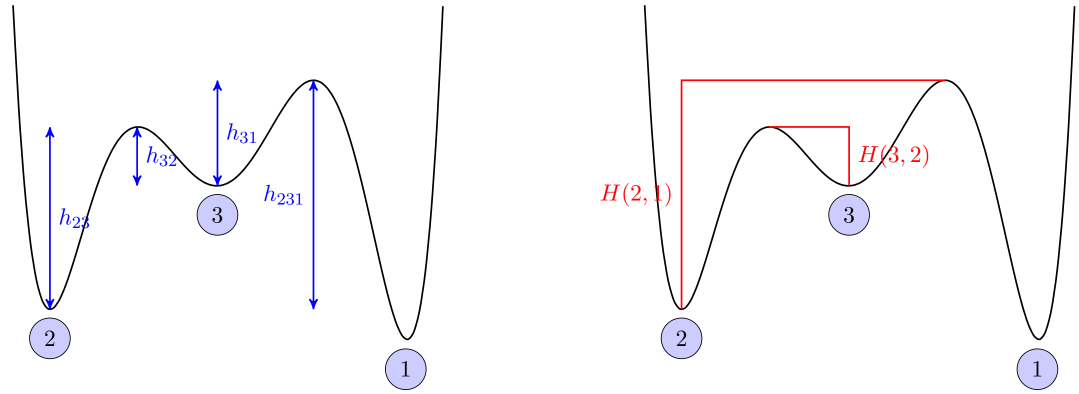

FIGURE 1. Definition of communication heights and metastable hierarchy.

Definition 2.1 (Communication heights)**.** *Let $i \neq j \in \mathcal{X}$. For $p \geqslant 1$, the $(p+1)$-step* communication height *from i to j is defined inductively by*

$$h_{ik_1\dots k_pj} = h_{ik_1\dots k_p} \vee (h_{ik_1} - h_{k_1i} + h_{k_1k_2} - h_{k_2k_1} + \dots + h_{k_pj}) \tag{2.4}$$

(see Figure 1). We define the communication height *from i to $j \neq i$ by*

$$H(i,j) = \min_{\gamma : i \to j} h_\gamma \;, \tag{2.5}$$

where the minimum runs over all paths $\gamma = (i, k_1, \dots, k_p, j)$ of length $p+1 \geqslant 1$. Any such path realising the minimum in (2.5) *is called a* minimal path from i to j. *If $i \notin A \subset \mathcal{X}$, we define the communication height from i to A as*

$$H(i,A) = \min_{j \in A} H(i,j) \;. \tag{2.6}$$

Communication heights can be equivalently defined in terms of heights of saddles, by

$$h_{ik_1\dots k_pj} + V_i = V_{(i,k_1)} \vee V_{(k_1,k_2)} \vee \dots \vee V_{(k_p,j)} \;. \tag{2.7}$$

Thus $H(i,j) + V_i$ is the minimum over all paths γ from i to j of the maximal saddle height encountered along γ.

Assumption 2.2 (Metastable hierarchy)**.** The elements of $\mathcal{X} = \{1, \dots, n\}$ can be ordered in such a way that if $\mathcal{M}_k = \{1, \dots, k\}$,

$$H(k, \mathcal{M}_{k-1}) \leqslant \min_{i<k} H(i, \mathcal{M}_k \setminus \{i\}) - \theta \;, \qquad k = 2, \dots, n \tag{2.8}$$

for some $\theta > 0$. We say that the order $1 \prec 2 \prec \dots \prec n$ defines the *metastable hierarchy* of $\mathcal{X}$ (see Figure 1). Furthermore, for each k there is a unique edge $e^*(k)$ such that any minimal path $\gamma : k \to \mathcal{M}_{k-1}$ reaches height $H(k, \mathcal{M}_{k-1}) + V_k$ only on the edge $e^*(k)$. Finally, any non-minimal path $\gamma : k \to \mathcal{M}_{k-1}$ reaches at least height $V_{e^*(k)} + \theta$.

Condition (2.8) means that in the lower-triangular part of the matrix of communication heights $H(i,j)$, the minimum of each row is smaller than the minimum of the row above. Such an ordering will typically only exist if L admits no nontrivial symmetry group.

The following result is essentially equivalent to [11, Theorem 1.2], but we will provide a new proof that will be needed for the symmetric case.

Theorem 2.3 (Asymptotic behaviour of eigenvalues)**.** *If Assumption 2.2 holds, then for sufficiently small ε, the eigenvalues of L are given by $\lambda_1 = 0$ and*

$$\lambda_k = -\frac{c_{e^*(k)}}{m_k}\,\mathrm{e}^{-H(k,\mathcal{M}_{k-1})/\varepsilon}\bigl[1+\mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\bigr]\;, \qquad k=2,\dots,n\;. \tag{2.9}$$

Furthermore, let $\tau_{\mathcal{M}_{k-1}} = \inf\{t>0\colon X_t \in \mathcal{M}_{k-1}\}$ be the first-hitting time of $\mathcal{M}_{k-1}$. Then for $k=2,\dots,n$,

$$\mathbb{E}^i\bigl[\tau_{\mathcal{M}_{k-1}}\bigr] = \frac{1}{|\lambda_k|}\bigl[1+\mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\bigr] \tag{2.10}$$

holds for all initial values $i \in \mathcal{X}\setminus\mathcal{M}_{k-1}$.

2.3 Symmetry groups and their representations

Let G be a finite group of bijections $g:\mathcal{X}\to\mathcal{X}$. We denote by $\pi(g)$ the permutation matrix

$$\pi(g)_{ab} = \begin{cases} 1 & \text{if } g(a)=b\;,\\ 0 & \text{otherwise}\;. \end{cases} \tag{2.11}$$

We assume that the generator L is *invariant* under G, that is,

$$\pi(g)L = L\pi(g) \quad \forall g\in G\;. \tag{2.12}$$

This is equivalent to assuming $L_{ab} = L_{g(a)g(b)}$ for all $a,b\in\mathcal{X}$ and all $g\in G$.

Let us recall a few definitions from basic group theory.

Definition 2.4.

1. *For $a\in\mathcal{X}$, $O_a=\{g(a)\colon g\in G\}\subset\mathcal{X}$ is called the* orbit *of a.*
2. *For $a\in\mathcal{X}$, $G_a=\{g\in G\colon g(a)=a\}\subset G$ is called the* stabiliser *of a.*
3. *For $g\in G$, $\mathcal{X}^g=\{a\in\mathcal{X}\colon g(a)=a\}\subset\mathcal{X}$ is called the* fixed-point set *of g.*

The following facts are well known:

- The orbits form a partition of $\mathcal{X}$, denoted $\mathcal{X}/G$.
- For any $a\in\mathcal{X}$, G_a is a subgroup of G.
- For any $a\in\mathcal{X}$, the map $\varphi: gG_a\mapsto g(a)$ provides a bijection from the set G/G_a of left cosets to the orbit O_a of a, and thus $|G|/|G_a|=|O_a|$.
- For any $g\in G$ and any $a\in\mathcal{X}$, one has $G_{g(a)}=gG_ag^{-1}$, i.e. stabilisers of a given orbit are conjugated.
- *Burnside's lemma:* $\sum_{g\in G}|\mathcal{X}^g| = |G||\mathcal{X}/G|$.

We will denote the orbits of G by $A_1,\dots,A_m$. The value of the communication height $H(a,A_j)$ is the same for all $a\in A_i$, and we will denote it $H(A_i,A_j)$. Similarly, we write V_{A_i} for the common value of all V_a, $a\in A_i$. We shall make the following two non-degeneracy assumptions:

Assumption 2.5 (Metastable order of orbits)**.** Let $\mathcal{M}_k = A_1\cup\dots\cup A_k$. One can order the orbits in such a way that

$$H(A_k,\mathcal{M}_{k-1}) \leqslant \min_{i<k} H(A_i,\mathcal{M}_k\setminus A_i)-\theta\;, \qquad k=2,\dots,m \tag{2.13}$$

for some $\theta>0$. We indicate this by writing $A_1\prec A_2\prec\dots\prec A_m$. Furthermore, for each $k=2,\dots,m$, there is an edge $e^*(k)\in E$ such that

$$H(A_k,\mathcal{M}_{k-1})+V_{A_k} = V_{(a,b)} \quad\Leftrightarrow\quad \exists g\in G\colon (g(a),g(b))=e^*(k)\;. \tag{2.14}$$

Assumption 2.6 (Absence of accidental degeneracy)**.** Whenever there are elements a_1, b_1, a_2, $b_2 \in \mathcal{X}$ such that $h_{a_1b_1} = h_{a_2b_2}$, there exists $g \in G$ such that $g(\{a_1, b_1\}) = \{a_2, b_2\}$.

We make the rather strong Assumption 2.6 mainly to simplify the expressions for eigenvalues; the approach we develop here can be applied without this assumption.

Direct transitions between two orbits A_i and A_j are dominated by those edges (a, b) for which h_{ab} is minimal. We denote the minimal value

$$h^*(A_i, A_j) = \inf\{h_{ab} \colon a \in A_i, b \in A_j\} \; . \tag{2.15}$$

Note that $h^*(A_i, A_j)$ may be infinite (if there is no edge between the orbits), and that $H(A_i, A_j) \leqslant h^*(A_i, A_j)$. By decreasing, if necessary, the value of $\theta > 0$, we may assume that

$$h_{ab} > h^*(A_i, A_j), \; a \in A_i, \; b \in A_j \quad \Rightarrow \quad h_{ab} \geqslant h^*(A_i, A_j) + \theta \; . \tag{2.16}$$

Assumption 2.6 implies the following property of the matrix elements of L:

Lemma 2.7. *For all $a, b \in \mathcal{X}$, belonging to different orbits, $L_{ah(b)} = L_{ab}$ if and only if $h \in G_a G_b$.*

PROOF: By Assumption 2.6, $L_{ah(b)} = L_{ab}$ if and only if there is a $g \in G$ such that $g(a) = a$ and $g(b) = h(b)$. This is equivalent to the existence of a $g \in G_a$ such that $g(b) = h(b)$, i.e. $b = g^{-1}h(b)$. This in turn is equivalent to $h \in G_a G_b$. $\square$

By Lemma 2.7, if $h^*(A_i, A_j)$ is finite, each $a \in A_i$ is connected to exactly $|G_a G_b|/|G_b|$ states in $A_j \ni b$ with transition rate $L_{ab} = [c_{ab}/m_a] \, \mathrm{e}^{-h^*(A_i,A_j)/\varepsilon}$. Observe that

$$\begin{aligned} \varphi : G_a G_b / G_b &\to G_a/(G_a \cap G_b) \\ g G_b &\mapsto g(G_a \cap G_b) \end{aligned} \tag{2.17}$$

is a bijection, and therefore the number n_j^a of states in A_j communicating with a can be written in either of the two equivalent forms

$$n_j^a = \frac{|G_a G_b|}{|G_b|} = \frac{|G_a|}{|G_a \cap G_b|} \; . \tag{2.18}$$

The map π defined by (2.11) is a morphism from G to $\mathrm{GL}(n, \mathbb{C})$, and thus defines a *representation* of G (of dimension $\dim \pi = n$). In what follows, we will draw on some facts from representation theory of finite groups (see for instance [24]):

- A representation of G is called *irreducible* if there is no proper subspace of $\mathbb{C}^n$ which is invariant under all $\pi(g)$.
- Two representations π and π' of dimension d of G are called *equivalent* if there exists a matrix $S \in \mathrm{GL}(d, \mathbb{C})$ such that $S\pi(g)S^{-1} = \pi'(g)$ for all $g \in G$.
- Any finite group G has only finitely many inequivalent irreducible representations $\pi^{(0)}, \dots, \pi^{(r-1)}$. Here $\pi^{(0)}$ denotes the *trivial representation*, $\pi^{(0)}(g) = 1 \; \forall g \in G$.
- Any representation π of G can be decomposed into irreducible representations:

$$\pi = \bigoplus_{p=0}^{r-1} \alpha^{(p)} \pi^{(p)} \; , \qquad \alpha^{(p)} \geqslant 0 \; , \quad \sum_{p=0}^{r-1} \alpha^{(p)} \dim(\pi^{(p)}) = \dim(\pi) = n \; . \tag{2.19}$$

  This means that we can find a matrix $S \in \mathrm{GL}(n, \mathbb{C})$ such that all matrices $S\pi(g)S^{-1}$ are block diagonal, with $\alpha^{(p)}$ blocks given by $\pi^{(p)}(g)$. This decomposition is unique up to equivalence and the order of factors.

- For any irreducible representation $\pi^{(p)}$ contained in π, let $\chi^{(p)}(g) = \operatorname{Tr} \pi^{(p)}(g)$ denote its *characters*. Then

$$P^{(p)} = \frac{\dim(\pi^{(p)})}{|G|} \sum_{g \in G} \overline{\chi^{(p)}(g)} \pi(g) \tag{2.20}$$

is the projector on the invariant subspace of $\mathbb{C}^n$ associated with $\pi^{(p)}$. In particular,

$$\alpha^{(p)} \dim(\pi^{(p)}) = \operatorname{Tr} P^{(p)} = \frac{\dim(\pi^{(p)})}{|G|} \sum_{g \in G} \overline{\chi^{(p)}(g)} \chi(g) , \tag{2.21}$$

where $\chi(g) = \operatorname{Tr} \pi(g)$. Note that for the representation defined by (2.11), we have $\chi(g) = |\mathcal{X}^g|$.

Example 2.8 (Irreducible representations of the dihedral group)**.** The dihedral group D_N is the group of symmetries of a regular N-gon. It is generated by r, the rotation by $2\pi/N$, and s, one of the reflections preserving the N-gon. In fact

$$D_N = \bigl\{ \mathrm{id}, r, r^2, \dots, r^{N-1}, s, rs, r^s, \dots, r^{N-1}s \bigr\} \tag{2.22}$$

is entirely specified by the conditions $r^N = \mathrm{id}$, $s^2 = \mathrm{id}$ and $rs = sr^{-1}$. If N is even, then D_N has 4 irreducible representations of dimension 1, specified by $\pi(r) = \pm 1$ and $\pi(s) = \pm 1$. In addition, it has $\frac{N}{2} - 1$ irreducible representations of dimension 2, equivalent to

$$\pi(r) = \begin{pmatrix} \mathrm{e}^{2\,\mathrm{i}\,\pi k/N} & 0 \\ 0 & \mathrm{e}^{-2\,\mathrm{i}\,\pi k/N} \end{pmatrix} , \qquad \pi(s) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \qquad k = 1, \dots \frac{N}{2} - 1 . \tag{2.23}$$

The associated characters are given by

$$\chi(r^i s^j) = \operatorname{Tr} \pi(r^i s^j) = 2 \cos\biggl(\frac{2\pi i k}{N}\biggr) \delta_{j0} , \qquad i = 0, \dots, N-1,\ j = 0, 1 . \tag{2.24}$$

There are no irreducible representations of dimension larger than 2. If N is odd, there are 2 irreducible representations of dimension 1, specified by $\pi(r) = 1$ and $\pi(s) = \pm 1$, and $(N-1)/2$ irreducible representations of dimension 2.

3 Results

We are now going to use the decomposition (2.19) of the representation (2.11) to characterise the eigenvalues of L. It follows from (2.12) and (2.20) that

$$P^{(p)} L = L P^{(p)} , \qquad p = 0, \dots, r-1 , \tag{3.1}$$

so that the r images $P^{(p)}\mathbb{C}^n$ (where $n = |\mathcal{X}|$) are invariant subspaces for L. We can thus determine the eigenvalues of L by restricting the analysis to each restriction $L^{(p)}$ of L to the subspace $P^{(p)}\mathbb{C}^n$.

3.1 The trivial representation

Let us start by the restriction $L^{(0)}$ of L to the subspace $P^{(0)}\mathbb{C}^n$ associated with the trivial representation $\pi^{(0)}$.

Proposition 3.1 (Matrix elements of $L^{(0)}$ for the trivial representation)**.** *The subspace $P^{(0)}\mathbb{C}^n$ has dimension m and is spanned by the vectors $u_i^{(0)} = 1_{A_i}$, $i = 1,\dots m$. The off-diagonal matrix element of $L^{(0)}$ for transitions between the orbits A_i and A_j is given by*

$$L_{ij}^{(0)} := \frac{\langle u_i, Lu_j\rangle}{\langle u_i, u_i\rangle} = \frac{c_{ij}^*}{m_i^*}\,\mathrm{e}^{-h^*(A_i,A_j)/\varepsilon}[1+\mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})] , \tag{3.2}$$

with

$$c_{ij}^* = \frac{c_{ab}}{|G_a\cap G_b|} , \qquad m_i^* = \frac{m_a}{|G_a|} , \tag{3.3}$$

where $a \in A_i$ and $b \in A_j$ are such that $h_{ab} = h^*(A_i, A_j)$. Furthermore, $L^{(0)}$ is a generator, and thus its diagonal elements are given by

$$L_{ii}^{(0)} =: -\sum_{j\neq i} L_{ij}^{(0)} . \tag{3.4}$$

The basis vectors u_i are indicator functions on the orbits A_i. Thus if the initial distribution μ is uniform on each A_i, then it stays uniform on each A_i for all times. The process X_t is then equivalent to the process on $\{1,\dots,m\}$ with transition probabilities given by $L^{(0)}$. Applying Theorem 2.3 on the asymmetric case to this process, which is possible thanks to Assumption 2.5, we thus obtain the following Kramers formula for the eigenvalues of $L^{(0)}$.

Theorem 3.2 (Eigenvalues associated with the trivial representation)**.** *If Assumptions 2.5 and 2.6 hold true, then for ε small enough, the spectrum of $L^{(0)}$ consists in m eigenvalues of geometric multiplicity 1, given by $\lambda_1^{(0)} = 0$ and*

$$\lambda_k^{(0)} = \frac{c_{i(k)j(k)}^*}{m_k^*}\,\mathrm{e}^{-H(A_k,\mathcal{M}_{k-1})/\varepsilon}\big[1+\mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\big] , \qquad k = 2,\dots,m , \tag{3.5}$$

where $i(k)$ and $j(k)$ are such $e^*(k) = (a,b)$ with $a \in A_{i(k)}$ and $b \in A_{j(k)}$ (cf (2.14)). Furthermore, for $2 \leqslant k \leqslant m$, let μ be a probability distribution supported on $\mathcal{X}\setminus\mathcal{M}_{k-1}$ which is uniform on each A_j. Then

$$\mathbb{E}^\mu\big[\tau_{\mathcal{M}_{k-1}}\big] = \frac{1}{|\lambda_k|}\big[1+\mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\big] . \tag{3.6}$$

The main difference between the Kramers formula (3.5) of the symmetric case and its equivalent (2.9) for the asymmetric case is that the eigenvalues are multiplied by an extra factor $|G_c|/|G_a\cap G_b|$, $c \in A_k$, $a \in A_{i(k)}$ and $b \in A_{j(k)}$, which accounts for the symmetry.

3.2 Other irreducible representations of dimension 1

Theorem 3.2 only accounts for a small subset of m eigenvalues of the generator, associated with distributions that are uniform on each orbit A_i. The other eigenvalues of L will be associated to the rate at which non-uniform initial distributions approach the uniform one.

Lemma 3.3. *Let $\pi^{(p)}$ be an irreducible representation of dimension 1 of G, let A_i be an orbit of G and fix any $a \in A_i$. Denote by π_i the permutation induced by G on A_i and let $P_i^{(p)}$ be the associated projector, cf. (2.20). Then one of two following cases holds:*

- *either $\pi^{(p)}(h) = 1$ for all $h \in G_a$, and then $\operatorname{Tr} P_i^{(p)} = 1$;*
- *or $\sum_{h\in G_a}\pi^{(p)}(h) = 0$, and then $\operatorname{Tr} P_i^{(p)} = 0$.*

Let us call *active* (with respect to the representation $\pi^{(p)}$) the orbits A_i such that $\operatorname{Tr} P_i^{(p)} = 1$, and *inactive* the other orbits. The restriction $L^{(p)}$ of L to the subspace $P^{(p)}\mathbb{C}^n$ has dimension equal to the number of active orbits, and the following result describes its matrix elements.

Proposition 3.4 (Matrix elements for an irreducible representation of dimension 1)**.** *For each orbit A_i fix an $a_i \in A_i$. The subspace $P^{(p)}\mathbb{C}^n$ is spanned by the vectors $(u_i^{(p)})_{A_i \text{ active}}$ with components*

$$(u_i^{(p)})_a = \begin{cases} \overline{\pi^{(p)}(h)} & \text{if } a = h(a_i) \in A_i \;, \\ 0 & \text{otherwise} \;. \end{cases} \tag{3.7}$$

The off-diagonal matrix elements of $L^{(p)}$ between two active orbits A_i and A_j are again given by

$$L_{ij}^{(p)} = \frac{\langle u_i^{(p)}, L u_j^{(p)} \rangle}{\langle u_i^{(p)}, u_i^{(p)} \rangle} = L_{ij}^{(0)} = \frac{c_{ij}^*}{m_i^*} \, \mathrm{e}^{-h^*(A_i,A_j)/\varepsilon} [1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})] \;. \tag{3.8}$$

The diagonal elements of $L^{(p)}$ are given by

$$L_{ii}^{(p)} = L_{ii}^{(0)} - \sum_{gG_{a_i} \in G/G_{a_i} \setminus G_{a_i}} (1 - \pi^{(p)}(g)) L_{a_i g(a_i)} \;. \tag{3.9}$$

Using Assumption 2.6, we can obtain a more explicit expression for the diagonal matrix elements. For each orbit A_i, we can define a unique *successor* $s(i)$, which labels the orbit which is easiest to reach in one step from A_i:

$$\inf_{j \neq i} h^*(A_i, A_j) = h^*(A_i, A_{s(i)}) \;. \tag{3.10}$$

As a consequence of (3.4), we have

$$L_{ii}^{(0)} = -\frac{c_{is(i)}^*}{m_i^*} \, \mathrm{e}^{-h^*(A_i,A_{s(i)})/\varepsilon} [1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})] \;. \tag{3.11}$$

There are different cases to be considered, depending on whether it is easier, starting from $a \in A_i$, to reach states outside A_i or in $A_i \setminus a$. Let a^* be such that $h(a, a^*) = \inf_b h(a,b)$. Then

$$L_{ii}^{(p)} = \begin{cases} L_{ii}^{(0)} [1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})] & \text{if } a^* \notin A_i \;, \\ -2[1 - \operatorname{Re} \pi^{(p)}(k)] L_{aa^*} [1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})] & \text{if } a^* = k(a) \in A_i \text{ and } k \neq k^{-1} \;, \\ -[1 - \pi^{(p)}(k)] L_{aa^*} [1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})] & \text{if } a^* = k(a) \in A_i \text{ and } k = k^{-1} \;. \end{cases} \tag{3.12}$$

Relation (3.9) and the fact that not all orbits are active for a nontrivial representation imply that the matrix $L^{(p)}$ is not a generator if $p \neq 0$. We can however add a cemetery state to the set of active orbits, and thus associate to $L^{(p)}$ a Markovian jump process on the augmented space. The cemetery state is absorbing, which reflects the fact that all nonzero initial conditions in $P^{(p)}\mathbb{C}^n$ are asymmetric and will converge to the symmetric invariant distribution.

Theorem 3.5 (Eigenvalues associated with nontrivial irreducible representations of dimension 1)**.** *Let $\pi^{(p)}$ be a nontrivial irreducible representation of G of dimension* 1*, and let n_p be the number of active orbits associated with $\pi^{(p)}$. For sufficiently small ε, the spectrum of $L^{(p)}$ consists in n_p eigenvalues of geometric multiplicity* 1*. They can be determined by applying Theorem 2.3 to the augmented process defined by $L^{(p)}$, and ignoring the eigenvalue* 0*.*

3.3 Irreducible representations of dimension larger than 1

Lemma 3.6. *Let $\pi^{(p)}$ be an irreducible representation of G of dimension $d \geqslant 2$, and let A_i be an orbit of G. Denote by π_i the permutation induced by G on A_i, and let $P_i^{(p)}$ be the associated projector, cf. (2.20). Then for arbitrary $a \in A_i$,*

$$\operatorname{Tr}(P_i^{(p)}) = d\alpha_i^{(p)} , \qquad \alpha_i^{(p)} = \frac{1}{|G_a|} \sum_{h \in G_a} \chi^{(p)}(h) \in \{0, 1, \dots, d\} . \tag{3.13}$$

Here $\chi^{(p)}(h) = \operatorname{Tr} \pi^{(p)}(h)$ denotes the characters of the irreducible representation.

Let us again call *active* (with respect to the irreducible representation $\pi^{(p)}$) those orbits for which $\operatorname{Tr}(P_i^{(p)}) > 0$.

Proposition 3.7 (Matrix elements of $L^{(p)}$ for an irreducible representation $\pi^{(p)}$ of dimension larger than 1)**.** *The subspace $P^{(p)}\mathbb{C}^n$ is spanned by the vectors $(u_i^a)_{i=1,\dots,m,a\in A_i}$ with components*

$$(u_i^a)_b = \begin{cases} \dfrac{d}{|G_a|} \displaystyle\sum_{g \in G_a} \overline{\chi^{(p)}(gh)} & \text{if } b = h(a) \in A_i , \\ 0 & \text{otherwise} . \end{cases} \tag{3.14}$$

The matrix elements of $L^{(p)}$ between two different active orbits A_i and A_j are given by

$$\frac{\langle u_i^{h_1(a)}, L u_j^{h_2(b)} \rangle}{\langle u_i^{h_1(a)}, u_i^{h_1(a)} \rangle} = \frac{c_{ij}^*}{\alpha_i^{(p)} m_i^*} \, \mathrm{e}^{-h^*(A_i,A_j)/\varepsilon} \, M_{h_1(a)h_2(b)}^{(p)} [1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})] , \tag{3.15}$$

where $a \in A_i$, $b \in A_j$, $h_1, h_2 \in G$, and

$$M_{h_1(a)h_2(b)}^{(p)} = \frac{1}{|G_a G_b|} \sum_{g \in G_a G_b} \chi^{(p)}(h_1 g h_2^{-1}) . \tag{3.16}$$

The diagonal blocks of $L^{(p)}$ are given by the following expressions. Let $a \in A_i$ and let a^* be such that $h(a, a^*) = \inf_b h(a, b)$. Then

$$\frac{\langle u_i^{h_1(a)}, L u_i^{h_2(a)} \rangle}{\langle u_i^{h_1(a)}, u_i^{h_1(a)} \rangle} = \begin{cases} \dfrac{L_{ii}^{(0)}}{\alpha_i^{(p)}} M_{h_1(a)h_2(a)}^{(p)} [1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})] & \text{if } a^* \notin A , \\ \\ -\dfrac{L_{aa^*}}{\alpha_i^{(p)}} M_{h_1(a)h_2(a)}^{(p)} [1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})] & \text{if } a^* \in A , \end{cases} \tag{3.17}$$

where

$$M_{h_1(a)h_2(a)}^{(p)} = \frac{1}{|G_a|} \sum_{g \in G_a} \chi^{(p)}(h_1 g h_2^{-1}) \tag{3.18}$$

if $a^* \notin A_i$, while for $a^* = k(a) \in A_i$,

$$M_{h_1(a)h_2(a)}^{(p)} = \begin{cases} \dfrac{1}{|G_a|} \displaystyle\sum_{g \in G_a} \big[2\chi^{(p)}(h_1 g h_2^{-1}) - \chi^{(p)}(h_1 k g h_2^{-1}) - \chi^{(p)}(h_1 k^{-1} g h_2^{-1}) \big] & \text{if } k \neq k^{-1}, \\ \dfrac{1}{|G_a|} \displaystyle\sum_{g \in G_a} \big[\chi^{(p)}(h_1 g h_2^{-1}) - \chi^{(p)}(h_1 k g h_2^{-1}) \big] & \text{if } k = k^{-1}. \end{cases} \tag{3.19}$$

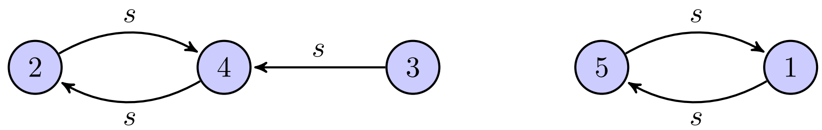

FIGURE 2. Example of graph of successors, with two cycles $(2, 4)$ and $(1, 5)$.

In order to apply this result, we have to choose, for each orbit A_i, $d\alpha_i^{(p)}$ linearly independent vectors among the $(u_i^a)_{a\in A_i}$.

This result shows that in an appropriate basis, the matrix $L^{(p)}$ has a block structure, with one block $L_{ij}^{(p)}$ for each pair of active orbits. Each block has the same exponential weight as in the one-dimensional case, but the prefactors are multiplied by a nontrivial matrix $M^{(p)}$ depending only on the representation and on the stabilisers of the two orbits.

In order to determine the eigenvalues, recall the definition (3.10) of the successor $s(i)$ of an orbit i. We define an oriented graph on the set of orbits, with oriented edges $i \to s(i)$ (see Figure 2). Assumption 2.6 implies that each orbit is either in a cycle of length 2, or in no cycle. If i is in a cycle of length 2 and $V_i < V_{s(i)}$, we say that i is *at the bottom of a cycle*. We will need the following assumption:

Assumption 3.8. Whenever (i, j) form a cycle in the graph of successors, $L_{jj}^{(p)}$ is invertible and the leading coefficient of the matrix

$$L_{ii}^{(p)} - L_{ij}^{(p)}\bigl(L_{jj}^{(p)}\bigr)^{-1}L_{ji}^{(p)} \tag{3.20}$$

has the same exponent as the leading coefficient of $L_{ii}^{(p)}$.

Note that this assumption will not hold in the one-dimensional case whenever $j = s(i)$. The reason it holds generically in the present case is that there is no particular reason that the matrix $L^{(p)}$ is a generator. In fact the row sums will typically be different from zero for each active orbit, which can be viewed as the fact that each active orbit communicates with a cemetery state. We will give an example in the next section. Under this assumption, we obtain the following characterisation of eigenvalues.

Theorem 3.9 (Eigenvalues associated with representations of dimension larger than 1)**.** *If Assumptions 2.5, 2.6 and 3.8 hold and ε is small enough, then the spectrum of $L^{(p)}$ consists, up to multiplicative errors $1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})$, in*

- *the eigenvalues of the matrices* (3.20) *for all orbits A_i such that i is at the bottom of a cycle and $s(i)$ is active;*
- *the eigenvalues of all other diagonal blocks $L_{ii}^{(p)}$.*

4 Examples

We discuss in this section two applications of the previous results, which are motivated by Example 1.2. In Appendix A, we show how the local minima and saddles of that system can be computed for small coupling γ. Here we determine the eigenvalues of the associated markovian jump processes, for the cases $N = 4$, which is relatively simple and can be solved in detail, and $N = 8$, which is already substantially more involved (the case $N = 6$ features degenerate saddles, so we do not discuss it here).

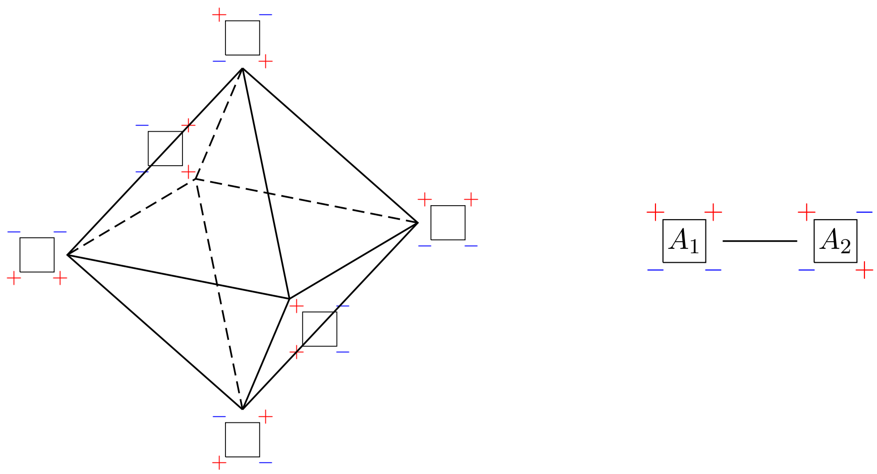

FIGURE 3. The graph $\mathcal{G} = (\mathcal{X}, E)$ for the case $N = 4$ has 6 nodes and 12 edges, forming an octaeder. The associated graph on the set of orbits has two sites and one edge.

4.1 The case $N = 4$

As explained in Appendix A, for $0 \leqslant \gamma < 2/5$ the system described in Example 1.2 admits 6 local minima, connected by 12 saddles of index 1. The potential (1.3) is invariant under the symmetry group $G = D_4 \times \mathbb{Z}_2 = \langle r, s, c \rangle$, which has order 16 and is generated by the rotation $r : (x_1, x_2, x_3, x_4) \mapsto (x_2, x_3, x_4, x_1)$, the reflection $s : (x_1, x_2, x_3, x_4) \mapsto (x_4, x_3, x_2, x_1)$, and the sign change $c : x \mapsto -x$. The local minima form two orbits

$$\begin{aligned} A_1 &= \big\{(1,1,-1,-1), (1,-1,-1,1), (-1,-1,1,1), (-1,1,1,-1)\big\} + \mathcal{O}(\gamma) \\ &= \big\{a, r(a), r^2(a), r^3(a)\big\} \\ A_2 &= \big\{(1,-1,1,-1), (-1,1,-1,1)\big\} + \mathcal{O}(\gamma) = \big\{b, r(b)\big\} \;, \end{aligned} \tag{4.1}$$

where we have chosen $a = (1,1,-1,-1) + \mathcal{O}(\gamma)$ and $b = (1,-1,1,-1) + \mathcal{O}(\gamma)$ as representatives. The associated stabilisers are

$$\begin{aligned} G_a &= \big\{\mathrm{id}, r^2 s, sc, r^2 c\big\} \\ G_b &= \big\{\mathrm{id}, rs, r^2, r^3 s, sc, rc, r^2 sc, r^3 c\big\} \;. \end{aligned} \tag{4.2}$$

The graph of connections forms an octaeder as shown in Figure 3. Note in particular that (2.18) is satisfied. Indeed, $|G_a \cap G_b| = 2$, and each site in A_1 has $|G_a|/|G_a \cap G_b| = 2$ neighbours in A_2, while each site in A_2 has $|G_b|/|G_a \cap G_b| = 4$ neighbours in A_1. The associated graph in terms of orbits is also shown in Figure 3.

The analysis of the potential (1.3) shows that the transition probabilities are of the form

$$L_{ab} = \frac{c_{ab}}{m_a}\,\mathrm{e}^{-h_{ab}/\varepsilon} \;, \qquad L_{ba} = \frac{c_{ab}}{m_b}\,\mathrm{e}^{-h_{ba}/\varepsilon} \;, \qquad L_{aa'} = \frac{c_{aa'}}{m_a}\,\mathrm{e}^{-h_{aa'}/\varepsilon} \;, \tag{4.3}$$

where the exponents satisfy

$$h_{ba} < h_{aa'} < h_{ab} \tag{4.4}$$

whenever $0 < \gamma < 2/5$. We set $\theta = (h_{aa'} - h_{ba}) \wedge (h_{ab} - h_{aa'})$. The generator L is of the form

$$L = \begin{pmatrix} L^{11} & L^{12} \\ L^{21} & L^{22} \end{pmatrix} \;, \tag{4.5}$$

with blocks

$$L^{11} = \begin{pmatrix} -2L_{aa'} - 2L_{ab} & L_{aa'} & 0 & L_{aa'} \\ L_{aa'} & -2L_{aa'} - 2L_{ab} & L_{aa'} & 0 \\ 0 & L_{aa'} & -2L_{aa'} - 2L_{ab} & L_{aa'} \\ L_{aa'} & 0 & L_{aa'} & -2L_{aa'} - 2L_{ab} \end{pmatrix} , \tag{4.6}$$

$$L^{12} = \begin{pmatrix} L_{ab} & L_{ab} \\ L_{ab} & L_{ab} \\ L_{ab} & L_{ab} \\ L_{ab} & L_{ab} \end{pmatrix} , \qquad L^{21} = \begin{pmatrix} L_{ba} & L_{ba} & L_{ba} & L_{ba} \\ L_{ba} & L_{ba} & L_{ba} & L_{ba} \end{pmatrix} , \qquad L^{22} = \begin{pmatrix} -4L_{ba} & 0 \\ 0 & -4L_{ba} \end{pmatrix} .$$

We can now apply the results of Section 3. From the known irreducible representations of the dihedral group D_4 (cf. Example 2.8) and the fact that c commutes with r and s, we deduce that G has 8 irreducible representations of dimension 1, given by

$$\pi_{\rho\sigma\tau}(r^i s^j c^k) = \rho^i \sigma^j \tau^k , \qquad \rho, \sigma, \tau = \pm 1 , \tag{4.7}$$

and two irreducible representation of dimension 2, that we denote $\pi_{1,\pm}$, with characters

$$\chi_{1,\pm}(r^i s^j c^k) = 2\cos(i\pi/2)\delta_{j0}(\pm 1)^k . \tag{4.8}$$

Applying Lemma 3.3 and Lemma 3.6, we obtain Table 1 for active and inactive orbits.

	A_1	A_2	αd
π_{+++}	1	1	2
π_{++-}	0	0	0
π_{+-+}	0	0	0
π_{+--}	0	0	0
π_{-++}	1	0	1
π_{-+-}	0	0	0
π_{--+}	0	0	0
π_{---}	0	1	1
$\pi_{1,+}$	0	0	0
$\pi_{1,-}$	2	0	2
$\lvert A\rvert$	4	2	6

Table 1. Active and inactive orbits and number of eigenvalues for the different irreducible representations when $N = 4$.

Table 1 shows that the permutation representation π induced by G on $\mathcal{X} = A_1 \cup A_2$ admits the decomposition

$$\pi = 2\pi_{+++} \oplus \pi_{-++} \oplus \pi_{---} \oplus \pi_{1,-} . \tag{4.9}$$

We can now determine the eigenvalues associated with each irreducible representation:

- Trivial representation π_{+++}: The associated subspace has dimension 2, and is spanned by the vectors $(1,1,1,1,0,0)^{\mathrm{T}}$ and $(0,0,0,0,1,1)^{\mathrm{T}}$. The matrix in this basis is given by

$$L^{(0)} = \begin{pmatrix} -2L_{ab} & 2L_{ab} \\ 4L_{ba} & -4L_{ba} \end{pmatrix} , \tag{4.10}$$

as can be checked by a direct computation, and is compatible with Proposition 3.1. The eigenvalues of $L^{(0)}$ are 0 and $-4L_{ba} - 2L_{ab}$, which is also compatible with Theorem 3.2 (giving the leading-order behaviour $-4L_{ba}[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})]$). In particular, we conclude that if μ is the uniform distribution on A_2, then we have the Eyring–Kramers formula

$$\mathbb{E}^{\mu}\bigl[\tau_{A_1}\bigr] = \frac{1}{4}\frac{m_b}{c_{ab}}\,\mathrm{e}^{h_{ba}/\varepsilon}\bigl[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\bigr] . \tag{4.11}$$

Note the prefactor 1/4, which is due to the symmetry.

- Representation π_{-++}: From (3.7) we see that the associated subspace is spanned by the vector $(1, -1, 1, -1, 0, 0)^{\mathrm{T}}$. A direct computation shows that the corresponding eigenvalue is $-4L_{aa'} - 2L_{ab}$, which is also compatible with (3.12), where we have to apply the second case, and use the fact that $\pi_{-++}(r) = -1$.
- Representation π_{---}: From (3.7) we see that the associated subspace is spanned by the vector $(0, 0, 0, 0, 1, -1)^{\mathrm{T}}$. A direct computation shows that the corresponding eigenvalue is $-4L_{ba}$, and the same result is obtained by applying (3.12) (first case).
- Representation $\pi_{1,-}$: From (3.14) we obtain that the associated subspace is spanned by the vectors $(2, 0, -2, 0, 0, 0)^{\mathrm{T}}$ and $(0, 2, 0, -2, 0, 0)^{\mathrm{T}}$. The associated matrix is

$$L^{1,-} = \begin{pmatrix} -2L_{aa'} - 2L_{ab} & 0 \\ 0 & -2L_{aa'} - 2L_{ab} \end{pmatrix} \tag{4.12}$$

and thus $-2L_{aa'} - 2L_{ab}$ is an eigenvalue of multiplicity 2. The leading-order behaviour $-2L_{aa'}[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})]$ is also obtained using (3.17) with $a^* = r(a)$ and (3.19) (first case), which shows that $M = 2\mathbb{1}$.

In summary, to leading order the eigenvalues of the generator are given by

$$0\ ,\ -2L_{aa'}\ ,\ -2L_{aa'}\ ,\ -4L_{aa'}\ ,\ -4L_{ba}\ ,\ -4L_{ba}\ . \tag{4.13}$$

They appear in groups with the same exponent, and possibly different prefactors. Note in particular that the spectral gap is given by $2L_{aa'}$, which is smaller than in the case of an asymmetric double-well, where it would be L_{ba}. This is due to the fact that the slowest process in the system is the internal dynamics of the orbit A_1.

4.2 The case $N = 8$

In the case $N = 8$, the potential is invariant under the group $G = D_8 \times \mathbb{Z}_2$, which has order 32. As explained in Appendix A, there are 182 local minima, connected by 560 saddles of index 1. The local minima form 12 orbits, of cardinality varying between 2 and 32 depending on the size of their stabiliser, see Table 2.

Local minima occur in two types:

- those with 4 coordinates equal to $1 + \mathcal{O}(\gamma)$, and 4 coordinates equal to $-1 + \mathcal{O}(\gamma)$; we denote these coordinates $+$ and $-$;
- and those with 3 coordinates equal to $\pm\alpha$ and 5 coordinates equal to $\pm\beta$, where $\alpha = 5/\sqrt{19} + \mathcal{O}(\gamma)$ and $\beta = -3/\sqrt{19} + \mathcal{O}(\gamma)$.

These local minima are connected according to the following rules:

$$\begin{array}{ll} 3 \times (\alpha \longleftrightarrow +) & 3 \times (-\alpha \longleftrightarrow -) \\ 1 \times (\beta \longleftrightarrow +) & 1 \times (-\beta \longleftrightarrow -) \\ 4 \times (\beta \longleftrightarrow -) & 4 \times (-\beta \longleftrightarrow +)\ , \end{array} \tag{4.14}$$

A	$\lvert A\rvert$	a	G_a
A_1	8	$(+,+,+,+,-,-,-,-)$	$\{\mathrm{id}, r^4s, r^4c, sc\}$
A_2	4	$(+,+,-,-,+,+,-,-)$	$\{\mathrm{id}, r^2s, r^4, r^6s, sc, r^2c, r^4sc, r^6c\}$
A_3	16	$(+,+,+,-,-,+,-,-)$	$\{\mathrm{id}, r^3s\}$
A_4	16	$(+,-,-,-,+,+,+,-)$	$\{\mathrm{id}, sc\}$
A_5	8	$(+,-,-,+,-,+,+,-)$	$\{\mathrm{id}, r^4s, r^4c, sc\}$
A_6	16	$(+,+,-,+,-,+,-,-)$	$\{\mathrm{id}, sc\}$
A_7	2	$(+,-,+,-,+,-,+,-)$	$\{\mathrm{id}, rs, r^2, r^3s, r^4, r^5s, r^6, r^7s,$ $sc, rc, r^2sc, r^3c, r^4sc, r^5c, r^6sc, r^7c\}$
A_8	32	$(\alpha,\alpha,\beta,\beta,\beta,\alpha,\beta,\beta)$	$\{\mathrm{id}\}$
A_9	16	$(\alpha,\alpha,\alpha,\beta,\beta,\beta,\beta,\beta)$	$\{\mathrm{id}, r^3s\}$
A_{10}	16	$(\beta,\alpha,\beta,\beta,\alpha,\beta,\alpha,\beta)$	$\{\mathrm{id}, r^3s\}$
A_{11}	16	$(\beta,\alpha,\beta,\alpha,\beta,\beta,\beta,\alpha)$	$\{\mathrm{id}, r^3s\}$
A_{12}	32	$(\alpha,\beta,\alpha,\alpha,\beta,\beta,\beta,\beta)$	$\{\mathrm{id}\}$

TABLE 2. Orbits A_i for the case $N = 8$ with their cardinality, one representative a and its stabiliser G_a. The symbols $\pm$ stand for $\pm 1 + \mathcal{O}(\gamma)$, while $\alpha = \pm 5/\sqrt{19} + \mathcal{O}(\gamma)$ and $\beta = \mp 3/\sqrt{19} + \mathcal{O}(\gamma)$. Stabilisers of other elements $a' = g(a)$ of any orbit are obtained by conjugation with g.

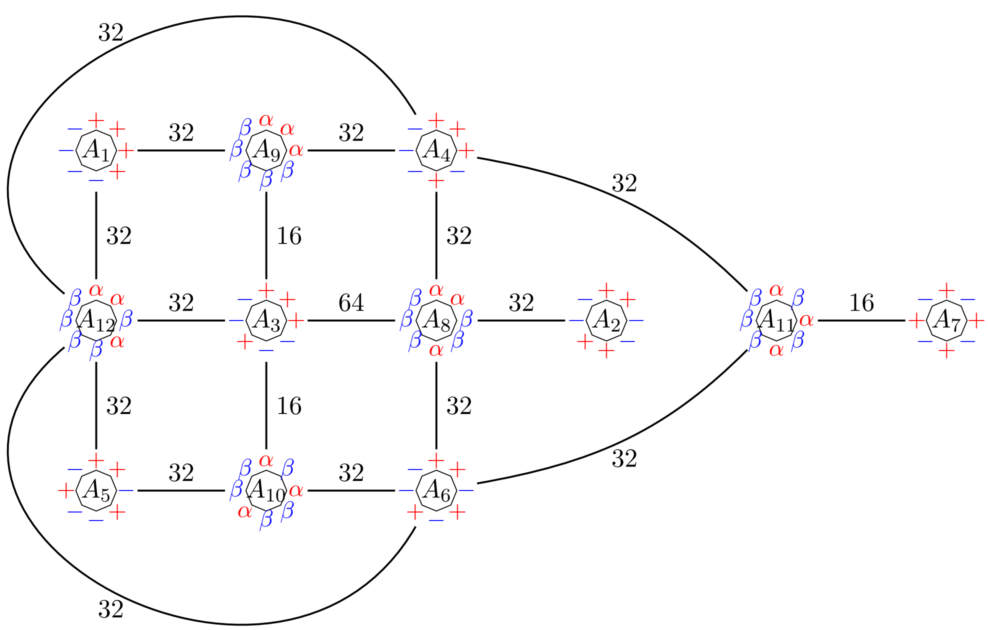

FIGURE 4. Graph on the set of orbits for the case $N = 8$. Each node displays a particular representative of the orbit. Figures next to the edges denote the total number of connections between elements of the orbits. Note that there is a kind of hysteresis effect, in the sense that going around a loop on the graph, following the connection rules, one does not necessarily end up with the same representative of the orbit.

meaning that each α and one of the βs are connected with a $+$, and so on. A major simplification will arise from the fact that there are no connections among sites of a same orbit.

We do not attempt to draw the full graph, which has 182 vertices and 560 edges. However, Figure 4 shows the graph on the set of orbits. The metastable hierarchy has been established by computing the height of saddles to second order in γ with the help of computer algebra.

The group $G = D_8 \times \mathbb{Z}_2$ has again 8 irreducible representations of dimension 1, given by

$$\pi_{\rho\sigma\tau}(r^i s^j c^k) = \rho^i \sigma^j \tau^k \;, \qquad \rho, \sigma, \tau = \pm 1 \;, \tag{4.15}$$

In addition, it has 6 irreducible representation of dimension 2 deduced from those of D_8, cf. (2.23). We denote them $\pi_{l,\pm}$, $l = 1, 2, 3$, and their characters satisfy (see (2.24))

$$\chi_{l,\pm}(r^i s^j c^k) = 2\cos(il\pi/4)\delta_{j0}(\pm 1)^k \;. \tag{4.16}$$

Applying Lemma 3.3 and Lemma 3.6, we obtain Table 3 of active and inactive orbits.

	A_1	A_2	A_3	A_4	A_5	A_6	A_7	A_8	A_9	A_{10}	A_{11}	A_{12}	αd
π_{+++}	1	1	1	1	1	1	1	1	1	1	1	1	12
π_{++-}	0	0	1	0	0	0	0	1	1	1	1	1	6
π_{+-+}	0	0	0	0	0	0	0	1	0	0	0	1	2
π_{+--}	0	0	0	1	0	1	0	1	0	0	0	1	4
π_{-++}	1	1	0	1	1	1	0	1	0	0	0	1	7
π_{-+-}	0	0	0	0	0	0	0	1	0	0	0	1	2
π_{--+}	0	0	1	0	0	0	0	1	1	1	1	1	6
π_{---}	0	0	1	1	0	1	1	1	1	1	1	1	9
$\pi_{1,+}$	0	0	2	2	0	2	0	4	2	2	2	4	20
$\pi_{1,-}$	2	0	2	2	2	2	0	4	2	2	2	4	24
$\pi_{2,+}$	2	0	2	2	2	2	0	4	2	2	2	4	24
$\pi_{2,-}$	0	2	2	2	0	2	0	4	2	2	2	4	22
$\pi_{3,+}$	0	0	2	2	0	2	0	4	2	2	2	4	20
$\pi_{3,-}$	2	0	2	2	2	2	0	4	2	2	2	4	24
$\lvert A\rvert$	8	4	16	16	8	16	2	32	16	16	16	32	182

Table 3. Active and inactive orbits and number of eigenvalues for the different irreducible representations when $N = 8$. There are 182 eigenvalues in total, 48 associated with 1-dimensional irreducible representations, and 134 associated with 2-dimensional irreducible representations.

It is now possible to determine the eigenvalues associated with each irreducible representation. The trivial representation π_{+++} will yield 12 eigenvalues, which are given by Theorem 3.2. The only difference with the Eyring–Kramers formula of the asymmetric case is an extra factor of the form $|G_c|/|G_a \cap G_b|$, where (a, b) is the highest edge of an optimal path from A_k to $\mathcal{M}_{k-1}$, and $c \in A_k$. For instance, the optimal path from A_7 to $\mathcal{M}_6$ is $A_7 \to A_{11} \to A_4$, and its highest edge is $A_7 \to A_{11}$. We thus obtain

$$\lambda_7^{(0)} = 8\frac{c_{a_7 a_{11}}}{m_{a_7}}\,\mathrm{e}^{-H(A_7,A_{11})/\varepsilon}\bigl[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\bigr] \tag{4.17}$$

where $a_7 \in A_7$ and $a_{11} \in A_{11}$, because $|G_{a_7}| = 16$ and $|G_{a_7} \cap G_{a_{11}}| = 2$ (cf. Table 2).

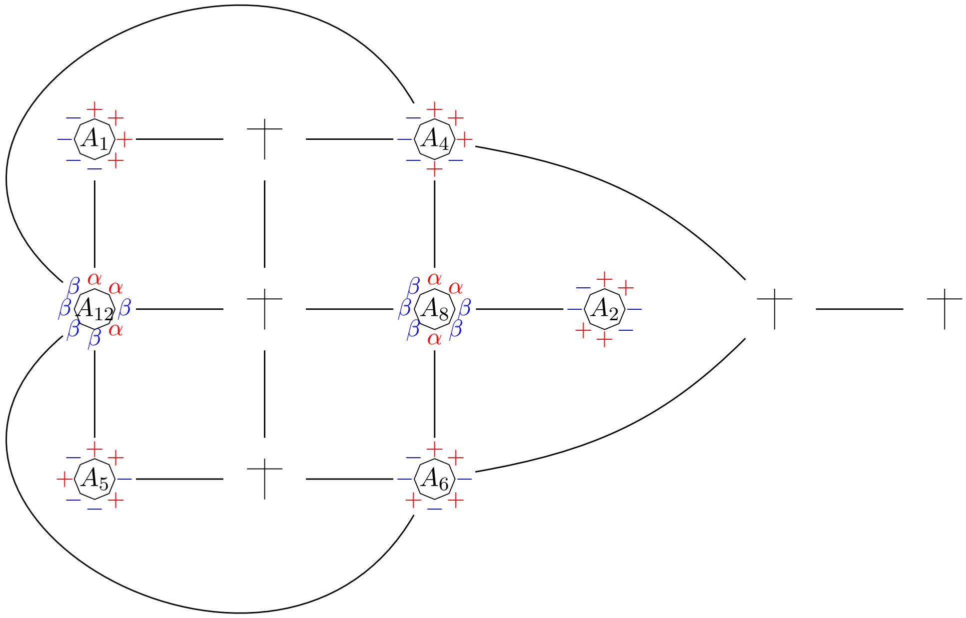

FIGURE 5. Graph for the case $N = 8$ associated with the representation π_{-++}.

The eigenvalues associated with other irreducible representations of dimension 1 can be deduced from the metastable hierarchy of the corresponding set of active orbits. For instance, Figure 5 shows the graph obtained for the representation π_{-++}, which yields 7 eigenvalues. An important difference to the previous case arises from the fact that some communication heights relevant for the eigenvalues are associated with transitions to the cemetery state. In particular, A_1 is no longer at the bottom of the hierarchy (which is occupied by the cemetery state), and thus there will be an eigenvalue of order $\mathrm{e}^{-H(A_1,A_9)/\varepsilon}$, because A_9 is the successor of A_1 of the form

$$\lambda_1^{(-++)} = -4\frac{c_{a_1a_9}}{m_{a_1}}\,\mathrm{e}^{-H(A_1,A_9)/\varepsilon}\big[1+\mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\big] \;. \tag{4.18}$$

Eigenvalues associated with irreducible representations of dimension 2 are given by Theorem 3.9. The graph of successors is shown in Figure 6. Observe that A_1 is at the bottom of the cycle containing A_1 and A_9. For instance, for the representation $\pi_{1,-}$, applying Proposition 3.7 with the choice of basis $(u_i^a, u_i^{a'})$ with $a' = r^2(a)$ for each orbit, we obtain

$$\begin{aligned}
L_{11}^{(1,-)} &= L_{11}^{(0)}\mathbb{1}[1+\mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})]\;, & L_{11}^{(0)} &= -4\frac{c_{a_1a_9}}{m_{a_1}}\,\mathrm{e}^{-H(A_1,A_9)/\varepsilon}\;,\\
L_{19}^{(1,-)} &= L_{11}^{(0)}M_{19}[1+\mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})]\;, & & \\
L_{91}^{(1,-)} &= L_{99}^{(0)}M_{91}[1+\mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})]\;, & L_{99}^{(0)} &= -2\frac{c_{a_9a_1}}{m_{a_9}}\,\mathrm{e}^{-H(A_9,A_1)/\varepsilon}\;,\\
L_{99}^{(1,-)} &= L_{99}^{(0)}\mathbb{1}[1+\mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})]\;, & &
\end{aligned} \tag{4.19}$$

where

$$M_{19} = \frac{1}{4}\begin{pmatrix} 2+\sqrt{2} & \sqrt{2} \\ -\sqrt{2} & 2+\sqrt{2}\end{pmatrix}\;, \qquad M_{91} = \frac{1}{4}\begin{pmatrix} 2+\sqrt{2} & -\sqrt{2} \\ \sqrt{2} & 2+\sqrt{2}\end{pmatrix}\;. \tag{4.20}$$

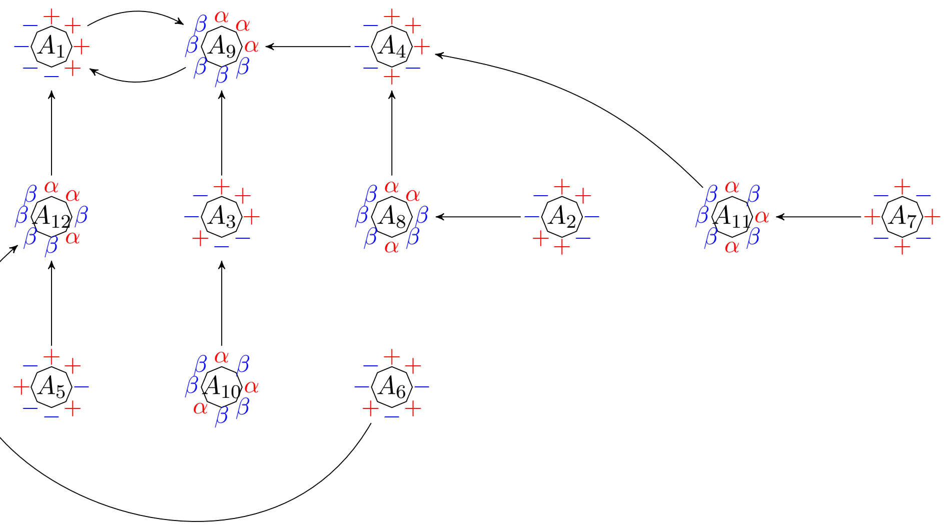

FIGURE 6. The graph of successors for $N = 8$.

Thus by Theorem 3.9, the eigenvalues associated with A_1 are those of the matrix

$$L_{11}^{(1,-)} - L_{19}^{(1,-)} \big(L_{99}^{(1,-)}\big)^{-1} L_{91}^{(1,-)} = -(2-\sqrt{2}) \frac{c_{a_1 a_9}}{m_{a_1}} \,\mathrm{e}^{-H(A_1,A_9)/\varepsilon}\, \mathbb{1}[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})] \;. \tag{4.21}$$

We thus obtain a double eigenvalue given by the Eyring–Kramers law with an extra factor of $(2-\sqrt{2})$.

5 Proofs – Group theory

In this section, we give the proofs of the different expressions for the matrix elements of L restricted to the subspaces $P_i^{(p)}\mathbb{C}^n$ associated with the irreducible representations $\pi^{(p)}$. Although we have introduced the results by starting with the trivial representation, then moving to other representations of dimension 1, and finally to higher-dimensional representations, it will be more straightforward to give directly proofs in the case of a general irreducible representation of arbitrary dimension d, and then to particularize to the cases $d = 1$ and $p = 0$.

To simplify notations, we will fix an irreducible representation $\pi = \pi^{(p)}$, orbits $A = A_i$, $B = A_j$, and elements $a \in A$ and $b \in B$. We write $\alpha_i = \alpha_i^{(p)}$ and $\chi = \chi^{(p)}$. Recall that $\pi_i(g)$ denotes the permutation matrix induced by g on the orbit A (we will consider π_i as a linear map on $\mathbb{C}^n$ which is identically zero on $\mathcal{X} \setminus A$). The associated projector $P_i = P_i^{(p)}$ is given by (cf. (2.20))

$$P_i = \frac{d}{|G|} \sum_{g\in G} \overline{\chi(g)} \pi_i(g) \;. \tag{5.1}$$

The only nonzero matrix elements of P_i are those between elements in A, and they can be written as

$$(P_i)_{ah(a)} = \frac{d}{|G|} \sum_{g\in G_a} \overline{\chi(gh)} \qquad \forall a \in A, \forall h \in G \;. \tag{5.2}$$

We write $P_j = P_j^{(p)}$ for the similarly defined projector associated with the orbit B.

Proof of Lemma 3.6. Taking the trace of (5.1), we obtain

$$\alpha_i d = \operatorname{Tr}(P_i) = \frac{d}{|G|} \sum_{g\in G} \overline{\chi(g)} \operatorname{Tr}(\pi_i(g)) \;. \tag{5.3}$$

Note that $\operatorname{Tr}(\pi_i(g)) = |A^g| = |A| 1_{g\in G_a}$. Therefore,

$$\alpha_i = \frac{|A|}{|G|} \sum_{g\in G_a} \overline{\chi(g)} = \frac{1}{|G_a|} \sum_{g\in G_a} \overline{\chi(g)} \;. \tag{5.4}$$

Since we have at the same time $\alpha_i \in \mathbb{N}_0$ and $\overline{\chi(g)} \in [-d,d]$, so that $\alpha_i \in [-d,d]$, we conclude that necessarily $\alpha_i \in \{0,1,\dots d\}$. □

Proof of Lemma 3.3. In the particular case $d=1$, Lemma 3.6 reduces to

$$\alpha_i = \frac{1}{|G_a|} \sum_{g\in G_a} \overline{\chi(g)} \in \{0,1\} \;. \tag{5.5}$$

This leaves only two possibilities: either $\alpha_i = 1$ and all $\chi(g) = \pi(g)$ are equal to 1 for $g \in G_a$, or $\alpha_i = 0$ and the above sum is equal to 0. □

Note that in the particular case of the trivial representation $\pi = \pi^{(0)}$, we are always in the case $\alpha_i = 1$. Thus all orbits are active for the trivial representation.

We now proceed to construct basis vectors for $P_i\mathbb{C}^n$. Let e^a denote the canonical basis vector of $\mathbb{C}^n$ associated with $a \in A$, and let $u^a \in \operatorname{im} P_i$ be defined by

$$u^a = \frac{|G|}{|G_a|} P_i e^a \;. \tag{5.6}$$

By (5.2), its nonzero components are given by

$$(u^a)_{h(a)} = \frac{|G|}{|G_a|} (P_i)_{ah(a)} = \frac{d}{|G_a|} \sum_{g\in G_a} \overline{\chi(gh)} \;. \tag{5.7}$$

This expression is equivalent to (3.14). For one-dimensional representations, it reduces to (3.7). Indeed $\chi(gh) = \pi(gh) = \pi(g)\pi(h)$ in dimension 1, and we can apply Lemma 3.3. For the trivial representation, $(u^a)_{h(a)}$ is identically equal to 1.

In order to compute matrix elements of L, we introduce the inner product on $\mathbb{C}^n$

$$\langle u, v\rangle = \frac{1}{|G|} \sum_{g\in G} \overline{u_{g(a)}} v_{g(a)} = \frac{|G_a|}{|G|} \sum_{g\in G/G_a} \overline{u_{g(a)}} v_{g(a)} \;, \tag{5.8}$$

where $g \in G/G_a$ is a slight abuse of notation for $gG_a \in G/G_a$ (it means that we pick one representative for each coset gG_a). Strictly speaking, only the restriction of $\langle\cdot,\cdot\rangle$ to the orbit A is an inner product, since it is not positive definite on all of $\mathbb{C}^n$.

Lemma 5.1. *The vector u^a is normalised in such a way that $\langle u^a, u^a\rangle = \alpha_i d$. Furthermore, for v^b defined in an analogous way,*

$$\frac{\langle u^a, Lv^b\rangle}{\langle u^a, u^a\rangle} = \frac{d}{\alpha_i |G||G_b|} \sum_{g\in G} \sum_{g'\in G} \overline{\chi(g)} \chi(g') L_{g(a)g'(b)} \;. \tag{5.9}$$

PROOF: We start by computing the norm of u^a:

$$\langle u^a, u^a\rangle = \frac{|G|^2}{|G_a|^2}\langle P_i e^a, P_i e^a\rangle = \frac{|G|^2}{|G_a|^2}\langle e^a, P_i{}^* P_i e^a\rangle = \frac{|G|^2}{|G_a|^2}\langle e^a, P_i e^a\rangle$$
$$= \frac{|G|}{|G_a|}\sum_{g\in G/G_a} \overline{e^a_{g(a)}}(P_i e^a)_{g(a)} = \frac{|G|}{|G_a|}(P_i)_{aa} = \frac{d}{|G_a|}\sum_{h\in G_a}\overline{\chi(h)} = \alpha_i d\ , \tag{5.10}$$

where we have used the fact that P_i is a hermitian projector. Before turning to the numerator of (5.9), note that for a matrix $M \in \mathbb{C}^{n\times n}$ one has

$$\langle e^a, Me^b\rangle = \frac{|G_a|}{|G|}M_{ab}\ . \tag{5.11}$$

Therefore,

$$\langle u^a, Lv^b\rangle = \frac{|G|^2}{|G_a||G_b|}\langle P_i e^a, LP_j e^b\rangle = \frac{|G|^2}{|G_a||G_b|}\langle e^a, P_i L P_j e^b\rangle$$
$$= \frac{|G|}{|G_b|}(P_i L P_j)_{ab}\ . \tag{5.12}$$

Now we have

$$(P_i L P_j)_{ab} = \sum_{g\in G/G_a}\sum_{g'\in G/G_b}(P_i)_{ag(a)}L_{g(a)g'(b)}(P_j)_{g'(b)b}$$
$$= \frac{d^2}{|G|^2}\sum_{g\in G/G_a}\sum_{g'\in G/G_b}\sum_{h\in G_a}\sum_{h'\in G_b}\overline{\chi(gh)}\ \overline{\chi((g')^{-1}h')}L_{g(a)g'(b)}\ . \tag{5.13}$$

Since $\overline{\chi((g')^{-1}h')} = \chi(g'(h')^{-1})$, the result follows by replacing first $(h')^{-1}$ by h' in the sum, and then gh by g and $g'h'$ by g'. □

The expression (5.9) for the matrix elements can be simplified with the help of the following identity.

Lemma 5.2. *For any $h \in G$,*

$$\frac{d}{|G|}\sum_{g\in G}\overline{\chi(g)}\chi(hg) = \chi(h)\ . \tag{5.14}$$

PROOF: Let G act on a set X such that $G_x = \{\mathrm{id}\}$ for all $x \in X$. By (5.2) we have

$$(P_X)_{x,h(x)} = \frac{d}{|G|}\overline{\chi(h)}\ . \tag{5.15}$$

This implies

$$(P_X^2)_{xh(x)} = \sum_{g\in G}(P_X)_{xg(x)}(P_X)_{g(x)h(x)} = \frac{d^2}{|G|^2}\sum_{g\in G}\overline{\chi(g)}\chi(h^{-1}g)\ . \tag{5.16}$$

Since P_X is a projector, the two above expressions are equal. □

Corollary 5.3. *The expressions* (5.9) *of the matrix elements simplify to*

$$\frac{\langle u^a, Lv^b\rangle}{\langle u^a, u^a\rangle} = \frac{1}{\alpha_i|G_b|}\sum_{g\in G}\chi(g)L_{ag(b)}\ . \tag{5.17}$$

PROOF: This follows by setting $g' = gh$ in (5.9), using $L_{g(a)gh(b)} = L_{ah(b)}$ and applying the lemma. This is possible since $\chi(gh) = \mathrm{Tr}(\pi(g)\pi(h)) = \mathrm{Tr}(\pi(h)\pi(g)) = \chi(hg)$. □

By the non-degeneracy Assumption 2.6, the sum in (5.17) will be dominated by a few terms only. Using this, general matrix elements of L can be rewritten as follows.

Proposition 5.4. *Let A and B be two different orbits, and assume that $a \in A$ and $b \in B$ are such that $h_{ab} = h^*(A, B)$, the minimal exponent for transitions from A to B. Then for any $h_1, h_2 \in G$,*

$$\frac{\langle u^{h_1(a)}, Lv^{h_2(b)}\rangle}{\langle u^{h_1(a)}, u^{h_1(a)}\rangle} = \frac{L_{ab}}{\alpha_i|G_b|}\sum_{g\in G_aG_b}\chi(h_1gh_2^{-1})[1+\mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})]\ . \tag{5.18}$$

Furthermore, elements of diagonal blocks can be written as

$$\frac{\langle u^{h_1(a)}, Lu^{h_2(a)}\rangle}{\langle u^{h_1(a)}, u^{h_1(a)}\rangle} = \frac{1}{\alpha_i|G_a|}\sum_{g\in G_a}\biggl[\chi(h_1gh_2^{-1})L_{aa} + \sum_{k\in G/G_a\setminus G_a}\chi(h_1kgh_2^{-1})L_{ak(a)}\biggr]\ . \tag{5.19}$$

PROOF: It follows from (5.17) that

$$\begin{aligned}\frac{\langle u^{h_1(a)}, Lv^{h_2(b)}\rangle}{\langle u^{h_1(a)}, u^{h_1(a)}\rangle} &= \frac{1}{\alpha_i|G_{h_2(b)}|}\sum_{g\in G}\chi(g)\underbrace{L_{h_1(a)\,gh_2(b)}}_{=L_{a\,h_1^{-1}gh_2(b)}} \\ &= \frac{1}{\alpha_i|G_b|}\sum_{k\in G_aG_b}\chi(h_1kh_2^{-1})L_{ab}[1+\mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})]\ ,\end{aligned} \tag{5.20}$$

where we have set $k = h_1^{-1}gh_2$, and used (2.16) and Lemma 2.7. This proves (5.18). Relation (5.19) follows from (5.17) after replacing $g \in G$ by kg, with $g \in G_a$ and $k \in G/G_a$, and singling out the term $k = \mathrm{id}$. □

Expression (5.18) is equivalent to (3.15) in Proposition 3.7, taking into account the definition (3.3) of c^*_{ij} and m^*_i. Particularising to one-dimensional representations yields (3.8) and (3.2).

It thus remains to determine the diagonal blocks. For one-dimensional representations, using $\chi(kg) = \pi(kg) = \pi(k)\pi(g)$ and Lemma 3.3 in (5.19) shows that

$$L^{(p)}_{ii} := \frac{\langle u^a, Lu^a\rangle}{\langle u^a, u^a\rangle} = L_{aa} + \sum_{k\in G/G_a\setminus G_a}\pi(k)L_{ak(a)}\ . \tag{5.21}$$

Subtracting $L^{(0)}$ for the trivial representation from $L^{(p)}$ proves (3.9). Furthermore, let $\mathbf{1}$ be the constant vector with all components equal to 1. Since L is a generator, we have

$$0 = L\mathbf{1} = \sum_{j=1}^m Lu^{(0)}_j \qquad \Rightarrow \qquad 0 = \sum_{j=1}^m L^{(0)}_{ij}\ , \tag{5.22}$$

which proves (3.4).

Finally let a^* be such that $h(a, a^*) = \inf_b h(a, b)$. We distinguish two cases:

1. Case $a^* \notin A$. Then the right-hand side of (5.21) is dominated by the first term, and we have $L^{(p)}_{ii} = L_{aa}[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})]$. The sum inside the brackets in (5.19) is also dominated by the first term, which implies the first lines in (3.17) and in (3.12).
2. Case $a^* = k_0(a) \in A$. Relation (3.11) implies that $L^{(0)}_{ii}$ is negligible with respect to L_{aa^*}, and thus

$$L_{aa} = -\sum_{k\in G/G_a\setminus G_a} L_{ak(a)}[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})] \; . \tag{5.23}$$

Thus for one-dimensional representations, we obtain from (5.21) that

$$L^{(p)}_{ii} := \frac{\langle u^a, Lu^a\rangle}{\langle u^a, u^a\rangle} = -\sum_{k\in G/G_a\setminus G_a} (1-\pi(k))L_{ak(a)}[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})] \; . \tag{5.24}$$

The sum is dominated by $k = k_0$ and $k = k_0^{-1}$, which implies the last two lines of (3.12). For general representations, we obtain from (5.19) that

$$\frac{\langle u^{h_1(a)}, Lu^{h_2(a)}\rangle}{\langle u^{h_1(a)}, u^{h_1(a)}\rangle} = -\frac{1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})}{\alpha_i|G_a|} \sum_{g\in G_a} \sum_{k\in G/G_a\setminus G_a} \bigl[\chi(h_1 g h_2^{-1}) - \chi(h_1 k g h_2^{-1})\bigr] L_{ak(a)} \; , \tag{5.25}$$

which implies the second line in (3.17).

6 Proofs – Estimating eigenvalues

6.1 Block-triangularisation

We consider in this section a generator $L \in \mathbb{R}^{n\times n}$ with matrix elements $L_{ij} = \mathrm{e}^{-h_{ij}/\varepsilon}$, satisfying Assumption 2.2 on existence of a metastable hierarchy. In this section, we have incorporated the prefactors in the exponent, i.e., we write h_{ij} instead of $h_{ij} - \varepsilon\log(c_{ij}/m_i)$ and V_i instead of $V_i + \varepsilon\log(m_i)$.

In addition, we assume the *reversibility condition for minimal paths*

$$V_i + H(i,j) = V_j + H(j,i) + \mathcal{O}(\varepsilon\,\mathrm{e}^{-\theta/\varepsilon}) \qquad \forall i,j \in \{2,\dots,n\} \; . \tag{6.1}$$

If the reversibility assumption (2.3) holds, then (6.1) is satisfied. However (6.1) is slightly weaker, because it only concerns minimal transition paths. We do not assume reversibility for site 1, since this will allow us to cover situations associated with nontrivial representations. Thus the first row of L may be identically zero, making 1 an absorbing state.

Our aim is to construct a linear change of variables transforming L into a triangular matrix. The change of variables is obtained by combining $n-1$ elementary transformations to block-triangular form. Given some $1 \leqslant m < n$, we write L in the form

$$L = \begin{pmatrix} L^{11} & L^{12} \\ L^{21} & A \end{pmatrix} \; , \tag{6.2}$$

with blocks $L^{11} \in \mathbb{R}^{(n-m)\times(n-m)}$, $A \in \mathbb{R}^{m\times m}$, $L^{12} \in \mathbb{R}^{(n-m)\times m}$ and $L^{21} \in \mathbb{R}^{m\times(n-m)}$, and we assume $\det(A) \neq 0$. We would like to construct matrices $S, T \in \mathbb{R}^{n\times n}$ satisfying

$$LS = ST \tag{6.3}$$

where T is block-triangular. More precisely, we impose that

$$S = \begin{pmatrix} \mathbb{1} & S^{12} \\ 0 & 1 \end{pmatrix} \qquad \text{and} \qquad T = \begin{pmatrix} T^{11} & 0 \\ T^{21} & \tilde{A} \end{pmatrix} , \tag{6.4}$$

with blocks of the same dimensions as the blocks of L. Plugging (6.4) into (6.3) yields the relations

$$\begin{aligned} T^{11} &= L^{11} - S^{12}L^{21} , \\ \tilde{A} &= A + L^{21}S^{12} , \\ T^{21} &= L^{21} , \end{aligned} \tag{6.5}$$

and

$$L^{11}S^{12} - S^{12}A - S^{12}L^{21}S^{12} + L^{12} = 0 . \tag{6.6}$$

If we manage to prove that (6.6) admits a solution, then we will have shown that L is similar to the block-diagonal matrix T, and the eigenvalues of L are those of T^{11} and $\tilde{A}$. In the sequel, the size of matrices is measured in the operator sup-norm,

$$\|L\| = \sup_{\|x\|_\infty = 1} \|Lx\|_\infty , \qquad \|x\|_\infty = \sup_i |x_i| . \tag{6.7}$$

Proposition 6.1. *If* $\|L^{12}A^{-1}\|$ *is sufficiently small, then* (6.6) *admits a solution* S^{12}*, such that* $\|S^{12}\| = \mathcal{O}(\|L^{12}A^{-1}\|)$*.*

Proof: For fixed blocks A, L^{21}, consider the function

$$\begin{aligned} f : \mathbb{R}^{(n-m)\times m} \times \mathbb{R}^{(n-m)\times n} &\to \mathbb{R}^{(n-m)\times m} \\ (X, (L^{11}, L^{12})) &\mapsto L^{11}XA^{-1} - X - XL^{21}XA^{-1} + L^{12}A^{-1} . \end{aligned} \tag{6.8}$$

Then $f(0,0) = 0$, and the Fréchet derivative of f with respect to X at $(0,0)$ is given by $\partial_X f(0,0) = -\operatorname{id}$. Hence the implicit-function theorem applies, and shows the existence of a map $X^* : \mathbb{R}^{(n-m)\times n} \to \mathbb{R}^{(n-m)\times m}$ such that $f(X^*, (L^{11}, L^{12})) = 0$ in a neighbourhood of $(0,0)$. Then $S^{12} = X^*(L^{11}, L^{12})$ solves (6.6). Furthermore, $\|S^{12}\| = \mathcal{O}(\|L^{12}A^{-1}\|)$ follows from the expression for the derivative of the implicit function. □

The first-order Taylor expansion of S^{12} reads

$$S^{12} = L^{12}A^{-1} + \mathcal{O}\Big(\|L^{12}A^{-1}\| \big[\|L^{11}A^{-1}\| + \|L^{21}L^{12}A^{-2}\|\big]\Big) . \tag{6.9}$$

We will start by analysing the first-order approximation obtained by using $S_0^{12} = L^{12}A^{-1}$. The resulting transformed matrix is

$$T_0 = \begin{pmatrix} T_0^{11} & 0 \\ L^{21} & \tilde{A}_0 \end{pmatrix} = \begin{pmatrix} L^{11} - L^{12}A^{-1}L^{21} & 0 \\ L^{21} & A + L^{21}L^{12}A^{-1} \end{pmatrix} \tag{6.10}$$

Lemma 6.2. *The matrix* T_0^{11} *is still a generator.*

Proof: The fact that L is a generator implies $L^{11}\mathbf{1} + L^{12}\mathbf{1} = 0$ and $L^{21}\mathbf{1} + A\mathbf{1} = 0$, where $\mathbf{1}$ denotes the constant vector of the appropriate size. It follows that

$$L^{12}A^{-1}L^{21}\mathbf{1} = L^{12}A^{-1}(-A\mathbf{1}) = -L^{12}\mathbf{1} = L^{11}\mathbf{1} , \tag{6.11}$$

and thus $T_0^{11}\mathbf{1} = 0$. □

We will see that T_0^{11} can be interpreted as the generator of a jump process in which the sites $i > n-m$ have been "erased". Our strategy will be to show that this reduced process has the same communication heights as the original one, and then to prove that higher-order terms in the expansion of S^{12} do not change this fact. We can then apply the same strategy to the block T^{11}, and so on until the resulting matrix is block-triangular with blocks of size m. The diagonal blocks of this matrix then provide the eigenvalues of L.

6.2 The one-dimensional case

We consider in this section the case $m = 1$, which allows to cover all one-dimensional representations. The lower-right block A of L is then a real number that we denote a ($= L_{nn}$), and we write $\tilde{a}$ instead of $\tilde{A}$.

The first-order approximation

The matrix elements of T_0^{11} are given by (c.f. (6.10))

$$T^0_{ij} = L_{ij} - \frac{1}{a} L_{in} L_{nj} \;, \qquad i,j = 1,\dots n-1 \;. \tag{6.12}$$

Assumption 2.2 implies that there is a unique successor $k = s(n) \in \{1, n-1\}$ such that $h_{nk} = \min_{j \in \{1,n-1\}} h_{nj}$. Since L is a generator, we have $a = -\operatorname{e}^{-h_{nk}/\varepsilon}[1 + \mathcal{O}(\operatorname{e}^{-\theta/\varepsilon})]$, and thus $T^0_{ij} = \operatorname{e}^{-\tilde{h}_{ij}/\varepsilon}$ where

$$\tilde{h}_{ij} = \tilde{h}^0_{ij} + \mathcal{O}(\varepsilon \operatorname{e}^{-\theta/\varepsilon}) \qquad \text{with} \qquad \tilde{h}^0_{ij} = h_{ij} \wedge (h_{in} - h_{nk} + h_{nj}) \;. \tag{6.13}$$

The new exponent $\tilde{h}^0_{ij}$ can be interpreted as the lowest cost to go from site i to site j, possibly visiting n in between.

We denote by $\widetilde{H}^0(i,j)$ the new communication height between sites $i,j \in \{1,\dots,n-1\}$, defined in the same way as $H(i,j)$ but using $\tilde{h}^0_{ij}$ instead of h_{ij} (p-step communication heights are defined analogously). In order to show that the new communication heights are in fact equal to the old ones, we start by establishing a lower bound.

Lemma 6.3. *For all $i \neq j \in \{1,\dots,n-1\}$,*

$$\tilde{h}^0_{ij} \geqslant h_{ij} \wedge h_{inj} \;, \tag{6.14}$$

with equality holding if $i = k$ or $j = k$. As a consequence, $\widetilde{H}^0(i,j) \geqslant H(i,j)$ for these i,j.

PROOF: Recall from Definition 2.1 that the two-step communication height $i \to n \to j$ is given by $h_{inj} = h_{in} \vee (h_{in} - h_{ni} + h_{nj})$. We consider three cases:

- If $i = k$, then $h_{knj} = h_{kn} - h_{nk} + h_{nj}$ because $h_{nj} > h_{nk}$, and thus $\tilde{h}^0_{kj} = h_{kj} \wedge h_{knj}$.
- If $j = k$, then $h_{ink} = h_{in}$ because $h_{nk} < h_{ni}$, and thus $\tilde{h}^0_{ik} = h_{ik} \wedge h_{in} = h_{ik} \wedge h_{ink}$.
- If $i \neq k \neq j$, then $h_{in} - h_{nk} + h_{nj} > h_{inj}$ because $h_{nk} < h_{ni}, h_{nj}$ and (6.14) holds.

The consequence on communication heights follows by comparing maximal heights along paths from i to j. $\square$

Proposition 6.4. *For all $i \neq j \in \{1,\dots,n-1\}$ and sufficiently small ε,*

$$\widetilde{H}^0(i,j) = H(i,j) + \mathcal{O}(\varepsilon \operatorname{e}^{-\theta/\varepsilon}) \;. \tag{6.15}$$

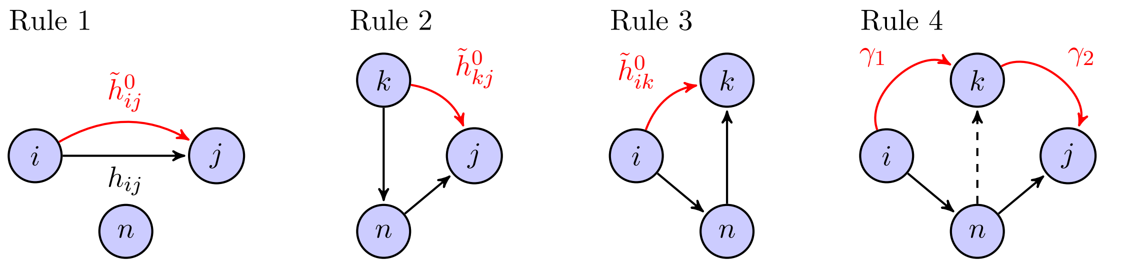

FIGURE 7. Replacement rules for minimal paths.

PROOF: Let γ be a minimal path between two sites i_0 and j_0. In view of Lemma 6.3, it is sufficient to construct a path $\tilde\gamma$ from i_0 to j_0, which does not include n, such that $\tilde h^0_{\tilde\gamma} = h_\gamma$. This new path is obtained by applying the following replacement rules (see Figure 7):

1. leave as is each segment $i \to j$ with $i, j \neq k, n$;
2. replace any segment $k \to n \to j$ with $j \neq k, n$ by $k \to j$;
3. replace any segment $i \to n \to k$ with $i \neq k, n$ by $i \to k$;
4. replace any segment $i \to n \to j$ with $i, j \neq k, n$ by the concatenation of a minimal path $\gamma_1 : i \to k$ and a minimal path $\gamma_2 : k \to j$. If one of these paths contains n, apply rules 2. or 3.

It is sufficient to show that each of these modifications leaves invariant the local communication height.

1. Segment $i \to j$ with $i, j \neq k, n$: $h_{ij} \leqslant h_{inj}$ because the path is minimal; thus either $h_{ij} \leqslant h_{in}$ and thus $\tilde h^0_{ij} = h_{ij} \wedge (h_{in} - h_{nk} + h_{nj}) = h_{ij}$ because $h_{nk} < h_{nj}$. Or $h_{ij} \leqslant h_{in} - h_{ni} + h_{nj} < h_{in} - h_{nk} + h_{nj}$ and thus again $\tilde h^0_{ij} = h_{ij}$.
2. Segment $k \to n \to j$ with $j \neq k, n$: Then $\tilde h^0_{kj} = h_{kj} \wedge (h_{kn} - h_{nk} + h_{nj}) = h_{kn} - h_{nk} + h_{nj}$ because the path $k \to n \to j$ is minimal, and we have seen in the previous lemma that this is equal to h_{knj}. Thus $\tilde h^0_{kj} = h_{knj}$.
3. Segment $i \to n \to k$ with $i \neq k, n$: Here $\tilde h^0_{ik} = h_{ik} \wedge h_{in}$. We have seen in the previous lemma that $h_{in} = h_{ink}$, which must be smaller than h_{ik} because the path is minimal. We conclude that $\tilde h^0_{ik} = h_{ink}$.
4. Segment $i \to n \to j$ with $i, j \neq k, n$: In this case we have $\tilde h^0_{ikj} = h_{inj} + \mathcal{O}(\varepsilon\, \mathrm{e}^{-\theta/\varepsilon})$. Indeed,
   - By minimality of the path, $h_{in} \leqslant H(i,k) \vee (H(i,k) - H(k,i) + h_{kn})$. The reversibility assumption (6.1) and the minimality of γ_1 and $n \to k$ yield
   $$\begin{aligned} H(i,k) - H(k,i) + h_{kn} &= V_n - V_i + h_{nk} + \mathcal{O}(\varepsilon\, \mathrm{e}^{-\theta/\varepsilon}) \\ &= h_{in} - h_{ni} + h_{nk} + \mathcal{O}(\varepsilon\, \mathrm{e}^{-\theta/\varepsilon}) \\ &< h_{in} + \mathcal{O}(\varepsilon\, \mathrm{e}^{-\theta/\varepsilon}) \end{aligned} \tag{6.16}$$
   and thus $h_{in} \leqslant H(i,k) \leqslant h_{ik}$ for sufficiently small ε. This implies
   $$\tilde h^0_{ik} = h_{ik} \wedge h_{in} = h_{in}\ . \tag{6.17}$$
   - Minimality also yields $h_{nj} \leqslant h_{nk} \vee (h_{nk} - h_{kn} + H(k,j)) = h_{nk} - h_{kn} + H(k,j)$, where we have used $h_{nj} > h_{nk}$. Thus $h_{kn} - h_{nk} + h_{nj} \leqslant H(k,j) \leqslant h_{kj}$, which implies
   $$\tilde h^0_{kj} = h_{kn} - h_{nk} + h_{nj}\ . \tag{6.18}$$

- By assumption (6.1),

$$\begin{aligned} h_{kn} - h_{nk} + h_{ni} &= H(k,i) - H(i,k) + h_{in} + \mathcal{O}(\varepsilon\,\mathrm{e}^{-\theta/\varepsilon}) \\ &\leqslant H(k,i) + \mathcal{O}(\varepsilon\,\mathrm{e}^{-\theta/\varepsilon}) \\ &\leqslant h_{ki} + \mathcal{O}(\varepsilon\,\mathrm{e}^{-\theta/\varepsilon})\;, \end{aligned} \tag{6.19}$$

  since $h_{in} \leqslant H(i,k)$, so that

$$\tilde{h}^0_{ki} = h_{kn} - h_{nk} + h_{ni} + \mathcal{O}(\varepsilon\,\mathrm{e}^{-\theta/\varepsilon})\;. \tag{6.20}$$

Combining (6.17), (6.18) and (6.20), we obtain $\tilde{h}^0_{ikj} = h_{inj} + \mathcal{O}(\varepsilon\,\mathrm{e}^{-\theta/\varepsilon})$, concluding the proof. □

The full expansion

It remains to extend the previous results from the first-order approximation S^{12}_0 to the exact solution S^{12}.

Proposition 6.5. *For sufficiently small ε, the matrix S^{12} satisfying* (6.6) *is given by the convergent series*

$$S^{12} = \sum_{p=0}^{\infty} \frac{1}{a^{p+1}} \bigl(L^{11}\bigr)^p L^{12} \bigl[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\bigr]\;. \tag{6.21}$$

PROOF: First observe that by Assumption 2.2, $\|L^{21}A^{-1}\| = |a|^{-1}\|L^{21}\| = \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})$. Thus by Proposition 6.1, (6.6) admits a solution S^{12} of order $\mathrm{e}^{-\theta/\varepsilon}$. This solution satisfies

$$S^{12} = \frac{1}{a}L^{12} + \frac{1}{a}L^{11}S^{12} - \frac{S^{12}L^{21}}{a}S^{12}\;. \tag{6.22}$$

Note that $S^{12}L^{21}/a$ is a scalar of order $\mathrm{e}^{-\theta/\varepsilon}$. It follows that

$$S^{12} = \frac{1}{a}\Bigl[\mathbb{1} - \frac{1}{a}L^{11}\Bigr]^{-1} L^{12}\bigl[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\bigr]\;, \tag{6.23}$$

and the conclusion follows by writing the inverse as a geometric series. □

Plugging (6.21) into (6.5), we obtain

$$T^{11} = L^{11} + \sum_{p=0}^{\infty} \frac{1}{a^{p+1}} \bigl(L^{11}\bigr)^p L^{12}L^{21} \bigl[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\bigr]\;. \tag{6.24}$$

L^{11} and the term $p=0$ correspond to the first-order approximation T^{11}_0. It follows that the matrix elements of T^{11} are of the form $\mathrm{e}^{-\tilde{h}_{ij}/\varepsilon}$ where

$$\tilde{h}_{ij} = \tilde{h}^0_{ij} \wedge \inf_{\substack{p\geqslant 1\\ 1\leqslant l_1,\dots,l_p\leqslant n-1}} \Bigl(h_{il_1} + h_{l_1l_2} + \dots + h_{l_pn} + h_{nj} - (p+1)h_{nk}\Bigr) + \mathcal{O}(\varepsilon\,\mathrm{e}^{-\theta/\varepsilon})\;. \tag{6.25}$$

In order to control the remainder terms, we establish the following estimate.

Lemma 6.6. *For any $p \geqslant 1$, any $i, l_1, \dots, l_p \in \{1,\dots,n-1\}$ and $j \in \{1,\dots,n\}$,*

$$h_{il_1} + h_{l_1l_2} + \dots + h_{l_pj} - ph_{nk} \geqslant h_{il_1\dots l_pj} + p\theta\;, \tag{6.26}$$

$$h_{il_1} + h_{l_1l_2} + \dots + h_{l_pn} + h_{nj} - (p+1)h_{nk} \geqslant h_{il_1\dots l_pnj} + p\theta\;. \tag{6.27}$$

Proof: We prove first (6.26) for $p = 1$. If $h_{il} > h_{il} - h_{li} + h_{lj}$ then $h_{ilj} = h_{il}$. This implies $h_{il} + h_{lj} - h_{nk} = h_{ilj} + (h_{lj} - h_{nk}) \geqslant h_{ilj} + \theta$, where we have used (2.8). Otherwise $h_{ilj} = h_{il} - h_{li} + h_{lj}$, and then $h_{il} + h_{lj} - h_{nk} = h_{ilj} + (h_{li} - h_{nk}) \geqslant h_{ilj} + \theta$. The proof easily extends by induction to general p, using the definition (2.4) of communication heights and the fact that $h_{ij} - h_{nk} \geqslant \theta$ for $i = 1, \dots n-1$.

To prove the second inequality (6.27) for $p = 1$, we use that if $h_{iln} \geqslant h_{il} - h_{li} + h_{ln} - h_{nl} + h_{nj}$, then $h_{ilnj} = h_{iln}$ and thus $h_{il} + h_{ln} + h_{nj} - 2h_{nk} = (h_{il} + h_{ln} - h_{nk}) + (h_{nj} - h_{nk})$ so that the conclusion follows from (6.26) and the fact that $h_{nj} \geqslant h_{nk}$. Otherwise we have $h_{ilnj} = h_{il} - h_{li} + h_{ln} - h_{nl} + h_{nj}$ and $h_{il} + h_{ln} + h_{nj} - 2h_{nk} = h_{ilnj} + (h_{li} - h_{nk}) + (h_{nl} - h_{nk})$, which is greater or equal $h_{ilnj} + \theta$. The proof then extends by induction to general p. □

Corollary 6.7. *For all $i \neq j \in \{0, \dots, n-1\}$,*

$$\tilde{h}_{ij} = \tilde{h}^0_{ij} \wedge R_{ij} + \mathcal{O}(\varepsilon\,\mathrm{e}^{-\theta/\varepsilon}) \qquad \text{where } R_{ij} \geqslant H(i,j) + \theta\ . \tag{6.28}$$

Proof: This follows directly from (6.25), (6.27) and the definition (2.5) of the communication height $H(i,j)$. □

Corollary 6.8. *Communication heights are preserved to leading order in ε, that is,*

$$\widetilde{H}(i,j) = H(i,j) + \mathcal{O}(\varepsilon\,\mathrm{e}^{-\theta/\varepsilon}) \qquad \forall i,j \in \{1, \dots, n-1\}\ . \tag{6.29}$$

Proof: Corollary 6.7 and Proposition 6.4 directly yield $\widetilde{H}(i,j) \leqslant H(i,j) + \mathcal{O}(\varepsilon\,\mathrm{e}^{-\theta/\varepsilon})$ since $\tilde{h}_{ij} \leqslant \tilde{h}^0_{ij} + \mathcal{O}(\varepsilon\,\mathrm{e}^{-\theta/\varepsilon})$ implies that maximal heights encountered along paths do not increase. To show equality, consider an optimal path $\tilde{\gamma} : i \to j$. Relation (6.28) applied to each segment of $\tilde{\gamma}$ shows that γ is also an optimal path for the original generator. □

Note that this result shows in particular that assumption (6.12) on reversibility for optimal paths is satisfied by the new communication heights. We can now state the main result of this section, which characterises the eigenvalues of a generator admitting a metastable hierarchy.

Theorem 6.9 (Eigenvalues of a metastable generator)**.** *Let L be a generator satisfying Assumption 2.2 on existence of a metastable hierarchy and the reversibility condition for minimal paths* (6.1)*. For sufficiently small ε, the eigenvalues of L are given by $\lambda_1 = 0$ and*

$$\lambda_k = -\,\mathrm{e}^{-H(k,\mathcal{M}_{k-1})/\varepsilon}\bigl[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\bigr]\ , \qquad k = 2, \dots, n\ . \tag{6.30}$$

Proof: Since L is a generator, necessarily $\lambda_1 = 0$. Furthermore, L has the same eigenvalues as

$$T = \begin{pmatrix} T^{11} & 0 \\ T^{12} & \tilde{a} \end{pmatrix}\ , \tag{6.31}$$

where $\tilde{a} = a + L^{21}S^{12}$. Assumption 2.2 and the fact that L is a generator imply that

$$a = \mathrm{e}^{-h_{nk}/\varepsilon}\bigl[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\bigr]\ , \tag{6.32}$$

with $h_{nk} = h_{ns(n)} = H(n, \mathcal{M}_{n-1})$. Furthermore, we have $\|L^{21}\| = \mathcal{O}(a)$ and Proposition 6.1 shows that $\|S^{12}\| = \mathcal{O}(\|L^{12}a^{-1}\|) = \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})$. Thus $\tilde{a} = a(1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon}))$, which proves (6.30) for $k = n$.

The remaining eigenvalues $\lambda_2, \dots, \lambda_{n-1}$ are those of T^{11}. Adding, if necessary, a cemetery state, we can make T^{11} a generator (meaning that we add an identically zero first row to T^{11} and a first column such that the row sums are all zero). Corollary 6.8 shows that T^{11} admits the same metastable hierarchy as L, up to negligible error terms. Thus the result follows by induction on the size of L. □

We have thus proved Relation (2.9) in Theorem 2.3, and by extension the corresponding statements in Theorem 3.2 and Theorem 3.5.

6.3 The higher-dimensional case

We consider now the case of an irreducible representation of dimension $d \geqslant 2$. Then the generator L has a block structure, with blocks whose dimensions are multiples of d. We add a cemetery state to the system in such a way that the row sums of L vanish. We associate with L an auxiliary matrix L_* which has only one element $\mathrm{e}^{-h^*(A_i,A_j)/\varepsilon}$ for each pair (i,j) of active orbits, plus the cemetery state.

Applying to L the triangularisation algorithm described in Section 6.1 changes the blocks of L to leading order according to

$$L_{ij} \mapsto \widetilde{L}_{ij} = L_{ij} - L_{in}L_{nn}^{-1}L_{nj} \ . \tag{6.33}$$

The algorithm induces a transformation on L_* which is equivalent to the one-dimensional algorithm discussed in the previous section. Thus we conclude from Theorem 6.9 that communication heights of L_* are preserved.

Let us examine the following two cases.

- Assume $j = s(i)$ is the successor of i. Then
  - If $n \neq s(i)$, then $\widetilde{L}_{ij} = L_{ij}[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})]$, because L_{nj} is at most of order L_{nn}, and L_{in} is negligible with respect to L_{ij}.
  - If $n = s(i)$, then either $j \neq s(n)$, and then again $\widetilde{L}_{ij} = L_{ij}[1+\mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})]$, because L_{nj} is negligible with respect to L_{nn}. Or $j = s(n)$, and then $L_{in}L_{nn}^{-1}L_{nj}$ is comparable to L_{ij}.

  We thus conclude that $\widetilde{L}_{ij} = L_{ij}[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})]$, unless the graph of successors contains a path $i \to n \to j$, in which case the leading term of L_{ij} is modified according to (6.33).
- Consider now the case $j = i$. By the previous point, L_{ii} is modified to leading order by the triangularisation algorithm if and only if the graph of successors contains a cycle $i \to n \to i$. Note that in this case, the modification involves the two matrices L_{in} and L_{ni}. These matrices cannot have been modified to leading order at a previous step. Indeed, L_{in} has been modified if and only if there exists a $m \succ n$ such that the graph of successors contains a path $i \to m \to n$. Assumption 2.6 implies that this is incompatible with the fact that the graph contains $i \to n \to i$. A similar argument applies to L_{ni}.

It follows that at each step of the triangularisation algorithm, the diagonal blocks L_{ii} are preserved to leading order, unless i is at the bottom of a cycle in the graph of successors. This proves Theorem 3.9.

7 Proofs – Expected first-hitting times

The results involving expected first-hitting times are all based on a combination of the Feynman–Kac and Dynkin formulas. One version of the Feynman–Kac formula (see for instance [20, Section 1.3]) states that for every bounded measurable $f : \mathcal{X} \to \mathbb{R}$,

$$\mathbb{E}^x\bigl[\mathrm{e}^{\lambda t} f(X_t)\bigr] = \bigl(\mathrm{e}^{t(L+\lambda\mathbb{1})} f\bigr)(x) := \sum_{y\in\mathcal{X}} \bigl[\mathrm{e}^{t(L+\lambda\mathbb{1})}\bigr]_{xy} f(y) \ . \tag{7.1}$$

In other words $u(t,\cdot) = \mathbb{E}^{\cdot}\bigl[\mathrm{e}^{\lambda t} f(X_t)\bigr]$ satisfies the differential equation $\partial_t u = (L + \lambda\mathbb{1})u$. This result can be extended to stopping times, in a similar way as in Dynkin's formula.

Proposition 7.1 ("Dynkin–Feynman–Kac formula"). *Fix $A \subset \mathcal{X}$ and a bounded measurable function $g : A \to \mathbb{R}$. Then for any $\lambda \in \mathbb{C}$ such that $\mathbb{E}^x\big[|\mathrm{e}^{\lambda\tau_A}|\big] < \infty$, the function $h^\lambda_{A,g} : \mathcal{X} \to \mathbb{C}$ defined by*

$$h^\lambda_{A,g}(x) = \mathbb{E}^x\big[\mathrm{e}^{\lambda\tau_A}\, g(X_{\tau_A})\big] \tag{7.2}$$

satisfies the boundary value problem

$$\begin{aligned} (Lh)(x) &= -\lambda h(x) \qquad && x \in A^c \;, \\ h(x) &= g(x) && x \in A \;. \end{aligned} \tag{7.3}$$

Conversely, if h satisfies the boundary value problem (7.3) *and $\mathbb{E}^x\big[|\mathrm{e}^{\lambda\tau_A}|\big] < \infty$, then $h = h^\lambda_{A,g}$.*

Proof: By the Markov property, for all $x \in A^c$ and $t, s \geqslant 0$,

$$\mathbb{E}^x\big[\mathbb{E}^{X_t}\big[1_{\{\tau_A \geqslant s\}} g(X_{\tau_A})\big]\big] = \mathbb{E}^x\big[\mathbb{E}^x\big[1_{\{\tau_A \geqslant t+s\}} g(X_{\tau_A}) \;\big|\; \mathcal{F}_t\big]\big] = \mathbb{E}^x\big[1_{\{\tau_A \geqslant t+s\}} g(X_{\tau_A})\big] \;. \tag{7.4}$$

Integrating this against $\lambda\,\mathrm{e}^{\lambda s}$ from 0 to ∞ yields

$$\begin{aligned} \mathbb{E}^x\big[\mathbb{E}^{X_t}\big[\mathrm{e}^{\lambda\tau_A}\, g(X_{\tau_A})\big]\big] &= \mathbb{E}^x\big[1_{\{\tau_A \geqslant t\}}\, \mathrm{e}^{\lambda(\tau_A - t)}\, g(X_{\tau_A})\big] + \mathbb{E}^x\big[1_{\{\tau_A < t\}} g(X_{\tau_A})\big] \\ &= \mathrm{e}^{-\lambda t}\, \mathbb{E}^x\big[\mathrm{e}^{\lambda\tau_A}\, g(X_{\tau_A})\big] + \mathbb{E}^x\big[1_{\{\tau_A < t\}}\big(1 - \mathrm{e}^{\lambda(\tau_A - t)}\big) g(X_{\tau_A})\big] \;, \end{aligned} \tag{7.5}$$

and thus

$$\mathbb{E}^x\big[h^\lambda_{A,g}(X_t)\big] = \mathrm{e}^{-\lambda t}\, h^\lambda_{A,g}(x) + \mathcal{O}(t^2) \;. \tag{7.6}$$

By definition of the generator, it follows that

$$(Lh^\lambda_{A,g})(x) = \frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}^x\big[h^\lambda_{A,g}(X_t)\big]\Big|_{t=0} = -\lambda h^\lambda_{A,g}(x) \;. \tag{7.7}$$

If $x \in A$, then $\tau_A = 0$ so that clearly $h^\lambda_{A,g}(x) = g(x)$. This proves that $h^\lambda_{A,g}(x)$ satisfies (7.3). To prove the converse, let $h(x)$ satisfy (7.3). By the Feynman–Kac formula (7.1),

$$\mathbb{E}^x\big[\mathrm{e}^{\lambda t}\, h(X_t)\big] = h(x) + \mathbb{E}^x\bigg[\int_0^t \mathrm{e}^{\lambda s}[(L + \lambda\mathbb{1})h](X_s)\,\mathrm{d}s\bigg] \;. \tag{7.8}$$

Evaluating this in $t \wedge \tau_A$ and taking the limit $t \to \infty$, which is justified by Lebesgue's dominated convergence theorem, we obtain

$$\mathbb{E}^x\big[\mathrm{e}^{\lambda\tau_A}\, g(X_{\tau_A})\big] = h(x) + \mathbb{E}^x\bigg[\int_0^{\tau_A} \mathrm{e}^{\lambda s}\, \underbrace{[(L + \lambda\mathbb{1})h](X_s)}_{=0}\,\mathrm{d}s\bigg] = h(x) \;, \tag{7.9}$$

which proves the result. $\square$

In particular, for $g(x) = 1_A(x)$, we see that $h^\lambda_A(x) = \mathbb{E}^x\big[\mathrm{e}^{\lambda\tau_A}\big]$ satisfies the equation

$$\begin{aligned} (Lh^\lambda_A)(x) &= -\lambda h^\lambda_A(x) \qquad && x \in A^c \;, \\ h^\lambda_A(x) &= 1 && x \in A \;. \end{aligned} \tag{7.10}$$

Note that $h^0_A(x) = 1$ for all $x \in \mathcal{X}$. Consider now the function

$$w_A(x) = \frac{\mathrm{d}}{\mathrm{d}\lambda} h^\lambda_A(x)\Big|_{\lambda=0} = \mathbb{E}^x[\tau_A] \;. \tag{7.11}$$

Evaluating the derivative of (7.10) in $\lambda = 0$, and using the fact that $w_A(x) = 0$ for all $x \in A$, we obtain the relation

$$\sum_{y\in A^c} L_{xy} w_A(y) = -1 \; . \tag{7.12}$$

If we set $B = A^c$ and write L as

$$L = \begin{pmatrix} L_{AA} & L_{AB} \\ L_{BA} & L_{BB} \end{pmatrix} \; , \tag{7.13}$$

then (7.12) reads

$$w_A = -L_{BB}^{-1}\mathbf{1} \; . \tag{7.14}$$

Proposition 7.2 (Expected first-hitting time)**.** *If L satisfies the assumptions of Theorem 2.3 and $A = \mathcal{M}_k = \{1, \dots k\}$ with $k \geqslant 1$, then*

$$\mathbb{E}^x[\tau_A] = \frac{1}{|\lambda_{k+1}|}[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})] \tag{7.15}$$

holds for all $x \in A^c$.

Proof: The proof is by induction on the size $m = n - k$ of L_{BB}. The result is obviously true if $m = 1$, since the lower-right matrix element of L is equal to the eigenvalue λ_n, up to an error $1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})$. Thus assume $m > 1$ and write

$$L_{BB} = \begin{pmatrix} L^{11} & L^{12} \\ L^{21} & a \end{pmatrix} \; , \tag{7.16}$$

with blocks $L^{11} \in \mathbb{R}^{(m-1)\times(m-1)}$, $L^{12} \in \mathbb{R}^{(m-1)\times 1}$, $L^{21} \in \mathbb{R}^{1\times(m-1)}$ and $a \in \mathbb{R}$. Using (6.3) and (6.4), we see that

$$\begin{aligned} L_{BB}^{-1}\mathbf{1} = ST^{-1}S^{-1} &= \begin{pmatrix} 1\!\!1 & S_{12} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} (T^{11})^{-1} & 0 \\ -\tilde{a}^{-1}L^{21}(T^{11})^{-1} & \tilde{a}^{-1} \end{pmatrix} \begin{pmatrix} 1\!\!1 & -S_{12} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{1} \\ 1 \end{pmatrix} \\ &= \begin{pmatrix} 1\!\!1 & S_{12} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} (T^{11})^{-1} & 0 \\ -\tilde{a}^{-1}L^{21}(T^{11})^{-1} & \tilde{a}^{-1} \end{pmatrix} \begin{pmatrix} \mathbf{1} - S^{12} \\ 1 \end{pmatrix} \\ &= \begin{pmatrix} 1\!\!1 & S_{12} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} (T^{11})^{-1}[\mathbf{1} + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})] \\ \tilde{a}^{-1}\bigl[1 - L^{21}(T^{11})^{-1}\mathbf{1}(1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon}))\bigr] \end{pmatrix} \; . \end{aligned} \tag{7.17}$$

By induction, we may assume that

$$(T^{11})^{-1}\mathbf{1} = \frac{1}{|\lambda_{k+1}|}\mathbf{1}\bigl[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\bigr] \; , \tag{7.18}$$

which implies

$$L^{21}(T^{11})^{-1}\mathbf{1} = \frac{L^{21}\mathbf{1}}{|\lambda_{k+1}|}\bigl[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\bigr] = \frac{|\lambda_n|}{|\lambda_{k+1}|}\bigl[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\bigr] \, . \tag{7.19}$$

Plugging this into (7.17) and using the fact that $|\lambda_{k+1}|/|\lambda_n| = \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})$ we obtain

$$L_{BB}^{-1}\mathbf{1} = \begin{pmatrix} 1\!\!1 & S_{12} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} |\lambda_{k+1}|^{-1}\mathbf{1}\bigl[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\bigr] \\ |\lambda_{k+1}|^{-1}\bigl[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\bigr] \end{pmatrix} = \frac{1}{|\lambda_{k+1}|}\mathbf{1}\bigl[1 + \mathcal{O}(\mathrm{e}^{-\theta/\varepsilon})\bigr] \; , \tag{7.20}$$

which concludes the proof. □

This completes the proof of Theorem 2.3, and thus also of Theorem 3.2 and Theorem 3.5.

A Critical points of the constrained system

We give in this appendix a brief description of how we obtained the local minima and saddles of index 1 for Example 1.2 (a more detailed analysis of this system will be published elsewhere). The case $N = 4$ was first studied in [16].

We look for extrema of the potential

$$V_\gamma(x) = \sum_{i\in\mathbb{Z}/N\mathbb{Z}} U(x_i) + \frac{\gamma}{4} \sum_{i\in\mathbb{Z}/N\mathbb{Z}} (x_{i+1} - x_i)^2 \tag{A.1}$$

where $U(x) = \frac{1}{4}x^4 - \frac{1}{2}x^2$, under the constraint

$$\sum_{i\in\mathbb{Z}/N\mathbb{Z}} x_i = 0 \; . \tag{A.2}$$

We will apply a perturbative argument in γ, and thus start by considering the case $\gamma = 0$. Then the extremalisation problem is equivalent to solving $\nabla V_0(x) = \lambda\mathbf{1}$ on $\{\sum x_i = 0\}$, or equivalently

$$f(x_i) = \lambda \qquad \forall i \in \mathbb{Z}/N\mathbb{Z} \; , \tag{A.3}$$

where $f(x) = U'(x) = x^3 - x$ and λ is the Lagrange multiplier. There are three cases to consider:

1. If $|\lambda| > 2/(3\sqrt{3})$, then $f(x) = \lambda$ admits only one real solution, different from zero, and the constrained problem has no solution.
2. If $|\lambda| = 2/(3\sqrt{3})$, then $f(x) = \lambda$ admits two real solutions, given by $\pm 1/\sqrt{3}$ and $\mp 2/\sqrt{3}$. Then solutions exist only if N is a multiple of 3 (and they may give rise to degenerate families of stationary points).
3. If $|\lambda| < 2/(3\sqrt{3})$, then $f(x) = \lambda$ admits three different real solutions α_0, α_1 and α_2. We denote by $n_i \in \mathbb{N}_0$ the number of x_i equal to α_i, and reorder the α_i in such a way that $n_0 \leqslant n_1 \leqslant n_2$. Then the constrained problem is equivalent to

$$\begin{aligned} \alpha_0 + \alpha_1 + \alpha_2 &= 0 \\ \alpha_0\alpha_1\alpha_2 &= \lambda \\ \alpha_0\alpha_1 + \alpha_0\alpha_2 + \alpha_1\alpha_2 &= -1 \\ n_0\alpha_0 + n_1\alpha_1 + n_2\alpha_2 &= 0 \end{aligned} \tag{A.4}$$

with $n_0 + n_1 + n_2 = N$. This can be seen to be equivalent to

$$(\alpha_0, \alpha_1, \alpha_2) = \pm \frac{1}{R^{1/2}} (n_2 - n_1, n_0 - n_2, n_1 - n_0) \tag{A.5}$$

where $R = n_0^2 + n_1^2 + n_2^2 - n_0n_1 - n_0n_2 - n_1n_2$.

This shows that if N is not a multiple of 3, then all solutions of the constrained problem can be indexed by ordered triples (n_0, n_1, n_2) of non-negative integers whose sum is N. By examining the Hessian of the potential (taking into account the constraint), one can prove the following result.

Theorem A.1. *Assume $N \geqslant 5$ is not a multiple of 3. Then for $\gamma = 0$*

1. *all local minima are given by ordered triples $(0, n_1, N - n_1)$ with $3n_1 > N$;*
2. *all saddles of index 1 are given by ordered triples $(1, n_1, N - n_1 - 1)$ with $3n_1 > N$.*

If $N = 4$, then all local minima are given by the triple $(0,2,2)$ and all saddles of index 1 by the triple $(1,1,2)$.

In the case $N = 4$,

- the triple $(0,2,2)$ yields 6 local minima, having each two coordinates equal to 1 and two coordinates equal to -1;
- the triple $(1,1,2)$ yields 12 saddles of index 1, having each two coordinates equal to 0, one coordinate equal to 1 and the other one equal to -1.

One can check the octahedral structure of the associated graph by constructing paths from each saddle to two different local minima, along which the potential decreases. For instance, the path $\{(1,t,-t,-1)\colon -1 \leqslant t \leqslant 1\}$ interpolates between the local minima $(1,-1,1,-1)$ and $(1,1,-1,-1)$ via the saddle $(1,0,0,-1)$, and the value of the potential along this path is $2U(t)$, which is decreasing in $|t|$ on $[-1,1]$.

In the case $N = 8$,

- the triple $(0,4,4)$ yields $\binom{8}{4} = 70$ local minima, having each four coordinates equal to 1 and four coordinates equal to -1;
- the triple $(0,3,5)$ yields $2\binom{8}{3} = 112$ local minima, having three coordinates equal to $\pm\alpha = \pm 5/\sqrt{19}$ and five coordinates equal to $\pm\beta = \mp 3/\sqrt{19}$;
- and the triple $(1,3,4)$ yields $2\frac{8!}{1!3!4!} = 560$ saddles of index 1, with one coordinate equal to $\mp 1/\sqrt{7}$, three coordinates equal to $\pm 3/\sqrt{7}$ and four coordinates equal to $\mp 2/\sqrt{7}$.

The connection rules stated in Section 4.2 can again be checked by constructing paths along which the potential decreases.

	$\gamma = 0$	$\gamma > 0$		V_γ
a	$(1,1,-1,-1)$	$(x,x,-x,-x)$	$x = \sqrt{1-\gamma}$	$-(1-\gamma)^2$
b	$(1,-1,1,-1)$	$(x,-x,x,-x)$	$x = \sqrt{1-2\gamma}$	$-(1-2\gamma)^2$
a–a'	$(1,0,-1,0)$	$(x,0,-x,0)$	$x = \sqrt{1-\gamma}$	$-\frac{1}{2}(1-\gamma)^2$
a–b	$(1,-1,0,0)$	$(x,-x,y,-y)$	$x,y = \frac{\sqrt{2-\gamma}\pm\sqrt{2-5\gamma}}{\sqrt{8}}$	$-\frac{1}{8}(4-12\gamma+7\gamma^2)$

TABLE 4. Local minima and saddles of index 1 for the case $N = 4$, with the value of the potential. The relevant heights are $h_{ab} = V_\gamma(a\text{–}b) - V_\gamma(a)$, $h_{ba} = V_\gamma(a\text{–}b) - V_\gamma(b)$, and $h_{aa'} = V_\gamma(a\text{–}a') - V_\gamma(a)$.

Since the Hessian is nondegenerate at the stationary points listed by Theorem A.1, the implicit-function theorem applies, and shows that these points persist, with the same stability, for sufficiently small positive γ. In the case $N = 4$, the coordinates can even be computed explicitly (Table 4), drawing on the fact that they keep the same symmetry as for $\gamma = 0$.

The value of the potential at the stationary points can then be computed, exactly for $N = 4$ and perturbatively to second order in γ for $N = 8$, which allows to determine the metastable hierarchy.

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