Preliminary version

RIGHT ORDER SPECTRAL GAP ESTIMATES FOR GENERATING SETS OF $\mathbb{Z}_4$

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Abstract. Using coupling arguments, a distance method and Zeifman's method we give sharp estimates on the spectral gap for a special case of the class of Markov chains on generating n-tuples of Abelian groups. In our case the group is $\mathbb{Z}_4^n$.

Keywords: Markov chains, spectral gap, coupling

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1. Introduction

This paper treats a special case of a problem which in its most general form has been posed by D. Aldous in a survey talk on the ICM 1994. It is basically concerned with the problem of the speed of convergence of some algorithms used in computer algebra packages in order to produce random elements from a group G. Generally speaking the setting is as follows: We are given a finite, directed, labelled graph $\mathcal{G} = (V, E)$ that is reversible (i.e. if $i \to j \in V$ then also $j \to i \in V$) and a finite group G. Moreover let Γ be a set that generates G (and assume $|\Gamma| \geq 1$). Classically one would proceed in the following way to produce a random element from G. Start with the identity and successively choose random elements from Γ and multiply by them from the right.

A new algorithm proposed by Celler et. al. [?] suggests to run a Markov chain on V^G with $|V| > |\Gamma|$, instead. More precisely, they propound to start with labelling the first $|\Gamma|$ vertices of V with the elements of Γ and the rest by the identity. The random walk then proceeds by selecting randomly an edge from V (i.e. with the uniform distribution on all edges) and if this edge is $i \to j$ by replacing x_j (the element associated with vertex j) by $x_i x_j$ with probability $1/2$ and by $x_i x_j^{-1}$ with probability $1/2$.

In particular, if $\mathcal{G} = K_n$, the complete directed graph on n vertices, this walk has the uniform probability on all admissible n-tuples from G, i.e. all $x \in G^n$ with $\langle x \rangle = G$ as its invariant measure. This does not quite imply that also the distribution of any coordinate of the walk converges to the uniform distribution on G. For example if $n = 2$, $\mathcal{G} = K_2$, and $G = \mathbb{Z}_2$ the fact that the first coordinate of the walk is 0 automatically implies that the other is 1. But as n gets larger the difference between the uniform distribution on G (in each coordinate) and the one induced by the uniform distribution on all admissible configurations becomes more and more negligible.

Aldous' question now concerns the speed of convergence of this walk. In the two papers [?] and [?] Diaconis and Saloff-Coste analyse the above walk for different choices of $\mathcal{G}$ and G. In particular, for $\mathcal{G} = K_n$ and $G = \mathbb{Z}_2$ they show in [?] that about $\mathcal{O}(n^2 logn)$ steps of the walk suffice to come close for convergence to stationarity.

In this paper we will be concerned with the case where $\mathcal{G} = K_n$ but $G = \mathbb{Z}_4$ (the case $\mathcal{G} = K_n$ and $G = \mathbb{Z}_3$ has been studied in a previous paper by one of the authors (see [?]). By applying a new technique – the so-called distance method, which has its roots in the theory of diffusions on manifolds – we are even able to show that the spectral gap of the above chain is of order $\mathcal{O}(\frac{1}{n})$ (implying that after $\mathcal{O}(n\ln(n))$ steps the walk is already close to the invariant measure.

In order to agree on some notation let Q be an irreducible Markov chain on the finite state space X, and $L = Id - Q$ its (discrete) infinitesimal generator. By irreducibility there exists a uniquely determined stationary distribution π of Q (that is $\pi Q = \pi$) that charges any point in X. Assume that Q is reversible with respect to π, that is the detailed balance equations

$$\pi(y)Q(y,x) = \pi(x)Q(x,y)$$

are fulfilled for every pair $x, y \in X$.
This especially implies that the eigenvalues of Q and hence the eigenvalues of L are real. We write the latter in the form

$$0 = \lambda_0 < \lambda_1 \leq \ldots \leq \lambda_{|X|-1} \leq 2.$$

The spectral gap is defined by $\operatorname{gap}(L) = \lambda_1 \vee (2 - \lambda_{|X|-1})$.
For complex-valued functions f, g on X the scalar product on $L^2(\pi)$ is defined by

$$\langle f, g\rangle_{L^2(\pi)} = \sum_{x\in X} f(x)\overline{g(x)}\pi(x)$$

and the corresponding norm on $L^2(\pi)$ is denoted by $\|f\|_{L^2(\pi)}$.
The minimax characterisation of eigenvalues, see [?] p. 176, then yields that

$$\lambda_1 = \inf\left\{ \mathcal{E}(f,f) \,:\, \|f\|_{L^2(\pi)} = 1,\, E_\pi(f) = 0 \right\}.$$

Lower bounds on λ_1 yield upper bounds for the rate of convergence of the underlying continuous-time Markov chain. In general for discrete-time Markov chains one also has to take care of the negative eigenvalues. However, by adding some holding (e.g. using $1/2(Q + Id)$ instead of Q) one can achieve that the modified chain has its smallest eigenvalue bounded away from -1 as far as we want to.
In this paper we will mainly use a so-called distance method. The idea of this method is to compare a given unknown eigenfunction of the second-largest eigenvalue with a positive (distance) function. If the transition matrix satisfies some contraction principle with respect to the distance function, we obtain an upper estimate of the second-largest eigenvalue. A more explicit explanation will be given in the third paragraph. For the origins of this method applied to time-continuous Markov processes the reader is referred to [?], [?]. For first applications for discrete-time Markov-chains see [?]. Moreover we will use a method due to Zeifman, cf. [?], that allows estimates on the rate of convergence for birth and death Markov chains.
The rest of the paper is organised as follows. Section 2 contains a statement of the results. In Section 3 we will explain our main tools, namely the distance method mentioned above and its connection to path coupling of Markov chains. Section 4 finally contains the rather technical proofs.

2. Results

Let us return to the Markov chain on $\mathbb{Z}_4^n$ described in the introduction. So, more precisely, the state space of the walk is given by

$$X = \left\{ x \in \mathbb{Z}_4^n \,:< \{x_1, \ldots, x_n\} >= \mathbb{Z}_4 \right\},$$

where $< A >$ denotes the group generated by the set A. Given that the Markov chain is in state $g = (g_1, \dots, g_n)$, we choose an edge (i, j) in the edge set of K_n uniformly at random. Then with probability 1/2 the element g_j is replaced by $g_i g_j$ or $g_i g_j^{-1}$ respectively.

So all in all the transition probabilities of the walk Y_n described by this procedure are given by

$$P(Y_{n+1} = (g_1, \dots g'_j, \dots, g_n) | Y_n = (g_1, \dots g_j, \dots, g_n)) =$$
$$\left(\frac{1}{n(n-1)} \sum_{i \neq j, g_i g_j = g'_j} 1\right) + \left(\frac{1}{n(n-1)} \sum_{i \neq j, g_i g_j^{-1} = g'_j} 1\right).$$

Before we state our result let us finally introduce two more notations. For $x \in X$ we define

$$n_1(x) = |\{ 1 \leq i \leq n \, : \, x_i \in \{1, 3\}\}| ,$$

and

$$n_2(x) = |\{ 1 \leq i \leq n \, : \, x_i = 2\}| .$$

Moreover, we let $n(x) = (n_1(x), n_2(x))$.

For this random walk we have the following results.

Theorem 2.1. *For the random walk Y_n described above the following bounds on the spectral gap $\lambda_1(Q)$ hold true*

$$\frac{c_1}{n} \geq \lambda_1(Q) \geq \frac{c_2}{n}. \tag{1}$$

Also, the largest eigenvalue $\lambda_{|X|-1}$ of L satisfies

$$\lambda_{|X|-1} \leq 2 - \frac{c}{n}. \tag{2}$$

3. The distance method

Let $\beta \neq 1$ be an eigenvalue of Q with corresponding eigenfunction f. Assume that there exists a function $d : X \to \mathbb{R}^+$ such that $[Qd](x) \leq \alpha d(x)$ for all $x \in X$ and some $\alpha \leq 1$. Let

$$m := \max \left\{ \frac{|f(x)|}{d(x)} \, : \, x \in X \right\}.$$

Choose $x \in X$ such that $|f(x)| / d(x) = m$. Then we have

$$\begin{aligned} |\beta f(x)| &= |[Qf](x)| = \left| \sum_{y \in X} Q(x, y) f(y) \right| \\ &\leq \sum_{y \in X} Q(x, y) |f(y)| = \sum_{y \in X} Q(x, y) \frac{|f(y)|}{d(y)} d(y) \\ &\leq \frac{|f(x)|}{d(x)} [Qd](x) \leq \alpha |f(x)| . \end{aligned}$$

Dividing by $|f(x)|$ we conclude $|\beta| \leq \alpha$. Thus we arrive at

Proposition 3.1. *Let $d : X \to \mathbb{R}^+$ be a function, such that $[Qd](x) \leq \alpha d(x)$ for all $x \in X$ and a fixed $\alpha \leq 1$. Then for all eigenvalues $\beta \neq 1$ of Q, $|\beta| \leq \alpha$.*

We obtain a similar result to Proposition 3.1 by using couplings.

Proposition 3.2. *Let $d : X \times X \to \mathbb{R}^+$ be a function, such that for some coupling $\widetilde{Q}$ of (Q, Q) the inequality $[\widetilde{Q}d](x, y) \leq \alpha d(x, y)$ for all $x \neq y$ and some $\alpha \leq 1$ holds true. Then any eigenvalue $\beta \neq 1$ of Q satisfies, $|\beta| \leq \alpha$.*

Proof. Similarly to Proposition 3.1 we define

$$m := \max\left\{ \frac{|f(y) - f(x)|}{d(x, y)} \; : \; x \neq y \in X \right\}.$$

Let (x, y) be such that $|g(x, y)| / d(x, y) = m$, where $g(x, y) = f(y) - f(x)$. We conclude

$$|\beta g(x, y)| = \left| \left[\widetilde{Q}g\right](x, y) \right| \leq m \left[\widetilde{Q}d\right](x, y) \leq m\alpha d(x, y).$$

Hence $|\beta| \leq \alpha$. □

Remark 3.3. *The basic trick of the distance methode is to find a distance functions that models "the landscape" given by $|f(y) - f(x)|$ as close as possible and on the other hand still allows for a nice coupling.*

In the applications we will use the distance method in the following way. Suppose that there is a set $M \subset X \times X$ of the form $M = \dot{\bigcup}_{i=1}^{k} M_i \times M_i$, such that there is a coupling $\widetilde{Q}$ keeping the "levels" $M_j \times M_j$ fixed, that is a coupling for which $(x, y) \in M_i \times M_i$ and $\widetilde{Q}((x, y), (x', y')) > 0$ implies $(x', y') \in M_j \times M_j$ for some j. Thus, the bivariate coupled chain never escapes from M. In other words, at the same time the two particles are in the same M_j. Assume that there is a contraction of $\widetilde{Q}$ on M with respect to some function $d : X \times X \to \mathbb{R}_0^+$, i.e. $[\widetilde{Q}d](x, y) \leq \alpha d(x, y)$ for some $\alpha < 1$ for all $(x, y) \in M_i \times M_i$, $i \in \{1, 2, \ldots, k\}$ (indeed d may even depend on j). If there is an eigenfunction f to an eigenvalue β that is non-constant on some M_i, we obtain the estimate $|\beta| \leq \alpha$.

Otherwise, if all eigenfunctions f for β are constant on each M_i, we may identify all points in each M_i and analyze an induced Markov chain. If, for example, $Q(x, M_j) = Q(y, M_j)$ for all $x, y \in M_i$ and $i, j \in \{1, 2, \ldots, k\}$ we can consider the induced Markov chain given by $K(i, j) := Q(x, M_j)$, where $x \in M_i$ is arbitrary. It is known that the spectrum of K is contained in the spectrum of Q. However, if we are interested in the second-largest or the smallest eigenvalue the non-existence of non-constant eigenfunctions on the sets M_i yields that the second-largest or the smallest eigenvalue of K must coincide with those of Q.

4. Proofs

Before we step into the details let us quickly exhibit the principal structure of the proof. It is basically split into two parts depending on whether the eigenfunctions to β_1 are all constant on the "level sets" of $n(\cdot)$, or not. So we distinguish between

A) There is an eigenfunction f to the eigenvalue β_1 of Q such that $f(x) = f(y)$ for all $x, y \in X$ satisfying $n(x) = n(y)$. In this case, the analysis of the Markov chain Q can be reduced to that of an associated Markov chain on a subset of the two-dimensional lattice. See (3) for the definition of the transition probabilities on the state space $Y = \{ (i, j) \; : \; i \geq 1, \, j \geq 0, \, i + j \leq n\}$. Figure 1 illustrates the state space for the case $n = 7$.

and

B) For all eigenfunctions f to β_1 of Q there exist $x, y \in X$ such that $n(x) = n(y)$ and $f(x) \neq f(y)$.

The analysis of this case is split into different subcases. If x and y not only have the same index $n(\cdot)$ but also the same number of 1's, then x can be obtained by a permutation of y. As a permutation is nothing but the product of several transpositions, there also have to be x and y with $f(x) \neq f(y)$ such that x can be obtained from y by a simple transposition. According to in which arguments x and y differ we obtain four different subcases (as 1 and 3 can be treated identically). On the other hand, if e.g. x contains more 1's than y (and thus y contains more 3's) by the same sort of reduction argument we can assume that x contains exactly one more 1 than y and that they differ in precisely one position (say the first), where x is 1 while y is 3.

These cases will be treated at the end of this section.

Let us now turn to the proof of the main theorem.

4.1. **Proof of Proposition 2.1. Proof** of (1). As indicated above the proof is divided into several parts

Case A) There exists an eigenfunction f to β_1 of Q such that for all $x, y \in X$ with $n(x) = n(y)$ we have $f(x) = f(y)$. In this case the analysis of the Markov chain reduces to the analysis of the Markov chain K on the two-dimensional grid, where K is given by

$$K((i,j),(i',j')) := P\left(\, n(X_t) = (i',j') \mid n(X_{t-1}) = (i,j)\,\right).$$

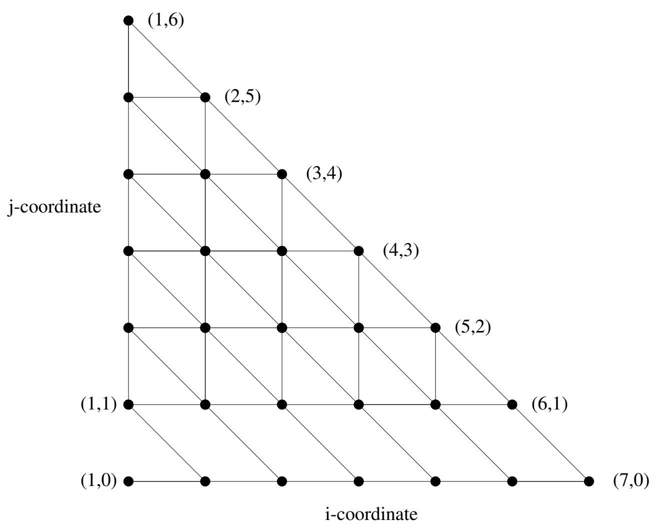

FIGURE 1. State space Y in the case $n = 7$.

More precisely on the state space

$$Y = \{\,(i,j) \,:\, i \geq 1,\ j \geq 0,\ i + j \leq n\,\}$$

the transition probabilities are

$$
\begin{aligned}
K\left((i,j),(i+1,j)\right) &= \tfrac{(n-i-j)i}{n(n-1)} && \rightarrow \\
K\left((i,j),(i-1,j)\right) &= \tfrac{i(i-1)}{2n(n-1)} && \leftarrow \\
K\left((i,j),(i,j+1)\right) &= \tfrac{(n-i-j)j}{n(n-1)} && \uparrow \\
K\left((i,j),(i,j-1)\right) &= \tfrac{j(j-1)}{n(n-1)} && \downarrow \\
K\left((i,j),(i+1,j-1)\right) &= \tfrac{ij}{n(n-1)} && \searrow \\
K\left((i,j),(i-1,j+1)\right) &= \tfrac{i(i-1)}{2n(n-1)} && \nwarrow \\
K\left((i,j),(i,j)\right) &= \tfrac{ij}{n(n-1)} + \tfrac{n-i-j}{n} && \bullet
\end{aligned}
\tag{3}
$$

Here the arrows to the right side illustrate to which neighboring point the particle is moving, e.g. '$\rightarrow$' means a move to the right (increment of the first coordinate) and '$\bullet$' indicates that the particle stays at its current position. Using the minimax characterization (see e.g. [?]) it is straightforward to check that the second-largest eigenvalue of Q coincides with that of K.
Therefore we estimate the spectral gap of the Markov chain K on the grid defined in (3).

Proposition 4.1. *The first positive eigenvalue λ_1 of the discrete generator $L = I - K$, where K is given by (3) satisfies*

$$\lambda_1 \geq \frac{2}{9}\frac{1}{n}.$$

Proof. Again, we differentiate between two cases.

If there is an eigenfunction f of K such that $f((i,j)) = f((i,j'))$ for all i,j,j' with $(i,j) \in Y$ and $(i,j') \in Y$. Similar to the above reduction, in this case we can reduce the problem for estimating the second-largest eigenvalue of the chain K to that of the one-dimensional chain M with state space $Z = \{1,2,\dots,n\}$ with transition probabilities

$$
\begin{aligned}
M(i,i+1) &= \frac{(n-i)i}{n(n-1)} \\
M(i,i-1) &= \frac{i(i-1)}{2n(n-1)}.
\end{aligned}
$$

This chain can and has been studied bei Zeifman's method (cf. [?], [?]). In [?] it has been shown that indeed the Assumptions of Theorem 1 in [?] are fulfilled implying that for any $\varepsilon > 0$ there is N such that $\lambda_1(M) \geq (1-\varepsilon)/(n-1)$ for all $n \geq N$, cf. [?].

If, on the other hand, for any eigenfunction f of K there exists $(i,j) \in Y$ and $(i,j') \in Y$ such that $f((i,j)) \neq f((i,j'))$ we may apply a path coupling argument. To this end let us first introduce the coupling $\widetilde{K}$ of K that we will use. For i,j such that

$n-i-2j+1 \geq 0$ we let

$$
\begin{array}{rll}
\widetilde{K}\left([(i,j),(i,j-1)],[(i+1,j),(i+1,j-1)]\right) = \frac{(n-i-j)i}{n(n-1)} & \rightarrow & \rightarrow \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i-1,j),(i-1,j-1)]\right) = \frac{i(i-1)}{2n(n-1)} & \leftarrow & \leftarrow \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i,j+1),(i,j)]\right) = \frac{(n-i-(j-1))(j-1)}{n(n-1)} & \uparrow & \uparrow \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i,j-1),(i,j-2)]\right) = \frac{(j-1)(j-2)}{n(n-1)} & \downarrow & \downarrow \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i+1,j-1),(i+1,j-1)]\right) = \frac{i}{n(n-1)} & \searrow & \rightarrow \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i+1,j-1),(i+1,j-2)]\right) = \frac{i(j-1)}{n(n-1)} & \searrow & \searrow \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i-1,j+1),(i-1,j)]\right) = \frac{i(i-1)}{2n(n-1)} & \nwarrow & \nwarrow \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i,j),(i,j-1)]\right) = \frac{(n-i-j)(n-1)+ij}{n(n-1)} & \bullet & \bullet \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i,j+1),(i,j-1)]\right) = \frac{n-i-2j+1}{n(n-1)} & \uparrow & \bullet \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i,j-1),(i,j-1)]\right) = \frac{2(j-1)}{n(n-1)} & \downarrow & \bullet
\end{array}
$$

For i,j such that $n-i-2j+1 < 0$ we let

$$
\begin{array}{rll}
\widetilde{K}\left([(i,j),(i,j-1)],[(i+1,j),(i+1,j-1)]\right) = \frac{(n-i-j)i}{n(n-1)} & \rightarrow & \rightarrow \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i-1,j),(i-1,j-1)]\right) = \frac{i(i-1)}{2n(n-1)} & \leftarrow & \leftarrow \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i,j+1),(i,j)]\right) = \frac{(n-i-j)j}{n(n-1)} & \uparrow & \uparrow \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i,j-1),(i,j-2)]\right) = \frac{(j-1)(j-2)}{n(n-1)} & \downarrow & \downarrow \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i+1,j-1),(i+1,j-1)]\right) = \frac{i}{n(n-1)} & \searrow & \rightarrow \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i+1,j-1),(i+1,j-2)]\right) = \frac{i(j-1)}{n(n-1)} & \searrow & \searrow \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i-1,j+1),(i-1,j)]\right) = \frac{i(i-1)}{2n(n-1)} & \nwarrow & \nwarrow \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i,j),(i,j-1)]\right) = \frac{(n-i-j+1)(n-1)+(j-1)(i-2)}{n(n-1)} & \bullet & \bullet \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i,j),(i,j)]\right) = \frac{2j+i-n-1}{n(n-1)} & \bullet & \uparrow \\
\widetilde{K}\left([(i,j),(i,j-1)],[(i,j-1),(i,j-1)]\right) = \frac{2(j-1)}{n(n-1)} & \downarrow & \bullet
\end{array}
$$

Consider the set

$$S = \{\, [(i,j),(i,j')] \;:\; (i,j) \in Y,\ (i,j') \in Y \,\}.$$

and observe that the coupling presented above guarantees that the coupled process will never leave S given that it starts in S. For this reason it is clearly not necessary to define transition probabilities for elements not in S. Next, we need to proivide a distance function for neighboring elements in Y. For $(i,j),(i,j-1) \in Y$ we define,

$$d((i,j),(i,j-1)) = \begin{cases} \frac{1}{i(j+1)} & : \quad (i,j) \neq (1,1) \\ \frac{5}{4} & : \quad (i,j) = (1,1). \end{cases}$$

For elements $(i,j_1),(i,j_2) \in Y$ with $j_1 < j_2$ we define

$$d((i,j_1),(i,j_2)) = \sum_{l=j_1+1}^{j_2} d((i,l),(i,l-1)). \tag{4}$$

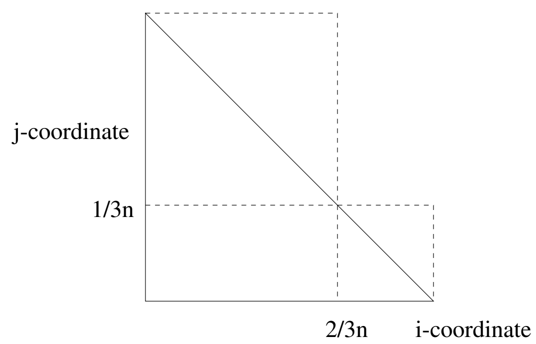

FIGURE 2. The rectangles cover the triangular state space.

Now we show an estimate of the type

$$\left[\widetilde{K}d\right]((i,j),(i,j-1)) \leq \alpha d((i,j),(i,j-1)), \tag{5}$$

for all $(i,j),(i,j-1) \in Y$ for some fixed $\alpha < 1$. Using (4) and the linearity of $\widetilde{K}$ for $(i,j_2),(i,j_1) \in Y$ this clearly yields

$$\left[\widetilde{K}d\right]((i,j_2),(i,j_1)) \leq \alpha d((i,j_2),(i,j_1)),$$

for all $(i,j_2),(i,j_1) \in Y$ with $j_1 < j_2$.
In the following considerations we will use the abbreviation $d(i,j-1) = d((i,j),(i,j-1))$.
Let us distinguish the following cases: **Case I:** $n-i-2j<0$.
Case Ia: $i \geq 2$, $j \geq 2$.
According to the distance method sketched in Section 3 and our goal to bound the spectral gap by c/n we need to show that the following expression is bounded from above by $-cn$,

$$\begin{aligned} & n(n-1)[\widetilde{K}d]((i,j),(i,j-1)) \\ = \; & (n-i-j)id(i+1,j-1) + \frac{i(i-1)}{2}d(i-1,j-1) + (n-i-j)jd(i,j) + (j-1)(j-2)d(i,j-2) \\ & + i(j-1)d(i+1,j-2) + \frac{i(i-1)}{2}d(i-1,j) + (n-i-j+1)(n-1)d(i,j-1) \\ & + (i-2)(j-1)d(i,j-1). \end{aligned}$$

Using the function

$$f : (i,j) \mapsto 2n(n-1)\left[\frac{[\widetilde{K}d]((i,j),(i,j-1))}{d(i,j-1)} - 1\right]$$

we obtain

$$f(i,j) \;=\; -\frac{1}{2}\frac{4nij - 3i^2 + i^3 + 2ni + 2nj - 6i^2j}{(i+1)(j+1)} + \mathcal{O}(1).$$

As both nominator and denominator of f are linear functions in j one quickly checks that the function $j \mapsto f(i,j)$ is either monotonly decreasing or increasing (depending on the fixed value of i). We give estimates for $f(i,j)$ in each of the two rectangles indicated in Figure 2.
Case Ia1: $i \leq 2/3n$.

Using the monotonicity of the function $j \mapsto f(i,j)$we have

$$f(i,j) \leq f(i,2) \vee f(i,n).$$

Note that

$$f(i,2) = -\frac{1}{6}\frac{4n+10ni-15i^2+i^3}{i} \leq -n + \mathcal{O}(1),$$

and

$$f(i,n) = -\frac{1}{2}\frac{2n^2-6i^2n+2in+i^3+4n^2i}{(n+1)(i+1)} \leq -\frac{2}{9}n + \mathcal{O}(1).$$

for all $2 \leq i \leq 2/3n$.

Case Ia2: $2/3n < i \leq n$**.** Again using the monotonicity of $j \mapsto f(i,j)$, we obtain that

$$f(i,j) \leq f(i,2) \vee f(i,n/3).$$

Estimating $f(i,2)$ and $f(i,n/3)$ we conclude that

$$f(i,j) \leq -\frac{1}{2}n + O(1),$$

for all $2/3n \leq i \leq n$. Combining the estimates of the subcases shows that

$$f(i,j) \leq -\frac{2}{9}n + \mathcal{O}(1),$$

for all $i \geq 2$, $j \geq 2$ with $i+j \leq n$.

Case Ib: $i=1$, $j \geq 2$**.** Here we obtain

$$\frac{[\widetilde{K}d]((1,j),(1,j-1))}{d(1,j-1)} - 1 = -\frac{1}{4n(n-1)}\frac{3jn+n-j-1}{j+1} \leq -\frac{1}{4(n-1)},$$

for all $2 \leq j \leq n$.

Case Ic: $i \geq 2$, $j=1$**.** The condition $n-i-2j<0$ implies that $i \geq n-1$ and hence $i = n-1$, since $i+j \leq n$. Therefore, we only need to compute

$$2n(n-1)\left[\frac{[\widetilde{K}d]((n-1,1),(n-1,0))}{d(n-1,0)} - 1\right] = -\frac{1}{4}n^2 + O(n).$$

Case II: $n-i-2j \geq 0$**.**

Case IIa: $i \geq 2$, $j \geq 2$**.**

The expression that we have to estimate is given by

$$\begin{aligned} n(n-1)[\widetilde{K}d]((i,j),(i,j-1)) \quad &= \quad (n-i-j)id(i+1,j-1) + \frac{i(i-1)}{2}d(i-1,j-1) \\ &\quad +(n-i-j+1)(j-1)d(i,j) + (j-1)(j-2)d(i,j-2) \\ &\quad +i(j-1)d(i+1,j-2) + i(i-1)/2d(i-1,j) \\ &\quad +(n-i-j)(n-1)d(i,j-1) + ijd(i,j-1) \\ &\quad +(n-i-2j+1)[d(i,j-1)+d(i,j)]. \end{aligned}$$

Defining the function

$$f : (i,j) \mapsto 2n(n-1)\left[\frac{[\widetilde{K}d]((i,j),(i,j-1))}{d(i,j-1)} - 1\right],$$

we obtain

$$f(i,j) \quad = \quad -\frac{-2n+4j^2-i^2-4i^2j+4j^2i+i^3+2nij}{(i+1)(j+1)} + O(1).$$

Our aim is to give an upper estimate for the expression to the right side under the condition $n-i-2j \geq 0$, $i \geq 2$ and $j \geq 2$. For the sake of convenience we will consider the function $h(i,j) := f(i-1, j-1)$ rather than f. Considering h as a function of j for fixed i, we obtain that the first derivative has zeros $j = 1/2\sqrt{i^2-2n}$ and $j = -1/2\sqrt{i^2-2n}$. Clearly, the negative value for j is not acceptable.

Case IIa1: $i < \sqrt{2n}$. In this case $h'(i,\cdot)$ has no zeros at all, so that the function $h(i,\cdot)$ is monotone. Thus

$$\max_{3 \leq j \leq n/2+1} h(i,j) \leq h(i,3) \vee h(i, n/2+1).$$

Note that

$$h(i,3) = -\frac{1}{3}\frac{36i + 4ni - 12i^2 - 6n + i^3}{i} \leq -\frac{2}{3}n$$

for all $3 \leq i \leq n$. Moreover, we have

$$h(i, n/2+1) = -2\frac{2n^2 i - 2ni^2 - n^2 + i^3}{i(n+2)} + \mathcal{O}(1) \leq -3n + \mathcal{O}(1)$$

for all $3 \leq i \leq \sqrt{2n}$.

Case IIa2: $i \geq \sqrt{2n}$. As $h(i,\cdot)$ has two local extrema, one with a positive and one with a negative j one readily sees that in this case the function $j \mapsto h(i,j)$, $j \geq 1$, is concave. Therefore $h(i,j)$ is maximal for $j_0 = 1/2\sqrt{i^2-2n}$. Writing i in the form $i = \alpha(i)\sqrt{n}$ we have

$$h(i,j_0) = -2\frac{2i^2-4n}{\sqrt{i^2-2n}} + 4i + 2\frac{n}{i} - 2n = -2g(\alpha(i)) - 2n,$$

where g denotes the concave function defined by

$$g(x) = \sqrt{n}\left[\frac{(2x^2-4)}{\sqrt{x^2-2}} - 2x - \frac{1}{x}\right].$$

Note that $\lim_{x \to \sqrt{2}} g(x) = -2^{3/2}\sqrt{n} - 2^{-1/2}\sqrt{n}$ and $g(\sqrt{n}) = O(1)$. This yields that

$$\max_{\sqrt{2n} \leq i \leq n} h(i,j_0) \leq \sup_{\sqrt{2} \leq \alpha \leq \sqrt{n}} [-2g(\alpha) - 2n] \leq -2n + O(\sqrt{n}).$$

Case IIb: $i \geq 3$, $j = 1$. Here we have that

$$\frac{[\widetilde{K}d]((i,1),(i,0))}{d(i,0)} - 1 \quad = \quad -\frac{1}{4n(n-1)}\frac{2(i-1)n + 2 - i^2 + i^3}{i+1} \leq -\frac{n+5}{4n(n-1)},$$

for all $3 \leq i \leq n$.

Cases IIc: $i = 2$, $j = 1$ and $i = 1$, $j = 1$.

Here we compute

$$\frac{[\widetilde{K}d]((2,1),(2,0))}{d(2,0)} - 1 = -\frac{1}{3(n-1)}$$

and

$$\frac{[\widetilde{K}d]((1,1),(1,0))}{d(1,0)} - 1 = -\frac{1}{5(n-1)} - \frac{3}{5n(n-1)}.$$

Case IId: $i = 1$, $j \geq 2$.

$$\begin{aligned}\frac{[\widetilde{K}d]((1,j),(1,j-1))}{d(1,j-1)} - 1 &= -\frac{1}{2n(n-1)}\frac{(j-1)n + 4j^2 + 3j - 1}{j+1} \\ &\leq -\frac{1}{6(n-1)} - \frac{7}{2n(n-1)}.\end{aligned}$$

□

This finishes the analysis of the spectral gap in part A.

Let us now turn to part B, that is the case where for every eigenfunction f to the second largest eigenvalue of Q there are $x, y \in X$ with $n(x) = n(y)$ but $f(x) \neq f(y)$. Let us first consider the case where these x and y, although having the same signature $n(\cdot)$ contain a different number of 1's, say x has more 1's than y. Then there must also exist x and y with the above properties such that x contains exactly one more 1 than y does (otherwise f would be constant on such x and y). Finally, by permutation we may assume that these x and y are such that $x = (1, x_2, x_3, \ldots, x_n)$ and $y = (3, x_2, x_3, \ldots, x_n)$.
For such pairs (x, y) as described above we define a rather obvious coupling. Without loss of generality we assume that $x = (1, x_2, \ldots, x_n)$, and $y = (3, y_2 \ldots y_n)$ with $x_j = y_j$ for $j \geq 2$. We define the coupling $\widetilde{Q}$ by

$$\begin{aligned}\widetilde{Q}((x,y),[(2,x_2\ldots x_n),(2,y_2\ldots y_n)]) &:= \frac{i-1}{2n(n-1)} \\ \widetilde{Q}((x,y),[(0,x_2\ldots x_n),(0,y_2\ldots y_n)]) &:= \frac{i-1}{2n(n-1)} \\ \widetilde{Q}((x,y),(x',y')) &:= Q(x,x') = Q(y,y'),\end{aligned}$$

where (x', y') satisfy the same conditions as (x, y), that is there is a uniqe i such that $(x'_i, y'_i) \in \{(1,3),(3,1)\}$.
For fixed $c \in]0,1[$ we define a distance d on pairs x, y with $n_1(x) = n_1(y)$ as follows

$$d(x,y) = \prod_{j=1}^{cn-n_1(x)} (1 + j/n)\,.$$

Since d actually depends on the number of 1's and 3's only we may write $d(x, y) = d(n_1(x))$.

Let us now see that the coupling $\widetilde{Q}$ contracts the function d. First consider the case that $2 \leq n_1(x) \leq cn - 1$.

$$\begin{aligned}\left[\widetilde{Q}d\right](x,y) &= \frac{(i-1)^2}{n(n-1)}d(i-1) + \frac{i(n-i)}{n(n-1)}d(i+1) \\ &\quad + \left[1 - \frac{(i-1)^2}{n(n-1)} - \frac{i(n-i)}{n(n-1)}\right] d(i).\end{aligned}$$

Note that we have used that with probability $(i-1)/[n(n-1)]$ the pair x, y hits the diagonal and d is zero in this case. Multiplying by $n(n-1)/d(i)$ and subtracting 1 gives

$$\frac{n(n-1)}{d(i)}\left[\widetilde{Q}d\right](x,y)-1 = (i-1)^2\frac{d(i-1)}{d(i)}+i(n-i)\frac{d(i+1)}{d(i)} + \left[-(i-1)^2-i(n-i)\right].$$

Note that

$$\frac{d(i-1)}{d(i)} = 1+(cn-i+1)/n$$

and

$$\frac{d(i+1)}{d(i)} = 1/[1+(cn-i)/n].$$

Setting $c=1/10$ we arrive at

$$\frac{n(n-1)}{d(i)}\left[\widetilde{Q}d\right](x,y)-1 = \frac{1}{10n(11n-10i)}\left(121i^2n^2-220i^3n+100i^4-10in^3+450i^2n-300i^3-132in^2\right) +\mathcal{O}(1)$$

Consider the function

$$f := i\mapsto (121i^2n^2-220i^3n+100i^4-10in^3+450i^2n-300i^3-132in^2.$$

A simple observation shows that f is a convex function on the interval $[2,n/10]$. Thus h is maximal at the interval points. This yields using that $h(n/10-1)=-17n^3+\mathcal{O}(n^2)$, $h(2)=-20n^3+\mathcal{O}(n^2)$ and $11n-10i\geq 10n$ for $2\leq i\leq n/10$,

$$\frac{n(n-1)}{d(i)}\left[\widetilde{Q}d\right](x,y)-1 \leq -\frac{17}{100}n+\mathcal{O}(1).$$

Let us now turn to the borderline cases: If $n_1(x)=1$, a straightforward calculation shows that

$$\frac{n(n-1)}{d(1)}\left[\widetilde{Q}d\right](x,y)-1 \leq -\frac{1}{11}n+\mathcal{O}(1).$$

For $n_1(x)=n/10$ we quickly check that

$$\frac{n(n-1)}{d(n/10)}\left[\widetilde{Q}d\right](x,y)-1 \leq -\frac{9}{100}n+\mathcal{O}(1).$$

If finally $n_1(x)\geq n/10+1$, we obtain

$$\frac{n(n-1)}{d(i)}\left[\widetilde{Q}d\right](x,y)-1 = 1-\frac{i-1}{n(n-1)}\leq 1-\frac{1}{10n}+\mathcal{O}(n^{-2}).$$

The considerations show that in the situation described above the spectral gap $\lambda_1(Q)$ is bounded from below by $\frac{1}{11n}$.

It remains to show what happens if for each eigenfunction f to β_1 there exists $x,y\in X$ with $n(x)=n(y)$, $f(x)\neq n(y)$, and x and y contain the same number of 1's. Obviously then y is nothing but a permutation of x. As we decompose any permutation into a number of transpositions, there also have to be x and y with the above properties such that x differs from y by a transposition of two coordinates (without loss of generality the first two), only. We distinguish four different cases

Case I: $x = (03\,*)$, $y = (30\,*)$
Case II: $x = (31\,*)$, $y = (13\,*)$
Case III: $x = (02\,*)$, $y = (20\,*)$
Case IV: $x = (12\,*)$, $y = (21\,*)$.

Here $*$ indicates that the configurations x and y agree in the third to n'th coordinate. The other two cases $x = (23\,*)$, $y = (32\,*)$, and $x = (01\,*)$, $y = (10\,*)$ do not need a special consideration here, since the rôles of 1 and 3 are completely identical.

The treatment of the different cases is somewhat technical, but not at all complicated. It basically consists of coming up with an appropriate distance function and a coupling and showing that the distance is contracted by the coupling by a factor $1 - \frac{const}{n}$. As indeed the calculations are very similar in all of the four cases, we will only show them in detail in one case and in the other cases limit ourselves to presenting the coupling, the distance, and the results.

In all four cases we will use the same distance function

$$d(x, y) := d(n(x)) := \prod_{r=1}^{\frac{1}{6}n-n_1(x)} \theta(r) \prod_{r=1}^{\frac{1}{6}n-n_2(x)} \theta(r)$$

where

$$\theta(r) = \frac{n-6r}{n} + \frac{4}{21}\frac{r}{n}.$$

The idea behind this choice of the distance function is the following. In all four cases there is a natural coupling bewtween the Markov chain starting in x and the one starting in y. As, first theses couplings may leave a certain case and enter another one, but never leave the set of x and y's with $n(x) = n(y)$, the distance function $d(x, y)$ is reasonably defined. Second, these natural couplings only work well, in the sense that they bring the chains together with probability of order $\frac{1}{n}$ if there are enough 1's, 3's, and 2's. Luckily with a large number of zeros the tendency of creating new 1's, 3's, and 2's dominates the tendency of their elimination. The distance d takes account of this creation phenomenon. The constants $\frac{1}{6}$ and $\frac{4}{21}$ in the definition of d are somehow arbitrarily taken from a small intervall of possible parameters. Their only justification is that they work.

Let us now turn to the analysis of the different cases.

Case I: $x = (03\,*)$**,** $y = (30\,*)$ Here we couple the Markov chain starting in x to the chain starting in y in the following way. Recall, that the transition mechanism in principle is to take random indices i and j and then to replace x_j by $x_i x_j$ with probability 1/2 and by $x_i x_j^{-1}$ with probability 1/2.

So, if the walk in x "proposes" to replace x_j by $x_i x_j$ or by $x_i x_j^{-1}$ with $i, j \geq 3$ the walk in y will do the same. If $i = 1$ and $j \geq 3$ for the walk in x , the walk in y takes $i = 2$ and the same j and then does the same as the x-walk does. Vice versa, if $i = 2$ and $j \geq 3$ for the walk in x, the walk in y takes $i = 1$ and the same j and again does the same. If finally the x-walk chooses $j = 1$ (or $j = 2$, resp.) and any i, then the walk in y will choose $j = 2$ (or $j = 1$, resp.) and the same i and then do the same as the x-walk does. Note that in the last case the two walks actually might meet, namely when the 3 in the second component of x is met by a one (and the same holds true for the 3 in the first component of y).

Also notice that the coupling – let us call it $\overline{Q}$ – might actually leave Case I and enter, for example, Case IV (which doesn't matter since the distance function there is the same), but it will never leave the set of x and y which can be obtained by a transposition form each other.

By the definition of $\overline{Q}$ and the distance d

$$\frac{2n(n-1)}{d(x,y)}\Big([\overline{Q}d](x,y) - d(x,y)\Big) \tag{6}$$

$$= -\frac{1}{28n(4n-3k)(4n-3l)}\Big(864nkl^2 - 579n^2kl + 192n^2k^2l - 288nk^3l + 1056n^2kl^2 - 828nkl^3 - 252nk^2l^2 + 468nk^2l - 196n^3kl - 324k^3l + 684nk^3 + 108k^4l + 484n^3k \tag{7}$$

$$\tag{8}$$

VEREINFACHUNG

HALLO MATTHIAS! Hier geht die neue Vereinfachung los, die jetzt auch die anderen 3 Fälle x=(12..) y=(21..) usw. (siehe unten) abhandelt:

Next we consider the cases that x and y having Hamming distance 2 look as follows

i) $x = (12x_3 \dots x_n)$, $y = (21y_3 \dots y_n)$,
ii) $x = (01x_3 \dots x_n)$, $y = (10y_3 \dots y_n)$,
iii) $x = (02x_3 \dots x_n)$, $y = (20y_3 \dots y_n)$,

where in each of these cases $x_i = y_i$ for $i \geq 3$.
The distance for x, y such that $n(x) = (i,j)$, $n(y) = (i,j)$ is defined by

$$d(x,y) = \begin{cases} \frac{1}{i} & : \text{ for } x,y \text{ as in cases } i) \text{ and } ii) \\ \frac{1}{i} + \frac{2}{3n} & : \text{ for } x,y \text{ as in case } iii). \end{cases}$$

The coupling that we use is the very natural one. The Hamming distance keeps the value 2 until the two particles meet.
For all three cases we need to show that there is a contraction, i.e. for $\widetilde{Q}$ denoting the coupling kernel,

$$[\widetilde{Q}d](x,y) \leq (1-\alpha)d(x,y),$$

for all x, y as in $i) - iii)$ for some $\alpha > 0$. Transforming the equation from above we have to show that

$$\Big[[\widetilde{Q}d](x,y) - d(x,y)\Big] / d(x,y) \leq -\alpha.$$

We define $d_1(i,j) = 1/i$ and $d_2(i,j) = 1/i + 2/(3n)$. Thus for $n(x) = n(y) = (i,j)$ we have

$$d(x,y) = \begin{cases} d_1(i,j) & : \text{ for } x,y \text{ as in cases } i) \text{ and } ii) \\ d_2(i,j) & : \text{ for } x,y \text{ as in case } iii). \end{cases}$$

Case i). $x = (12...)$, $y = (21...)$. The term of interest is given by

$$
\begin{aligned}
f_1(i,j) \; := \; & \Big[(n-i-j)id_1(i+1,j) + (n-i-j)jd_1(i,j+1) + (i-1)^2/2d_1(i-1,j) \\
& +(i-1)/2d_2(i-1,j) + j(j-1)d(i,j-1) + i(j-1)d(i+1,j-1) \\
& (i-1)^2/2d_1(i-1,j+1) + ijd_1(i,j) - (i+j)(n-1)d_1(i,j)\Big]/d_1(i,j) \qquad (9) \\
= \; & \frac{1}{6}\frac{(2i^2+3in-6n^2-2+3n)i}{n(i+1)} \\
\leq \; & \frac{-n}{6}\frac{i}{i+1} \leq -\frac{n}{12}.
\end{aligned}
$$

Here are more details for (9). 1st summand: 1 or 3 is added to a zero component with prob. $i(n-i-j)/(2n(n-1)$.
2nd summand: 2 is added to zero component 3rd summand: 1 or 3 is added to a 1 or 3 (except the component x_1 resp. y_2) such that the new component is zero.
4th summand: 1 or 3 is added to the first component x_1 resp. y_2 such that we get to case iii).
5th summand: 2 is added to another 2.
6th summand: 1 is added to a component 2 except the component $x_2 = 2$, $y_1 = 2$. (if we add 1 to the component $x_2 = 2$, $y_1 = 2$ we are done by the previous case: DAS IST UNSERE 1. VEREINFACHUNG).
7th summand: 1 or 3 is added to a 1 or 3 (except the component $x_1 = 2$, $y_2 = 1$) to give a 2 component
8th summand: 2 is added to a 1 or 3. 9th summand: results from the transformation shown above.

Case ii). $x = (01...)$, $y = (10...)$. The term of interest is given by

$$
\begin{aligned}
f_2(i,j) \; := \; & \Big[(n-i-j-1)id_1(i+1,j) + (n-i-j)jd_1(i,j+1) + (i-1)^2/2d_1(i-1,j) \\
& +j(j-1)d(i,j-1) + ijd(i+1,j-1) \\
& (i-1)^2/2d_1(i-1,j+1) + (i-1)/2d_2(i-1,j+1) \\
& +ijd_1(i,j) - (i+j)(n-1)d_1(i,j)\Big]/d_1(i,j) \\
= \; & \frac{1}{6}\frac{(2i^2+3in-6n^2-2+3n)i}{n(i+1)} \\
(10) \quad \leq \; & \frac{-n}{6}\frac{i}{i+1} \leq -\frac{n}{12}.
\end{aligned}
$$

In case ii) we get exactly the same term as in case i).

Case $iii)$. $x = (02...)$, $y = (20...)$. The term of interest is given by

$$\begin{aligned}
f_3(i,j) \;&:=\; \Big[(n-i-j-1)id_2(i+1,j) + id_1(i+1,j) \\
&\quad +(n-i-j-1)jd_2(i,j+1) + i(i-1)/2d_2(i-1,j) \\
&\quad +(j-1)^2 d_2(i,j-1) + i(j-1)d_2(i+1,j-1) \\
&\quad +id_1(i+1,j-1) + +i(i-1)/2d_2(i-1,j+1) + ijd_2(i,j) \\
&\quad -(i+j)(n-1)d_2(i,j)\Big]/d_2(i,j) \\
&= \; -\frac{4i^3 - 6i^2 n + 4i^2 j + 2i^2 + 3in^2 + 6ijn - 2i - 6in + 4ij - 3n + 6jn}{(i+1)(3n+2i)}.
\end{aligned}$$

We show that the function

$$h(i,j) := \frac{4i^3 - 6i^2 n + 4i^2 j + 3in^2 + 6ijn}{(i+1)(3n+2i)}$$

is positive of order n for $1 \leq i \leq n$, $0 \leq j \leq n$. More precisely assume that we would know that $h(i,j) \geq cn$ where c is a positive constant. Then we have

$$f_3(i,j) \leq -cn + \mathcal{O}(1).$$

The derivate of the function $j \mapsto h(i,j)$, i fixed, is given by $2i/(i+1)$. Thus $j \mapsto h(i,j)$ is increasing in j for each i. Thus for each i, $h(i,j)$ is smallest for $j = 1$. We thus arrive at

$$h(i,j) \geq h(i,1) = \frac{i(4i^2 - 6in + 4i + 6n + 3n^2)}{(i+1)(3n+2i)}.$$

Since $1/2 \leq i/(i+1) \leq 1$ we neglect the factor $i/(i+1)$. The function

$$i \mapsto \frac{4i^2 - 6in + 4i + 6n + 3n^2}{3n + 2i}$$

is minimal for $i_0 = -3/2n + 1/2\sqrt{21}n$. We obtain

$$\begin{aligned}
h(i_0,1) \;&=\; -\frac{n(15\sqrt{21}n - 69n - 2\sqrt{21} + 6)}{-3n + \sqrt{21}n + 2} \\
&\approx\; -n\frac{-0,2614n - 2\sqrt{21} + 6}{1,5826n + 2} \approx 0,16n + \mathcal{O}(1).
\end{aligned}$$