

## $L_2$ DISCREPANCY OF LINEARLY DIGIT SCRAMBLED ZAREMBA POINT SETS

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ABSTRACT. We give an exact formula for the  $L_2$  discrepancy of a class of generalized two-dimensional Hammersley point sets in base  $b$ , namely generalized Zaremba point sets. For the construction of such point sets one needs sequences of permutations of the form  $\pi_l(k) = \alpha k + l \pmod{b}$  for  $k, l \in \{0, \dots, b-1\}$ . As a corollary we obtain a condition on these sequences which yields the best possible order of  $L_2$  discrepancy of generalized Zaremba point sets in the sense of Roth's lower bound, with very small leading constants.

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### 1. Introduction

For a point set  $\mathcal{P} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$  of  $N \geq 1$  points in the unit-square  $[0, 1]^2$  the  $L_2$  discrepancy is defined by

$$L_2(\mathcal{P}) := \left( \int_0^1 \int_0^1 |E(x; y; \mathcal{P})|^2 dx dy \right)^{1/2},$$

where the so-called *discrepancy function* is given by  $E(x; y; \mathcal{P}) = A([0, x) \times [0, y); N; \mathcal{P}) - Nxy$ , where  $A([0, x) \times [0, y); N; \mathcal{P})$  denotes the number of indices  $1 \leq M \leq N$  for which  $\mathbf{x}_M \in [0, x) \times [0, y)$ . The  $L_2$  discrepancy is a quantitative measure for the irregularity of distribution of  $\mathcal{P}$ , i.e., the deviation from ideal uniform distribution. See [5, 6, 16, 18, 19, 20] for more information on  $L_2$  discrepancy and its relation to numerical integration.

The asymptotic behavior of the minimal possible  $L_2$  discrepancy of an  $N$ -element point set as  $N$  tends to infinity is well-known. It was first shown by

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Roth [23] that there is a constant  $c > 0$  with the following property: for any  $N \in \mathbb{N}$  and for any  $N$ -element point set  $\mathcal{P}$  in  $[0, 1)^2$  we have

$$L_2(\mathcal{P}) \geq c\sqrt{\log N}. \quad (1)$$

On the other hand it is known that there is a constant  $C > 0$  such that for all  $N \in \mathbb{N}$ ,  $N \geq 2$ , there exists an  $N$ -element point set  $\mathcal{P}$  in  $[0, 1)^2$  with

$$L_2(\mathcal{P}) \leq C\sqrt{\log N} + O(1). \quad (2)$$

Today a lot of explicit constructions of point sets are known which achieve an upper bound of the form (2); see, for example, [1, 4, 9, 10, 11, 12, 13, 15, 17, 22, 25] and [2, 3, 5] for corresponding results in arbitrary dimension  $s \geq 2$ .

If one is interested in the constants  $c$  and  $C$  in (1) and (2) for large  $N$  it is advisable to study the constants  $\underline{c}$  and  $\bar{c}$  defined as

$$\underline{c} := \liminf_{N \rightarrow \infty} \inf_{\substack{\mathcal{P} \subset [0, 1)^s \\ \#\mathcal{P} = N}} \frac{L_2(\mathcal{P})}{\sqrt{\log N}} \quad \text{and} \quad \bar{c} := \limsup_{N \rightarrow \infty} \inf_{\substack{\mathcal{P} \subset [0, 1)^s \\ \#\mathcal{P} = N}} \frac{L_2(\mathcal{P})}{\sqrt{\log N}}.$$

In [14] it is shown that (1) holds with  $c = 7/(216\sqrt{\log 2}) = 0.038925\dots$ . Furthermore, a construction presented in [12] shows that (2) holds with  $C = 0.17907\dots$  for infinitely many  $N$ . Therefore the best estimates for  $\underline{c}$  and  $\bar{c}$  known so far are

$$0.038925\dots \leq \underline{c} \leq \bar{c} \leq 0.17907\dots \quad (3)$$

The value  $C = 0.17907\dots$  can be achieved with so-called generalized Hammersley point sets whose definition will be presented now.

Throughout the paper the base  $b \geq 2$  is an integer and  $\mathfrak{S}_b$  is the set of all permutations of  $\{0, \dots, b-1\}$ .

**DEFINITION 1** (generalized Hammersley point set). Let  $b \geq 2$  and  $n \geq 1$  be integers and let  $\Sigma = (\sigma_0, \dots, \sigma_{n-1}) \in \mathfrak{S}_b^n$ . For an integer  $1 \leq N \leq b^n$ , write  $N-1 = \sum_{r=0}^{n-1} a_r(N)b^r$  in the  $b$ -adic system and define  $S_b^\Sigma(N) := \sum_{r=0}^{n-1} \sigma_r(a_r(N))b^{-r-1}$ . Then the *generalized two-dimensional Hammersley point set in base  $b$*  consisting of  $b^n$  points associated to  $\Sigma$  is defined by

$$\mathcal{H}_{b,n}^\Sigma := \left\{ \left( S_b^\Sigma(N), \frac{N-1}{b^n} \right) : 1 \leq N \leq b^n \right\}.$$

If we choose in the above definition  $\sigma_i = \text{id}$  — the identity in  $\mathfrak{S}_b$  — for all  $i \in \{0, \dots, n-1\}$ , then we obtain the classical two-dimensional Hammersley point set in base  $b$ .

A lot of sequences of permutations  $\Sigma = (\sigma_0, \dots, \sigma_{n-1}) \in \mathfrak{S}_b^n$  are known which achieve an order  $O(\sqrt{\log N})$  for the  $L_2$  discrepancy of  $\mathcal{H}_{b,n}^\Sigma$ , see [9, 10, 11, 12, 15, 25] and the references therein.

Here we deal with sequences of permutations of the following form: for  $\sigma \in \mathfrak{S}_b$  and  $l \in \{0, \dots, b-1\}$  let  $\sigma_l(k) := \sigma(k) + l \pmod{b}$  for all  $k \in \{0, \dots, b-1\}$ . We call  $\sigma_l$  the *shifted permutation  $\sigma$  with shift  $l$* .

**DEFINITION 2** (generalized Zaremba point set). Let  $\sigma \in \mathfrak{S}_b$ . A generalized Hammersley point set  $\mathcal{H}_{b,n}^\Sigma$  where  $\Sigma \in \{\sigma_l : 0 \leq l < b\}^n$  is called a *generalized Zaremba point set*.

This terminology goes back to White [25] who considered sequences  $\Sigma$  of the form

$$(\text{id}_0, \text{id}_1, \dots, \text{id}_{b-1}, \text{id}_0, \text{id}_1, \dots, \text{id}_{b-1}, \dots) \quad (4)$$

of length  $n$  and who gave an exact formula for the  $L_2$  discrepancy of the corresponding generalized Hammersley point set, which he named *Zaremba point set*. This result is generalized in [11] to arbitrary sequences  $\Sigma \in \{\text{id}_l : 0 \leq l < b\}^n$ . The main result in [11] states that

$$(L_2(\mathcal{H}_{b,n}^\Sigma))^2 = n \frac{(b^2 - 1)(3b^2 + 13)}{720b^2} + O(1) \quad (5)$$

whenever the permutations  $\text{id}_l$  for  $0 \leq l < b$  appear with the same frequency in the sequence  $\Sigma$ . It is interesting that the specific order of the  $\text{id}_l$ 's is of no importance contrary to (4). This observation was already made in [15].

It is the aim of this paper to generalize the results from [11] to sequences of permutations  $\Sigma$  belonging to  $\{\pi_l : 0 \leq l < b\}^n$ , where  $\pi$  is a linear permutation in  $\mathfrak{S}_b$ , i.e., of the form  $\pi(k) = \alpha k \pmod{b}$  for some  $\alpha \in \{1, \dots, b-1\}$  with  $\gcd(\alpha, b) = 1$ . This generalization allows a drastic improvement of the leading factor  $\frac{(b^2-1)(3b^2+13)}{720b^2}$  in Formula (5).

Doing so, we continue to explore the  $L_2$  discrepancy of various classes of Hammersley point sets with the help of an exact formula for the discrepancy function first used in [9] and then in [10, 11, 12] (see Lemma 3 below). Apart from number theory, permutations  $\pi_l$  are of interest since they are widely used in quasi-Monte Carlo methods under the name *linear digit scramblings*, to improve Halton sequences and  $(0, s)$ -sequences (so-called Faure sequences); see for instance [8, 18].

The paper is organized as follows. In Section 2 we present the main results of the paper and in Section 3 we provide some auxiliary results which are necessary for the proofs in Section 4. We close this introductory section with some notations which are used throughout the paper.

**Basic Notations.** The analysis of the  $L_2$  discrepancy is based on special functions which have been first introduced by Faure [7] and which are defined as follows:

For  $\sigma \in \mathfrak{S}_b$  let  $\mathcal{Z}_b^\sigma = (\sigma(0)/b, \sigma(1)/b, \dots, \sigma(b-1)/b)$ . For  $h \in \{0, 1, \dots, b-1\}$  and  $x \in [(k-1)/b, k/b)$ , where  $k \in \{1, \dots, b\}$ , we define

$$\varphi_{b,h}^\sigma(x) = \begin{cases} A([0, h/b); k; \mathcal{Z}_b^\sigma) - hx & \text{if } 0 \leq h \leq \sigma(k-1), \\ (b-h)x - A([h/b, 1); k; \mathcal{Z}_b^\sigma) & \text{if } \sigma(k-1) < h < b, \end{cases}$$

where here for a sequence  $X = (x_M)_{M \geq 1}$  we denote by  $A(I; k; X)$  the number of indices  $1 \leq M \leq k$  such that  $x_M \in I$ . Further, the function  $\varphi_{b,h}^\sigma$  is extended to the reals by periodicity. Note that  $\varphi_{b,0}^\sigma = 0$  for any  $\sigma$  and that  $\varphi_{b,h}^\sigma(0) = 0$  for any  $\sigma \in \mathfrak{S}_b$  and any  $0 \leq h < b$ .

For  $r \in \mathbb{N}$  define  $\varphi_b^{\sigma, (r)} := \sum_{h=0}^{b-1} (\varphi_{b,h}^\sigma)^r$  and we simply write  $\varphi_b^\sigma := \varphi_b^{\sigma, (1)}$ . Note that  $\varphi_b^\sigma$  is continuous (see [1, Propriété 3.3] and [7, Propriété 3.2.2]), piecewise linear on the intervals  $[k/b, (k+1)/b)$  and  $\varphi_b^\sigma(0) = \varphi_b^\sigma(1)$ .

Further, for our purpose, we will need the integrals  $\Phi_b^\sigma := (1/b) \int_0^1 \varphi_b^\sigma(x) dx$  and  $\Phi_b^{\sigma, (2)} := (1/b) \int_0^1 \varphi_b^{\sigma, (2)}(x) dx$ .

## 2. The results

First we state a generalization of [11, Theorem 1] and of [15, Theorem 1].

**PROPOSITION 1.** *Let  $\pi \in \mathfrak{S}_b$  be linear and let  $\Sigma = (\sigma_0, \dots, \sigma_{n-1}) \in \{\pi_l : 0 \leq l < b\}^n$ . For  $0 \leq l < b$  define  $\lambda_l := \#\{0 \leq i < n : \sigma_i = \pi_l\}$ . Then we have*

$$\begin{aligned} (L_2(\mathcal{H}_{b,n}^\Sigma))^2 &= \left( \sum_{l=0}^{b-1} \lambda_l \Phi_b^{\pi_l} \right)^2 + n \Phi_b^{\pi, (2)} + \sum_{l=0}^{b-1} \lambda_l \Phi_b^{\pi_l} \\ &\quad + \sum_{l=0}^{b-1} \frac{\lambda_l}{b} \left[ \varphi_b^{\pi, (2)} \left( \frac{\pi^{-1}(l)}{b} \right) - 2F_b^\pi(l) - b(\Phi_b^{\pi_l})^2 \right] + O(1), \end{aligned}$$

where  $F_b^\pi(l) := (1/b) \sum_{h,j=0}^{b-1} \varphi_{b,h}^\pi(\pi^{-1}(l)/b) \varphi_{b,h}^\pi(j/b)$ .

The proof of this result will be presented in Section 4. Although the idea for the proof is the same as for  $\pi = \text{id}$  in [11], the proof is much more sophisticated and a lot of technical difficulties must be overcome before to reach the proposed formula. A short outline is given below, just before Lemma 4.

The following result provides a choice of  $\Sigma$  which yields the best possible order of  $L_2$  discrepancy with respect to Roth's lower bound (1). This result generalizes [11, Corollary 1] (see formula (5)).

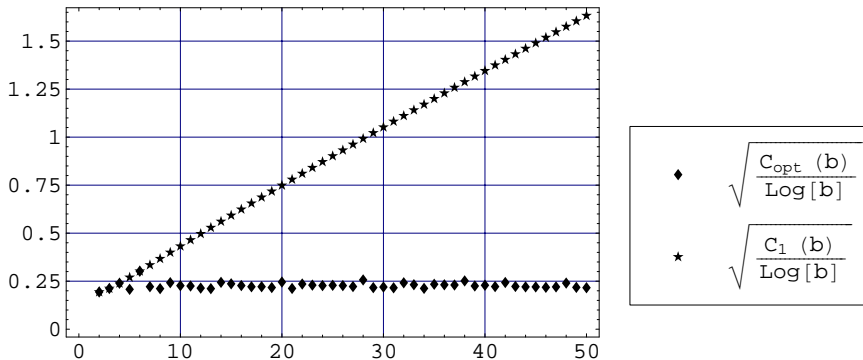


FIGURE 1. Comparison of  $\sqrt{C_{\text{opt}}(b)/\log b}$  and  $\sqrt{C_1(b)/\log b}$  for  $b = 2, \dots, 50$ .

**THEOREM 1.** *Let  $\pi \in \mathfrak{S}_b$  be linear and let  $\Sigma \in \{\pi_l : 0 \leq l < b\}^n$  be such that  $\lambda_l = \lfloor n/b \rfloor + \theta_l$  with  $\theta_l \in \{0, 1\}$  for all  $0 \leq l < b$ . Then we have*

$$(L_2(\mathcal{H}_{b,n}^\Sigma))^2 = n(\Phi_b^{\pi, (2)} - (\Phi_b^\pi)^2) + O(1).$$

Thus we obtain the optimal order  $O(\sqrt{n})$  for the  $L_2$  discrepancy of  $\mathcal{H}_{b,n}^\Sigma$  whenever the permutations  $\pi_l$  for  $0 \leq l < b$  appear with the same frequency in the sequence  $\Sigma$ , independently of the specific order of the  $\pi_l$ 's.

The result of Theorem 1 yields a drastic improvement of [11, Corollary 1] (see formula (5)) when we use the “optimal” linear permutation  $\pi(k) = \alpha k \pmod{b}$  instead of  $\pi(k) = \text{id}$  (i.e.  $\alpha = 1$ ). For  $\alpha = 1$  we have  $\Phi_b^{\pi, (2)} - (\Phi_b^\pi)^2 = \frac{(b^2-1)(3b^2+13)}{720b^2} =: C_1(b)$ . Let now  $C_{\text{opt}}(b) := \min\{\Phi_b^{\pi, (2)} - (\Phi_b^\pi)^2 : 1 \leq \alpha < b \text{ and } \gcd(\alpha, b) = 1\}$ . Using results from [12] the value  $\Phi_b^{\pi, (2)} - (\Phi_b^\pi)^2$  for a given permutation  $\pi$  can easily be calculated, for example with MATHEMATICA. A comparison of the two quantities  $C_{\text{opt}}(b)$  and  $C_1(b)$  for  $b = 2, \dots, 50$  can be found in Figure 1. To compare the result also with the constants  $\underline{c}$  and  $\bar{c}$  from (3) we plot  $\sqrt{C_{\text{opt}}(b)/\log b}$  and  $\sqrt{C_1(b)/\log b}$ , respectively. Notice that the constants  $C_{\text{opt}}(b)$  are very close to the analogous constants in [12], even though a bit larger.

In Theorem 1 we require  $b$  permutations to obtain the optimal order of  $L_2$  discrepancy. The following result shows that the optimal order can be obtained with only one permutation.

**THEOREM 2.** *If  $b \in \mathbb{N}$ ,  $b \geq 2$ ,  $\alpha \in \{1, \dots, b-1\}$  with  $\gcd(\alpha, b) = 1$  and  $l \in \{0, \dots, b-1\}$  are chosen such that  $\Phi_b^{\pi_l} = 0$ , then with  $\Sigma = (\pi_l, \dots, \pi_l)$  we have  $L_2(\mathcal{H}_{b,n}^\Sigma) = O(\sqrt{n})$ .*

For  $\alpha = 1$  there exist infinitely many  $b \geq 2$  and corresponding  $l$  such that  $\Phi_b^{\pi_l} = \Phi_b^{\text{id}_l} = 0$ ; see [10, Corollary 1] for a necessary and sufficient condition. Many further examples of  $(b, \alpha, l)$  for which  $\Phi_b^{\pi_l} = 0$  can be found numerically, for example using MATHEMATICA. Until now we were not able to give a characterization of those  $(b, \alpha, l)$  which yield  $\Phi_b^{\pi_l} = 0$ . Finding such a characterization remains open for the moment.

### 3. Auxiliary results

In this section we provide the main tools for the proof of Proposition 1. For the sake of completeness, we give short hints for the proofs of lemmas concerned with shifts and already proved in [10].

For  $\sigma = \text{id}$ , the identity in  $\mathfrak{S}_b$ , we have

$$\varphi_{b,h}^{\text{id}}(x) = \begin{cases} (b-h)x & \text{if } x \in [0, h/b], \\ h(1-x) & \text{if } x \in [h/b, 1], \end{cases} \quad (6)$$

from which one obtains (see [9, Lemma 3] for details) that for  $x \in [\frac{k}{b}, \frac{k+1}{b}]$ ,  $0 \leq k < b$ , we have

$$\varphi_b^{\text{id}}(x) = \frac{b(b-2k-1)}{2} \left(x - \frac{k}{b}\right) + \frac{k(b-k)}{2}. \quad (7)$$

Considering shifts of general permutations, we will need extensions of formulas (6) and (7). First, recall from [1, Propriété 3.4] that

$$(\varphi_{b,h}^\sigma)'(k/b+0) = (\varphi_{b,h}^{\text{id}})'(\sigma(k)/b+0). \quad (8)$$

(Here and later on by  $f'(x+0)$  we mean the right-derivative of the function  $f$  at  $x$ .) Then, using that the functions  $\varphi_{b,h}^\sigma$  are continuous and piecewise linear, it is easy to see that

$$\varphi_{b,h}^\sigma(l/b) = (1/b) \sum_{k=0}^{l-1} (\varphi_{b,h}^\sigma)'(k/b+0), \quad (9)$$

from which we deduce  $\varphi_b^\sigma(l/b) = (1/b) \sum_{k=0}^{l-1} (\varphi_b^\sigma)'(k/b+0)$ , and, using (8) and (6),

$$\varphi_b^\sigma\left(\frac{l}{b}\right) = l \frac{b-1}{2} - \sum_{i=0}^{l-1} \sigma(i). \quad (10)$$

These two last properties were proved directly in [1, Propriété 3.5 (i)]. Since  $\varphi_b^\sigma$  is linear on intervals  $[l/b, (l+1)/b]$  we obtain from (10) that for all  $x \in [l/b, (l+1)/b]$  we have

$$\varphi_b^\sigma(x) = b \frac{b - 2\sigma(l) - 1}{2} \left(x - \frac{l}{b}\right) + l \frac{b-1}{2} - \sum_{i=0}^{l-1} \sigma(i). \quad (11)$$

In [12, Lemma 5] it has been shown that

$$\Phi_b^\sigma = \frac{1}{b^2} \left( \sum_{i=0}^{b-1} \sigma(i)i - b \left(\frac{b-1}{2}\right)^2 \right). \quad (12)$$

In the following we assume that  $\pi \in \mathfrak{S}_b$  is linear, i.e.,  $\pi(k) = \alpha k \pmod{b}$  for some  $\alpha \in \{1, \dots, b-1\}$  with  $\gcd(\alpha, b) = 1$ . In this case we have that  $\pi^{-1}$  is linear as well, that  $\pi^{-1}(l + \pi(k)) = \pi^{-1}(l) + k \pmod{b}$  and that  $(\pi_l)^{-1} = (\pi^{-1})_{b-\pi^{-1}(l) \pmod{b}}$ .

**LEMMA 1.** *For any  $0 \leq k, l < b$  we have*

$$(\varphi_b^{\pi_l})' \left( \frac{k}{b} + 0 \right) = (\varphi_b^\pi)' \left( \frac{k + \pi^{-1}(l)}{b} + 0 \right).$$

**Proof.** With (8) and with  $\varphi_b^\sigma = \sum_{h=0}^{b-1} \varphi_{b,h}^\sigma$  we obtain

$$\begin{aligned} (\varphi_b^{\pi_l})' \left( \frac{k}{b} + 0 \right) &= (\varphi_b^{\text{id}})' \left( \frac{\pi_l(k)}{b} + 0 \right) = (\varphi_b^{\text{id}})' \left( \frac{\pi(k) + l}{b} + 0 \right) \\ &= (\varphi_b^\pi)' \left( \frac{\pi^{-1}(\pi(k) + l)}{b} + 0 \right) = (\varphi_b^\pi)' \left( \frac{k + \pi^{-1}(l)}{b} + 0 \right). \end{aligned} \quad \square$$

The following lemma gives a relation between the functions  $\varphi_b^\sigma$  and  $\varphi_b^{\sigma_l}$ .

**LEMMA 2.** *For any  $0 \leq l < b$  and  $x \in [0, 1]$  we have*

$$\varphi_b^{\pi_l}(x) = \varphi_b^\pi \left( x + \frac{\pi^{-1}(l)}{b} \right) - \varphi_b^\pi \left( \frac{\pi^{-1}(l)}{b} \right). \quad (13)$$

**Proof.** Both sides of (13) coincide in  $x = 0$ , are continuous and linear on intervals of the form  $[k/b, (k+1)/b]$  and also their right derivatives at  $k/b$ ,  $0 \leq k < b$  coincide by Lemma 1. Hence (13) is a proper equation.  $\square$

**REMARK 1.** For an arbitrary permutation  $\sigma$ , it can be shown by recursion that Lemma 2 becomes: For any  $x \in [\frac{k}{b}, \frac{k+1}{b}]$ ,  $0 \leq k < b$ ,

$$\varphi_b^{\sigma_l}(x) = \varphi_b^\sigma \left( x - k + \frac{\sigma^{-1}(l + \sigma(k))}{b} \right) - B_k,$$

where  $B_k = \sum_{h=0}^k \varphi_b^\sigma \left( \frac{\sigma^{-1}(l + \sigma(h))}{b} \right) - \sum_{h=0}^{k-1} \varphi_b^\sigma \left( \frac{\sigma^{-1}(l + \sigma(h) + 1)}{b} \right)$ . Apart from the interest of linear digit scramblings  $\pi_l$  in applications, the complexity of that formula is a reason for choosing, at first, linear permutations.

The following lemma provides a formula for the discrepancy function of generalized Hammersley point sets.

**LEMMA 3.** For integers  $1 \leq \lambda, N \leq b^n$  we have

$$E \left( \frac{\lambda}{b^n}; \frac{N}{b^n}; \mathcal{H}_{b,n}^\Sigma \right) = \sum_{j=1}^n \varphi_{b,\varepsilon_j}^{\sigma_{j-1}} \left( \frac{N}{b^j} \right),$$

where the  $\varepsilon_j = \varepsilon_j(\lambda, n, N)$  can be given explicitly.

A proof of this result together with formulas for  $\varepsilon_j = \varepsilon_j(\lambda, n, N)$  can be found in [9, Lemma 1].

**REMARK 2.** Let  $0 \leq x, y \leq 1$  be arbitrary. Since all points from  $\mathcal{H}_{b,n}^\Sigma$  have coordinates of the form  $\alpha b^{-n}$  for some  $\alpha \in \{0, 1, \dots, b^n - 1\}$ , we have

$$E(x; y; \mathcal{H}_{b,n}^\Sigma) = E(x(n); y(n); \mathcal{H}_{b,n}^\Sigma) + b^n(x(n)y(n) - xy), \quad (14)$$

where for  $0 \leq x \leq 1$  we define  $x(n) := \min\{\alpha b^{-n} \geq x : \alpha \in \{0, \dots, b^n\}\}$ .

In the following we will give a series of lemmas with further, more involved properties of the functions  $\varphi_{b,h}^\sigma$  and  $\varphi_b^{\sigma,(r)}$  functions. Before going on, as stated in Section 2, we briefly outline the unfolding of the proof of Proposition 1. In Section 4, after the proof of our last lemma (Lemma 8), the proof of Proposition 1 starts with the consideration of the two-dimensional integral involving (14). This term can be easily split into three sums. The first one,  $\Sigma_1$ , is the most important one, with a priori  $n^2$  terms, and needs the whole series of lemmas (excepted Lemma 7 which is required for  $\Sigma_2$ ) culminating in Lemma 8 which can be viewed as a discrete version of Proposition 1. The third sum  $\Sigma_3$  is trivial, but  $\Sigma_2$  has a lot of technical complications which require a careful analysis to be overcome. Nevertheless, the exact computation of  $\Sigma_2$  is necessary in view of Theorem 1, since it contains a priori  $n$  terms. Finally, putting the three sums together yields the result of Proposition 1.



**LEMMA 4.** For  $1 \leq N \leq b^n$ ,  $1 \leq j_1 < \dots < j_k \leq n$  and  $r_1, \dots, r_k \in \mathbb{N}$  we have

$$\sum_{\lambda=1}^{b^n} \prod_{i=1}^k \left( \varphi_{b, \varepsilon_{j_i}}^{\sigma_{j_i-1}} \left( \frac{N}{b^{j_i}} \right) \right)^{r_i} = b^{n-k} \prod_{i=1}^k \varphi_b^{\sigma_{j_i-1}, (r_i)} \left( \frac{N}{b^{j_i}} \right).$$

A proof of this result can be found in [9, Lemma 2].

**LEMMA 5.** For  $0 \leq h, k < n$ ,  $h \neq k$  and  $0 \leq l, m < b$  we have

$$\begin{aligned} & \sum_{N=1}^{b^n} \varphi_b^{\pi_l} \left( \frac{N}{b^h} \right) \varphi_b^{\pi_m} \left( \frac{N}{b^k} \right) \\ &= b^n \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{\pi^{-1}(l)}{b} \right) \right) \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{\pi^{-1}(m)}{b} \right) \right). \end{aligned}$$

*Proof.* We use the abbreviation  $l' = \pi^{-1}(l)$  and  $m' = \pi^{-1}(m)$ . Using Lemma 2 we have

$$\begin{aligned} & \sum_{N=1}^{b^n} \varphi_b^{\pi_l} \left( \frac{N}{b^h} \right) \varphi_b^{\pi_m} \left( \frac{N}{b^k} \right) \\ &= \sum_{N=1}^{b^n} \varphi_b^\pi \left( \frac{N}{b^h} + \frac{l'}{b} \right) \varphi_b^\pi \left( \frac{N}{b^k} + \frac{m'}{b} \right) + b^n \varphi_b^\pi \left( \frac{l'}{b} \right) \varphi_b^\pi \left( \frac{m'}{b} \right) \\ & \quad - \varphi_b^\pi \left( \frac{m'}{b} \right) \sum_{N=1}^{b^n} \varphi_b^\pi \left( \frac{N}{b^h} + \frac{l'}{b} \right) - \varphi_b^\pi \left( \frac{l'}{b} \right) \sum_{N=1}^{b^n} \varphi_b^\pi \left( \frac{N}{b^k} + \frac{m'}{b} \right). \quad (15) \end{aligned}$$

From the periodicity of  $\varphi_b^\pi$  we obtain

$$\begin{aligned} \sum_{N=1}^{b^n} \varphi_b^\pi \left( \frac{N}{b^h} + \frac{l'}{b} \right) &= b^{n-h} \sum_{N=0}^{b^h-1} \varphi_b^\pi \left( \frac{N}{b^h} + \frac{l'}{b} \right) = b^{n-h} \sum_{N=0}^{b^{h-1}-1} \sum_{t=0}^{b-1} \varphi_b^\pi \left( \frac{N}{b^h} + \frac{t}{b} \right) \\ &= b^{n-h} \sum_{N=0}^{b^{h-1}-1} b \int_0^1 \varphi_b^\pi(x) dx = b^{n+1} \Phi_b^\pi, \quad (16) \end{aligned}$$

since for fixed  $0 \leq N < b^{h-1}$  we have  $\sum_{t=0}^{b-1} \varphi_b^\pi \left( \frac{N}{b^h} + \frac{t}{b} \right) = b \int_0^1 \varphi_b^\pi(x) dx$  as shown in [12, Proof of Lemma 4, p. 405].

Without loss of generality we may assume that  $h < k$ . Then we have

$$\sum_{N=1}^{b^n} \varphi_b^\pi \left( \frac{N}{b^h} + \frac{l'}{b} \right) \varphi_b^\pi \left( \frac{N}{b^k} + \frac{m'}{b} \right)$$

$$\begin{aligned}
&= b^{n-k} \sum_{N=0}^{b^k-1} \varphi_b^\pi \left( \frac{N}{b^k} + \frac{l'}{b} \right) \varphi_b^\pi \left( \frac{N}{b^k} + \frac{m'}{b} \right) \\
&= b^{n-k} \sum_{N=0}^{b^{k-1}-1} \varphi_b^\pi \left( \frac{N}{b^k} + \frac{l'}{b} \right) \sum_{t=0}^{b-1} \varphi_b^\pi \left( \frac{N}{b^k} + \frac{t}{b} \right) \\
&= b^{n-k} b \int_0^1 \varphi_b^\pi(x) dx \sum_{N=0}^{b^{k-1}-1} \varphi_b^\pi \left( \frac{N}{b^k} + \frac{l'}{b} \right) \\
&= \int_0^1 \varphi_b^\pi(x) dx \sum_{N=0}^{b^n-1} \varphi_b^\pi \left( \frac{N}{b^k} + \frac{l'}{b} \right) \\
&= b^n \left( \int_0^1 \varphi_b^\pi(x) dx \right)^2 = b^n (b\Phi_b^\pi)^2. \tag{17}
\end{aligned}$$

Now the result follows from inserting (16) and (17) into (15).  $\square$

**LEMMA 6.** For  $1 \leq k \leq n$  we have

$$\sum_{N=1}^{b^n} \varphi_b^{\pi_l, (2)} \left( \frac{N}{b^k} \right) = b^n \left( b\Phi_b^{\pi, (2)} + \frac{b(b^2-1)}{36b^{2k}} + \varphi_b^{\pi, (2)} \left( \frac{\pi^{-1}(l)}{b} \right) - 2F_b^\pi(l) \right),$$

where  $F_b^\pi(l) := (1/b) \sum_{h,j=0}^{b-1} \varphi_{b,h}^\pi(\pi^{-1}(l)/b) \varphi_{b,h}^\pi(j/b)$ .

*Proof.* Again we write  $l' = \pi^{-1}(l)$ . We have

$$\begin{aligned}
\varphi_b^{\pi_l, (2)} \left( \frac{N}{b^k} \right) &= \sum_{h=0}^{b-1} \left( \varphi_{b,h}^{\pi_l} \left( \frac{N}{b^k} \right) \right)^2 = \sum_{h=0}^{b-1} \left( \varphi_{b,h}^\pi \left( \frac{N}{b^k} + \frac{l'}{b} \right) - \varphi_{b,h}^\pi \left( \frac{l'}{b} \right) \right)^2 \\
&= \varphi_b^{\pi, (2)} \left( \frac{N}{b^k} + \frac{l'}{b} \right) + \varphi_b^{\pi, (2)} \left( \frac{l'}{b} \right) - 2 \sum_{h=0}^{b-1} \varphi_{b,h}^\pi \left( \frac{N}{b^k} + \frac{l'}{b} \right) \varphi_{b,h}^\pi \left( \frac{l'}{b} \right).
\end{aligned}$$

By using the periodicity of  $\varphi_b^{\pi, (2)}$  we obtain

$$\sum_{N=1}^{b^n} \varphi_b^{\pi, (2)} \left( \frac{N}{b^k} + \frac{l'}{b} \right) = \sum_{N=1}^{b^n} \varphi_b^{\pi, (2)} \left( \frac{N}{b^k} \right) = b^n \left( b\Phi_b^{\pi, (2)} + \frac{b(b^2-1)}{36b^{2j}} \right),$$

where the last equality is [12, Lemma 4, Equation (8)].

Furthermore we have

$$\sum_{N=1}^{b^n} \sum_{h=0}^{b-1} \varphi_{b,h}^\pi \left( \frac{N}{b^k} + \frac{l'}{b} \right) \varphi_{b,h}^\pi \left( \frac{l'}{b} \right) = \sum_{h=0}^{b-1} \varphi_{b,h}^\pi \left( \frac{l'}{b} \right) \sum_{N=1}^{b^n} \varphi_{b,h}^\pi \left( \frac{N}{b^k} + \frac{l'}{b} \right).$$

Using the periodicity of  $\varphi_{b,h}^\pi$ , we obtain for the innermost sum

$$\begin{aligned} \sum_{N=1}^{b^n} \varphi_{b,h}^\pi \left( \frac{N}{b^k} + \frac{l'}{b} \right) &= b^{n-k} \sum_{N=0}^{b^k-1} \varphi_{b,h}^\pi \left( \frac{N}{b^k} \right) \\ &= b^{n-k} \sum_{j=0}^{b-1} \sum_{N=jb^{k-1}+1}^{(j+1)b^{k-1}} \varphi_{b,h}^\pi \left( \frac{N}{b^k} \right). \end{aligned}$$

For  $j/b \leq x \leq (j+1)/b$  we have

$$\varphi_{b,h}^\pi(x) = b \left( x - \frac{j}{b} \right) \left[ \varphi_{b,h}^\pi \left( \frac{j+1}{b} \right) - \varphi_{b,h}^\pi \left( \frac{j}{b} \right) \right] + \varphi_{b,h}^\pi \left( \frac{j}{b} \right).$$

Therefore we have

$$\begin{aligned} &\sum_{N=1}^{b^n} \varphi_{b,h}^\pi \left( \frac{N}{b^k} + \frac{l'}{b} \right) \\ &= b^{n-k} \sum_{j=0}^{b-1} b \left[ \varphi_{b,h}^\pi \left( \frac{j+1}{b} \right) - \varphi_{b,h}^\pi \left( \frac{j}{b} \right) \right] \sum_{N=jb^{k-1}+1}^{(j+1)b^{k-1}} \left( \frac{N}{b^k} - \frac{j}{b} \right) \\ &\quad + b^{n-1} \sum_{j=0}^{b-1} \varphi_{b,h}^\pi \left( \frac{j}{b} \right) \\ &= b^{n-k} \sum_{j=0}^{b-1} \left[ \varphi_{b,h}^\pi \left( \frac{j+1}{b} \right) - \varphi_{b,h}^\pi \left( \frac{j}{b} \right) \right] \frac{b+b^k}{2b} + b^{n-1} \sum_{j=0}^{b-1} \varphi_{b,h}^\pi \left( \frac{j}{b} \right) \\ &= b^{n-1} \sum_{j=0}^{b-1} \varphi_{b,h}^\pi \left( \frac{j}{b} \right). \end{aligned}$$

Hence we have

$$\sum_{h=0}^{b-1} \sum_{N=1}^{b^n} \varphi_{b,h}^\pi \left( \frac{N}{b^k} + \frac{l'}{b} \right) \varphi_{b,h}^\pi \left( \frac{l'}{b} \right) = b^{n-1} \sum_{h=0}^{b-1} \varphi_{b,h}^\pi \left( \frac{l'}{b} \right) \sum_{j=0}^{b-1} \varphi_{b,h}^\pi \left( \frac{j}{b} \right) = b^n F_b^\pi(l).$$

The result follows.  $\square$

**LEMMA 7.** For  $0 \leq h \leq n$  and  $0 \leq l < b$  we have

$$\sum_{N=1}^{b^n} N \varphi_b^\pi \left( \frac{N}{b^h} + \frac{\pi^{-1}(l)}{b} \right) = b^{2n} \frac{b\Phi_b^\pi}{2} + b^{n+h} f_b^\pi(l) + b^n g_b^\pi(l),$$

where  $g_b^\pi(l) = \frac{b}{2}\Phi_b^\pi - \frac{b^2+1}{24} + \frac{l(b-1)}{4} - \frac{1}{2}\sum_{i=0}^{l-1}\pi(i)$  and

$$\begin{aligned} f_b^\pi(l) &= -\frac{b}{2}\Phi_b^\pi + \frac{(b-1)^2(1-5b)}{24b} + \frac{1}{2b^2}\sum_{i=0}^{b-1}i^2\pi(i) + \frac{(b-1)l(l-2)}{2b} \\ &\quad - \left(l - \frac{1}{2}\right)\frac{1}{b}\sum_{i=0}^{l-1}\pi(i) + \frac{1}{b}\sum_{i=0}^{l-1}i\pi(i). \end{aligned}$$

*Proof.* Again we write  $l' = \pi^{-1}(l)$ . Splitting up the range of summation yields

$$\sum_{N=1}^{b^n} N\varphi_b^\pi\left(\frac{N}{b^h} + \frac{l'}{b}\right) = \sum_{k=0}^{b^{n-h+1}-1} \sum_{N=kb^{h-1}+1}^{(k+1)b^{h-1}} N\varphi_b^\pi\left(\frac{N}{b^h} + \frac{l'}{b}\right).$$

For  $0 \leq k < b^{n-h+1}$  let  $k = qb + r$  with integers  $0 \leq r < b$  and  $0 \leq q < b^{n-h}$ . Then for  $kb^{h-1} + 1 \leq N \leq (k+1)b^{h-1}$  we have  $r/b \leq N/b^h - q \leq (r+1)/b$ . Hence,

- if  $0 \leq r < b - l$ , then

$$N/b^h - q + l'/b \in \left[\frac{r+l'}{b}, \frac{r+l'+1}{b}\right] \subseteq [0, 1);$$

- if  $b - l' \leq r < b$ , then

$$N/b^h - q + l'/b - 1 \in \left[\frac{r+l'-b}{b}, \frac{r+l'-b+1}{b}\right] \subseteq [0, 1).$$

Using the periodicity of  $\varphi_b^\pi$  and Equation (11) we therefore obtain

$$\begin{aligned} \sum_{N=1}^{b^n} N\varphi_b^\pi\left(\frac{N}{b^h} + \frac{l'}{b}\right) &= \sum_{r=0}^{b-1} \sum_{q=0}^{b^{n-h}-1} \sum_{N=qb^h+r}^{qb^h+(r+1)b^{h-1}} N\varphi_b^\pi\left(\frac{N}{b^h} - q + \frac{l'}{b}\right) \\ &= \sum_{r=0}^{b-l'-1} \sum_{q=0}^{b^{n-h}-1} \sum_{N=qb^h+r}^{qb^h+(r+1)b^{h-1}} N\varphi_b^\pi\left(\frac{N}{b^h} - q + \frac{l'}{b}\right) \\ &\quad + \sum_{r=b-l'}^{b-1} \sum_{q=0}^{b^{n-h}-1} \sum_{N=qb^h+r}^{qb^h+(r+1)b^{h-1}} N\varphi_b^\pi\left(\frac{N}{b^h} - q + \frac{l'}{b} - 1\right) \\ &= \sum_{r=0}^{b-l'-1} \sum_{q=0}^{b^{n-h}-1} \sum_{N=qb^h+r}^{qb^h+(r+1)b^{h-1}} N \left(\frac{b(b-2\pi(r+l'))-1}{2}\right) \left(\frac{N}{b^h} - q - \frac{r}{b}\right) \end{aligned}$$

$$\begin{aligned}
 & + \frac{(r+l')(b-1)}{2} - \sum_{i=0}^{r+l'-1} \pi(i) \\
 & + \sum_{r=b-l'}^{b-1} \sum_{q=0}^{b^n-h-1} \sum_{N=qb^h+rbb^{h-1}+1}^{qb^h+(r+1)b^{h-1}} N \left( \frac{b(b-2\pi(r+l'-b)-1)}{2} \left( \frac{N}{b^h} - q - \frac{r}{b} \right) \right. \\
 & \quad \left. + \frac{(r+l'-b)(b-1)}{2} - \sum_{i=0}^{r+l'-b-1} \pi(i) \right) \\
 & = \Sigma_1 + \Sigma_2 + \Sigma_3 + \Sigma_4,
 \end{aligned}$$

where:

$$\begin{aligned}
 \Sigma_1 & := \sum_{r=0}^{b-l'-1} \frac{(b-2\pi(r+l')-1)b^n(b^h+b)(2b-3b^{h+1}+3b^{n+1}+b^h(4+6r))}{24b^{2+h}} \\
 \Sigma_2 & := \sum_{r=0}^{b-l'-1} \left( \frac{(r+l')(b-1)}{2} - \sum_{i=0}^{r+l'-1} \pi(i) \right) \frac{b^n(b-b^{h+1}+b^{n+1}+b^h(1+2r))}{2b^2} \\
 \Sigma_3 & := \sum_{r=b-l'}^{b-1} \frac{(b-2\pi(r+l'-b)-1)b^n(b^h+b)(2b-3b^{h+1}+3b^{n+1}+b^h(4+6r))}{24b^{2+h}} \\
 \Sigma_4 & := \sum_{r=b-l'}^{b-1} \left( \frac{(r+l'-b)(b-1)}{2} - \sum_{i=0}^{r+l'-b-1} \pi(i) \right) \\
 & \quad \times \frac{b^n(b-b^{h+1}+b^{n+1}+b^h(1+2r))}{2b^2}
 \end{aligned}$$

Now tedious calculations using (12) lead to the desired result.  $\square$

#### 4. The proofs of the main results

First we show a discrete version of Proposition 1.

**LEMMA 8.** *For  $\Sigma = (\sigma_0, \dots, \sigma_{n-1}) \in \{\pi_l : 0 \leq l < b\}^n$  let  $\lambda_l := \#\{0 \leq i < n : \sigma_i = \pi_l\}$ . Then we have*

$$\frac{1}{b^{2n}} \sum_{\lambda, N=1}^{b^n} E \left( \frac{\lambda}{b^n}; \frac{N}{b^n}; \mathcal{H}_{b,n}^\Sigma \right) = \sum_{l=0}^{b-1} \frac{\lambda_l}{b} \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{\pi^{-1}(l)}{b} \right) \right) \quad (18)$$

and

$$\begin{aligned}
 & \frac{1}{b^{2n}} \sum_{\lambda, N=1}^{b^n} \left( E \left( \frac{\lambda}{b^n}; \frac{N}{b^n}; \mathcal{H}_{b,n}^\Sigma \right) \right)^2 \tag{19} \\
 &= \left( \sum_{l=0}^{b-1} \frac{\lambda_l}{b} \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{\pi^{-1}(l)}{b} \right) \right) \right)^2 + n\Phi_b^{\pi, (2)} + \frac{1}{36} \left( 1 - \frac{1}{b^{2n}} \right) \\
 &+ \sum_{l=0}^{b-1} \frac{\lambda_l}{b} \left[ \varphi_b^{\pi, (2)} \left( \frac{\pi^{-1}(l)}{b} \right) - 2F_b^\pi(l) - \frac{1}{b} \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{\pi^{-1}(l)}{b} \right) \right)^2 \right].
 \end{aligned}$$

*Proof.* We just give the (much more involved) proof of (19). Equation (18) can be shown in the same way.

When  $\lambda_l \neq 0$ , let  $h_i^{(l)}$  for  $1 \leq i \leq \lambda_l$  ( $1 \leq h_i^{(l)} \leq n$ ) be the integers such that  $\sigma_{h_i^{(l)}-1} = \pi_l$ , i.e.  $\sigma_{h_1^{(l)}-1} = \dots = \sigma_{h_{\lambda_l}^{(l)}-1} = \pi_l$ . Using Lemma 3 and Lemma 4 we have

$$\begin{aligned}
 & \frac{1}{b^{2n}} \sum_{\lambda, N=1}^{b^n} \left( E \left( \frac{\lambda}{b^n}; \frac{N}{b^n}; \mathcal{H}_{b,n}^\Sigma \right) \right)^2 = \frac{1}{b^{2n}} \sum_{\lambda, N=1}^{b^n} \sum_{i,j=1}^n \varphi_{b,\varepsilon_i}^{\sigma_{i-1}} \left( \frac{N}{b^i} \right) \varphi_{b,\varepsilon_j}^{\sigma_{j-1}} \left( \frac{N}{b^j} \right) \\
 &= \frac{1}{b^{2n}} \sum_{i=1}^n \sum_{N=1}^{b^n} \sum_{\lambda=1}^{b^n} \left( \varphi_{b,\varepsilon_i}^{\sigma_{i-1}} \left( \frac{N}{b^i} \right) \right)^2 \\
 &+ \frac{1}{b^{2n}} \sum_{\substack{i,j=1 \\ i \neq j}}^n \sum_{N=1}^{b^n} \sum_{\lambda=1}^{b^n} \varphi_{b,\varepsilon_i}^{\sigma_{i-1}} \left( \frac{N}{b^i} \right) \varphi_{b,\varepsilon_j}^{\sigma_{j-1}} \left( \frac{N}{b^j} \right) \\
 &= \frac{1}{b^{2n}} \sum_{i=1}^n \sum_{N=1}^{b^n} b^{n-1} \varphi_b^{\sigma_{i-1}, (2)} \left( \frac{N}{b^i} \right) \\
 &+ \frac{1}{b^{2n}} \sum_{\substack{i,j=1 \\ i \neq j}}^n \sum_{N=1}^{b^n} b^{n-2} \varphi_b^{\sigma_{i-1}} \left( \frac{N}{b^i} \right) \varphi_b^{\sigma_{j-1}} \left( \frac{N}{b^j} \right) \\
 &= \frac{1}{b^{2n}} \sum_{l=0}^{b-1} \sum_{i=1}^{\lambda_l} \sum_{N=1}^{b^n} b^{n-1} \varphi_b^{\pi_l, (2)} \left( \frac{N}{b^{h_i^{(l)}}} \right) \\
 &+ \frac{1}{b^{2n}} \sum_{\substack{l,m=0 \\ l \neq m}}^{b-1} \sum_{i=1}^{\lambda_l} \sum_{j=1}^{\lambda_m} \sum_{N=1}^{b^n} b^{n-2} \varphi_b^{\pi_l} \left( \frac{N}{b^{h_i^{(l)}}} \right) \varphi_b^{\pi_m} \left( \frac{N}{b^{h_j^{(m)}}} \right)
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{1}{b^{2n}} \sum_{l=0}^{b-1} \sum_{\substack{i,j=1 \\ i \neq j}}^{\lambda_l} \sum_{N=1}^{b^n} b^{n-2} \varphi_b^{\pi_l} \left( \frac{N}{b^{h_i^{(l)}}} \right) \varphi_b^{\pi_l} \left( \frac{N}{b^{h_j^{(l)}}} \right) \\
 & =: A + B + C.
 \end{aligned}$$

Using Lemma 5 we get (again we write  $l' = \pi^{-1}(l)$  and  $m' = \pi^{-1}(m)$ )

$$B = \frac{1}{b^2} \sum_{\substack{l,m=0 \\ l \neq m}}^{b-1} \lambda_l \lambda_m \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{l'}{b} \right) \right) \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{m'}{b} \right) \right)$$

and

$$C = \frac{1}{b^2} \sum_{l=0}^{b-1} \lambda_l (\lambda_l - 1) \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{l'}{b} \right) \right)^2.$$

For  $A$  we use Lemma 6 and the fact that  $\sum_{l=0}^{b-1} \lambda_l = n$  to obtain

$$\begin{aligned}
 A & = \frac{1}{b^{2n}} \sum_{l=0}^{b-1} \sum_{i=1}^{\lambda_l} \sum_{N=1}^{b^n} b^{n-1} \varphi_b^{\pi_l, (2)} \left( \frac{N}{b^{h_i^{(l)}}} \right) \\
 & = \frac{1}{b} \sum_{l=0}^{b-1} \sum_{i=1}^{\lambda_l} \left( b\Phi_b^{\pi, (2)} + \frac{b(b^2-1)}{36b^{2h_i^{(l)}}} + \varphi_b^{\pi, (2)} \left( \frac{l'}{b} \right) - 2F_b^\pi(l) \right) \\
 & = n\Phi_b^{\pi, (2)} + \frac{1}{36} \left( 1 - \frac{1}{b^{2n}} \right) + \sum_{l=0}^{b-1} \frac{\lambda_l}{b} \left( \varphi_b^{\pi, (2)} \left( \frac{l'}{b} \right) - 2F_b^\pi(l) \right).
 \end{aligned}$$

Overall we obtain

$$\begin{aligned}
 & \frac{1}{b^{2n}} \sum_{\lambda, N=1}^{b^n} \left( E \left( \frac{\lambda}{b^n}; \frac{N}{b^n}; \mathcal{H}_{b,n}^\Sigma \right) \right)^2 \\
 & = \left( \sum_{l=0}^{b-1} \frac{\lambda_l}{b} \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{l'}{b} \right) \right) \right)^2 - \sum_{l=0}^{b-1} \frac{\lambda_l}{b^2} \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{l'}{b} \right) \right)^2 \\
 & \quad + n\Phi_b^{\pi, (2)} + \frac{1}{36} \left( 1 - \frac{1}{b^{2n}} \right) + \sum_{l=0}^{b-1} \frac{\lambda_l}{b} \left( \varphi_b^{\pi, (2)} \left( \frac{l'}{b} \right) - 2F_b^\pi(l) \right) \\
 & = \left( \sum_{l=0}^{b-1} \frac{\lambda_l}{b} \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{l'}{b} \right) \right) \right)^2 + n\Phi_b^{\pi, (2)} + \frac{1}{36} \left( 1 - \frac{1}{b^{2n}} \right) \\
 & \quad + \sum_{l=0}^{b-1} \frac{\lambda_l}{b} \left[ \varphi_b^{\pi, (2)} \left( \frac{l'}{b} \right) - 2F_b^\pi(l) - \frac{1}{b} \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{l'}{b} \right) \right)^2 \right].
 \end{aligned}$$

□

Now we give the proof of Proposition 1.

**P r o o f.** Again we use the abbreviation  $l' = \pi^{-1}(l)$ . Using (14) we obtain

$$\begin{aligned}
 (L_2(\mathcal{H}_{b,n}^\Sigma))^2 &= \int_0^1 \int_0^1 (E(x(n); y(n); \mathcal{H}_{b,n}^\Sigma) + b^n(x(n)y(n) - xy))^2 dx dy \\
 &= \frac{1}{b^{2n}} \sum_{\lambda, N=1}^{b^n} \left( E\left(\frac{\lambda}{b^n}; \frac{N}{b^n}; \mathcal{H}_{b,n}^\Sigma\right) \right)^2 \\
 &\quad + 2b^n \sum_{\lambda, N=1}^{b^n} \int_{\frac{\lambda-1}{b^n}}^{\frac{\lambda}{b^n}} \int_{\frac{N-1}{b^n}}^{\frac{N}{b^n}} E\left(\frac{\lambda}{b^n}; \frac{N}{b^n}; \mathcal{H}_{b,n}^\Sigma\right) \left(\frac{\lambda}{b^n} \frac{N}{b^n} - xy\right) dx dy \\
 &\quad + b^{2n} \sum_{\lambda, N=1}^{b^n} \int_{\frac{\lambda-1}{b^n}}^{\frac{\lambda}{b^n}} \int_{\frac{N-1}{b^n}}^{\frac{N}{b^n}} \left(\frac{\lambda}{b^n} \frac{N}{b^n} - xy\right)^2 dx dy \\
 &=: \Sigma_1 + \Sigma_2 + \Sigma_3.
 \end{aligned}$$

The term  $\Sigma_1$  has been evaluated in Lemma 8 and straightforward calculus shows that  $\Sigma_3 = (1 + 18b^n + 25b^{2n})/(72b^{2n})$ . So it remains to deal with  $\Sigma_2$ .

Evaluating the integral appearing in  $\Sigma_2$  we obtain

$$\begin{aligned}
 \Sigma_2 &= \frac{1}{b^{3n}} \sum_{\lambda, N=1}^{b^n} (\lambda + N) E\left(\frac{\lambda}{b^n}; \frac{N}{b^n}; \mathcal{H}_{b,n}^\Sigma\right) - \frac{1}{2b^{3n}} \sum_{\lambda, N=1}^{b^n} E\left(\frac{\lambda}{b^n}; \frac{N}{b^n}; \mathcal{H}_{b,n}^\Sigma\right) \\
 &=: \Sigma_4 - \Sigma_5.
 \end{aligned}$$

The term  $\Sigma_5$  can be obtained from Lemma 8, Equation (18). For  $\Sigma_4$  we have

$$\begin{aligned}
 \Sigma_4 &= \frac{1}{b^{3n}} \sum_{\lambda, N=1}^{b^n} \lambda E\left(\frac{\lambda}{b^n}; \frac{N}{b^n}; \mathcal{H}_{b,n}^\Sigma\right) + \frac{1}{b^{3n}} \sum_{\lambda, N=1}^{b^n} N E\left(\frac{\lambda}{b^n}; \frac{N}{b^n}; \mathcal{H}_{b,n}^\Sigma\right) \\
 &=: \frac{1}{b^{3n}} (\Sigma_{4,1} + \Sigma_{4,2}).
 \end{aligned}$$

As to  $\Sigma_{4,2}$ , with Lemma 3, Lemma 4, Equation (13) and Lemma 7 we obtain

$$\begin{aligned}
 \Sigma_{4,2} &= b^{n-1} \sum_{l=0}^{b-1} \sum_{i=1}^{\lambda_l} \sum_{N=1}^{b^n} N \left( \varphi_b^\pi \left( \frac{N}{b^{h_i^{(l)}}} + \frac{l'}{b} \right) - \varphi_b^\pi \left( \frac{l'}{b} \right) \right) \\
 &= b^{2n-1} \sum_{l=0}^{b-1} \sum_{i=1}^{\lambda_l} \left( b^{n+1} \frac{\Phi_b^\pi}{2} + b^{h_i^{(l)}} f_b^\pi(l) + g_b^\pi(l) - \frac{b^n + 1}{2} \varphi_b^\pi \left( \frac{l'}{b} \right) \right)
 \end{aligned}$$



$$= b^{3n} \frac{\Phi_b^\pi}{2} n + b^{2n-1} \sum_{l=0}^{b-1} \sum_{i=1}^{\lambda_l} \left( b^{h_i^{(l)}} f_b^\pi(l) + g_b^\pi(l) - \frac{b^n + 1}{2} \varphi_b^\pi \left( \frac{l'}{b} \right) \right),$$

where again the integers  $h_i^{(l)}$  satisfy  $\sigma_{h_1^{(l)}-1} = \dots = \sigma_{h_{\lambda_l}^{(l)}-1} = \pi_l$  if  $\lambda_l \neq 0$ .

We turn to  $\Sigma_{4,1}$ . Let  $g : [0, 1]^2 \rightarrow [0, 1]^2$  be defined by  $g(x, y) = (y, x)$  and for  $\Sigma = (\sigma_0, \dots, \sigma_{n-1})$  define  $\Gamma = (\gamma_0, \dots, \gamma_{n-1}) := (\sigma_{n-1}^{-1}, \dots, \sigma_0^{-1})$ . Then it is easy to see (for details see [9, Proof of Theorem 4]) that  $\mathcal{H}_{b,n}^\Sigma = g \left( \mathcal{H}_{b,n}^\Gamma \right)$ . Therefore we obtain

$$\Sigma_{4,1} = \sum_{\lambda, N=1}^{b^n} \lambda E \left( \frac{\lambda}{b^n}; \frac{N}{b^n}; \mathcal{H}_{b,n}^\Sigma \right) = \sum_{\lambda, N=1}^{b^n} \lambda E \left( \frac{N}{b^n}; \frac{\lambda}{b^n}; \mathcal{H}_{b,n}^\Gamma \right),$$

which will allow us to use the result for  $\Sigma_{4,2}$ . To this end, we must check the correspondences between  $\Sigma$  and  $\Gamma$ : For  $\Sigma \in \{\pi_l : 0 \leq l < b\}^n$  we also have  $\Gamma \in \{\pi_l : 0 \leq l < b\}^n$ . If  $l = 0$  we get  $(\pi_0)^{-1} = (\pi^{-1})_0$  and for  $0 < l < b$ , we get  $(\pi_l)^{-1} = (\pi^{-1})_{b-\pi^{-1}(l)}$  as remarked just before Lemma 1. Hence for  $l > 0$  and  $\lambda_l \neq 0$  we have  $\sigma_{h_1^{(l)}-1}^{-1} = \dots = \sigma_{h_{\lambda_l}^{(l)}-1}^{-1} = (\pi_l)^{-1} = (\pi^{-1})_{b-\pi^{-1}(l)}$ , so that  $\gamma_{n+1-h_1^{(l)}-1} = \dots = \gamma_{n+1-h_{\lambda_l}^{(l)}-1} = (\pi^{-1})_{b-\pi^{-1}(l)}$ . Further  $\gamma_{u_1^{(b-r)}-1} = \dots = \gamma_{u_{\lambda_{\pi(b-r)}}^{(b-r)}-1} = (\pi^{-1})_r$ , where  $u_i^{(b-r)} := n - h_i^{\pi(b-r)} + 1$ . Since  $\pi^{-1}$  is also linear we may use the formula for  $\Sigma_{4,2}$  and obtain

$$\begin{aligned} \Sigma_{4,1} &= b^{3n} \frac{\Phi_b^{\pi^{-1}}}{2} n + b^{2n-1} \\ &\quad \times \sum_{r=0}^{b-1} \sum_{i=1}^{\lambda_{\pi(b-r)}} \left( b^{u_i^{(b-r)}} f_b^{\pi^{-1}}(r) + g_b^{\pi^{-1}}(r) - \frac{b^n + 1}{2} \varphi_b^{\pi^{-1}} \left( \frac{\pi(r)}{b} \right) \right) \\ &= b^{3n} \frac{\Phi_b^\pi}{2} n + b^{2n-1} \\ &\quad \times \sum_{r=0}^{b-1} \sum_{i=1}^{\lambda_{\pi(b-r)}} \left( b^{n-h_i^{(\pi(b-r))+1}} f_b^{\pi^{-1}}(r) + g_b^{\pi^{-1}}(r) - \frac{b^n + 1}{2} \varphi_b^{\pi^{-1}} \left( \frac{\pi(r)}{b} \right) \right) \\ &= b^{3n} \frac{\Phi_b^\pi}{2} n + b^{2n-1} \\ &\quad \times \sum_{l=0}^{b-1} \sum_{i=1}^{\lambda_l} \left( b^{n-h_i^{(l)+1}} f_b^{\pi^{-1}}(b-l') + g_b^{\pi^{-1}}(b-l') - \frac{b^n + 1}{2} \varphi_b^{\pi^{-1}} \left( \frac{b-l}{b} \right) \right) \end{aligned}$$

where we have used that  $\Phi_b^{\pi^{-1}} = \Phi_b^\pi$  as shown in [12, Lemma 5]. Hence we have

$$\begin{aligned} \Sigma_4 &= \Phi_b^\pi n - \frac{b^n + 1}{2b^{n+1}} \sum_{l=0}^{b-1} \lambda_l \left( \varphi_b^\pi \left( \frac{l'}{b} \right) + \varphi_b^{\pi^{-1}} \left( \frac{b-l}{b} \right) \right) \\ &\quad + \frac{1}{b^{n+1}} \sum_{l=0}^{b-1} \sum_{i=1}^{\lambda_l} \left( b^{h_i^{(l)}} f_b^\pi(l) + b^{n-h_i^{(l)}+1} f_b^{\pi^{-1}}(b-l') \right) \\ &\quad + \frac{1}{b^{n+1}} \sum_{l=0}^{b-1} \lambda_l \left( g_b^\pi(l) + g_b^{\pi^{-1}}(b-l') \right). \end{aligned}$$

Now we obtain

$$\begin{aligned} (L_2(\mathcal{H}_{b,n}^\Sigma))^2 &= \left( \sum_{l=0}^{b-1} \frac{\lambda_l}{b} \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{l'}{b} \right) \right) \right)^2 + n\Phi_b^{\pi,(2)} + \frac{1}{36} \left( 1 - \frac{1}{b^{2n}} \right) \\ &\quad + \sum_{l=0}^{b-1} \frac{\lambda_l}{b} \left[ \varphi_b^{\pi,(2)} \left( \frac{l'}{b} \right) - 2F_b^\pi(l) - \frac{1}{b} \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{l'}{b} \right) \right)^2 \right] \\ &\quad + \Phi_b^\pi n - \frac{b^n + 1}{2b^{n+1}} \sum_{l=0}^{b-1} \lambda_l \left( \varphi_b^\pi \left( \frac{l'}{b} \right) + \varphi_b^{\pi^{-1}} \left( \frac{b-l}{b} \right) \right) \\ &\quad + \frac{1}{b^{n+1}} \sum_{l=0}^{b-1} \sum_{i=1}^{\lambda_l} \left( b^{h_i^{(l)}} f_b^\pi(l) + b^{n-h_i^{(l)}+1} f_b^{\pi^{-1}}(b-l') \right) \\ &\quad + \frac{1}{b^{n+1}} \sum_{l=0}^{b-1} \lambda_l \left( g_b^\pi(l) + g_b^{\pi^{-1}}(b-l') \right) \\ &\quad - \frac{1}{2b^n} \sum_{l=0}^{b-1} \frac{\lambda_l}{b} \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{l'}{b} \right) \right) + \frac{1 + 18b^n + 25b^{2n}}{72b^{2n}} \\ &= \left( \sum_{l=0}^{b-1} \frac{\lambda_l}{b} \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{l'}{b} \right) \right) \right)^2 + n\Phi_b^{\pi,(2)} + n\Phi_b^\pi \\ &\quad + \sum_{l=0}^{b-1} \frac{\lambda_l}{b} \left[ \varphi_b^{\pi,(2)} \left( \frac{l'}{b} \right) - 2F_b^\pi(l) - \frac{1}{b} \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{l'}{b} \right) \right)^2 \right] \\ &\quad - \frac{1}{2b} \sum_{l=0}^{b-1} \lambda_l \left( \varphi_b^\pi \left( \frac{l'}{b} \right) + \varphi_b^{\pi^{-1}} \left( \frac{b-l}{b} \right) \right) + O(1). \quad (20) \end{aligned}$$

From Lemma 2 it follows that

$$\Phi_b^\pi - \frac{1}{b}\varphi_b^\pi(l'/b) = \Phi_b^{\pi_l} \quad (21)$$

and from [12, Lemma 5] we know that  $\Phi_b^\pi = \Phi_b^{\pi^{-1}}$  and hence

$$\begin{aligned} n\Phi_b^\pi - \frac{1}{2b} \sum_{l=0}^{b-1} \lambda_l \left( \varphi_b^\pi \left( \frac{l'}{b} \right) + \varphi_b^{\pi^{-1}} \left( \frac{b-l}{b} \right) \right) \\ &= \sum_{l=0}^{b-1} \lambda_l \left( \Phi_b^\pi - \frac{1}{2b}\varphi_b^\pi \left( \frac{l'}{b} \right) - \frac{1}{2b}\varphi_b^{\pi^{-1}} \left( \frac{b-l}{b} \right) \right) \\ &= \frac{1}{2} \sum_{l=0}^{b-1} \lambda_l \Phi_b^{\pi_l} + \frac{1}{2} \sum_{l=0}^{b-1} \lambda_l \left( \Phi_b^{\pi^{-1}} - \frac{1}{b}\varphi_b^{\pi^{-1}} \left( \frac{b-l}{b} \right) \right) \\ &= \frac{1}{2} \sum_{l=0}^{b-1} \lambda_l \Phi_b^{\pi_l} + \frac{1}{2} \sum_{l=0}^{b-1} \lambda_l \Phi_b^{(\pi^{-1})\pi^{-1}(b-l \pmod{b})} \\ &= \frac{1}{2} \sum_{l=0}^{b-1} \lambda_l \Phi_b^{\pi_l} + \frac{1}{2} \sum_{l=0}^{b-1} \lambda_l \Phi_b^{(\pi_l)^{-1}} = \sum_{l=0}^{b-1} \lambda_l \Phi_b^{\pi_l}. \end{aligned}$$

The desired result follows from inserting this and (21) into (20).  $\square$

We give the proof of Theorem 1.

*Proof.* If  $\lambda_l = \lfloor n/b \rfloor + \theta_l$  with  $\theta_l \in \{0, 1\}$ , then from (20) we obtain

$$\begin{aligned} &(L_2(\mathcal{H}_{b,n}^\Sigma))^2 \\ &= n\Phi_b^{\pi,(2)} + \frac{n}{b^2} \sum_{l=0}^{b-1} \left[ \varphi_b^{\pi,(2)} \left( \frac{l'}{b} \right) - 2F_b^\pi(l) - \frac{1}{b} \left( b\Phi_b^\pi - \varphi_b^\pi \left( \frac{l'}{b} \right) \right)^2 \right] + O(1) \\ &= n(\Phi_b^{\pi,(2)} - (\Phi_b^\pi)^2) + \frac{n}{b^2} A + O(1), \text{ where} \end{aligned}$$

$$A := \sum_{l=0}^{b-1} \left[ \varphi_b^{\pi,(2)} \left( \frac{l'}{b} \right) - 2F_b^\pi(l) + 2\Phi_b^\pi \varphi_b^\pi \left( \frac{l'}{b} \right) - \frac{1}{b} \left( \varphi_b^\pi \left( \frac{l'}{b} \right) \right)^2 \right].$$

It remains to prove that  $A = 0$ . Writing everything with  $\varphi_{b,h}^\pi \left( \frac{l}{b} \right)$ , we get

$$A = \sum_{l,h=0}^{b-1} \left( \varphi_{b,h}^\pi \left( \frac{l}{b} \right) \right)^2 - \frac{2}{b} \sum_{h,j,l=0}^{b-1} \varphi_{b,h}^\pi \left( \frac{l}{b} \right) \varphi_{b,h}^\pi \left( \frac{j}{b} \right)$$

$$+ \frac{2}{b^2} \left( \sum_{l,h=0}^{b-1} \varphi_{b,h}^\pi \left( \frac{l}{b} \right) \right)^2 - \frac{1}{b} \sum_{l=0}^{b-1} \left( \sum_{h=0}^{b-1} \varphi_{b,h}^\pi \left( \frac{l}{b} \right) \right)^2.$$

Using (9) the above expression can be written as

$$\begin{aligned} A &= \frac{1}{b^2} \sum_{l,h=0}^{b-1} \sum_{k_1=0}^{l-1} (\varphi_{b,h}^\pi)' \left( \frac{k_1}{b} + 0 \right) \sum_{k_2=0}^{l-1} (\varphi_{b,h}^\pi)' \left( \frac{k_2}{b} + 0 \right) \\ &\quad - \frac{2}{b^3} \sum_{h,j,l=0}^{b-1} \sum_{k_1=0}^{l-1} (\varphi_{b,h}^\pi)' \left( \frac{k_1}{b} + 0 \right) \sum_{k_2=0}^{j-1} (\varphi_{b,h}^\pi)' \left( \frac{k_2}{b} + 0 \right) \\ &\quad + \frac{2}{b^4} \sum_{h_1,l,h_2,j=0}^{b-1} \sum_{k_1=0}^{l-1} (\varphi_{b,h_1}^\pi)' \left( \frac{k_1}{b} + 0 \right) \sum_{k_2=0}^{j-1} (\varphi_{b,h_2}^\pi)' \left( \frac{k_2}{b} + 0 \right) \\ &\quad - \frac{1}{b^3} \sum_{l=0}^{b-1} \left( \sum_{h=0}^{b-1} \sum_{k=0}^{l-1} (\varphi_{b,h}^\pi)' \left( \frac{k}{b} + 0 \right) \right)^2. \end{aligned}$$

In [12, Section 5] it is shown that

$$\begin{aligned} \sum_{h=0}^{b-1} (\varphi_{b,h}^\pi)' \left( \frac{k_1}{b} + 0 \right) (\varphi_{b,h}^\pi)' \left( \frac{k_2}{b} + 0 \right) &= \frac{b(b-1)(2b-1)}{6} \\ &\quad + \frac{b}{2} (\pi(k_1)(\pi(k_1)+1) + \pi(k_2)(\pi(k_2)+1)) - b^2 \max(\pi(k_1), \pi(k_2)) \end{aligned}$$

and  $\sum_{h=0}^{b-1} (\varphi_{b,h}^\pi)' \left( \frac{k}{b} + 0 \right) = b(b-1)/2 - b\pi(k)$ .

With these formulas and using the fact that  $\pi(b-k) = b - \pi(k)$ ,  $k \neq 0$ , one gets after tedious computations that  $A_0 = b^4 A$  consists of sums  $S_i$  whose summands are all polynomial in  $b, k, l, \pi(k), \pi(l)$  and  $\max(k, l), \max(\pi(k), \pi(l))$ . These polynomials will be denoted by  $p_i$ . Furthermore, we can single out polynomials in  $b$  from the sums. The sums are then dependent on  $\pi$  while the polynomials depend only on  $b$  but not on  $\pi$ . I.e., we can make an ansatz for  $A_0$ , for which we then subsequently want to determine the  $p_i$ :

$$A_0 = A_0(\pi) = \sum_{i=0}^5 p_i(b) S_i(\pi),$$

where the  $p_i$  are polynomials in  $b$  and

$$S_0 \equiv 1, \quad S_i(\pi) := \sum_{k=0}^{b-1} k^i \pi(k)^i, \quad \text{for } i = 1, 2,$$

$$\begin{aligned}
 S_3(\pi) &:= \sum_{k,l=0}^{b-1} \max(k, l) \max(\pi(k), \pi(l)), \\
 S_4(\pi) &:= \sum_{k,l=0}^{b-1} kl \max(\pi(k), \pi(l)), \\
 S_5(\pi) &:= S_1(\pi)^2.
 \end{aligned}$$

Any linear dependencies between the  $S_i$  (which we were not able to show directly) will appear as additional dimensions to the solution space of the ansatz.

Now, to determine the  $p_i$ , we first solve the following linear equation system for fixed  $b$ , where  $b$  is large enough such that there exist at least as many  $\pi$  as  $S_i$ :

$$(S_i(\pi))_{\pi, i} (x_i)_i = (A_0(\pi))_{\pi}.$$

The left hand side matrix is in  $\mathbb{Z}^{\varphi(b) \times b}$ , where  $\varphi(b)$  is the Euler phi function.

Since by the ansatz the system is solvable, we obtain as particular solution the values of  $p_i$  at the fixed  $b$ , i.e., the vector  $(p_i(b))_i$ . If the left hand side matrix is of full rank we have a unique solution, otherwise we additionally have a nullspace  $N_b$  (which we consider in a canonical form).

Repeating this for sufficiently many  $b$  we can derive the  $p_i$  by interpolation. Note that the degrees of the  $p_i$  are bounded by the maximum degree of terms inside the sums plus the depth with which they are nested. (In this application the bound is 8.)

Similarly we also derive a basis of the nullspace and get

$$A_0(\pi) = \sum_i \left( p_i(b) + \sum_j \lambda_j q_{i,j}(b) \right) S_i(\pi),$$

for some polynomials  $q_{i,j}$  and arbitrarily chosen  $\lambda_j \in \mathbb{Q}$ , where

$$0 = \sum_i q_{i,j}(b) S_i(\pi),$$

and with  $j$  ranging over the maximum of dimensions of the  $N_b$ . So at least one  $S_i$  is linearly dependent. We repeat the process with this  $S_i$  excluded and  $A_0$  multiplied with  $\text{lcm}_j(q_{i,j})$ . In the iteration the dimension of the nullspaces is now reduced by one, so the algorithm terminates after finitely many steps.

By an implementation in MATHEMATICA we observe that, in fact, in this application

$$S_4 = -bS_3 + S_2 + bS_1 + \frac{b^3(b-1)^2}{2}$$

$$4S_5 = 4b^2S_3 - 5bS_2 + b^2(5b - 8)S_1 - \frac{4b^2(40b^4 - 72b^3 + 31b^2 + 1)}{72}.$$

The matrices  $(S_i(\pi))_{\pi; i=0,1,2,3}$  are of full rank for  $b = 20, \dots, 35$  and any choices of  $\pi$ . Furthermore all right hand side vectors  $A_0(\pi)$  evaluate to zero. So finally we obtain that all  $p_i$  are identically zero, and thus  $A_0 = 0$  and the same holds for  $A$ .  $\square$

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