General discrepancy estimates II: the Haar function system

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1. Introduction. Discrepancy is the central quantitative concept of the theory of uniform distribution of sequences modulo one. It measures how well the empirical distribution of a set $\mathcal{P} = \{\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_{N-1}\}$ in $[0, 1]^s$, $s \geq 1$, approximates uniform distribution on the *s*-dimensional unit cube (see [3]). The most important notion is the rectangle discrepancy.

DEFINITION 1. Let \mathcal{P} be a finite point set in $[0,1]^s$, $\mathcal{P} = \{\mathbf{x}_0, \mathbf{x}_1, \dots, \dots, \mathbf{x}_{N-1}\}$. The (extreme) rectangle discrepancy $D_N(\mathcal{P})$ of \mathcal{P} is defined as

$$D_N(\mathcal{P}) := \sup_{J \in \mathcal{J}} \left| \frac{A(J,N)}{N} - \lambda_s(J) \right|.$$

Here \mathcal{J} denotes the class of all subintervals of $[0,1[^s \text{ of the form } J = \prod_{i=1}^s [u_i, v_i]; A(J, N)$ represents the number of $n, 0 \leq n < N$, for which $\mathbf{x}_n \in J$; and λ_s stands for Lebesgue measure on $[0,1]^s$.

Discrepancy is a numerical quantity that has found numerous interesting applications. The latter range from the assessment of pseudorandom number generators to error bounds for integration methods in higher dimensions. For a comprehensive exposition of the current state of research in these fields of numerical analysis, the reader is referred to the monograph of Niederreiter [8].

In applications we are restricted to finite rational point sets \mathcal{P} : when using computers we have to cope with finite precision arithmetics. Niederreiter [4, 8] proved a general theorem to estimate the rectangle discrepancy for this kind of point sets. This estimate is the very basis of the *serial test*, the most important theoretical criterion in pseudorandom number generation.

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The surveys of Eichenauer-Herrmann [1] and of Niederreiter [6, 7] contain extensive references. In Niederreiter's theorem, the rectangle discrepancy $D_N(\mathcal{P})$ is estimated by exponential sums. In [2], we have presented a new approach to this result. The method is based on the Walsh function system.

In this paper, we shall obtain estimates for the rectangle discrepancy in terms of Haar functions. These functions constitute one of the most important orthonormal systems of harmonic analysis. Their use in the quantitative theory of uniform distribution of sequences modulo one is not new. The monograph of Sobol' [10] contains a thorough discussion of quasi-Monte Carlo integration with the Haar function system.

We have based our technique on Fourier analysis with respect to the Haar system. The interested reader will find an outline of our approach in the proof of Theorem 1. The method is interesting in itself. It is open to generalizations.

2. Dyadic expansions and Haar functions. The Haar system is best presented in the terminology of dyadic expansions of real numbers. For a nonnegative integer k, let

$$k = \sum_{j=0}^{\infty} k_j \, 2^j, \quad k_j \in \{0, 1\},$$

be the unique dyadic expansion of k in base 2. Every number $x \in [0, 1]$ has a unique dyadic expansion

$$x = \sum_{j=0}^{\infty} x_j \, 2^{-j-1}, \quad x_j \in \{0, 1\},$$

under the condition that $x_j \neq 1$ for infinitely many j. In the following, this uniqueness condition will be assumed without further notice.

Notation. (i) Let $x \in [0, 1[$, with dyadic expansion $x = 0.x_0x_1...$, and let k be a nonnegative integer, $k = \sum_{j=0}^{\infty} k_j 2^j$. For $g \in \mathbb{N}$ we define

$$x(g) := 0.x_0 x_1 \dots x_{g-1}, \quad k(g) := \sum_{j=0}^{g-1} k_j 2^j$$

Then $x(g) \in \{a2^{-g} : 0 \le a < 2^g\}$ and $k(g) \in \{0, 1, \dots, 2^g - 1\}$. Further, put $x(0) := 0, \quad k(0) := 0.$

(ii) An interval of the form $[a2^{-g}, (a+1)2^{-g}], 0 \le a < 2^g, g \ge 0, a$ and g integers, is called an *elementary dyadic interval of length* 2^{-g} . A subinterval I of the s-dimensional torus $[0,1]^s$ is called an *elementary dyadic interval* if

it has the form

$$I = \prod_{i=1}^{s} [a_i 2^{-g_i}, (a_i + 1)2^{-g_i}],$$

with integers a_i and g_i , $0 \le a_i < 2^{g_i}$, $g_i \ge 0$.

(iii) Let $b_0, b_1, \ldots, b_{q-1}$ be arbitrary digits in $\{0, 1\}$. Let

$$I(b_0, b_1, \dots, b_{g-1}) := \{ x \in [0, 1[: x_j = b_j, \ \forall j : 0 \le j < g \}$$

denote the cylinder set of order g defined by $b_0, b_1, \ldots, b_{g-1}$. Then, for any elementary dyadic interval $I = [a2^{-g}, (a+1)2^{-g}]$ of length $2^{-g}, g \in \mathbb{N}$, there is a unique cylinder set $I(b_0, b_1, \ldots, b_{g-1})$ such that

$$I = I(b_0, b_1, \ldots, b_{g-1}).$$

We only have to observe that $a2^{-g} = 0.b_0b_1...b_{g-1}$ with suitable digits b_j .

The Haar functions constitute an important and widely used orthonormal function system in harmonic analysis. For the theory, the reader is referred to the monograph of Schipp *et al.* [9].

DEFINITION 2. Let $\{h_k : k \ge 0\}$ denote the system of Haar functions on the interval [0,1]. The k-th Haar function h_k is defined as follows:

$$h_0(x) := 1 \quad \forall x \in [0, 1[$$

If $k \ge 1, 2^g \le k < 2^{g+1}, k = 2^g + m, 0 \le m < 2^g$, then

$$h_k(x) := \begin{cases} 2^{g/2}, & x \in [m2^{-g}, m2^{-g} + 2^{-g-1}[, \\ -2^{g/2}, & x \in [m2^{-g} + 2^{-g-1}, (m+1)2^{-g}[, \\ 0, & \text{otherwise.} \end{cases}$$

Let H_k denote the k-th normalized Haar function,

$$H_k := 2^{-g/2} h_k$$
 if $2^g \le k < 2^{g+1}, g \ge 0$, and $H_0 := h_0$.

Remark 1. (i) We note that the number m in the definition of h_k is just the integer k(g).

(ii) The function H_k takes only the values -1, 0 and 1.

DEFINITION 3. Let $\{h_{\mathbf{k}} : \mathbf{k} = (k_1, k_2, \dots, k_s), k_i \geq 0\}$ denote the system of Haar functions on the *s*-dimensional torus $[0, 1]^s$. The **k**-th Haar function $h_{\mathbf{k}}$ is defined as

$$h_{\mathbf{k}}(\mathbf{x}) := \prod_{i=1}^{s} h_{k_i}(x_i), \quad \mathbf{x} = (x_1, \dots, x_s) \in [0, 1]^s.$$

In analogy to Definition 2, let

$$H_{\mathbf{k}}(\mathbf{x}) := \prod_{i=1}^{s} H_{k_i}(x_i), \quad \mathbf{x} = (x_1, \dots, x_s) \in [0, 1[^s, 1])$$

denote the **k**-th normalized Haar function on $[0, 1]^s$.

DEFINITION 4. Let h_k be the kth Haar function on [0, 1]. We define the fundamental domain D_k of h_k as the elementary dyadic interval

$$D_k := [k(g)2^{-g}, (k(g)+1)2^{-g}[$$

if $2^g \le k < 2^{g+1}$. For k = 0 we define $D_0 := [0, 1]$.

The fundamental domain $D_{\mathbf{k}}$ of the **k**-th Haar function $h_{\mathbf{k}}$ on $[0, 1[^{s}, \mathbf{k} = (k_{1}, \ldots, k_{s}))$, is defined to be the elementary dyadic interval

$$D_{\mathbf{k}} := \prod_{i=1}^{s} D_{k_i}.$$

Remark 2. The functions $h_{\mathbf{k}}$ and $H_{\mathbf{k}}$ vanish outside the fundamental domain $D_{\mathbf{k}}$ of $h_{\mathbf{k}}$.

The Haar coefficients of an integrable function f defined on [0, 1] will be denoted by $\hat{f}(k)$,

$$\widehat{f}(k) := \int_{[0,1[} f(x) h_k(x) dx.$$

Accordingly, the Haar coefficients of an integrable function f defined on $[0,1]^s$ will be denoted by $\hat{f}(\mathbf{k})$,

$$\widehat{f}(\mathbf{k}) := \int_{[0,1[^s]} f(\mathbf{x}) h_{\mathbf{k}}(\mathbf{x}) d\mathbf{x}$$

3. The discrepancy estimate. In step 3 of the proof of Theorem 1 we shall have to estimate the Haar coefficients of characteristic functions of certain subintervals of $[0, 1]^s$. For the necessary calculations, the reader will be referred to Lemmas 1–3.

LEMMA 1. Let $f(x) := \mathbf{1}_I(x) - \lambda(I)$, where I is a subinterval of the interval [0, 1].

(i) If I is an elementary dyadic interval of length $2^{-\alpha}$, then $\hat{f}(k) = 0$ for all $k \geq 2^{\alpha}$.

(ii) $IfI = [0, \beta], 0 < \beta < 1$, then $\widehat{f}(0) = 0$ and, for all k in the range $2^g \leq k < 2^{g+1}, g \geq 0$,

$$\widehat{f}(k) = \begin{cases} 2^{g/2}(\beta - \beta(g+1)) & \text{if } 2^g\beta(g) = k(g) \text{ and } \beta_g = 0, \\ 2^{g/2}(2^{-g-1} - (\beta - \beta(g+1))) & \text{if } 2^g\beta(g) = k(g) \text{ and } \beta_g = 1, \\ 0 & \text{if } 2^g\beta(g) \neq k(g). \end{cases}$$

Proof. Part (i) is shown as follows. Let $2^g \leq k < 2^{g+1}$, with $g \geq \alpha$. Define the digits a_0, \ldots, a_{g-1} by

$$0.a_0 \dots a_{g-1} := k(g)/2^g.$$

The Haar function h_k is zero outside its fundamental domain $D_k = I(a_0, \ldots, a_{g-1})$, which is an elementary dyadic interval of length 2^{-g} . Now, let

I be an arbitrary elementary dyadic interval of length $2^{-\alpha}$. If I does not contain D_k , then it is evident that $\hat{f}(k) = 0$. If D_k is a subinterval of I, then

$$\widehat{f}(k) = \int_{I} h_k(x) \, dx = \int_{D_k} h_k(x) \, dx = \int_{0}^{1} h_k(x) \, dx = 0.$$

To prove part (ii), consider k such that $2^g \le k < 2^{g+1}$, $g \ge 0$. From part (i) we deduce that

$$\widehat{f}(k) = \int_{\beta(g)}^{\beta} h_k(x) \, dx$$

The result follows easily. \blacksquare

LEMMA 2. Let $f(x) := \mathbf{1}_I(x) - \lambda(I)$, where $I = [a2^{-\alpha}, b2^{-\alpha}], 0 \le a < b \le 2^{\alpha}, \alpha \ge 1$, with integers a, b and α . Define $\beta' := a2^{-\alpha}$ and $\beta'' := b2^{-\alpha}$. Then, for all k such that $2^g \le k < 2^{g+1}, g < \alpha$,

$$|\widehat{f}(k)| \begin{cases} = 0 & \text{if } k(g) \notin \{2^{g}\beta'(g), 2^{g}\beta''(g)\}, \\ \leq 2^{-1-g/2} & \text{if } k(g) \in \{2^{g}\beta'(g), 2^{g}\beta''(g)\}. \end{cases}$$

Proof. We have $\hat{f}(0) = 0$ and, for all $k \ge 1$,

$$\widehat{f}(k) = \widehat{\mathbf{1}}_{I}(k) = \widehat{\mathbf{1}}_{[0,\beta''[}(k) - \widehat{\mathbf{1}}_{[0,\beta'[}(k)$$

If $b = 2^{\alpha}$, i.e. $\beta'' = 1$, then $\widehat{\mathbf{1}}_{[0,\beta''[}(k) = 0$ for all $k \ge 1$. The result follows directly from Lemma 1. If $b < 2^{\alpha}$, then we have to consider two cases. In the first case, if k(g) equals neither $2^{g}\beta'(g)$ nor $2^{g}\beta''(g)$, then $\widehat{f}(0) = 0$. If k(g) equals exactly one of these two numbers, we can apply Lemma 1 directly. If $k(g) = 2^{g}\beta'(g) = 2^{g}\beta''(g)$, then a short calculation gives the result.

Remark 3. In Lemma 2, we have proved the following. There are at most two numbers k in $[2^g, 2^{g+1}]$ such that $\widehat{f}(k) \neq 0$. If k equals one of them, then $|\widehat{f}(k)| \leq 2^{-g/2-1}$.

DEFINITION 5. Let k be a nonnegative integer. Define

(i)
$$\varrho_{\text{Haar}}(k) := \begin{cases} 1 & \text{if } k = 0, \\ 2^{-g/2} & \text{if } 2^g \le k < 2^{g+1}, \ g \ge 0, \end{cases}$$

(ii)
$$\varrho_{\text{Haar}}^{\text{rect}}(k) := \begin{cases} 1 & \text{if } k = 0, \\ 2^{-g/2-1} & \text{if } 2^g \le k < 2^{g+1}, g \ge 0 \end{cases}$$

(iii) If $\mathbf{k} = (k_1, \dots, k_s)$ with nonnegative integer coordinates k_i , then let

$$\varrho_{\mathrm{Haar}}(\mathbf{k}) := \prod_{i=1}^{s} \varrho_{\mathrm{Haar}}(k_i),$$

and, analogously,

$$\varrho_{\text{Haar}}^{\text{rect}}(\mathbf{k}) := \prod_{i=1}^{s} \varrho_{\text{Haar}}^{\text{rect}}(k_i).$$

Remark 4. We observe that $H_{\mathbf{k}} = \rho_{\text{Haar}}(\mathbf{k})h_{\mathbf{k}}$.

LEMMA 3. Let $f(\mathbf{x}) := \mathbf{1}_G(\mathbf{x}) - \lambda_s(G)$, where

$$G := \prod_{i=1}^{s} \left[\frac{a_i}{2^{\alpha}}, \frac{b_i}{2^{\alpha}} \right], \quad 0 \le a_i < b_i \le 2^{\alpha},$$

is a subinterval of $[0,1]^s$. Define

$$\Delta := \{ \mathbf{k} \in \mathbb{Z}^s : 0 \le k_i < 2^\alpha \ \forall i \} \quad and \quad \Delta^* := \Delta \setminus \{ \mathbf{0} \}.$$

Then:

(i) For all $\mathbf{k} \in \mathbb{Z}^s \setminus \Delta^*$ with nonnegative coordinates k_i , $1 \le i \le s$, we have $|\widehat{f}(\mathbf{k})| = 0$.

(ii) For all $\mathbf{k} \in \Delta^*$, $|\widehat{f}(\mathbf{k})| \le \varrho_{\text{Haar}}^{\text{rect}}(\mathbf{k})$.

Proof. Let $\mathbf{k} = (k_1, \dots, k_s)$. We have $\widehat{f}(\mathbf{0}) = 0$ and, for all $\mathbf{k} \neq \mathbf{0}$, $\widehat{f}(\mathbf{k}) = \widehat{\mathbf{1}}_G(\mathbf{k})$. Further, $\widehat{\mathbf{1}}_G(\mathbf{k}) = \prod_{i=1}^s \widehat{\mathbf{1}}_{G_i}(k_i)$, where $G_i := [a_i q^{-\alpha}, b_i q^{-\alpha}]$. The result follows directly from Lemma 2.

THEOREM 1. Let $\mathcal{P} = {\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_{N-1}}$ be a finite point set in $[0, 1]^s$, with \mathbf{x}_n of the form $\mathbf{x}_n = \mathbf{y}_n / M \mod 1$, $\mathbf{y}_n \in \mathbb{Z}^s$. Suppose that $M = 2^{\alpha}$, with some positive integer α . Let

(1)
$$S_N(H_{\mathbf{k}}) := \frac{1}{N} \sum_{n=0}^{N-1} H_{\mathbf{k}}(\mathbf{x}_n),$$

 $H_{\mathbf{k}}$ the **k**-th normalized Haar function on $[0, 1]^{s}$. Let

$$B := \sup_{\mathbf{k}\in\Delta^*} |S_N(H_{\mathbf{k}})|,$$

where the domain Δ^* has been defined in Lemma 3. Then

(2)
$$D_N(\mathcal{P}) \le 1 - \left(1 - \frac{1}{M}\right)^s + B\left(\log_2 M + \frac{1}{2}\right)^s$$

R e m a r k 5. The numerical quantity $B = B(\mathcal{P})$ is closely related to the *nonuniformity* $\varphi_{\infty}(\mathcal{P})$ of the point set \mathcal{P} . The nonuniformity is a measure of the evenness of the distribution of \mathcal{P} in $[0, 1]^s$. It has been introduced by Sobol' (see [10, 11, 5]). Its definition is as follows:

$$\varphi_{\infty}(\mathcal{P}) := N \sup_{\mathbf{k} \neq \mathbf{0}} |S_N(H_{\mathbf{k}})|.$$

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Hence $B \leq (1/N)\varphi_{\infty}(\mathcal{P})$. It is known that

$$\frac{1}{N}\varphi_{\infty}(\mathcal{P}) \le 2^{s}D_{N}(\mathcal{P})$$

(see [5, inequality (2.8), p. 968]). Inequality (2) yields an upper bound for $D_N(\mathcal{P})$ in terms of $\varphi_{\infty}(\mathcal{P})$:

$$D_N(\mathcal{P}) \le 1 - \left(1 - \frac{1}{M}\right)^s + \frac{1}{N}\varphi_{\infty}(\mathcal{P})\left(\log_2 M + \frac{1}{2}\right)^s.$$

Proof of Theorem 1. For an arbitrary Borel subset E of $\left[0,1\right[^s$ we define

$$R_N(E) := \frac{1}{N} \sum_{n=0}^{N-1} (\mathbf{1}_E(\mathbf{x}_n) - \lambda_s(E)) \quad \left(= \frac{A(E,N)}{N} - \lambda_s(E) \right).$$

The proof of Theorem 1 is structured as follows:

Step 1: Discretization of the problem: we approximate an arbitrary subinterval C of $[0, 1]^s$ by an appropriate set G.

Step 2: Estimation of the discretization error $|R_N(C) - R_N(G)|$.

Step 3: Estimation of $|R_N(G)|$.

Step 1. Let C be an arbitrary subinterval of $[0, 1]^s$. We define

$$\Gamma := \frac{1}{M} \mathbb{Z}^s \bmod 1.$$

For a point $\mathbf{p} \in \Gamma$, $\mathbf{p} = (p_1, \ldots, p_s)$, we let

$$I_{\mathbf{p}} := \prod_{i=1}^{s} \left[p_i, p_i + 1/M \right[$$

denote the elementary dyadic interval of sidelength M^{-1} defined by the point **p**. We approximate C by a finite union G of elementary dyadic intervals $I_{\mathbf{p}}$:

(3)
$$G := G(C) := \bigcup_{\mathbf{p} \in \Gamma \cap C} I_{\mathbf{p}}.$$

Let us consider the following *discretization principle*:

$$|R_N(C)| \le |R_N(C) - R_N(G)| + |R_N(G)|.$$

We observe that

$$A(C,N) = A(G,N).$$

Hence the *discretization error* is given by

$$|R_N(C) - R_N(G)| = |\lambda_s(C) - \lambda_s(G)|.$$

Step 2. C is a subinterval of $[0, 1]^s$,

$$C = \prod_{i=1}^{s} [u_i, v_i], \quad 0 \le u_i < v_i \le 1.$$

We consider two subcases. The idea stems from Niederreiter [8, Proof of Theorem 3.10, p. 34].

Case 1: $G = \emptyset$. In this case, there is some $i, 1 \leq i \leq s$, such that $v_i - u_i < 1/M$. But then

$$|R_N(C)| = \lambda_s(C) < \frac{1}{M} \le 1 - \left(1 - \frac{1}{M}\right)^s.$$

Hence the estimate (2) trivially holds.

Case 2: $G \neq \emptyset$. Then G is an s-dimensional subinterval of the form

$$G := \prod_{i=1}^{s} \left[\frac{a_i}{M}, \frac{b_i}{M} \right]$$

where

$$a_i := \min\{a \in \{0, 1, \dots, M - 1\} : u_i \le a/M\}$$

$$b_i := \min\{a \in \{1, \dots, M\} : v_i \le a/M\}.$$

Lemma 3.9 in [8] implies the following bound for the discretization error:

$$|\lambda_s(C) - \lambda_s(G)| \le 1 - \left(1 - \frac{1}{M}\right)^s.$$

S t e p = 3. Lemma 3(i) implies that the function

$$f(\mathbf{x}) := \mathbf{1}_G(\mathbf{x}) - \lambda_s(G)$$

is a Haar polynomial. In other words, the Haar series of f is finite. We have

(4)
$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \Delta^*} \widehat{\mathbf{1}}_G(\mathbf{k}) h_{\mathbf{k}}(\mathbf{x}) \quad \forall \mathbf{x} \in [0, 1]^s$$

From this identity it follows that

(5)
$$R_N(G) = \sum_{\mathbf{k}\in\Delta^*} \widehat{\mathbf{1}}_G(\mathbf{k}) S_N(h_{\mathbf{k}}),$$

where

(6)
$$S_N(h_{\mathbf{k}}) := \frac{1}{N} \sum_{n=0}^N h_{\mathbf{k}}(\mathbf{x}_n).$$

Consider the set

$$\Delta(\mathbf{g}) := \{ \mathbf{k} \in \mathbb{Z}^s : \forall i, \ 1 \le i \le s : 2^{g_i} \le k_i < 2^{g_i+1} \},\$$

where $\mathbf{g} = (g_1, \ldots, g_s) \in \mathbb{Z}^s$, and all coordinates g_i are nonnegative. From Remark 3 we know that there are at most $2^{\sharp\{i:g_i \geq 1\}}$ points \mathbf{k} in the set $\Delta(\mathbf{g})$

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such that $\widehat{\mathbf{1}}_G(\mathbf{k}) \neq 0$. We deduce from Lemma 3(ii) that

$$|\widehat{\mathbf{1}}_G(\mathbf{k})| \le 2^{-s} \prod_{i=1}^s 2^{-g_i/2} \quad \forall \, \mathbf{k} \in \Delta(\mathbf{g})$$

Further, we observe that

$$H_{\mathbf{k}} = \prod_{i=1}^{s} 2^{-g_i/2} h_{\mathbf{k}} \quad \forall \, \mathbf{k} \in \Delta(\mathbf{g})$$

We now consider a suitable partition of the summation domain Δ^* . For $u, 0 \leq u < s$, let

$$\Delta_u := \{ \mathbf{k} \in \Delta^* : \sharp \{ i : k_i = 0 \} = u \}.$$

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Then

$$\Delta^* = \bigcup_{u=0}^{s-1} \Delta_u \quad \text{(disjoint union)}.$$

Let

$$\Box := \{ \mathbf{g} \in \mathbb{Z}^s : \forall i, 1 \le i \le s : 0 \le g_i < \alpha \},$$

and, for $t, 0 \le t \le s$,
$$\Box := \{ \mathbf{g} \in \Box : \sharp \{i: a_i = 0\} = t \}$$

$$\Box_t := \{ \mathbf{g} \in \Box : \sharp \{ i : g_i = 0 \} = t \}.$$

Then

$$\Delta_0 = \bigcup_{t=0}^s \bigcup_{\mathbf{g} \in \square_t} \Delta(\mathbf{g}) \quad \text{(disjoint union)}.$$

As a consequence,

$$\Big|\sum_{\mathbf{k}\in\Delta_0}\widehat{\mathbf{1}}_G(\mathbf{k})\,S_N(h_{\mathbf{k}})\Big|\leq B\sum_{t=0}^s 2^{-t}\sharp\Box_t=B\left(\alpha-\frac{1}{2}\right)^s.$$

In the very same manner we obtain the estimate

$$\Big|\sum_{\mathbf{k}\in\Delta_u}\widehat{\mathbf{1}}_G(\mathbf{k})S_N(h_{\mathbf{k}})\Big|\leq B\binom{s}{u}\left(\alpha-\frac{1}{2}\right)^{s-u}.$$

This ends the proof of Theorem 1. \blacksquare

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