Discrete charging of metallic grains: Statistics of addition spectra

Yshai Avishai∗, Daniel Berend† and Luba Bromberg‡

Abstract

We analyze the statistics of electrostatic energies (and their differences) for a quantum dot system composed of a finite number $K$ of electron islands (metallic grains) with random capacitance-inductance matrix $C$, for which the total charge is discrete, $Q = Ne$ (where $e$ is the charge of an electron and $N$ is an integer). The analysis is based on a generalized charging model, where the electrons are distributed among the grains such that the electrostatic energy $E(N)$ is minimal. Its second difference (inverse compressibility) $\chi_N = E(N + 1) - 2E(N) + E(N - 1)$ represents the spacing between adjacent Coulomb blockade peaks appearing when the conductance of the quantum dot is plotted against gate voltage. The statistics of this quantity has been the focus of experimental and theoretical investigations during the last two decades. We provide an algorithm for calculating the distribution function corresponding to $\chi_N$ and show that this function is piecewise polynomial.

1 Introduction

The physics exposed in the addition spectra of quantum dots is rather rich, and hence its investigation is at the focus of both experimental and theoretical studies. After the origin of Coulomb-blockade peaks has been elucidated,

∗Departments of Physics, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel
†Departments of Mathematics and Computer Science, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel
‡Department of Mathematics, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel
investigation is directed toward more subtle questions such as their heights, widths, and spacings. The underlying physics is related to the ground-state energy, chemical potential, and inverse compressibility of quantum dots composed of a few metallic electron islands coupled capacitively and inductively to each other.

The present work concentrates on the distribution of spacings between Coulomb-blockade peaks in large semiconductor quantum dots. In particular, we are interested in fluctuations of these quantities with the number \( N \) of electrons on the dot. The main problem can be stated as follows: According to the simplest picture (charging model), in which the quantum dot is regarded as a single-electron island whose coupling with the leads is through its capacitance \( C \), the total potential energy of a quantum dot with \( N \) electrons and charge \( Q = Ne \) is \( Q^2/2C - V_gQ \), where \( V_g \) is the gate voltage and \( e \) is the electron charge. The position of the \( N \)-th Coulomb-blockade peak occurs at a gate voltage \( V_g = Ne^2/C \). This peak position is then a linear function of \( N \), and therefore the spacing between two adjacent peaks should be a constant \( e^2/C \), independent of \( N \). This is not always confirmed experimentally. The situation is even more intriguing if the quantum dot is large and might contain more than a single electron puddle. As indicated in a series of recent experiments [1], the spacing between adjacent Coulomb blockade peaks occasionally vanishes; namely, Coulomb blockade peaks tend to bunch. The problem is therefore to explain why the results predicted from a simple charging model deviate substantially from the experimental observation.

In [2], a generalized charging model has been tested, where it is assumed that the large dot used in the experiments [1] could be divided into a set of potential wells (metallic grains) with random capacitances and random mutual inductances. This casts the question of Coulomb blockade peak spacing distribution into the problem of elucidating the statistics of the addition spectrum of a relatively simple physical system. It consists of \( K \) metallic grains (or capacitors), such that the number of electrons on the \( i \)-th grain
is \( n_i \) \((i = 1, 2, \ldots, K)\), the total number of electrons being \( N \). The charging model for such a system (at zero temperature) is based on the assumption that the distribution of electrons among the grains is determined by requiring that the electrostatic energy \( E(N) \) of a dot containing \( N \) electrons is minimal. It is useful at this point to recall the basic facts pertaining to the energy of the electrostatic field of conductors [4]. The electrostatic energy of the system is a bilinear form in the numbers \( n_i \). This form is given by a \( K \times K \) matrix \( W = \frac{1}{2}C^{-1} \). Here \( C \) (matrix elements \( c_{ij}; \ i, j = 1, 2 \ldots K \)) is a positive-definite symmetric matrix of capacitance and inductance coefficients. Physically, the matrix \( C \) has positive diagonal entries and negative (more precisely, non-positive) non-diagonal entries [4],

\[
c_{ij} = c_{ji}, \quad c_{ii} > 0, \quad c_{ij} \leq 0 \ (i \neq j).
\]  

(1)

On the other hand, all the elements of \( C^{-1} \) are non-negative. More precisely, with \( w_{ij}; \ i, j = 1, 2 \ldots K \) the elements of the matrix \( W = \frac{1}{2}C^{-1} \), one has,

\[
w_{ii} > 0, \quad w_{ij} \geq 0 \ (i \neq j).
\]  

(2)

The off-diagonal entries \( c_{ij}, i \neq j \), decay as an inverse power of the distance between the grains, while the diagonal entries \( c_{ii} \) are proportional to the geometrical size of the grains. The notion of randomness enters when we recall that experimentally, the sizes of the grains, as well as the distances between them, are random quantities. This means that the elements of the matrix \( C \) are random numbers (subject, of course, to the required symmetries (1)). The spacing between Coulomb blockade peaks is equal to the second difference of the ground state energy. In other words, the distribution of spacing peaks is determined by the statistics of the inverse compressibility,

\[
\chi_N \equiv E(N + 1) - 2E(N) + E(N - 1).
\]  

(3)

When two Coulomb blockade peaks coincide, the second difference \( \chi_N \) vanishes. Note that, on the average (and on a large scale), the energy \( E(N) \) grows
quadratically with \( N \). Therefore, one would expect the second difference to stay finite and \( N \) independent. However, there is no simple relation such as 
\[ E(N) = aN + bN^2. \]
The deviation of \( E(N) \) from exact quadratic behavior makes its second difference \( \chi_N \) non-constant, and a fluctuating quantity. It is precisely these fluctuations which we intend to study. As we shall see, the fact that electron charge is quantized makes this task non-trivial.

Having explained the physical motivation, we then pose the mathematical problem: what is the distribution \( p(\chi) \) of inverse compressibility for a given system of metallic grains with random capacitive matrix \( C \)? As a crude approximation it was assumed in [3] that the metallic grains are indeed very far apart, and the matrix \( C \) is nearly diagonal, its \( K \) diagonal elements (capacitances) being random numbers. The energy of the system in the diagonal case is given by
\[
E(N) = \min \sum_{i=1}^{K} \frac{1}{2c_i} n_i^2, \quad \text{(subject to } \sum_{i=1}^{K} n_i = N). \tag{4}
\]

The minimum in (4) is taken over all possible partitions \((n_i)_{i=1}^{K}\) of \( N \). It was first proved that the minimum problem (4) has the following convenient feature: If \( n_1, n_2, \ldots, n_K \) are the argument values bringing \( E(N) \) to its minimal value for some \( N \), then the minimum for \( N + 1 \) is obtained by retaining all \( n_i \)'s, except for one which is increased by 1. This allowed an exact determination of the distribution function according to which the sequence \( \chi_N \) is distributed. For a random set of capacitors \((c_1, c_2, \ldots, c_K - \text{random numbers with probability distribution } P(c_1, c_2, \ldots, c_K))\), the distribution of the inverse compressibility \( F(\chi) \) was calculated in [3].

Our next goal is to study this problem for general positive-definite matrices \( C \). The problem turns out to be quite harder. To begin with, it is no longer true that the optimal solution for \( N + 1 \) is obtained in a simple manner from that for \( N \). That is, for each \( N \) we need to re-distribute the \( N \) electrons between the grains, and it may well happen that, although the \( n_i \)'s grow in general with \( N \), some of them will actually decrease infinitely of-
ten as $N$ increases by 1 each time. Namely, there will exist infinitely many values of $N$ for which the optimal value of some $n_i$ decreases as $N$ grows to $N+1$. Thus, the problem entails new behavioral patterns with respect to the diagonal case.

Our main result in this paper is an algorithm for calculating the distribution function corresponding to $(\chi_N)$. Moreover, we show that this function is piecewise polynomial. We state the result in Section 2. Section 3 is a short digression, discussing a few notions which arise in the proof. The proof of the main theorem is given in Section 4.

## 2 The Main Results

Mathematically, our problem is as follows. Let $C = (c_{ij})_{i,j=1}^K$ be a positive-definite matrix, with positive diagonal elements and non-positive off-diagonal elements. Assume that the sum of elements in every row of $C$ is positive and that all entries of $\frac{1}{2}C^{-1} = W = (w_{ij})_{i,j=1}^K$ are non-negative. Put

$$E(N) = \min \left\{ \sum_{i,j=1}^K w_{ij}n_in_j : n_i \in \mathbb{Z}_+, \sum_{i=1}^K n_i = N \right\}, \quad N \in \mathbb{N},$$

(5)

where $\mathbb{N}$ is the set of positive integers and $\mathbb{Z}_+ = \mathbb{N} \cup \{0\}$. We want to understand the statistical behavior of the sequence $E(N)$, and in particular that of the second difference sequence

$$\chi_N = E(N+1) - 2E(N) + E(N-1).$$

(6)

To formulate our main result, we need a few definitions and notations.

**Definition 2.1** Let $(x_n)_{n=1}^\infty$ be a sequence of real numbers and $F$ a distribution function. The sequence $(x_n)$ is *asymptotically $F$-distributed* if

$$\left| \frac{\{1 \leq n \leq M : x_n \leq x\}}{M} \right| \xrightarrow{M \to \infty} F(x)$$
for every continuity point $x$ of $F$ (where $|S|$ denotes the cardinality of a finite set $S$).

The definition almost coincides with [5, p.53, Def. 7.1], except that there the sequence $(x_n)$ is considered only modulo 1. Note that a sequence need not be asymptotically $F$-distributed for some $F$, as the following example shows.

Example 2.1 The sequence of numbers

$$0, \underbrace{1, \ldots, 1}_{10}, \underbrace{0, \ldots, 0}_{10^2}, \underbrace{1, \ldots, 1}_{10^3}, \ldots$$

is not asymptotically $F$-distributed for any $F$.

A stronger notion is obtained when we require not only long initial block of the sequence to behave approximately according to $F$, but rather require any long block to behave so. This leads to the following definition ([5, p.40, Def. 5.1] and [5, p.200, Def. 3.2].)

Definition 2.2 In the setup of Definition 2.1, $(x_n)$ is asymptotically well $F$-distributed if

$$\frac{|\{L < n \leq M : x_n \leq x\}|}{M - L} \xrightarrow{M - L \to \infty} F(x)$$

for every continuity point $x$ of $F$.

The following example demonstrates that the property of asymptotic well $F$-distribution is indeed strictly stronger than that of asymptotic $F$-distribution.

Example 2.2 The sequence of numbers

$$\underbrace{0, \ldots, 1}_{12}, \underbrace{0, 0}_{2}, \underbrace{1, 1}_{3}, \underbrace{0, 0, 0}_{3}, \underbrace{1, 1, 1}_{3}, \ldots$$
is asymptotically $F$-distributed, where $F$ is the distribution function

$$F(x) = \begin{cases} 
0, & x < 0, \\
\frac{1}{2}, & 0 \leq x < 1, \\
1, & x \geq 1, 
\end{cases}$$

but it is not asymptotically well $F$-distributed.

**Definition 2.3** A function $g : \mathbb{R} \to \mathbb{R}$ is *piecewise polynomial* if there exist intervals (finite or infinite) $I_j \subseteq \mathbb{R}$ and polynomials $Q_j$, $1 \leq j \leq m$, such that

$$g(x) = Q_j(x), \quad x \in I_j, \ 1 \leq j \leq m.$$ 

The *degree* of $g$ is $\max_{1 \leq j \leq m} \deg Q_j$.

Returning to our problem, let $b_i = \sum_{j=1}^{K} c_{ij}$, $1 \leq i \leq K$, be the row sums of the matrix $C$. Since the matrix $C$ is random, in the generic case the numbers $b_1, b_2, ..., b_K$ are linearly independent over the rationals. (That is, considered as vectors in the space $\mathbb{R}$ over the field of rational numbers $\mathbb{Q}$, they are independent.)

Now we can formulate our main result.

**Theorem 2.1** Let $C$ be a positive-definite symmetric matrix, with positive row sums $b_1, b_2, ..., b_K$ and let $W = \frac{1}{2}C^{-1}$. Suppose that $b_1, b_2, ..., b_K$ are linearly independent over the rationals. Then the sequence $(\chi_N)_{N=1}^{\infty}$ of the second differences, defined via (5) and (6), is asymptotically well $F$-distributed, where $F$ is a continuous piecewise polynomial function of degree at most $K - 1$, which can be effectively computed.

As mentioned in the introduction, a phenomenon which occurs in the general case dealt with here, but not in the special case of diagonal matrices $C$, is that, as we pass from $N$ to $N + 1$, there may be re-distribution of the $n_i$'s in the optimal solution. The following example is to that effect.
Example 2.3 Let
\[ C = \begin{pmatrix} 2 & 0 & -1 \\ 0 & 2 & -1 \\ -1 & -1 & 3 \end{pmatrix}, \quad W = \frac{1}{2} C^{-1} = \frac{1}{16} \begin{pmatrix} 5 & 1 & 2 \\ 1 & 5 & 2 \\ 2 & 2 & 4 \end{pmatrix}. \]

Then:
\[ E(N) = \frac{1}{16} \min_{n_1+n_2+n_3=N, n_i \geq 0} (5n_1^2 + 2n_1n_2 + 4n_1n_3 + 5n_2^2 + 4n_2n_3 + 4n_3^2). \]

Using the techniques in the beginning of Section 4, it is easy to verify that the optimal values of \( n_1, n_2, n_3 \) are given by
\[
(n_1, n_2, n_3) = \begin{cases} 
\left( \frac{N}{3}, \frac{N}{3}, \frac{N}{3} \right), & N \equiv 0 \pmod{3}, \\
\left( \frac{N-1}{3}, \frac{N-1}{3}, \frac{N+2}{3} \right), & N \equiv 1 \pmod{3}, \\
\left( \frac{N+1}{3}, \frac{N+1}{3}, \frac{N-2}{3} \right), & N \equiv 2 \pmod{3}.
\end{cases}
\]

Thus, for any non-negative integer \( K \), when passing from \( N = 3k + 1 \) to \( N = 3k + 2 \), the value of \( n_3 \) at the optimal point decreases from \( k+1 \) to \( k \).

3 Uniform Distribution Modulo 1

In this section we briefly discuss the notion of uniform distribution modulo 1 and recall a few related results, which will be needed in the proof of the Theorem 2.1.

Definition 3.1 A sequence \((x_n)_{n=1}^{\infty}\) of real numbers is uniformly distributed modulo 1 if
\[
\frac{|\{1 \leq n \leq N : a \leq \{x_n\} < b\}|}{N} \to b - a, \quad 0 \leq a < b \leq 1,
\]
where \( \{t\} \) is the fractional part of a real number \( t \) ([5, p.1, Def. 1.1]).

In terms of Definition 2.1 \((x_n)\) is uniformly distributed modulo 1 if and only if the sequence \((\{x_n\})\) of fractional parts is \(F\)-distributed, where \( F \) is the distribution function of the uniform distribution on \([0, 1]\):
\[
F(x) = \begin{cases} 
0, & x < 0, \\
x, & 0 \leq x \leq 1, \\
1, & x > 1.
\end{cases}
\]
The notion of uniform distribution modulo 1 has a multi-dimensional analogue. A sequence \((x_n)_{n=1}^{\infty}\) in \(\mathbb{R}^s\) is uniformly distributed modulo 1 in \(\mathbb{R}^s\) if
\[
\frac{|\{1 \leq n \leq N : a \leq \{x_n\} < b\}|}{N} \rightarrow \prod_{i=1}^{s} (b_i - a_i), \quad 0 \leq a < b \leq 1,
\]
where \(0 = (0, 0, \ldots, 0) \in \mathbb{R}^s\), \(a = (a_1, a_2, \ldots, a_s)\), and so forth, and inequalities between vectors in \(\mathbb{R}^s\) are to be understood component-wise ([5, p.47, Def. 6.1]).

The notion of uniform distribution modulo 1, both in the 1-dimensional and the multi-dimensional cases, has a stronger version, whereby the required property holds not only along initial blocks of the sequence, but along any blocks of larger and larger lengths ([5, p.40, Def. 5.1]. A sequence satisfying this stronger property is well distributed modulo 1. Obviously, well distribution modulo 1 is equivalent in the 1-dimensional case to \(F\)-distribution of the sequence of fractional parts for the function \(F\) given by ([7]). A basic example of a sequence which is uniformly distributed modulo 1 is \((n\alpha)_{n=1}^{\infty}\), where \(\alpha\) is an arbitrary irrational [5, p.8, Def 2.1]. In the multi-dimensional case, the sequence \((n\alpha_1, n\alpha_2, \ldots, n\alpha_s)_{n=1}^{\infty}\) is uniformly distributed modulo 1 in \(\mathbb{R}^s\) if and only if the numbers \(1, \alpha_1, \alpha_2, \ldots, \alpha_s\) are linearly independent over \(\mathbb{Q}\) ([5, pp. 48-49]). Moreover, for these sequences, well distribution is equivalent to uniform distribution.

Recall that the density of a set \(A \subseteq \mathbb{N}\) is given by
\[
D(A) = \lim_{M \to \infty} \frac{|A \cap [1, M]|}{M}
\]
if the limit exists. If, moreover, the limit
\[
BD(A) = \lim_{M-L \to \infty} \frac{|A \cap (L, M]|}{M}
\]
exists, then it is called the Banach density of \(A\).

We can rephrase the definition of uniform distribution modulo 1 using the notion of density of a set. Namely, \((x_n)_{n=1}^{\infty}\) is uniformly distributed modulo 1
if for every interval $I \subseteq [0, 1)$ we have

$$D(\{n : \{x_n\} \in I\}) = |I|,$$  \hspace{1cm} (8)

where $|I|$ denotes the length of $I$. Similarly, $(x_n)_{n=1}^{\infty}$ is well distributed modulo 1 if (8) continues to hold when the density of the left-hand side is replaced by Banach density.

### 4 Proof of Theorem 2.1

To avoid complicated notation, shall prove in Theorem 2.1 only that $(x_N)_{N=1}^{\infty}$ is asymptotically $F$-distributed, and not that it is asymptotically well $F$-distributed. As will be seen in the proof, our result depends on the fact that the sequence $(\{Nb_1\}, \{Nb_2\}, ..., \{Nb_{K-1}\})$ is uniformly distributed modulo 1 in $\mathbb{R}^{K-1}$. Since this sequence is actually well distributed modulo 1, the same proof shows that $(x_N)_{N=1}^{\infty}$ is actually well $F$-distributed.

Along with the sequence $E(N)$ from (5), it is very useful to consider the sequence $E_1(N)$, defined by

$$E_1(N) = \min \left\{ \sum_{i,j=1}^{K} w_{ij} x_i x_j : x_i \in \mathbb{R}, \sum_{i=1}^{K} x_i = N \right\}, \quad N \in \mathbb{N}. \hspace{1cm} (9)$$

Obviously, $E_1(N) \leq E(N)$ for each $N$. We shall refer to the minimum problems on the right hand side of (5) and of (9) as the constrained problem and the unconstrained problem, respectively.

Denote by $e$ the column $K$-vector with all entries 1.

**Lemma 4.1** The unique minimum of the unconstrained problem is

$$x_0 = \frac{N}{\sum_{i,j=1}^{K} c_{ij}} \cdot C e.$$

and the corresponding unconstrained minimum is $E_1(N) = \frac{N^2}{2 \sum_{i,j=1}^{K} c_{ij}}$. 

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Due to our assumption regarding the positivity of the row sums of $C$, all components of $x_0$ are positive. Multiplying all entries of $C$ by any constant $c > 0$ we obtain an equivalent problem. Taking $c = (\sum_{i,j=1}^{K} c_{ij})^{-1}$, we shall henceforth assume that $\sum_{i,j=1}^{K} c_{ij} = 1$. In particular, denoting $b = (b_1, b_2, ..., b_K)^t$, we have

$$x_0 = NCe = Nb$$

and

$$E_1(N) = \frac{N^2}{2}.$$  \hspace{1cm} (11)

**Proof of Lemma 4.1** Let $x \neq x_0$ be any feasible solution of the unconstrained problem. Putting $a = \frac{N}{\sum_{i,j=1}^{K} c_{ij}}$ and $y = x - x_0$, we obtain

$$x^tWx = (x_0 + y)^tW(x_0 + y) = x_0^tWx + 2x_0^tWy + y^tWy = x_0^tWx_0 + a1^tCC^{-1}y + y^tWy = x_0^tWx_0 + a1^tWy + y^tWy = x_0^tWx_0 + y^tWy > x_0^tWx_0.$$  

Consequently,

$$E_1(N) = \frac{N}{\sum_{i,j=1}^{K} c_{ij}} e^tCW \frac{N}{\sum_{i,j=1}^{K} c_{ij}} Ce = \frac{N^2}{2 \sum_{i,j=1}^{K} c_{ij}}.$$  

**Lemma 4.2** $E_1(N) \geq E(N) - \sum_{i,j=1}^{K} w_{ij}$ for every $N$.

**Proof** Let $x_0 = (x_{01}, x_{02}, ..., x_{0K})$ be the minimum point of the unconstrained problem. Let $r = \sum_{i=1}^{K} \{x_{0i}\}$ be the sum of fractional parts of all coordinates of $x_0$. Obviously, $r$ is an integer, $0 \leq r < K$. Let $i_1, i_2, ..., i_K$ be all integers between 1 and $K$, ordered so that $\{x_{0,i_1}\} \leq \{x_{0,i_2}\} \leq ... \leq \{x_{0,i_K}\}$ (where ties are resolved arbitrarily). Consider the vector $n = (n_1, n_2, ..., n_K)$ defined by

$$n_i = \begin{cases}  \lfloor x_{0,i} \rfloor, & i = i_1, i_2, ..., i_{K-r}, \\  \lfloor x_{0,i} \rfloor + 1, & \text{otherwise} \end{cases}.$$  

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As mentioned in Lemma 4.1, all \(x_0, i\)'s are positive, and hence \(n\) is a feasible solution of the constrained problem. Set \(y = n - x_0\). Since all coordinates of \(y\) lie in the interval \((-1, 1)\), as in the proof of Lemma 4.1 we have

\[
E(N) \leq n^t W n = x_0^t W x_0 + y^t W y \leq E_1(N) + \sum_{i,j=1}^K w_{ij} \tag{12}
\]

which proves the lemma.

**Lemma 4.3** There exists an effective constant \(\Delta = \Delta(C)\) such that, for every \(N\), the distance between the solution of the constrained problem and that of the unconstrained problem does not exceed \(\Delta\).

**Proof** Write \(W = P^{-1} D P\), where \(P\) is orthogonal and \(D\) diagonal. Let \(M\) be an upper bound on the eigenvalues of \(C\) (for example, the \(L^\infty\)-norm \(\max_{1 \leq i \leq K} \sum_{j=1}^K |c_{ij}| \) of \(C\)). Then \(M^{-1}\) is a lower bound for the eigenvalues of \(W\), namely for the diagonal entries of \(D\). Let \(F\) be the diagonal matrix with positive diagonal entries and \(F^2 = D\). Obviously, \(\|Fz\|_2 \geq M^{-1/2}\|z\|_2\) for every \(z \in \mathbb{R}^K\). Then for every \(y \in \mathbb{R}^K\) we have

\[
y^t W y = y^t P^{-1} F F P y = \|FPy\|_2^2 \geq \|Py\|_2^2 / M = \|y\|_2^2 / M.
\]

Now let \(x_0\) and \(n = x_0 + y\) be minimum points of the unconstrained problem and of the constrained problem, respectively. Then

\[
E(N) = n^t W n = x_0^t W x_0 + y^t W y,
\]

which implies by Lemma 4.2 that \(y^t W y \leq \sum_{i,j=1}^K w_{ij}\). Thus

\[
\|y\|_2^2 / M \leq \sum_{i,j=1}^K w_{ij},
\]

which yields the conclusion of the lemma with

\[
\Delta = \sqrt{M \sum_{i,j=1}^K w_{ij}}.
\]
Proof of Theorem 2.1. Lemmas 4.1-4.3 provide a simple algorithm for calculating $E(N)$ for each $N$ in constant time. Namely, we find the point $x_0$ yielding the optimal $E_1(N)$ according to Lemma 4.1, calculate the value of $n^t W n$ for all integral points $n$, with coordinate sum $N$, within distance $\Delta$ from $x_0$, and take the best of them. If the optimal point turns out to be $n = x_0 + y$, we shall refer to $y$ as the correction vector. We have $y = n - x_0 = l - \{x_0\}$, where $\{x_0\}$ denotes the vector of fractional parts of the coordinates of $x_0$ and $l$ belongs to some finite effective set $L$ of integer vectors. Since the sum of coordinates of the correction vector is always 0, the sum of coordinates of $l$ must equal that of $\{x_0\}$. Thus, $L$ consists of all integer vectors $l$, for which the vector $l - \{x_0\}$ is of norm not exceeding the bound in Lemma 4.3 and its coordinates sum vanishes. To emphasize the dependence of $L$ on $x_0$, we shall sometimes write $L(x_0)$ instead of $L$.

Now when choosing the optimal $l$ out of $L$, we first notice that, among any two candidates $l_1$ and $l_2$, the former will be better (or equal) than the latter if and only if

$$(x_0 + l_1 - \{x_0\})^t W (x_0 + l_1 - \{x_0\}) \leq (x_0 + l_2 - \{x_0\})^t W (x_0 + l_2 - \{x_0\}).$$

This inequality is easily seen to be equivalent to

$$2(l_2 - l_1)^t W \{x_0\} \leq l_2^t W l_2 - l_1^t W l_1.$$ 

Consequently, $l$ is the optimal choice if and only if

$$2(l' - l)^t W \{x_0\} \leq (l')^t W l' - l^t W l, \quad l' \in L. \quad (13)$$

To study the second differences

$$\chi_N = E(N + 1) - 2E(N) + E(N - 1),$$

we shall write each term on the right-hand side in the form $E_1(N + j) + d_j$ for an appropriate $d_j$. In fact, as in (12), denoting by $y_1, y_2$ and $y_3$ the correction vectors for $N - 1, N$ and $N + 1$, respectively, we have:

$$\chi_N = E_1(N + 1) - 2E_1(N) + E_1(N - 1) + y_3^t W y_3 - 2y_2^t W y_2 + y_1^t W y_1. \quad (14)$$
By (11):
\[ \chi_N = 1 + y'_3 W 2 y_3 - 2 y'_2 W y_2 + y'_1 W y_1. \] (15)
Let be \( x_0, x'_0, x''_0 \) the points yielding the optimal values of \( E_1(N - 1), E_1(N), E_1(N + 1) \), respectively. In view of (10):
\[ x'_0 = x_0 + b, \quad x''_0 = x_0 + 2b. \] (16)
For appropriate integer vectors \( p \in L(x_0), p' \in L(x'_0), p'' \in L(x''_0) \):
\[ y_1 = p - \{x_0\}, \quad y_2 = p' - \{x'_0\}, \quad y_3 = p'' - \{x''_0\}. \] (17)
The vectors \( p, p', p'' \) are determined by the system of inequalities:
\[
\begin{cases} 
2(l - p)' W \{x_0\} \leq l' Wl - p' W p, & l \in L(x_0), \\
2(l - p)' W \{x'_0\} \leq l' Wl - (p')' W p', & l \in L(x'_0), \\
2(l - p'')' W \{x''_0\} \leq l' Wl - (p'')' W p'', & l \in L(x''_0). \end{cases} \] (18)
Due to (16), it is natural to try to rewrite (18) in terms of \( \{x_0\} \) without referring to \( \{x'_0\} \) and \( \{x''_0\} \). Divide the \( K \)-dimensional torus \( T^K \), which we identify with \([0, 1)^K\), according to the vector \( b \), as follows.

The \( i \)-th coordinate \( x'_{0i} \) of \( \{x_0\} \) may be either \( x_{0i} + b_i \) or \( x_{0i} + b_i - 1 \), depending on whether \( x'_{0i} + b_i \) is smaller than 1 or not, respectively. Similarly, \( x''_{0i} \) may assume one of the three values \( x_{0i} + 2b_i - c \), where \( c = 0, 1, 2 \). Divide the circle \( T \) into three disjoint intervals (actually arcs), on each of which both \( \{x'_{0i}\} \) and \( \{x''_{0i}\} \) assume the same form in terms of \( \{x_{0i}\} \).
We have to distinguish between two cases:
1) If \( b_i \leq \frac{1}{2} \), write
\[ T = [0, 1 - 2b_i] \cup [1 - 2b_i, 1 - b_i] \cup [1 - b_i, 1]. \] (19)
If \( x_{0i} \) belongs to the first interval on the right-hand, then
\[ \{x'_{0i}\} = \{x_{0i}\} + b_i, \quad \{x''_{0i}\} = \{x_{0i}\} + 2b_i, \]
if it belongs to the second
\[ \{x'_{0i}\} = \{x_{0i}\} + b_i, \quad \{x''_{0i}\} = \{x_{0i}\} + 2b_i - 1, \]
if it belongs to the third.
and if it belongs to the third
\[ \{x'_{0i}\} = \{x_{0i}\} + b_i - 1, \quad \{x''_{0i}\} = \{x_{0i}\} + 2b_i - 1. \]

2) If \( b_i > \frac{1}{2} \), write
\[ T = [0, 1 - b_i) \cup [1 - b_i, 2 - 2b_i) \cup [2 - 2b_i, 1). \] (20)

This time, depending on the interval on the right-hand side containing \( \{x_{0i}\} \), we have either
\[ \{x'_{0i}\} = \{x_{0i}\} + b_i, \quad \{x''_{0i}\} = \{x_{0i}\} + 2b_i - 1, \]
or
\[ \{x'_{0i}\} = \{x_{0i}\} + b_i - 1, \quad \{x''_{0i}\} = \{x_{0i}\} + 2b_i - 1, \]
or
\[ \{x'_{0i}\} = \{x_{0i}\} + b_i - 1, \quad \{x''_{0i}\} = \{x_{0i}\} + 2b_i - 2. \]

Let \( I_{1i}, I_{2i}, I_{3i} \) be the intervals on the right-hand side of (19) or (20), depending on whether \( b_i \leq \frac{1}{2} \) or not, respectively. Denote:
\[ \Omega_{\eta_1, \eta_2, \ldots, \eta_{K-1}} = I_{1\eta_1} \times I_{2\eta_2} \times \ldots \times I_{K-1, \eta_{K-1}}, \quad \eta_1, \ldots, \eta_{K-1} \in \{1, 2, 3\}. \]
The sets \( \Omega_{\eta_1, \eta_2, \ldots, \eta_{K-1}} \) decompose the \((K - 1)\)-dimensional torus into a union of \(3^{K-1}\) disjoint boxes:
\[ T^{K-1} = \bigcup_{\eta_1=1}^{3} \bigcup_{\eta_2=1}^{3} \ldots \bigcup_{\eta_{K-1}=1}^{3} \Omega_{\eta_1, \eta_2, \ldots, \eta_{K-1}}. \]

The information provided by the vector \( \{x_0\} \) is partly redundant as the fact that \( \sum_{i=1}^{K} x_{0i} \) is an integer determines each component in terms of the others. To avoid this inconvenience, we shall eliminate, say, \( \{x_{0K}\} \). Divide \( T^{K-1} \) into \( K \) parts as follows:
\[ \Omega^s = \{(t_1, \ldots, t_{K-1}) \in T^{K-1} : s - 1 < \sum_{i=1}^{K-1} t_i \leq s\}, \quad s = 0, \ldots, K - 1. \] (21)
(Thus, $\Omega^0 = \{0\}$, while all other $\Omega^i$’s have non-empty interior.) Suppose that $(\{x_{01}\}, ..., \{x_{0,K-1}\}) \in \Omega^s$. Then:

$$\{x_{0K}\} = s - \{x_{01}\} - ... - \{x_{0,K-1}\}. \quad (22)$$

We need a further subdivision to ensure that, in each cell, both $\{x'_0\}$ and $\{x''_0\}$ assume the same form in terms of $\{x_{01}\}, ..., \{x_{0,K-1}\}$. To this end, we first split $T$ into three subintervals, similarly to (19) and (20), depending on whether $b_K \leq \frac{1}{2}$ or $b_K > \frac{1}{2}$, namely

$$T = [0, 1 - 2b_K) \cup [1 - 2b_K, 1 - b_K) \cup [1 - b_K, 1) \quad (23)$$

or

$$T = [0, 1 - b_K) \cup [1 - b_K, 2 - 2b_K) \cup [2 - 2b_K, 1). \quad (24)$$

Let $I_{K1}, I_{K2}, I_{K3}$ be the intervals in the splitting. Put:

$$\Omega^s_\eta = \{(t_1, ..., t_{K-1}) \in \Omega^s : s - \sum_{i=1}^{K-1} t_i \in I_{K\eta}\}, \quad \eta = 1, 2, 3. \quad (25)$$

Suppose $b_K \leq \frac{1}{2}$. If the point $(\{x_{01}\}, ..., \{x_{0,K-1}\})$ belongs to $\Omega^s_1$, then

$$\{x'_{0K}\} = s - \sum_{i=1}^{K-1} \{x_{0i}\} + b_K, \quad \{x''_{0K}\} = s - \sum_{i=1}^{K-1} \{x_{0i}\} + 2b_K,$$

if it belongs to $\Omega^s_2$, then

$$\{x'_{0K}\} = s - \sum_{i=1}^{K-1} \{x_{0i}\} + b_K, \quad \{x''_{0K}\} = s - \sum_{i=1}^{K-1} \{x_{0i}\} + 2b_K - 1,$$

and if it belongs to $\Omega^s_3$, then

$$\{x'_{0K}\} = s - \sum_{i=1}^{K-1} \{x_{0i}\} + b_K - 1, \quad \{x''_{0K}\} = s - \sum_{i=1}^{K-1} \{x_{0i}\} + 2b_K - 1.$$

If $b_K > \frac{1}{2}$, then we similarly find linear expressions for $\{x'_{0K}\}$ and $\{x''_{0K}\}$ in terms of the $\{x_{0i}\}$’s on each $\Omega^s_\eta$. 

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Denote:
\[ \Omega_{\eta_1 \eta_2 \cdots \eta_K}^s = \Omega_{\eta_1 \eta_2 \cdots \eta_{K-1}}^s \cap \Omega_{\eta_K}^s, \quad 0 \leq s \leq K - 1, \ 1 \leq \eta_i \leq 3. \]

Then
\[
T^{K-1} = \bigcup_{s=0}^{K-1} \bigcup_{\eta_1=1}^{3} \bigcup_{\eta_K=1}^{3} \Omega_{\eta_1 \cdots \eta_K}^s
\]
forms a decomposition of \( T^{K-1} \) into a disjoint union of \( K \cdot 3^K \) disjoint polytopes. The important property of this decomposition is that, if \( \{x_{01}\}, \ldots, \{x_{0,K-1}\} \) belongs to any cell \( \Omega_{\eta_1 \eta_2 \cdots \eta_K}^s \), the \( 2K + 1 \) numbers \( \{x_{0K}\}, \{x_{01}'\}, \ldots, \{x_{01}'',\}, \ldots, \{x_{0,K-1}'\}, \{x_{01}'',\}, \ldots, \{x_{0,K-1}'''\} \) depend linearly on the first \( K - 1 \) coordinates \( \{x_{01}\}, \ldots, \{x_{0,K-1}\} \). That is
\[
\begin{align*}
\{x_{0i}'\} &= \{x_{0i}\} + b_i - \alpha_i', \quad 1 \leq i \leq K - 1, \\
\{x_{0i}''\} &= \{x_{0i}\} + 2b_i - \alpha_i'', \quad 1 \leq i \leq K - 1, \\
\{x_{0K}'\} &= s - \sum_{i=1}^{K-1} \{x_{0i}\} + b_K - \alpha_K', \\
\{x_{0K}''\} &= s - \sum_{i=1}^{K-1} \{x_{0i}\} + 2b_K - \alpha_K'',
\end{align*}
\]
where \( \alpha_i' \in \{0, 1\}, \ \alpha_i'' \in \{0, 1, 2\}, \ i = 1, 2, \ldots, K \). Altogether, there exists a linear transformation \( T: \mathbf{R}^{K-1} \to \mathbf{R}^K \), and for each cell \( \Omega_{\eta_1 \eta_2 \cdots \eta_K}^s \) there exist vectors \( \mathbf{v}, \mathbf{v}', \mathbf{v}'' \in \mathbf{R}^K \), such that, denoting \( \mathbf{x} = (\{x_{01}\}, \ldots, \{x_{0,K-1}\}) \), we have
\[
\{x_0\} = Tx + \mathbf{v}, \quad \{x_0'\} = Tx + \mathbf{v}', \quad \{x_0''\} = Tx + \mathbf{v}''.
\]
On each cell \( \Omega_{\eta_1 \eta_2 \cdots \eta_K}^s \) we may now rewrite the system \( \mathbf{18} \), defining the optimal vectors \( \mathbf{p}, \mathbf{p}', \mathbf{p}'' \), in the form:
\[
\begin{cases}
2(l - \mathbf{p})^T W Tx \leq l' W l - \mathbf{p}' W \mathbf{p} - 2(l - \mathbf{p})^T W \mathbf{v}, & l \in L, \\
2(l - \mathbf{p}')^T W Tx \leq l' W l - (\mathbf{p}')^T W \mathbf{p}' - 2(l - \mathbf{p}')^T W \mathbf{v}', & l \in L', \\
2(l - \mathbf{p}'')^T W Tx \leq l' W l - (\mathbf{p}'')^T W \mathbf{p}'' - 2(l - \mathbf{p}'')^T W \mathbf{v}'', & l \in L''.
\end{cases}
\]
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Note that we have suppressed the dependence of the sets $L, L', L''$ on $x_0, x'_0, x''_0$. In fact, considering $L$, for example, it is clear that each candidate $l \in L$ must have sum of coordinates $s$ and, in view of Lemma 4.3, its norm is bounded above by $\Delta + \sqrt{K}$. Thus, taking

$$L = \{ l \in \mathbb{Z}^K : \|l\| \leq \Delta + \sqrt{K}, \sum_{i=1}^{K} l_i = s \},$$

$$L' = \{ l \in \mathbb{Z}^K : \|l\| \leq \Delta + \sqrt{K}, \sum_{i=1}^{K} l_i = s + 1 - \sum_{i=1}^{K} \alpha'_i \},$$

$$L'' = \{ l \in \mathbb{Z}^K : \|l\| \leq \Delta + \sqrt{K}, \sum_{i=1}^{K} l_i = s + 2 - \sum_{i=1}^{K} \alpha''_i \},$$

(where $l = (l_1, l_2, ..., l_K)$), we certainly do not miss any potentially optimal vectors $p, p', p''$ by restricting the search to $L, L', L''$, respectively.

For each choice of $\eta_1, ..., \eta_K, s$ and of the vectors $p, p', p''$, let $P_{\eta_1, ..., \eta_K}^{s}$ be the set of all points in $\Omega_{\eta_1}^{s} ... \Omega_{\eta_K}^{s}$ satisfying (29). Then

$$T^{K-1} = \bigcup_{s=0}^{K-1} \bigcup_{\eta_1=1}^{3} ... \bigcup_{\eta_K=1}^{3} \bigcup_{p \in L} P_{\eta_1}^{s} \bigcup_{p' \in L'} P_{\eta_2}^{s} \bigcup_{p'' \in L''} P_{\eta_3}^{s},$$

(30)

where the sets on the right-hand side are disjoint (up to sets of a smaller dimension).

By (17) and (28), for all points in each subpolytope $P_{\eta_1, ..., \eta_K}^{s}$ we have the same optimal correction vectors

$$y_1 = q - Tx, \quad y_2 = q' - Tx, \quad y_3 = q'' - Tx,$$

(31)

where $q = p - v, q' = p' - v', q'' = p'' - v''$. Hence, if the point $x$ belongs to $P_{\eta_1, ..., \eta_K}^{s}$, then $\chi_N$ depends linearly on the coordinates $\{x_0, ..., x_{K-1}\}$:

$$\chi_N = 1 + (q - Tx)^t W(q - Tx) - 2(q' - Tx)^t W(q - Tx) +$$

$$+ (q'' - Tx)^t W(q'' - Tx)$$

(32)

$$= 2(-q + 2q' - q'')^t W TX + const.$$
where \( const = 1 + q'Wq - 2(q')'Wq' + (q'')'Wq'' \). (Note that all coefficients on the right-hand side depend on \( \eta_1, ..., \eta_K, s, p, p', p'' \).)

We need to find the function \( F \) according to which the sequence \( (\chi_N)_{N=1}^{\infty} \) is asymptotically \( F \)-distributed. To simplify our notations, rewrite (30) in the form

\[
T^{K-1} = \bigcup_{i=1}^{r} P_i,
\]

where each \( P_i \) is one of the polytopes \( P_{\eta_1, ..., \eta_K}^{p, p', p''} \). Denote

\[
\theta_N = (\{Nb_1\}, ..., \{Nb_{K-1}\}), \quad N = 1, 2, ...
\]

and

\[
A_i = \{N \in \mathbb{N} : \theta_N \in P_i\}, \quad i = 1, 2, ..., r.
\]

(The \( A_i \)'s may intersect, as the \( P_i \)'s may intersect on sets of a smaller dimension. However, this will cause no problem as the intersections are sets of density 0 in \( \mathbb{N} \). Alternatively, we may first decide in some arbitrary way where to place “problematic” integers.)

Let \( \theta_N^{(i)} \) be the subsequence of \( \theta_N \), consisting of those elements \( \theta_N \) with \( N \in A_i, 1 \leq i \leq r \). That is, \( \theta_N^{(i)} \) is the \( N \)-th element of \( (\theta_N)_{N=1}^{\infty} \) which belongs to \( A_i \). Let \( (\chi_N^{(i)})_{N=1}^{\infty} \) be the corresponding subsequence of \( (\chi_N)_{N=1}^{\infty} \). If the point \( x \) lies in \( P_i \), then it belongs to the subsequence \( (\theta_N^{(i)})_{N=1}^{\infty} \). Thus, by (32) there are exist affine functions \( \psi_i : \mathbb{R}^{K-1} \to \mathbb{R} \) such that

\[
\chi_N^{(i)} = \psi_i(\theta_N^{(i)}), \quad 1 \leq i \leq r, \quad N = 1, 2, ...
\]

(33)

Since the numbers \( b_1, ..., b_K \) are linearly independent over \( \mathbb{Q} \), so are the numbers \( 1, b_1, ..., b_{K-1} \), and consequently the sequence \( (\theta_N) \) is uniformly distributed modulo 1 in \( \mathbb{R}^{K-1} \). Hence, each of the subsequences \( (\theta_N^{(i)})_{N=1}^{\infty}, 1 \leq i \leq r \), is uniformly distributed in \( P_i \). By (33) the sequence \( (\chi_N^{(i)})_{N=1}^{\infty} \) is the image of a uniformly distributed sequence in \( P_i \) under the mapping \( \psi_i \). Hence, letting \( (Y_1, Y_2, ..., Y_{K-1}) \) be a \((K-1)\)-dimensional random variable, uniformly
distributed in $P_i$, we see that $(\chi_N^{(i)})_{N=1}^{\infty}$ is $F_i$-distributed, where $F_i$ is the distribution function of $\psi_i(Y_1, Y_2, ..., Y_{K-1})$.

According to [3, Thm 2.3], $F_i$ is a piecewise polynomial function, each polynomial piece being of degree at most $K-1$, and can be effectively computed. Since $(\theta_N^{(i)})_{N=1}^{\infty}$ is uniformly distributed modulo 1 in $\mathbb{R}^{K-1}$, the density of each $A_i$ is the measure $d_i$ of the set $P_i$. As $P_i$ is a polytope, this measure can be effectively computed. By [2, Lemma 1], $(\chi_N)^{\infty}_{N=1}$ is asymptotically $F$-distributed, where $F = \sum_{i=1}^{r} d_i F_i$. This completes the proof.
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