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Scaling of the Thue–Morse Diffraction Measure

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We revisit the well-known and much studied Riesz product representation of the Thue–Morse diffraction measure, which is also the maximal spectral measure for the corresponding dynamical spectrum in the complement of the pure point part. The known scaling relations are summarised, and some new findings are explained. (changes marked in green introduced on March 21, 2016)

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1. Introduction

The Thue–Morse (TM) sequence is defined via the binary substitution $1 \mapsto 1\bar{1}$, $\bar{1} \mapsto \bar{1}1$; see [1, 2] and references therein for general background. The corresponding dynamical system is known to have mixed (pure point and singular continuous) spectrum [3–5], with a pure point part on the dyadic points and a singular continuous spectral measure in the form of a Riesz product. The latter coincides with the diffraction measure $\widehat{\gamma}$ of the TM Dirac comb with weights ± 1; compare [6] for details.

The Riesz product representation of the TM diffraction measure reads

$$\widehat{\gamma} = \prod_{n\geq 0} \left(1 - \cos(2^{n+1}\pi k)\right), \tag{1}$$

with convergence (as a measure, not as a function) in the vague topology; see [7] for general background. The singular continuous nature of $\widehat{\gamma}$ is traditionally proved [4, 8] by excluding pure points by Wiener's criterion [9, 10] and absolutely continuous parts by the Riemann–Lebesgue lemma [11]; compare [2, 6] and references therein for further material.

Since diffraction measures with singular continuous components do occur in practice [12], it is of interest to study such measures in more detail. Below, we use the TM paradigm to rigorously explore the scaling properties of "singular peaks" in a diffraction measure, combining methods from harmonic analysis and number theory; for further results of a similar type, we refer to [13–17] and references therein.

2. Uniform distribution properties

In what follows, arguments around uniform distribution will be important. Let us thus begin with a summary of equivalent characterisations.

Proposition 1. *Let $(x_n)_{n\in\mathbb{N}}$ be a sequence of real numbers in the interval $[0, 1]$. Then, the following properties are equivalent.*

1. *The sequence $(x_n)_{n\in\mathbb{N}}$ is uniformly distributed in the interval $[0, 1]$, also known as uniform distribution* mod 1.
2. *For every pair a, b of real numbers subject to the condition $0 \leq a < b \leq 1$, one has* $\lim_{N\to\infty} \frac{1}{N}\mathrm{card}(\{x_n \,|\, n \leq N\} \cap [a, b)) = b - a$.
3. *For every real-valued continuous function on the closed unit interval, one has* $\lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} f(x_n) = \int_0^1 f(x)\,\mathrm{d}x$.
4. *One has* $\lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} \mathrm{e}^{2\pi\mathrm{i}kx_n} = 0$ *for all wave numbers* $k \in \mathbb{Z} \setminus \{0\}$.

For details and proofs, we refer to [18, Chs. 1.1 and 1.2]. Let us note that the continuity condition in property 3 can be replaced by Riemann integrability [18, Cor. 1.1.1], but not by Lebesgue integrability (for obvious reasons).

Below, we particularly need uniform distribution properties of the sequence defined by multiples of $x_n = 2^n$, which was extensively studied in this context by Kac [19]. This is a special case of a classic family of sequences considered by Hardy and Littlewood [20], and by Weyl; see also [18, Thm. 1.4.1 and Notes to Ch. 1.4].

Lemma 1. *Let $(x_n)_{n\in\mathbb{N}}$ be a sequence of distinct integers. Then, the sequence $(x_n k)_{n\in\mathbb{N}}$ is uniformly distributed* mod 1 *for Lebesgue-almost all $k \in \mathbb{R}$. In particular, this holds for $x_n = \ell^n$ with any fixed integer $\ell \geq 2$.*

Consider the function $f(x) = \log(1 - \cos(2\pi x))$ on $[0, 1]$. It has singularities at $x = 0$ and $x = 1$, which are both integrable (via standard arguments). In fact, one has

$$\int_0^1 \log\left(1 - \cos(2\pi x)\right) \mathrm{d}x = -\log(2). \tag{2}$$

We also need a discrete analogue of this formula. Via $1 - \cos(2\vartheta) = 2 - (\sin(\vartheta))^2$ together with the well-known identity $\prod_{m=1}^{n-1} \sin\left(\pi\frac{m}{n}\right) = n/2^{n-1}$, one can derive that

$$\sum_{m=1}^{n-1} \log\left(1 - \cos(2\pi\tfrac{m}{n})\right) = \log\left(\frac{n^2}{2^{n-1}}\right) \tag{3}$$

holds for all $n \geq 1$.

In order to apply uniform distribution results, we set

$$f_0(x) = \begin{cases} f(x), & \text{if } 0 < x < 1, \\ 0, & \text{if } x = 0 \text{ or } x = 1, \end{cases}$$

which is Riemann integrable. By Proposition 1, we have

$$\lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} f_0(x_n) = -\log(2)$$

for any real-valued sequence $(x_n)_{n\in\mathbb{N}}$ that is uniformly

distributed mod 1. Alternatively, one may directly work with the function f itself if the sequence $(x_n)_{n\in\mathbb{N}}$ avoids the points $x=0$ and $x=1$.

3. Riesz product

A direct path to the Riesz product of the TM diffraction measure can be obtained as follows. Consider the recursion $v^{(n+1)} = v^{(n)}\overline{v^{(n)}}$ with initial condition $v^{(0)}=1$, which gives an iteration towards the one-sided fixed point v of the TM substitution on the alphabet $\{1,\bar{1}\}$. If we define the exponential sum

$$g_n(k) = \sum_{\ell=0}^{2^n-1} v_\ell \, \mathrm{e}^{-2\pi\,\mathrm{i}\,k\ell},$$

where $v = v_0v_1v_2\ldots$, the function g_n is then the Fourier transform of the weighted Dirac comb for $v^{(n)}$, when it is realised with the Dirac measures (of weight ±1) on the left endpoints of the unit intervals that represent the symbolic sequence of $v^{(n)}$. In particular, one has $g_0(k)=1$ and

$$g_{n+1}(k) = \left(1-\mathrm{e}^{-2\pi\,\mathrm{i}\,k2^n}\right) g_n(k)$$

for $n\geq 0$, so that

$$|g_{n+1}(k)|^2 = 2\,|g_n(k)|^2\left(1-\cos(2^{n+1}\pi k)\right).$$

One can then explicitly check that $f_n(k)=\frac{1}{2^n}|g_n(k)|^2 = \prod_{\ell=0}^{n-1}(1-\cos(2^{\ell+1}\pi k))$, which reproduces the Riesz product of Eq. (1) in the sense that $\lim_{n\to\infty} f_n = \widehat{\gamma}$ as measures in the vague topology.

As g_n corresponds to a chain of length 2^n, the growth rate $\beta(k)$ (when it is well-defined) is obtained as

$$\beta(k) = \lim_{n\to\infty}\frac{\log(f_n(k))}{n\log 2}.$$

Let us now consider the growth rate for various cases of the wave number k.

Case A. When $k=\frac{m}{2^r}$ with $r\geq 0$ and $m\in\mathbb{Z}$, all but finitely many factors of the Riesz product (1) vanish, so that no contribution can emerge from such values of k. In fact, these are the dyadic points, which support the pure point part of the dynamical spectrum. They are extinction points for the diffraction measure of the balanced weight case considered here; compare [5] for a discussion of this connection.

Case B. When $k\in\mathbb{R}$ is such that the sequence $(2^nk)_{n\in\mathbb{N}}$ is uniformly distributed mod 1, which is true for Lebesgue-almost all $k\in\mathbb{R}$ by Lemma 1, one obtains the growth rate

$$\begin{aligned}\beta(k) &= \lim_{N\to\infty}\frac{1}{N}\sum_{n=0}^{N-1}\frac{\log\left(1-\cos(2^{n+1}\pi k)\right)}{\log 2}\\ &= \int_0^1 \frac{\log\left(1-\cos(2\pi x)\right)}{\log 2}\,\mathrm{d}x = -1\end{aligned}$$

by uniform distribution and Eq. (2). Let us note that none of these sequences ever visits a dyadic point, so that the limit according to Proposition 1 applies. These values of the wave number k thus do not contribute to the TM measure.

Let us note that this argument shows that $\lim_{n\to\infty} f_n(k)=0$ pointwise for almost all $k\in\mathbb{R}$ and thus provides an alternative proof for the fact that the measure from Eq. (1) does not comprise an absolutely continuous part; compare Sect. 1 as well as [6, 11].

Case C. When $k=\frac{m}{3}$ with m not divisible by 3, one finds $f_n(k)=(3/2)^n$. Since this corresponds to a system (or sequence) of length 2^n, we have a growth rate of

$$\beta(k) = \frac{\log(3/2)}{\log 2} \approx 0.584963.$$

The same growth rate applies to all numbers of the form $k=\frac{m}{2^r3}$ with $r\geq 0$ and m not divisible by 3, because the factor 2^r in the denominator has no influence on the asymptotic scaling, due to the structure of the Riesz product (1). Note that the points of this form are dense in $\mathbb{R}$, but countable.

Similarly, when $k=\frac{m}{2^r5}$ with $r\geq 0$ and m not a multiple of 5, one finds

$$\beta(k) = \frac{\log(5/4)}{2\log 2} \approx 0.160964.$$

Case D. More generally, when $k=\frac{p}{2^rq}$ with $r\geq 0$, $q\geq 3$ odd and $\gcd(p,q)=1$, one can determine the growth rate explicitly. Recall that

$$U_q := (\mathbb{Z}/q\mathbb{Z})^\times = \{1\leq p<q \mid \gcd(p,q)=1\}$$

is the unit group of the residue class ring $\mathbb{Z}/q\mathbb{Z}$. If $S_q=\{2^n \bmod q \mid n\geq 0\}$ is the subgroup of U_q generated by the unit 2, one finds

$$\beta(k) = \frac{1}{\mathrm{card}(pS_q)}\sum_{n\in pS_q}\frac{\log\left(1-\cos\left(2\pi\frac{n}{q}\right)\right)}{\log 2} \tag{4}$$

by an elementary calculation. When $q=2m+1$, the integer $\mathrm{card}(S_q)$ is the multiplicative order of $2 \bmod q$, which is sequence A 002326 in [21].

When $\gcd(p,q)=1$, one has $\mathrm{card}(pS_q)=\mathrm{card}(S_q)$, even when the set pS_q is considered mod q. Let us note that formula (4) is written in such a way that it also holds for all p not divisible by q. If $\gcd(p,q)>1$, the set pS_q may be reduced mod q, which shows that the formula consistently gives $\beta(\frac{p}{q})$ in such cases.

Case E. When $\mathrm{card}(S_q)=q-1$, Eq. (3) leads to $\beta(\frac{1}{q})=g(q)$ with

$$g(q) = \frac{\log\left(\frac{q^2}{2^{q-1}}\right)}{\log\left(2^{q-1}\right)} = \frac{2\log(q)}{(q-1)\log 2} - 1. \tag{5}$$

For odd $q\geq 3$, the function $g(q)$ is positive precisely for $q=3$ and $q=5$, and negative otherwise; compare Fig. 1. In fact, also $\beta(\frac{1}{q})$ seems to be negative for all odd $q\geq 7$, though this does not hold for general $\beta(\frac{p}{q})$. Indeed, $\beta(\frac{3}{17})>0$, and all positive exponents for odd $7\leq q<1000$ are listed in the Table.

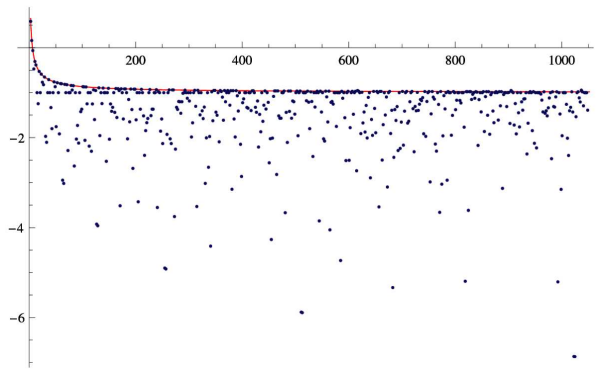

Fig. 1. Exponents $\beta(\frac{1}{q})$ according to Eq. (4) for all odd $3 \leq q < 1050$. Apart from $q = 3$ and $q = 5$, the exponents are negative. The solid line is the function g from Eq. (5). Exponents with large negative values emerge for $q = 2^r \pm 1$.

TABLE

Wave numbers $k = \frac{p}{q}$ with positive exponents, for all odd integers $5 < q < 1000$. For a given q, all $p \in U_q/S_q$ are considered (we choose the smallest element of the set $pS_q \bmod q$ as representative).

$\frac{p}{q}$	$\beta\left(\frac{p}{q}\right)$	$\frac{p}{q}$	$\beta\left(\frac{p}{q}\right)$	$\frac{p}{q}$	$\beta\left(\frac{p}{q}\right)$	$\frac{p}{q}$	$\beta\left(\frac{p}{q}\right)$	$\frac{p}{q}$	$\beta\left(\frac{p}{q}\right)$	$\frac{p}{q}$	$\beta\left(\frac{p}{q}\right)$
$\frac{3}{17}$	0.266	$\frac{25}{117}$	0.172	$\frac{37}{255}$	0.150	$\frac{65}{381}$	0.067	$\frac{47}{565}$	0.144	$\frac{65}{771}$	0.140
$\frac{5}{31}$	0.272	$\frac{19}{127}$	0.108	$\frac{43}{255}$	0.318	$\frac{47}{451}$	0.127	$\frac{81}{565}$	0.113	$\frac{161}{771}$	0.140
$\frac{11}{31}$	0.272	$\frac{21}{127}$	0.373	$\frac{53}{255}$	0.318	$\frac{65}{451}$	0.127	$\frac{61}{585}$	0.126	$\frac{69}{775}$	0.101
$\frac{5}{33}$	0.105	$\frac{27}{127}$	0.108	$\frac{91}{255}$	0.150	$\frac{67}{455}$	0.128	$\frac{97}{585}$	0.126	$\frac{83}{775}$	0.127
$\frac{7}{43}$	0.267	$\frac{43}{127}$	0.373	$\frac{37}{257}$	0.049	$\frac{69}{455}$	0.128	$\frac{53}{595}$	0.031	$\frac{111}{775}$	0.127
$\frac{11}{63}$	0.244	$\frac{19}{129}$	0.143	$\frac{43}{257}$	0.404	$\frac{53}{511}$	0.028	$\frac{87}{595}$	0.031	$\frac{117}{775}$	0.101
$\frac{13}{63}$	0.244	$\frac{11}{151}$	0.012	$\frac{45}{257}$	0.221	$\frac{75}{511}$	0.163	$\frac{51}{601}$	0.042	$\frac{57}{785}$	0.085
$\frac{11}{65}$	0.350	$\frac{35}{151}$	0.012	$\frac{23}{275}$	0.117	$\frac{83}{511}$	0.239	$\frac{63}{601}$	0.042	$\frac{137}{819}$	0.359
$\frac{11}{73}$	0.165	$\frac{25}{171}$	0.220	$\frac{49}{275}$	0.117	$\frac{85}{511}$	0.422	$\frac{53}{657}$	0.061	$\frac{145}{819}$	0.359
$\frac{13}{73}$	0.165	$\frac{19}{185}$	0.126	$\frac{25}{331}$	0.067	$\frac{87}{511}$	0.028	$\frac{101}{657}$	0.061	$\frac{67}{825}$	0.089
$\frac{13}{89}$	0.229	$\frac{17}{195}$	0.001	$\frac{35}{337}$	0.149	$\frac{107}{511}$	0.239	$\frac{51}{673}$	0.038	$\frac{173}{825}$	0.089
$\frac{19}{89}$	0.229	$\frac{41}{195}$	0.001	$\frac{57}{337}$	0.149	$\frac{109}{511}$	0.163	$\frac{57}{683}$	0.131	$\frac{67}{889}$	0.050
$\frac{9}{91}$	0.075	$\frac{17}{205}$	0.047	$\frac{49}{341}$	0.060	$\frac{171}{511}$	0.422	$\frac{71}{683}$	0.087	$\frac{95}{889}$	0.012
$\frac{19}{91}$	0.075	$\frac{31}{205}$	0.183	$\frac{57}{341}$	0.369	$\frac{43}{513}$	0.033	$\frac{103}{683}$	0.179	$\frac{129}{889}$	0.012
$\frac{11}{105}$	0.060	$\frac{19}{217}$	0.073	$\frac{71}{341}$	0.369	$\frac{77}{513}$	0.122	$\frac{111}{683}$	0.226	$\frac{157}{889}$	0.050
$\frac{17}{105}$	0.060	$\frac{37}{217}$	0.073	$\frac{73}{341}$	0.060	$\frac{83}{513}$	0.272	$\frac{113}{683}$	0.335	$\frac{83}{993}$	0.124
$\frac{17}{117}$	0.172	$\frac{35}{241}$	0.194	$\frac{31}{381}$	0.067	$\frac{85}{513}$	0.343	$\frac{55}{753}$	0.054	$\frac{149}{993}$	0.172

More generally, for any odd $q \geq 3$, one obtains (from case D) the formula

$$\frac{1}{q-1} \sum_{1<d|q} \operatorname{card}(S_d) \sum_{p \in U_d/S_d} \beta\left(\frac{p}{d}\right) = g(q). \tag{6}$$

Now, the Möbius inversion (with the Möbius function μ) leads to

$$\sum_{p \in U_q/S_q} \beta\left(\frac{p}{q}\right) = \frac{1}{\operatorname{card}(S_q)} \sum_{1 \neq d|q} \mu\left(\frac{q}{d}\right)(d-1)g(d), \tag{7}$$

while a simpler formula than Eq. (4) for the individual exponents seems difficult in general.

Case F. As is shown in [13] (by way of an explicit example), there are wave numbers k for which the exponent $\beta(k)$ does not exist. The construction is based on a suitable mixture of binary expansions for wave numbers with different exponents. Clearly, there are uncountably many such examples, though they still form a null set. Here, one can define a "spectrum" of exponents via the limits of all converging subsequences.

Case G. So far, we have identified countably many values of k, for which the scaling exponents can be calculated, while (due to case B) Lebesgue-almost all $k \in \mathbb{R}$ carry no singular peak. The remaining problem is to cope with the uncountably many wave numbers (of zero Lebesgue measure) that belong to the supporting set of the TM measure and may possess well-defined exponents.

The existence of such numbers can be understood via Diophantine approximation. Again, it is useful to start with the binary expansion of a wave number k, and then modify it in a suitable way. Consider first the example

$$k = \tfrac{1}{3} = 0.0101010101\ldots$$

If we now switch the binary digits at positions 2^r, with $r \in \mathbb{N}$, we obtain a different wave number k' that is irrational but nevertheless still has the same scaling exponent β as $k = \frac{1}{3}$, as longer and longer stretches of the binary expansion of k' agree with that of k. Clearly, via similar modifications, we can obtain uncountably many distinct irrational numbers with $\beta = \beta(\frac{1}{3})$.

The same strategy works for all other rational wave numbers k, and underlies the nature of the TM measure. In particular, this explains the existence of uncountably many "singular peaks", which together (in view of case B) still form a Lebesgue null set. These scaling exponents are accessible via our above arguments. It remains to decide in which sense the above analysis is complete.

4. Concluding remarks

An analogous approach works for all measures of the form of a classic Riesz product. In particular, the generalised Thue–Morse sequences from [22] can be analysed along these lines; compare also [3]. Likewise, the choice of different interval lengths is possible, though technically more complicated; compare [23] for some examples.

Higher-dimensional examples with purely singular continuous spectrum, such as the squiral tiling [24] or similar bijective block substitutions [8], may still lead to classic Riesz products, though they are now in more than one variable, and the analysis is hence more involved. Nevertheless, the scaling analysis will still lead to a better understanding of such measures.

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Note added on March 21, 2016

Our argument for Case B on the basis of uniform distribution modulo 1 of the sequence $\big(2^n x\big)_{n\in\mathbb{N}}$ for almost all $x \in \mathbb{R}$ is incomplete, because the function f defined by $f(x) = \log\big(1 - \cos(2\pi x)\big)$ is only Riemann integrable on $[0,1]$ in the generalised sense (meaning that it is an improper integral), which is insufficient here. However, f is properly integrable on $[0,1]$ in the Lebesgue sense and has an obvious 1-periodic extension to $\mathbb{R}$.

Consequently, rather than employing uniform distribution, one can argue with the dynamical system defined by the map T of the unit interval $[0,1]$ into itself, given by $x \mapsto 2x \bmod 1$. It is well-known that T leaves Lebesgue measure invariant and is ergodic relative to it, so that the Birkhoff sums satisfy

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=0}^{N-1} f(T^n(k)) = \int_0^1 f(x)\,\mathrm{d}x$$

for Lebesgue almost every $k \in \mathbb{R}$ by an application of the ergodic theorem.

This still gives the result of Case B for almost all wave numbers $k \in \mathbb{R}$, though it might be that they differ from the wave numbers with uniform distribution of $\big(2^n x\big)_{n\in\mathbb{N}}$ on a null set. This has no further consequence on the analysis presented in paper.