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Journal Item

THE SINGULAR CONTINUOUS DIFFRACTION MEASURE OF THE THUE-MORSE CHAIN

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ABSTRACT. The paradigm for singular continuous spectra in symbolic dynamics and in mathematical diffraction is provided by the Thue-Morse chain, in its realisation as a binary sequence with values in $\{\pm 1\}$. We revisit this example and derive a functional equation together with an explicit form of the corresponding singular continuous diffraction measure, which is related to the known representation as a Riesz product.

The Thue-Morse chain can be defined via the primitive substitution rule

$$\varrho : \begin{array}{l} 1 \mapsto 1\bar{1} \\ \bar{1} \mapsto \bar{1}1 \end{array}$$

on the two-letter alphabet $\{1, \bar{1}\}$; see [1, 10] for background. Let $v = v_0 v_1 v_2 \dots$ be the unique one-sided fixed point of ϱ with $v_0 = 1$. This infinite word satisfies

$$v_{2n} = v_n \quad \text{and} \quad v_{2n+1} = \bar{v}_n \tag{1}$$

for all $n \in \mathbb{N}_0$, where $\bar{\bar{1}} = 1$. Consider the bi-infinite word w, defined as

$$w_n = \begin{cases} v_n, & \text{for } n \geq 0, \\ v_{-n-1}, & \text{for } n < 0, \end{cases}$$

which is the unique reflection-symmetric fixed point of ϱ^2 with (admissible) seed $w_{-1} w_0 = 11$. It is cube-free and thus aperiodic. If S denotes the (two-sided) shift, defined by $(Sw)_n = w_{n+1}$, the Thue-Morse hull is the compact space $\mathbb{X} = \overline{\{S^m w \mid m \in \mathbb{Z}\}}$, where the closure is taken in the obvious product topology. Note that $\mathbb{X}$ coincides with the (discrete) local indistinguishability (or LI) class of w, and that the topological dynamical system $(\mathbb{X}, S)$ is strictly ergodic; see [10] for details.

Here, we consider the weighted Dirac comb

$$\omega = \sum_{n \in \mathbb{Z}} w_n \, \delta_n, \tag{2}$$

where δ_x denotes the normalised Dirac measure on $\mathbb{R}$, located at x, and $\bar{1} = -1$. In particular, ω is a translation bounded, signed measure on $\mathbb{R}$. The corresponding autocorrelation (or Patterson) measure γ, obtained by a volume-averaged convolution [6, 2] of ω with its reflected counterpart, reads

$$\gamma \;=\; \eta \, \delta_{\mathbb{Z}} \;:=\; \sum_{m \in \mathbb{Z}} \eta(m) \, \delta_m, \tag{3}$$

with the coefficients $\eta(m)$ obtained as the limits

$$\eta(m) \;=\; \lim_{N\to\infty} \frac{1}{2N+1} \sum_{\substack{-N\le k,\ell\le N\\ k-\ell=m}} w_k \, w_\ell \;=\; \lim_{N\to\infty} \frac{1}{2N+1} \sum_{n=-N}^{N} w_n \, w_{n-m} .$$

Note that these limits exist due to unique ergodicity, compare [10], with $\eta(0) = 1$. The autocorrelation coefficients satisfy $\eta(-m) = \eta(m)$ and, due to (1), the recursions

$$\eta(2m) = \eta(m) \quad \text{and} \quad \eta(2m+1) = -\frac{1}{2}\big(\eta(m) + \eta(m+1)\big), \tag{4}$$

valid for all $m \ge 0$. In particular, $\eta(1) = -\frac{1}{3}$, and all coefficients are uniquely specified.

By construction, η is a positive definite function on $\mathbb{Z}$, wherefore the Herglotz-Bochner theorem [8, Thm. I.7.6] guarantees the existence of a finite positive measure ν on $[0,1)$ with

$$\eta(m) \;=\; \int_0^1 e^{2\pi i m y} \, \mathrm{d}\nu(y) . \tag{5}$$

The diffraction measure $\widehat{\gamma}$ of the weighted Thue-Morse comb ω of (2) is the Fourier transform of γ. An elementary calculation shows that

$$\widehat{\gamma} = \nu * \delta_{\mathbb{Z}} \quad \text{and} \quad \nu = \widehat{\gamma}\big|_{[0,1)} .$$

In this formulation, the spectral properties of $\widehat{\gamma}$ follow immediately from those of ν. In particular, ν has a unique decomposition

$$\nu = \nu_{\mathrm{pp}} + \nu_{\mathrm{sc}} + \nu_{\mathrm{ac}}$$

into its pure point, singular continuous and absolutely continuous parts (relative to Lebesgue measure λ); see [12, Thms. I.13 and I.14].

It was first shown by Kakutani [7] that ν is a purely singular continuous measure, so $\nu = \nu_{\mathrm{sc}}$. Let us briefly adapt this to our setting. By Wiener's criterion [8, Cor. 7.11], $\nu_{\mathrm{pp}} = 0$ is equivalent to $\lim_{N\to\infty} \frac{1}{2N+1} \varSigma(N) = 0$, where

$$\varSigma(N) \;:=\; \sum_{m=-N}^{N} \big(\eta(m)\big)^2 .$$

When $N \ge 1$, we can use the recursion relations (4) to derive $\varSigma(4N) \le \frac{3}{2}\,\varSigma(2N)$. With $\alpha = \log_2(3/2) < 1$, one then obtains the estimate $\frac{1}{N}\varSigma(N) = \mathcal{O}(1/N^{1-\alpha})$. At this point, we know that $\nu = \nu_{\mathrm{sc}} + \nu_{\mathrm{ac}}$, and define the distribution function

$$F(x) := \nu\big([0,x]\big), \tag{6}$$

which is a continuous function of bounded variation on $[0,1]$. It satisfies $F(0) = 0$ and $F(x) + F(1-x) = 1$, the latter as a consequence of the symmetry of ν.

Following [7] and viewing ν as a Lebesgue-Stieltjes measure [9, Ch. X] with distribution function F, the two recursion relations (4) imply the identities

$$\begin{aligned} \mathrm{d}F(\tfrac{x}{2}) + \mathrm{d}F(\tfrac{x+1}{2}) \;&=\; \mathrm{d}F(x), \\ \mathrm{d}F(\tfrac{x}{2}) - \mathrm{d}F(\tfrac{x+1}{2}) \;&=\; -\cos(\pi x)\, \mathrm{d}F(x), \end{aligned} \tag{7}$$

for all $x \in [0,1]$. The left-hand sides are obtained from the corresponding sides of the recursions by a change of variables, followed by a split of the new integration region into two parts. The actual equality of the measures follows because we obtain equality of the integrals over arbitrary trigonometric polynomials, whence the Fourier uniqueness theorem [8, Thm. I.2.7] applies. The relations (7) must also hold for the two continuous components of ν separately, because $\nu_{\mathrm{sc}} \perp \nu_{\mathrm{ac}}$ by [9, Thm. VII.2.4].

Writing $\nu_{\mathrm{ac}} = g\lambda$ with $g \in L^1\big([0,1]\big)$, the identities (7) result in

$$\tfrac{1}{2}\big(g(\tfrac{x}{2}) + g(\tfrac{x+1}{2})\big) = g(x) \quad \text{and} \quad \tfrac{1}{2}\big(g(\tfrac{x}{2}) - g(\tfrac{x+1}{2})\big) = -\cos(\pi x)\, g(x),$$

this time for almost all $x \in [0,1]$. Defining now $\eta_{\mathrm{ac}}(m) = \int_0^1 e^{2\pi i m x} g(x)\,\mathrm{d}x$, we have $\eta_{\mathrm{ac}}(-m) = \eta_{\mathrm{ac}}(m)$ and inherit a set of recursions identical to (4), however with $\eta_{\mathrm{ac}}(0) = 0$ as a result of the Riemann-Lebesgue lemma [8, Thm. I.2.8], and hence $\eta_{\mathrm{ac}}(m) = 0$ for all $m \in \mathbb{Z}$. By the Fourier uniqueness theorem [8, Thm. I.2.7], this implies $g(x) = 0$ almost everywhere, and hence $\nu_{\mathrm{ac}} = 0$. Since ν itself cannot be the zero measure, we have $\nu = \nu_{\mathrm{sc}} \neq 0$, and the Thue-Morse diffraction measure $\widehat{\gamma}$ is a purely singular continuous, $\mathbb{Z}$-periodic, positive measure. It is the same for all Dirac combs of members of the hull $\mathbb{X}$.

The remainder of this note is concerned with an explicit calculation of ν, via its distribution function F, which does not seem to have been calculated in the literature so far. Adding the two equations for $\mathrm{d}F$ from (7), followed by integration, results in the functional equation

$$F(x) = \frac{1}{2}\int_0^{2x} \big(1 - \cos(\pi y)\big)\,\mathrm{d}F(y) \tag{8}$$

for the continuous function F, valid for $x \in [0, \frac{1}{2}]$. Since F is a continuous non-decreasing function on $[0,1]$, the difference $f(x) = F(x) - x$ defines a continuous function f of bounded variation, with $f(0) = 0$ and $f(x) + f(1-x) = 0$ for all $x \in [0,1]$. As such, f possesses a uniformly converging Fourier series of the form

$$f(x) = \sum_{m\geq 1} b_m \sin(2\pi m x),$$

with $b_m = 2\int_0^1 \sin(2\pi m x)\, f(x)\,\mathrm{d}x$. From Eqs. (5) and (6), one finds $\eta(m) = \pi m\, b_m$, so that

$$F(x) = x + \sum_{m\geq 1} \frac{\eta(m)}{m\pi} \sin(2\pi m x) \tag{9}$$

is a uniformly converging Fourier series representation of the Thue-Morse distribution function. This function satisfies the symmetry relation $F(x) + F(1-x) = 1$ for all $x \in [0,1]$, and is a solution of the integral equation (8).

To interpret (8) in a wider setting, let us introduce the space

$$D = \Big\{ G \in C\big([0,1],\mathbb{R}\big) \;\Big|\; \begin{array}{c} G(0)=0,\ G \text{ non-decreasing and} \\ G(x)+G(1-x)=1 \text{ on } [0,1] \end{array} \Big\} \tag{10}$$

of continuous, non-decreasing distribution functions on $[0,1]$ with the required symmetry, and define the mapping $\varPhi:\, D \longrightarrow D$ via $G \mapsto \varPhi(G)$ with

$$\big(\varPhi(G)\big)(x) = \begin{cases} \frac{1}{2}\int_0^{2x} \big(1-\cos(\pi y)\big)\,\mathrm{d}G(y), & \text{if } 0 \leq x \leq \frac{1}{2}, \\ 1 - \big(\varPhi(G)\big)(1-x), & \text{if } \frac{1}{2} < x \leq 1. \end{cases}$$

One can show that F of (9) is the only solution of $\varPhi(F) = F$ within D, because $\varPhi$ is a weak contraction with respect to the metric $d(G,H) := V(G-H)$, where V denotes the total variation of continuous functions on $[0,1]$; see [9, Ch. X] for background.

For a numerical high-precision computation of F, we employ a Volterra-type iteration within D, which is superior to using (9) directly. Starting from $F_0(x) = x$, where $F_0 \in D$, we set $F_{n+1} = \varPhi(F_n)$ for $n \geq 0$. This defines the (uniformly converging) sequence of distribution functions in D given by

$$F_n(x) = x + \sum_{m=1}^{2^n-1} \frac{c_m^{(n)}}{m\pi} \sin(2\pi m x). \tag{11}$$

Here, the coefficients $c_m^{(n)}$ satisfy the recursions

$$c_{2m}^{(n+1)} = c_m^{(n)} \quad \text{and} \quad c_{2m+1}^{(n+1)} = -\frac{1}{2}\bigl(c_m^{(n)} + c_{m+1}^{(n)}\bigr)$$

for $n \geq 1$ and $0 \leq m \leq 2^n - 1$, together with $c_0^{(1)} = 0$, $c_1^{(1)} = -\frac{1}{2}$ and $c_1^{(n+1)} = -\frac{1}{2}\bigl(1 + c_1^{(n)}\bigr)$. They approach the autocorrelation coefficients $\eta(m)$ via $\lim_{n\to\infty} c_m^{(n)} = \eta(m)$ for arbitrary $m \in \mathbb{N}$.

By construction, the distribution functions F_n represent absolutely continuous measures (although their limit does not). Writing $\mathrm{d}F_n(x) = f_n(x)\,\mathrm{d}x$, one finds $f_0(x) = 1$, and the functional equation (8) induces the recursion

$$f_{n+1}(x) \;=\; \bigl(1 - \cos(2\pi x)\bigr) f_n(2x) \;=\; 2\bigl(\sin(\pi x)\bigr)^2 f_n(2x)$$

for $n \geq 0$. This gives the well-known explicit representation

$$f_n(x) \;=\; \prod_{\ell=0}^{n-1} \bigl(1 - \cos(2^{\ell+1}\pi x)\bigr) \;=\; 2^n \prod_{\ell=0}^{n-1} \bigl(\sin(2^{\ell}\pi x)\bigr)^2 \tag{12}$$

of the Thue-Morse measure as a Riesz product; compare [11, Sec. 1.4.2].

The Volterra iteration leads to a sequence $(F_n)_{n\in\mathbb{N}_0}$ of continuous distribution functions that converge uniformly (on $[0,1]$) to F, which is continuous as well. The latter is shown in Figure 1 and resembles the classic middle-thirds Cantor measure in various aspect, though it has full support (see below). Note that the corresponding sequence $(\mathrm{d}F_n)_{n\in\mathbb{N}_0}$ of absolutely continuous measures is only vaguely convergent, with the limit being purely singular continuous. Therefore, it is somewhat misleading to show a density for the Thue-Morse measure, as is often found in the literature. Still, it may be instructive to inspect the sequence of densities f_n in order to get some intuition on the singular nature of the Thue-Morse measure, or to study some of its scaling properties; see [5] and references therein.

On initial inspection, the distribution function F seems to have a plateau around $x = \frac{1}{2}$, with exact value $\frac{1}{2}$. More generally, as suggested by the Riesz products (12), one might expect a plateau around any $x \in \bigl(\{0,1\} \cup \{m/2^k \mid k \in \mathbb{N},\, m \in \mathbb{N} \text{ odd}\}\bigr) \cap [0,1]$, because the densities f_n vanish at x for all sufficiently large n, with the order of this zero linearly increasing with n. However, these potential gaps are all closed (see below). The corresponding values of F can be calculated with the series expansion (9). Unlike the situation of the gap labelling theorem for one-dimensional Schrödinger operators [3], where one knows the values of the integrated

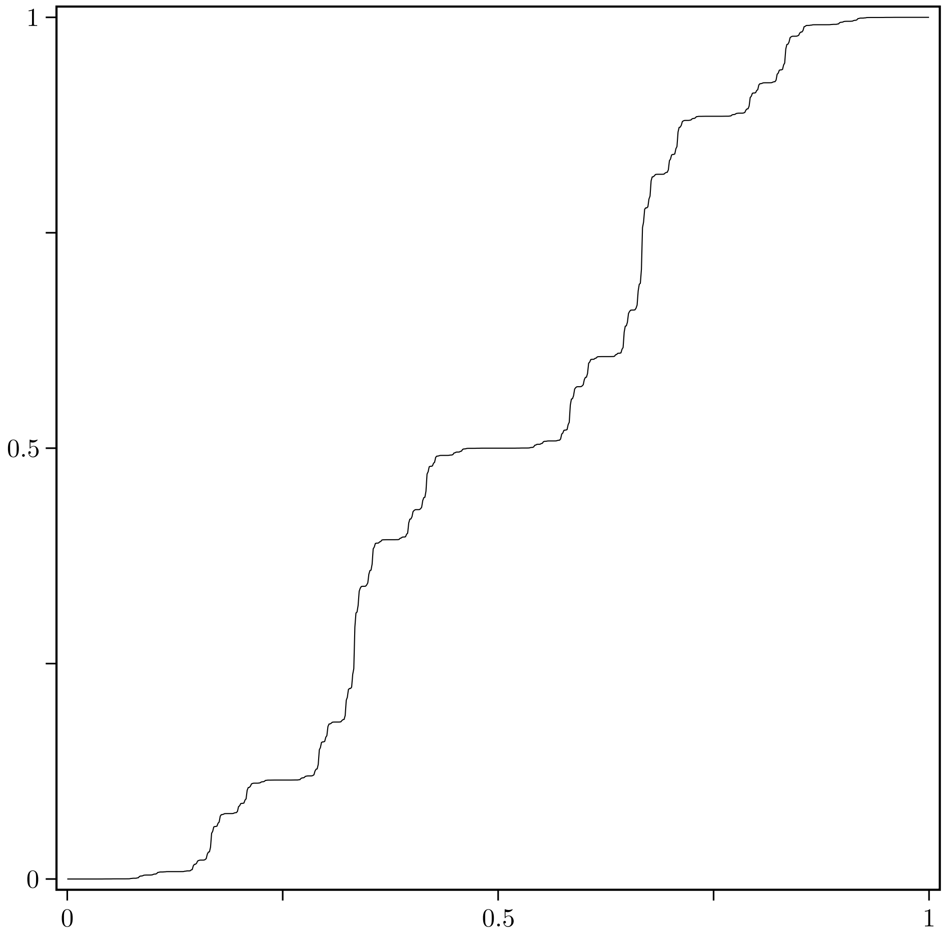

FIGURE 1. Distribution function F of the purely singular continuous diffraction measure of the Thue-Morse chain in the interval $[0, 1]$. Note that F is a strictly increasing function, despite the appearance of plateau-like regions.

density of states (IDOS) on the (always non-overlapping) plateaux but not their positions, we know the possible locations of the plateaux, but cannot see a topological constraint for the corresponding values of the distribution function (which can be determined from (9)).

It is interesting to note that the set of potential plateau locations coincides with the set of potential (but in our case extinct) Bragg peak positions, so the (extinct) Bragg peaks appear to 'repel' the continuous diffraction spectrum. Nevertheless, one has

$$\operatorname{supp}(\,\mathrm{d}F) = \operatorname{supp}(\nu) = [0, 1]$$

by [4, Prop. 28], which also implies that F is a strictly increasing function. In particular, as one can immediately see from (8), $F(x) = 0$ forces $F(2x) = 0$, which (when repeated) contradicts $F(1/2) = 1/2$ unless $x = 0$. This shows that there is no gap around 0 (and none around 1 by symmetry). The general argument uses that ν is a regular Borel measure; see [4] and references therein for details.

The methods used above can also be applied to other substitutions of constant length that fail to have pure point spectrum. This can be decided on the basis of Dekking's criterion; see [11, Sec. 6] for details. Although one still has to check Wiener's criterion and to find the analogue of the functional equation (7), this approach seems worth pursuing.

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