AUTOMORPHISM-INVARIANT POSITIVE DEFINITE FUNCTIONS ON FREE GROUPS

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ABSTRACT. In this article we raise some new questions about positive definite functions on free groups, and explain how these are related to more well-known questions. The article is intended as a survey of known results that also offers some new perspectives and interesting observations; therefore the style is expository.

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1. INTRODUCTION

Fix $r \ge 1$ and write $\mathbf{F} = \mathbf{F}_r$ for a free group on r generators $\{x_1, \ldots, x_r\}$. A central role in this paper will be played by the automorphism group $\operatorname{Aut}(\mathbf{F})$ of \mathbf{F} . It was proved by Nielsen [Nie24] that $\operatorname{Aut}(\mathbf{F})$ is generated by the following *elementary Nielsen moves:*

• For σ an element of the symmetric group S_r , we have $\alpha_{\sigma} \in \operatorname{Aut}(\mathbf{F})$ where

(1.1)
$$\alpha_{\sigma}(x_1,\ldots,x_r) \stackrel{\text{def}}{=} (x_{\sigma(1)},\ldots,x_{\sigma(r)}).$$

• We have $\iota \in Aut(\mathbf{F})$ where

(1.2)
$$\iota(x_1, x_2, \dots, x_r) = (x_1^{-1}, x_2, \dots, x_r).$$

• We have $\gamma \in \operatorname{Aut}(\mathbf{F})$ where

(1.3)
$$\gamma(x_1, x_2, \dots, x_r) = (x_1 x_2, x_2, \dots, x_r)$$

The other central concept of this paper is a *positive definite function* on a group.

Definition 1.1. Let Γ be any discrete group. A function $\tau : \Gamma \to \mathbf{C}$ is called *positive definite* if for any finite subset $S \subset \Gamma$, the matrix

$$[\tau(\gamma'\gamma^{-1})]_{\gamma,\gamma'\in S}$$

is positive semi-definite. In other words, for any vector $(\alpha_{\gamma})_{\gamma \in S} \in \mathbf{C}^{S}$ we have

$$\sum_{\gamma,\gamma'\in S} \tau(\gamma'\gamma^{-1})\alpha_{\gamma'}\overline{\alpha_{\gamma}} \ge 0.$$

If Γ is a discrete group, the group $\operatorname{Aut}(\Gamma)$ acts by precomposition on the collection of positive definite functions on Γ , giving rise to the notion of $\operatorname{Aut}(\Gamma)$ -invariant positive definite functions. Explicitly, a positive definite function τ is $\operatorname{Aut}(\Gamma)$ -invariant if

$$\tau(\alpha(\gamma)) = \tau(\gamma), \quad \forall \gamma \in \Gamma, \, \forall \alpha \in \operatorname{Aut}(\Gamma)$$

In this paper we are mainly interested in the case $\Gamma = \mathbf{F}$. Positive definite functions on free groups, without the Aut(\mathbf{F})-invariance condition, have been the subject of various investigations [DMFT80, Boz86, BT06], stemming in part from a fundamental construction of Haagerup in [Haa79]. See also the monograph [FTP83].

Our aim here is to explain what is known about $Aut(\mathbf{F})$ -invariant positive definite functions on \mathbf{F} , and identify some important questions about them.

Example 1.2. Let $\tau_{\lambda}(e) = 1$ and $\tau_{\lambda}(w) = 0$ for $w \neq e$. One can directly verify that this is a positive definite function on **F**, and that τ_{λ} is Aut(**F**)-invariant.

Example 1.3. Let $\tau_{\text{triv}}(w) = 1$ for all $w \in \mathbf{F}$. This is another $\text{Aut}(\mathbf{F})$ -invariant positive definite function on \mathbf{F} .

A rich family of examples that are the subject of much ongoing work arise from *word maps*. Throughout the rest of this paper, G will always refer to a compact topological group, and μ will be its probability Haar measure. In this paper, all topological groups are assumed to be Hausdorff¹. Denote $G^r \stackrel{\text{def}}{=} \underbrace{G \times G \times \ldots \times G}_{r \text{ times}}$. Any $w \in \mathbf{F}_r$ gives rise to a word map

$$w: G^r \to G$$

defined by substitutions. For example, if r = 2 and $w = x_1^2 x_2^{-2}$, then $w(g_1, g_2) = g_1^2 g_2^{-2}$. A related concept is that of the *w*-measure on *G*. The *w*-measure is the law of the random variable obtained by picking *r* independent elements of *G* according to the Haar measure, and evaluating the word map *w* at this random tuple. More formally, the *w*-measure on *G* is the pushforward measure

$$\mu_w = w_*(\mu^r),$$

where μ^r is the Haar measure on G^r . Word maps and measures give rise to Aut(**F**)-invariant positive definite functions on **F** as follows:

¹It is convenient to assume this so that we can identify Borel measures on G or G^r with elements of the continuous linear dual of continuous functions, without getting into technicalities.

$$au_{G,\pi}: \mathbf{F} \to \mathbf{C}$$

by

$$\tau_{G,\pi}(w) \stackrel{\text{def}}{=} \int_{g \in G} \operatorname{tr}(\pi(g)) d\mu_w = \int_{\mathbf{g} \in G^r} \operatorname{tr}(\pi(w(\mathbf{g}))) d\mu^r(\mathbf{g})$$

In other words, this function maps $w \in \mathbf{F}$ to the expected value of the character of π under the *w*-measure μ_w . This is a positive definite function on *w* as follows. Suppose $S \subset \mathbf{F}$ and we are given $\alpha_w \in \mathbf{C}$ for each $w \in S$. Then

(1.4)
$$\sum_{w,w'\in S} \tau_{G,\pi}(w'w^{-1})\alpha_{w'}\overline{\alpha_w} = \sum_{w,w'\in S} \alpha_{w'}\overline{\alpha_w} \int_{\mathbf{g}\in G^r} \operatorname{tr}(\pi([w'w^{-1}](\mathbf{g})))d\mu^r(\mathbf{g})$$
$$= \int_{\mathbf{g}\in G^r} \operatorname{tr}(A_{\mathbf{g}}A_{\mathbf{g}}^*)d\mu^r(\mathbf{g}),$$

where a superscript * means conjugate transpose and

$$A_{\mathbf{g}} = \sum_{w \in S} \alpha_w \pi(w(\mathbf{g})) \in \operatorname{End}(V).$$

Hence the quantity (1.4) is an integral of traces of non-negative operators and hence must be non-negative.

Moreover, $\tau_{G,\pi}$ is Aut(**F**)-invariant. This will follow from the following lemma that is folklore². In this paper, all proofs are given in the Appendix, and we mark all statements with proofs in the Appendix by a \star .

Lemma 1.5. \star The action of Aut(**F**) by precomposition on Hom(**F**, G) \cong G^r preserves the Haar measure μ^r .

The following two corollaries are immediate consequences of Lemma 1.5.

Corollary 1.6. If G is a compact topological group, $w \in \mathbf{F}$, and $\alpha \in \operatorname{Aut}(\mathbf{F})$, then the *w*-measure μ_w on G is equal to the $\alpha(w)$ -measure $\mu_{\alpha(w)}$ on G, namely,

$$\mu_w = \mu_{\alpha(w)}.$$

Corollary 1.7. If G is a compact topological group and π is a finite dimensional unitary representation of G, the positive definite function $\tau_{G,\pi}$ on **F** given in Example 1.4 is Aut(**F**)-invariant.

Note that this family of positive definite functions on \mathbf{F} coming from compact groups, includes, in particular, those coming from *finite* groups.

²See for example [Gol07] where a version is stated without a proof in the second sentence, and the unpublished paper [MP16, Section 2.5].

Remark 1.8. We point out that the construction given in Example 1.4 also works if μ^r is replaced by any Aut(**F**)-invariant Borel measure on G^r . These measures are by no means classified, and we will return to this point later in Question 6.4.

In light of Corollary 1.6, the following conjectures have been put forward:

Conjecture 1.9. Suppose w_1, w_2 are in **F**. If the w-measures μ_{w_1} and μ_{w_2} are the same on all compact groups G, does it follow that $w_2 \in Aut(\mathbf{F}).w_1$?

It has even been conjectured that:

Conjecture 1.10 (Shalev). If the w-measures μ_{w_1} and μ_{w_2} are the same on all <u>finite</u> groups G, then $w_2 \in \text{Aut}(\mathbf{F}).w_1$.

See [AV11, Question 2.2] where Conjecture 1.10 was posed as a question; the conjecture was made by Shalev in [Sha13, Conj. 4.2]. Of course Conjecture 1.9 is a direct consequence of Conjecture 1.10. In this paper we introduce the following related (weaker) question:

Question 1.11. Do Aut(**F**)-invariant positive definite functions on **F** separate Aut(**F**)orbits? In other words, if w_1, w_2 are in **F** and $\tau(w_1) = \tau(w_2)$ for all Aut(**F**)-invariant positive definite functions τ on **F**, does it follow that $w_2 \in Aut(\mathbf{F}).w_1$?

An affirmative answer to Question 1.11 could be viewed as an orbital analog of the Gelfand-Raikov Theorem [GR43]: for any locally compact topological group \mathcal{G} , the positive definite functions on \mathcal{G} separate elements of \mathcal{G} . Indeed, Question 1.11 could be asked for any locally compact topological group, but we restrict our attention here to the important special case of free groups.

To compare Question 1.11 and Conjectures 1.9 and 1.10, we introduce some equivalence relations on **F**. For $w_1, w_2 \in \mathbf{F}$ we say

- $w_1 \overset{\operatorname{Aut}(\mathbf{F})}{\sim} w_2$ if $w_2 \in \operatorname{Aut}(\mathbf{F}).w_1$
- $w_1 \stackrel{\text{FinGrp}}{\sim} w_2$ if $\mu_{w_1} = \mu_{w_2}$ on any finite group.
- $w_1 \overset{\mathbf{CptGrp}}{\sim} w_2$ if the measures $\mu_{w_1} = \mu_{w_2}$ on any compact group.
- $w_1 \overset{\text{PosDef}}{\sim} w_2$ if $\tau(w_1) = \tau(w_2)$ for all Aut(**F**)-invariant positive definite functions τ on **F**.

For $w_1, w_2 \in \mathbf{F}$, we have

(1.5) $w_1 \overset{\operatorname{Aut}(\mathbf{F})}{\sim} w_2 \Longrightarrow w_1 \overset{\operatorname{PosDef}}{\sim} w_2 \Longrightarrow w_1 \overset{\operatorname{CptGrp}}{\sim} w_2 \Longrightarrow w_1 \overset{\operatorname{FinGrp}}{\sim} w_2.$

The first and last implications above are obvious. The second implication follows immediately from the following lemma.

Lemma 1.12. \star For any compact topological group G, and $w \in \mathbf{F}$, the w-measure μ_w on G is determined uniquely by the map $\pi \mapsto \tau_{G,\pi}(w)$ where π runs over irreducible unitary representations of G and $\tau_{G,\pi}$ are the functions constructed in Example 1.4.

Remark 1.13. Section 8 in [PP15] discusses a few other related equivalence relations between words, where the focus is on word measures on finite groups and the profinite topology on the free group.

Notation. We write *e* for the identity element of a group. If *A* and *B* are elements of the same group, then $[A, B] = ABA^{-1}B^{-1}$ is their commutator. If *H* is a group, then [H, H] denotes its commutator subgroup. We write \emptyset for the empty set.

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2. A SURVEY

In this section we give a brief survey describing current knowledge about word measures on groups and Conjectures 1.9 and 1.10.

It has been known for a while that several properties of free words can be detected in finite quotients of free words and therefore also in word measures on finite groups. For example, if a word $w \in \mathbf{F}$ is *not* an *n*-th power (namely, if there is no $u \in \mathbf{F}$ with $w = u^n$) then there is a normal subgroup $N \leq \mathbf{F}$ such that wN is not an *n*-th power in $Q = \mathbf{F}/N$ – this result is attributed to Lubotzky in [Tho97]. It follows that if w_1 is an *n*-th power and w_2 is not, then for some finite group Q, there is an element $q \in Q$ which is not an *n*-th power, such that $q \in w_2(Q^r)$ but $q \notin w_1(Q^r)$. Thus $w_1 \not\prec w_2$. Consult [HMP19] for a different argument yielding this last result.

Similarly, Khelif [Khe04] shows that if $w \in \mathbf{F}$ is *not* a commutator of two words, then its image in some finite quotient of \mathbf{F} is a non-commutator. It follows that if w_1 is a commutator **FinGrp** and w_2 not, then $w_1 \not\sim w_2$.

However, the first significant progress on Conjecture 1.10 came from an important special case. If $w \in \operatorname{Aut}(\mathbf{F}).x_1$, then w is called *primitive*. A word is primitive in \mathbf{F}_r if and only if it is a member of a generating set of \mathbf{F}_r of size r. Since it is clear that $\mu_{x_1} = \mu$, i.e. Haar measure on G, for any compact G, it follows from Corollary 1.6 that if w is a primitive word then $\mu_w = \mu$ on any compact G, and in particular, on any finite G. The following theorem, asserting the converse, was conjectured to hold independently by several people including Avni, Gelander, Larsen, Lubotzky, and Shalev:

Theorem 2.1 (Puder-Parzanchevski). If $w \in \mathbf{F}_r$ and $\mu_w = \mu$ on every finite group, then w is primitive.

Theorem 2.1 was first proved by Puder [Pud14, Theorem 1.5] when r = 2 and then proved for general $r \ge 3$ by Puder and Parzanchevski in [PP15, Theorem 1.4']. Both papers rely on a careful analysis of the functions $\tau_{G,\pi}$ constructed in Example 1.4 when $G = S_n$, the symmetric group on n letters, and π is the standard n-dimensional representation of S_n by 0-1 matrices. Theorem 2.1 can be restated as the implication

$$w \stackrel{\mathbf{FinGrp}}{\sim} x_1 \implies w \stackrel{\mathrm{Aut}(\mathbf{F})}{\sim} x_1$$

and therefore establishes a basic instance of Conjecture 1.10.

The word x_1 , and by extension, the primitive words, have the property that whenever π is an *irreducible* representation of the compact group G, the values $\tau_{G,\pi}(x_1)$ of Example 1.4 are given by a very simple formula. Indeed, suppose that π is an irreducible unitary representation. Then

(2.1)
$$\tau_{G,\pi}(x_1) = \begin{cases} 1 & \text{if } \pi \text{ is the trivial representation} \\ 0 & \text{otherwise.} \end{cases}$$

This is a direct consequence of Schur orthogonality.

There is another type of words with a similarly general exact expression for $\tau_{G,\pi}(w)$, namely, surface words. An orientable surface word is one of the form

$$s_g = [x_1, x_2] \cdots [x_{2g-1}, x_{2g}]$$

where we assume $g \ge 1$ and $r \ge 2g$ (recall that r is the rank of the free group $\mathbf{F} = \mathbf{F}_r$). A non-orientable surface word is one of the form

$$t_g = x_1^2 \cdots x_g^2$$

where $g \ge 1$ and $r \ge g$. The reason for this naming is that the one-relator groups

$$\Gamma_g = \langle \mathbf{F}_{2g} | s_g \rangle, \quad \Lambda_g = \langle \mathbf{F}_g | t_g \rangle$$

are respectively, the fundamental groups of a closed <u>orientable</u> surface of genus g, and a closed <u>non-orientable</u> surface of genus g (the connected sum of g copies of the real projective plane $\mathbb{P}^2(\mathbf{R})$).

Frobenius [Fro96] proved the following result for finite groups, but the same proof applies to compact groups in general.

Theorem 2.2. Suppose that π is an irreducible representation of the compact group G on the vector space V. Then

$$\tau_{G,\pi}\left([x_1, x_2]\right) = \frac{1}{\dim V}.$$

An analogous result was later proved by Frobenius and Schur [FS06].

Theorem 2.3. Suppose that π is an irreducible unitary representation of the compact group G on the vector space V. Then $\tau_{G,\pi}(x_1^2)$ is in $\{-1,0,1\}$ and is called the Frobenius-Schur indicator of π , denoted by $FS(\pi)$. The Frobenius-Schur indicator is also given by

$$FS(\pi) = \begin{cases} 1 & \text{if } \pi \text{ is equivalent to a real representation} \\ 0 & \text{if } tr(\pi) \text{ is not real} \\ -1 & \text{if } tr(\pi) \text{ is real, but } \pi \text{ is not equivalent to a real representation.} \end{cases}$$

One also has the following basic observation.

Lemma 2.4. \star If $w_1, w_2 \in \mathbf{F}$, and w_1 and w_2 are generated by disjoint sets of the x_i , then

 $\mu_w = \mu_{w_1} * \mu_{w_2}.$

where * denotes convolution. Hence for π irreducible

$$\tau_{G,\pi}(w) = \frac{1}{\dim V} \tau_{G,\pi}(w_1) \tau_{G,\pi}(w_2).$$

From Lemma 2.4 and Theorems 2.2 and 2.3 it immediately follows that for irreducible π

(2.2)
$$\tau_{G,\pi}(s_g) = \frac{1}{(\dim V)^{2g-1}}$$

and

(2.3)
$$\tau_{G,\pi}(t_g) = \frac{FS(\pi)^g}{(\dim V)^{g-1}}.$$

By Lemma 1.12, this fully describes the word measures μ_{s_g} and μ_{t_g} on all compact groups. The following theorem was suggested as a line of inquiry at the 27th International Conference in Operator Theory in Timişoara, and has since been established to hold [MP19c].

Theorem 2.5 (Magee-Puder). If $w \in \mathbf{F}_r$ and $\mu_w = \mu_{sg}$ on every compact group, then $(r \ge 2g, and) w \in \operatorname{Aut}(\mathbf{F}_r).s_g$. In other words,

$$w \stackrel{\mathbf{CptGrp}}{\sim} s_g \implies w \stackrel{\mathrm{Aut}(\mathbf{F}_r)}{\sim} s_g$$

If $w \in \mathbf{F}_r$ and $\mu_w = \mu_{t_g}$ on every compact group, then $(r \ge g, and) w \in \operatorname{Aut}(\mathbf{F}_r).t_g$. In other words,

$$w \overset{\mathbf{CptGrp}}{\sim} t_g \implies w \overset{\mathrm{Aut}(\mathbf{F}_r)}{\sim} t_g$$

One may view this as a converse to the results of Frobenius and Schur: the formulas (2.2) and (2.3) uniquely characterize the orbits of s_g and t_g . The proof of Theorem 2.5 involves an analysis of the values $\tau_{G,\pi}(w)$ where G,π are one of the following:

- G = U(n), the group of $n \times n$ complex unitary matrices, and π is the *n*-dimensional defining representation of U(n). This relies on the results of the paper [MP19a].
- G = O(n), the group of $n \times n$ real orthogonal matrices, and π is the *n*-dimensional defining representation of O(n). The necessary analysis here comes from the work [MP19b].
- $G = S_{n,m}$ or $G = S^1 \wr S_n$ a generalized symmetric group, namely, the group of all $n \times n$ complex matrices such that any row or column contains exactly one non-zero entry, and the non-zero entries are taken from the *m*th roots of 1 or from the entire unit circle S^1 . The representation π is the standard one given by the definition of the group as a matrix group. The necessary analysis here is developed in [MP19c].

Independently, Hanany, Meiri and Puder obtained the following result [HMP19]:

Theorem 2.6 (Hanany-Meiri-Puder). Let $w_0 = x_1^m$ or $w_0 = [x_1, x_2]^m$ for some $m \in \mathbf{N}$. If $w \in \mathbf{F}_r$ induces the same measure as w_0 on every <u>finite</u> group, then $w \in \operatorname{Aut}(\mathbf{F}_r).w_0$. In other words,

(2.4)
$$w \overset{\operatorname{Fin}\operatorname{Grp}}{\sim} w_0 \Longrightarrow w \overset{\operatorname{Aut}(\mathbf{F}_r)}{\sim} w_0$$

In particular, Theorem 2.6 strengthens Theorem 2.5 in the case $w_0 = [x_1, x_2]$. It is an interesting question whether Theorem 2.5 can be proved for general g using only finite groups G. The proof of Theorem 2.6 relies on the results of Lubotzky [Tho97] and Khelif [Khe04] mentioned above, as well as on further developing the analysis of word measures on S_n from [PP15]. In fact, it is shown in [HMP19] that whenever (2.4) holds for some word $w_0 \in \mathbf{F}$, it also holds for every power of w_0 .

Rational Functions. A recurring theme in many of the works mentioned above is that for many "natural" families of groups and representations $\{(G_n, \pi_n)\}_{n \ge N_0}$, the function $\tau_{G_n, \pi_n}(w)$ is given by a rational function in n. For example, if std is the defining n-dimensional representation of U (n), then for $n \ge 2$

$$\tau_{U(n),\text{std}}\left([x_1, x_2]^2\right) = \frac{-4}{n^3 - n}$$

Indeed, this phenomenon occurs for natural series of representations of S_n [Nic94, LP10] and for the defining representations of generalized symmetric groups [MP19c]. Using the Weingarten calculus developed for computing integrals over Haar-random elements of classical compact Lie groups [Wei78, Col03, CŚ06], it is shown to hold also in the case of natural families of representations of U(n) [Răd06, MŚS07] and of O(n) and Sp(n) [MP19b]. The same phenomenon also occurs for natural families of representations of GL_n (\mathbb{F}_q), where \mathbb{F}_q is a fixed finite field [PW19].

These rational expressions depend on w, of course, but are Aut(**F**)-invariant. This means that they should have an "Aut(**F**)-invariant" interpretation, not relying on combinatorial properties of w, but rather on properties of w as an element of the abstract free group (with no given basis). Finding such interpretation for at least some of terms of the rational functions is one of the main results of [PP15] in the case of S_n , of [MP19a] in the case of U (n), of [MP19b] in the cases of O (n) and Sp (n) and of [MP19c] in the case of generalized symmetric groups.

One plausible strategy for proving Conjectures 1.9 and 1.10 is to gather a list of invariants of words which can be determined by word measures on groups, and then prove that this list separates $\operatorname{Aut}(\mathbf{F})$ -orbits. We have already mentioned above two invariants that can be determined by word measures on finite groups: whether w is an n-th power, and whether wis a simple commutator. Now we turn to a result of a similar type, but with a richer invariant that is detected. Given $w \in \mathbf{F}$, we define the *commutator length* of w, denoted $\operatorname{cl}(w)$, to be the minimum g for which we can solve the equation

$$w = [u_1, v_1] \cdots [u_g, v_g]$$

for $u_i, v_i \in \mathbf{F}$. If it is not possible to write w as the product of commutators (i.e., if $w \notin [\mathbf{F}, \mathbf{F}]$) then we say $cl(w) = \infty$. There is a related concept of stable commutator length. The stable commutator length of w, denoted scl(w), is defined by

$$\operatorname{scl}(w) \stackrel{\text{def}}{=} \lim_{m \to \infty} \frac{\operatorname{cl}(w^m)}{m}, \quad \text{if } w \in [\mathbf{F}, \mathbf{F}],$$

or ∞ otherwise. The existence of this limit follows from the subadditivity in m of $cl(w^m)$. Stable commutator length is an important object in geometric group theory and the theory of the free group: see the book of Calegari [Cal09a]. One of the fundamental results about scl is due to Calegari [Cal09b]:

Theorem 2.7 (Calegari). If $w \in \mathbf{F}$ then $\operatorname{scl}(w) \in \mathbf{Q} \cup \{\infty\}$.

The function scl : $\mathbf{F} \to \mathbf{Q} \cup \{\infty\}$ takes on infinitely many values when $r \ge 2$. For example, it is a result of Culler [Cul81] that $\operatorname{cl}([x_1, x_2]^n) = \lfloor \frac{n}{2} \rfloor + 1$ and hence

$$\operatorname{scl}([x_1, x_2]^k) = \lim_{m \to \infty} \frac{\operatorname{cl}([x_1, x_2]^{km})}{m} = \lim_{m \to \infty} \frac{\lfloor \frac{km}{2} \rfloor + 1}{m} = \frac{k}{2}$$

It is even known, by Calegari [Cal11], that if $r \ge 4$, scl(\mathbf{F}_r) contains a rational with any given denominator. The following theorem is proved in [MP19a, Cor. 1.11].

Theorem 2.8 (Magee-Puder). For $w \in \mathbf{F}$, knowing the word measure μ_w on every U(n) determines scl(w). As a consequence, for $w_1, w_2 \in \mathbf{F}$,

$$w_1 \overset{\mathbf{CptGrp}}{\sim} w_2 \implies \operatorname{scl}(w_1) = \operatorname{scl}(w_2)$$

The proof of Theorem 2.8 can be reinterpreted as the establishment of the following equality:

ī

$$\operatorname{scl}(w) = -\frac{1}{2} \sup_{k>0} \lim_{n \to \infty} \frac{\log \left| \tau_{\operatorname{U}(n), \operatorname{Sym}^k(\operatorname{std})}(w) \right|}{\log \left(n^k \right)}$$

where $\operatorname{Sym}^k(\operatorname{std})$ is the symmetric k^{th} power of the standard representation of $\operatorname{U}(n)$.

3. The GNS construction

In this section and the next one, we allow Γ to be any countable discrete group. The collection of positive definite functions τ on Γ form a convex cone that we will denote by $\mathcal{P}(\Gamma)$. The importance of positive definite functions on groups comes from their role in the Gelfand-Naimark-Segal (GNS) construction [GN43, Seg47]:

Theorem 3.1 (GNS construction). If $\tau : \Gamma \to \mathbf{C}$ is a positive definite function with $\tau(e) = 1$, then there is a **GNS triple** $(\pi_{\tau}, \mathcal{H}_{\tau}, \xi_{\tau})$ where

- \mathcal{H}_{τ} is a Hilbert space with inner product $\langle \bullet, \bullet \rangle_{\tau}$,
- $\pi_{\tau}: \Gamma \to U(\mathcal{H}_{\tau})$ is a homomorphism from Γ to the group of unitary operators $U(\mathcal{H}_{\tau})$ on \mathcal{H}_{τ} ,
- $\xi_{\tau} \in \mathcal{H}_{\tau}$ is a unit cyclic vector for the unitary representation π_{τ} , meaning that the linear span of $\{\pi_{\tau}(g)\xi_{\tau} : g \in \Gamma\}$ is dense in \mathcal{H}_{τ} , and

• we have $\tau(g) = \langle \pi_{\tau}(g)\xi_{\tau}, \xi_{\tau} \rangle_{\tau}$ for all $g \in \Gamma$.

The GNS triple associated to τ is unique up to unitary equivalence: if $(\pi_{\tau}, \mathcal{H}_{\tau}, \xi_{\tau})$ and $(\pi'_{\tau}, \mathcal{H}'_{\tau}, \xi'_{\tau})$ are two GNS triples, then there is a unitary intertwiner $u : \mathcal{H}_{\tau} \to \mathcal{H}'_{\tau}$ such that $u(\xi_{\tau}) = \xi'_{\tau}$ and for all $g \in \Gamma$, $\pi_{\tau}(g) = u^{-1}\pi'_{\tau}(g)u$.

Conversely, if $\pi : \Gamma \to U(\mathcal{H})$ is a unitary representation of Γ on a Hilbert space \mathcal{H} , and $\xi \in \mathcal{H}$ is a unit vector, then

$$\tau(w) = \langle \pi(w)\xi, \xi \rangle$$

is a positive definite function on Γ with $\tau(e) = 1$. Moreover, if ξ is cyclic then the GNS triple $(\pi_{\tau}, \mathcal{H}_{\tau}, \xi_{\tau})$ is equivalent, in the sense described above, to (π, \mathcal{H}, τ) .

Example 3.2 (Regular representation). The function τ_{λ} introduced in Example 1.2 is obtained as a matrix coefficient in the *regular representation* of **F**. Indeed let $\lambda : \mathbf{F} \to U(\ell^2(\mathbf{F}))$ denote the left regular representation. Then

$$\tau_{\lambda}(w) = \langle \lambda(w)\delta_e, \delta_e \rangle = \delta_{we} \quad \forall w \in \mathbf{F}.$$

Conversely, the GNS triple associated to λ is, up to isomorphism, $(\lambda, \ell^2(\mathbf{F}), \delta_e)$.

Example 3.3 (Trivial representation). The function τ_{triv} introduced in Example 1.3 is obtained as a matrix coefficient in the trivial representation triv : $\mathbf{F} \to U(\mathbf{C})$. Indeed, $1 \in \mathbf{C}$ is a cyclic vector for this representation. Thus

$$\tau_{\text{triv}}(w) = \langle \text{triv}(w)1, 1 \rangle = \langle 1, 1 \rangle = 1 \quad \forall w \in \mathbf{F}.$$

Example 3.4 (Compact group construction, continued). Let $\tau_{G,\pi}$ be the positive definite function constructed in Example 1.4. Recall that $\pi : G \to U(V)$ is a finite dimensional unitary representation of the compact group G. In this case, $\tau_{G,\pi}$ arises as a matrix coefficient in a subrepresentation of the direct integral³

$$\Pi_{G,\pi} = \int_{G^r}^{\oplus} \Pi_{\mathbf{g}} d\mu^r(\mathbf{g})$$

where $\Pi_{\mathbf{g}} : \mathbf{F} \to U(\text{End}(V)), \ \Pi_{\mathbf{g}}(w) A = \pi(w(\mathbf{g}))A$. The inner product on End(V) is given by $\langle A, B \rangle = \text{tr}(AB^*)$. The representation is generated by the cyclic vector

$$\xi = \int_{G^r}^{\oplus} \mathrm{Id}_{\mathrm{End}(V)} d\mu^r(\mathbf{g})$$

and \mathcal{H} is the closed linear span of $\{\Pi_{G,\pi}(w)\xi : w \in \mathbf{F}\}$. Then we have

$$\langle \Pi_{G,\pi}(w)\xi,\xi\rangle = \int_{G^r} \operatorname{tr}(\pi(w(\mathbf{g})))d\mu^r(\mathbf{g}) = \tau_{G,\pi}(w)$$

Example 3.5 (Characteristic subgroup construction). We now turn to yet another type of examples of Aut(**F**)-invariant positive definite functions on **F**. Let $\Lambda \leq \mathbf{F}$ be a *characteristic subgroup*, meaning that $\alpha(\Lambda) = \Lambda$ for any $\alpha \in \text{Aut}(\mathbf{F})$. As conjugation by elements of **F** gives

³The direct integral of representations is a generalization of the direct sum that uses a topological space with a Borel measure to index the summation, instead of a discrete set. For details see [Mac76, §2.4].

automorphisms, Λ is necessarily normal in **F**. Some examples of characteristic subgroups of **F** include

- The commutator subgroup [**F**, **F**].
- Groups in the derived series of **F**, for example, [[**F**, **F**], [**F**, **F**]].
- Groups in the lower or upper central series of **F**.
- If H is any group, the intersection of all kernels of homomorphisms $\mathbf{F} \to H$ (this may be trivial).

Note that $\operatorname{Aut}(\mathbf{F})$ acts by automorphisms on the group \mathbf{F}/Λ . We obtain an $\operatorname{Aut}(\mathbf{F})$ -invariant positive definite function on \mathbf{F} denoted by τ_{Λ} and given by

$$\tau_{\Lambda}(w) = \delta_{w\Lambda,e} = \begin{cases} 1 & \text{if } w \in \Lambda \\ 0 & \text{if } w \notin \Lambda. \end{cases}$$

Indeed, τ_{Λ} arises from the GNS triple (π, \mathcal{H}, ξ) where $\mathcal{H} = \ell^2(\mathbf{F}/\Lambda)$, π is the quasi-regular representation, and $\xi = \delta_e \in \ell^2(\mathbf{F}/\Lambda)$. It is clear that τ_{Λ} is Aut(**F**)-invariant since Λ is characteristic in **F**.⁴

Evidently, the subgroup of \mathbf{F} generated by an Aut(\mathbf{F})-orbit is characteristic. Therefore, the construction of Example 3.5 allows us to make a little progress on Question 1.11.

Proposition 3.6. \star If $w_1, w_2 \in \mathbf{F}$ and the orbits $\operatorname{Aut}(\mathbf{F}).w_1$ and $\operatorname{Aut}(\mathbf{F}).w_2$ generate different subgroups of \mathbf{F} then

$$w_1 \not\sim w_2.$$

We stress, however, that in general different $Aut(\mathbf{F})$ -orbits in \mathbf{F} may generate the same subgroup. This is illustrated in the following two examples:

Example 3.7. While $\operatorname{Aut}(\mathbf{F}).w$ and $\operatorname{Aut}(\mathbf{F}).w^{-1}$ generate the same subgroup, there is no reason for w and w^{-1} to be in the same orbit. For example, $w = x^2y^2xy^{-1}$ is not in the same orbit as its inverse.

Example 3.8. Let r = 2 and $w = x_1^2 x_2^3$. Let Λ be the group generated by Aut(\mathbf{F}_2).w. Then Λ also contains $w' = x_2^{-2} x_1^3$, since $(x_1, x_2) \mapsto (x_2^{-1}, x_1)$ is in Aut(\mathbf{F}_2). However,

$$ww' = x_1^2 x_2 x_1^3$$

is in Λ , and is primitive, since $x_1^2 x_2 x_1^3$ and x_1 generate \mathbf{F}_2 . Since Λ is characteristic, all primitive elements must be in Λ , and in particular, x_1 and x_2 are in Λ , so $\Lambda = \mathbf{F}_2$. However, w itself is not primitive: this can be inferred from Whitehead algorithm [LS77, Chapter I.4], or from the fact that $\tau_{S_3,\text{std}}(w) = 1.5 \neq 1 = \tau_{S_n,\text{std}}(x_1)$. I.e., $\text{Aut}(\mathbf{F}).w \neq \text{Aut}(\mathbf{F}).x_1$, but $\text{Aut}(\mathbf{F}).x_1$ and $\text{Aut}(\mathbf{F}).w$ generate the same group.

⁴More generally, if T is any positive definite function on \mathbf{F}/Λ , then $\tau(w) \stackrel{\text{def}}{=} T(w\Lambda)$ will be a positive definite function on \mathbf{F} . It will be $\operatorname{Aut}(\mathbf{F})$ -invariant if T is invariant under the induced action of $\operatorname{Aut}(\mathbf{F})$ on \mathbf{F}/Λ . Since classifying these T in general seems hard, we do not pursue this in detail here.

Before moving on, we address the following question. What does the GNS construction tell us about Aut(Γ)-invariant positive definite functions? We will denote by $\mathcal{P}_1(\Gamma)$ the elements τ of $\mathcal{P}(\Gamma)$ with $\tau(e) = 1$. Suppose that τ is an element of $\mathcal{P}_1(\Gamma)^{\operatorname{Aut}(\Gamma)}$, the elements of $\mathcal{P}_1(\Gamma)$ which are invariant under Aut(Γ). In this case, one can extend τ to a positive definite function τ^+ on the semidirect product $\Gamma \rtimes \operatorname{Aut}(\Gamma)$ by the formula

$$\tau^+(\gamma, \alpha) \stackrel{\text{def}}{=} \tau(\gamma).$$

Lemma 3.9. \star If $\tau \in \mathcal{P}_1(\Gamma)^{\operatorname{Aut}(\Gamma)}$, then τ^+ is a positive definite function on $\Gamma \rtimes \operatorname{Aut}(\Gamma)$.

Let $(\pi_{\tau^+}, \mathcal{H}_{\tau^+}, \xi_{\tau^+})$ be the associated GNS triple to τ^+ . Since $\langle \pi(e, \alpha)\xi_{\tau^+}, \xi_{\tau^+}\rangle = 1$, the cyclic vector ξ_{τ^+} is an invariant vector for the embedded copy of Aut(Γ) in $\Gamma \rtimes Aut(\Gamma)$ under $\alpha \mapsto (e, \alpha)$. The map $\tau \mapsto \tau^+$ gives a linear embedding of $\mathcal{P}_1(\Gamma)^{Aut(\Gamma)}$ into $\mathcal{P}_1(\Gamma \rtimes Aut(\Gamma))$.

Example 3.10 (Compact group construction, continued). Recall the notations of Examples 1.4 and 3.4. Let \mathcal{H}_0 denote the Hilbert space

$$\mathcal{H}_0 = \int_{G^r}^{\oplus} \operatorname{End}(V) d\mu^r(\mathbf{g}).$$

We will describe a unitary representation of $\mathbf{F} \rtimes \operatorname{Aut}(\mathbf{F})$ on this Hilbert space as follows. A vector in \mathcal{H}_0 is (an equivalence class) of an L^2 function $\mathbf{g} \mapsto B_{\mathbf{g}}$ for $\mathbf{g} \in G^r$ and $B_{\mathbf{g}} \in \operatorname{End}(V)$. We define for $(w, \alpha) \in \mathbf{F} \rtimes \operatorname{Aut}(\mathbf{F})$

$$\Pi_0(w,\alpha)\{\mathbf{g}\mapsto B_{\mathbf{g}}\}=\{\mathbf{g}\mapsto \pi(w(\mathbf{g}))B_{\alpha^{-1}(\mathbf{g})}\}.$$

It is straightforward to check this this gives a unitary representation of $\mathbf{F} \rtimes \operatorname{Aut}(\mathbf{F})$ on \mathcal{H}_0 , using Lemma 1.5. Now let $\Pi_{G,\pi}^+, \mathcal{H}_{G,\pi}^+$ be the subrepresentation of Π_0 generated by the vector

$$\xi_{G,\pi}^+ = \frac{1}{\sqrt{\dim V}} \int_{G^r}^{\oplus} \mathrm{Id}_{\mathrm{End}(V)} d\mu^r(\mathbf{g}).$$

Let $\tilde{\tau}_{G,\pi} = \frac{1}{\dim V} \tau_{G,\pi} \in \mathcal{P}_1(\mathbf{F})^{\operatorname{Aut}(\mathbf{F})}$. Now one has

$$\tilde{\tau}_{G,\pi}^+(w,\alpha) = \langle \Pi_0(w,\alpha)\xi_{G,\pi}^+,\xi_{G,\pi}^+\rangle = \frac{1}{\dim V} \int_{G^r} \operatorname{tr}(\pi(w(\mathbf{g})))d\mu^r(\mathbf{g}) = \tilde{\tau}_{G,\pi}(\alpha).$$

Thus we have constructed an explicit model for the GNS triple associated to $\tilde{\tau}_{G,\pi}^+$.

4. Extremal functions

To study $\mathcal{P}(\Gamma)$ it is convenient to introduce an operator algebra. We begin with $\mathbf{C}[\Gamma]$, the group algebra of Γ . We define a norm on $\mathbf{C}[\Gamma]$ by

$$|a\| = \sup_{\pi} \|\pi(a)\|$$

where π ranges over all cyclic *-representations⁵ of $\mathbf{C}[\Gamma]$. The completion of $\mathbf{C}[\Gamma]$ with respect to this norm is a C^* -algebra called the (full) group C^* -algebra of Γ , denoted by $C^*(\Gamma)$.

Any $\tau \in \mathcal{P}(\Gamma)$ extends to a continuous linear functional τ on $C^*(\Gamma)$ with $\|\tau\| = \tau(e)$. Therefore $\mathcal{P}_1(\Gamma)$ linearly embeds into the unit ball of the linear dual of $C^*(\Gamma)$. The set $\mathcal{P}_1(\Gamma)$ is closed in the weak-* topology and hence by the Banach-Alaoglu Theorem, $\mathcal{P}_1(\Gamma)$ is weak-* compact. Since $\mathcal{P}_1(\Gamma)$ is also obviously convex, the Krein-Milman Theorem tells us that $\mathcal{P}_1(\Gamma)$ is the (weak-*) closed convex hull of its extreme points that we will denote by hullext[$\mathcal{P}_1(\Gamma)$]. The classical relevance of the extreme points is the following result from [Seg47]:

Theorem 4.1. For $\tau \in \mathcal{P}_1(\Gamma)$, $\tau \in \text{ext}[\mathcal{P}_1(\Gamma)]$ if and only if the GNS representation π_{τ} is irreducible.

We may improve on the fact that $\mathcal{P}_1(\Gamma) = \overline{\operatorname{hullext}}[\mathcal{P}_1(\Gamma)]$ by means of Choquet theory. Since Γ is countable, $C^*(\Gamma)$ is separable, so $\mathcal{P}_1(\Gamma)$ is metrizable. Choquet's Theorem [Phe66, pg. 14] gives in the current context the following.

Theorem 4.2 (Choquet's Theorem for $\mathcal{P}_1(\Gamma)$). If $\tau \in \mathcal{P}_1(\Gamma)$, there is a (regular) Borel probability measure ν_{τ} supported on $\exp[\mathcal{P}_1(\Gamma)]$ such that for any $g \in \Gamma$,

$$\tau(g) = \int \tilde{\tau}(g) d\nu_{\tau}(\tilde{\tau}).$$

In this case, we say that ν_{τ} represents τ .

Recall we have seen as a consequence of the Krein-Milman Theorem that $\mathcal{P}_1(\Gamma) = \overline{\operatorname{hullext}}[\mathcal{P}_1(\Gamma)]$. Note that $\mathcal{P}_1(\Gamma)^{\operatorname{Aut}(\Gamma)}$ is a weak-* closed subset of $\mathcal{P}_1(\Gamma)$, since it is the intersection over $\alpha \in \operatorname{Aut}(\Gamma)$ and $g \in \Gamma$ of the sets of $\tau \in \mathcal{P}_1(\Gamma)$ such that

$$\tau(\alpha(g)) - \tau(g) = 0,$$

each of which is the vanishing locus of a weak-* continuous function on $\mathcal{P}_1(\Gamma)$. Hence $\mathcal{P}_1(\Gamma)^{\operatorname{Aut}(\Gamma)}$ is compact, and also convex, so the Krein-Milman Theorem gives

$$\mathcal{P}_1(\Gamma)^{\operatorname{Aut}(\Gamma)} = \overline{\operatorname{hull}}\operatorname{ext}[\mathcal{P}_1(\Gamma)^{\operatorname{Aut}(\Gamma)}].$$

This reduces Question 1.11 to the question of whether the functions in $\exp[\mathcal{P}_1(\mathbf{F})^{\operatorname{Aut}(\mathbf{F})}]$ separate $\operatorname{Aut}(\mathbf{F})$ -orbits. It also raises the interesting question of when our known examples of elements of $\mathcal{P}_1(\mathbf{F})^{\operatorname{Aut}(\mathbf{F})}$ are extremal.

Theorem 4.3. * Recall the notations from Example 1.4. Let π be an irreducible unitary representation of the compact group G. Then the function $\tilde{\tau}_{G,\pi} = \frac{1}{\dim V} \tau_{G,\pi}$ is in $\exp[\mathcal{P}_1(\mathbf{F})^{\operatorname{Aut}(\mathbf{F})}]$ if and only if the action by precomposition of $\operatorname{Aut}(\mathbf{F})$ on $G^r \cong \operatorname{Hom}(\mathbf{F}, G)$ is ergodic with respect to the Haar measure μ^r .

⁵A *-representation (π, V) of $\mathbf{C}[\Gamma]$ consists of a Hilbert space V and a **C**-algebra homomorphism π from $\mathbf{C}[\Gamma]$ to the bounded endomorphisms B(V) of V that also respects the star operations. The star operation on $\mathbf{C}[\Gamma]$ takes $\sum a_{\gamma}\gamma$ to $\sum \overline{a_{\gamma}}\gamma^{-1}$ and the star operation on B(V) is conjugate transpose. The *-representation (π, V) is cyclic if V contains a vector v such that $\pi(\mathbf{C}(\Gamma)).v$ is dense in V.

Fortunately, the action of $\operatorname{Aut}(\mathbf{F})$ on G^r has already been investigated by different researchers. The following theorem was proved by Goldman [Gol07] when G is a Lie group with simple factors of type U(1) or SU(2), and extended by Gelander in [Gel08] to the following.

Theorem 4.4 (Goldman, Gelander). Let G be a compact connected semisimple Lie group and suppose that $r \ge 3$. Then the action of $\operatorname{Aut}(\mathbf{F}_r)$ on G^r is ergodic with respect to the Haar measure μ^r .

Theorem 4.4 together with Theorem 4.3 allow us to produce many elements of $ext[\mathcal{P}_1(\mathbf{F})^{\operatorname{Aut}(\mathbf{F})}]$ using compact groups. The situation for finite groups is less clear. One important point is that when G is a finite non-trivial group, the action of $\operatorname{Aut}(\mathbf{F})$ on G^r will never be ergodic with respect to the Haar measure μ^r . The reason is that the subset

$$\operatorname{Epi}(\mathbf{F}, G) = \{ \phi \in \operatorname{Hom}(\mathbf{F}, G) : \phi(\mathbf{F}) = G \} \subset \operatorname{Hom}(\mathbf{F}, G)$$

is clearly invariant, and its complement has positive measure. Nonetheless, one could alter the definitions of $\tilde{\tau}_{G,\pi}$ to use the uniform measure on Epi(**F**, G) in place of μ^r . If Aut(**F**) acts transitively on Epi(**F**, G), this will yield elements of ext[$\mathcal{P}_1(\mathbf{F})^{\text{Aut}(\mathbf{F})}$]. However, it is a well-known open problem whether this is the case even for simple G:

Conjecture 4.5 (Wiegold's conjecture). If G is a finite simple group, and $r \ge 3$, then $\operatorname{Aut}(\mathbf{F}_r)$ acts transitively on $\operatorname{Epi}(\mathbf{F}_r, G)$.

The reader is invited to see the article of Lubotzky [Lub11] for a survey of Wiegold's conjecture and related questions. We also mention that it is proved in [HMP19] that two words induce the same measure on every finite group if and only if they induce the same measure on every finite group via epimorphisms.

5. A TOY PROBLEM

One of the philosophies of Voiculescu's Free Probability Theory introduced in [Voi91] is that one passes from classical probability problems involving commuting random variables to problems involving non-commutative random variables [VDN92, NS06, MS17]. In the same spirit, we may view the setup of the current paper as arising from a process by which one replaces

$$\mathbf{Z}^r \rightsquigarrow \mathbf{F}$$
$$\operatorname{Aut}(\mathbf{Z}^r) = \operatorname{GL}_r(\mathbf{Z}) \rightsquigarrow \operatorname{Aut}(\mathbf{F}).$$

In the setting of $\operatorname{GL}_r(\mathbf{Z})$ acting on \mathbf{Z}^r , we understand all the questions of this paper, and as we will see, they are connected to classical results concerning Borel measures on tori that are instructive to recall.

First we consider the extreme points of $\mathcal{P}_1(\mathbf{Z}^r)$. If $\tau \in \text{ext}[\mathcal{P}_1(\mathbf{Z}^r)]$, then the associated GNS triple $(\pi_{\tau}, \mathcal{H}_{\tau}, \xi_{\tau})$ has π_{τ} irreducible, so as \mathbf{Z}^r is abelian, \mathcal{H}_{τ} is one-dimensional, and

 $\langle \pi_{\tau}(\underline{x})\xi_{\tau},\xi_{\tau}\rangle = \exp(2\pi i\theta^{\tau}.\underline{x})$ for some

$$\theta^{\tau} = (\theta_1^{\tau}, \dots, \theta_r^{\tau}) \in [0, 1)^r,$$

where $t_{\tau} \underline{x}$ is the standard scalar (dot) product. Hence the correspondence $\tau \mapsto \theta^{\tau}$ identifies $\operatorname{ext}[\mathcal{P}_1(\mathbf{Z}^r)]$ with the torus $\mathbb{T}^r = (S^1)^r$. The weak-* topology on $\operatorname{ext}[\mathcal{P}_1(\mathbf{Z}^r)]$ corresponds to the standard metric topology on \mathbb{T}^r .

By Choquet's Theorem (Theorem 4.2) in this context, there is a regular Borel measure ν_{τ} on $\operatorname{ext}[\mathcal{P}_1(\mathbf{Z}^r)] = \mathbb{T}^r$ such that for any $\underline{x} \in \mathbf{Z}^r$

$$\tau(\underline{x}) = \int_{\text{ext}[\mathcal{P}_1(\mathbf{Z}^r)]} \tilde{\tau}(\underline{x}) d\nu_{\tau}(\tilde{\tau}) = \int_{\mathbb{T}^r} \exp(2\pi i\theta \cdot \underline{x}) d\nu_{\tau}(\theta).$$

In other words, $\tau(\underline{x})$ is simply the Fourier transform of ν_{τ} evaluated at \underline{x} .

In this case, as \mathbf{Z}^r is abelian, it is a consequence of the Stone-Weierstrass Theorem that ν_{τ} is uniquely determined by τ . It now follows that if τ is $\operatorname{GL}_r(\mathbf{Z})$ -invariant, so too is ν_{τ} . This reduces the classification of $\operatorname{GL}_r(\mathbf{Z})$ -invariant positive definite functions on \mathbf{Z}^r to the classification of $\operatorname{GL}_r(\mathbf{Z})$ -invariant Borel probability measures on \mathbb{T}^r . Moreover, the extreme points $\operatorname{ext}[\mathcal{P}_1(\mathbf{Z}^r)^{\operatorname{GL}_r(\mathbf{Z})}]$ correspond to extremal invariant measures, which by standard facts [Phe66, Prop 12.4] are the ergodic ones. One has the following classification of such measures by Burger [Bur91, Prop. 9]⁶.

Proposition 5.1. Any $\operatorname{GL}_r(\mathbf{Z})$ -invariant ergodic Borel probability measure on \mathbb{T}^d is either Lebesgue measure, or atomic and supported on a finite $\operatorname{GL}_r(\mathbf{Z})$ -orbit.

This can be read as a full classification of $\exp[\mathcal{P}_1(\mathbf{Z}^r)^{\operatorname{GL}_r(\mathbf{Z})}]$. While an analogous classification of $\exp[\mathcal{P}_1(\mathbf{F})^{\operatorname{Aut}(\mathbf{F})}]$ seems out of reach, it suggests that it would be interesting to pursue (see §6). Even further, we can show the following.

Theorem 5.2. \star For \mathbf{Z}^r , $\operatorname{GL}_r(\mathbf{Z})$, in place of \mathbf{F} , $\operatorname{Aut}(\mathbf{F})$, the hierarchy in (1.5) completely collapses. More concretely, for $\underline{x} = (x_1, \ldots, x_r)$, $\underline{y} = (y_1, \ldots, y_r) \in \mathbf{Z}^r$, $\underline{x} \in \operatorname{GL}_r(\mathbf{Z}) \cdot \underline{y}$ if and only if there is a finite abelian group G with uniform measure μ such that $\mu_{\underline{x}} = \mu_{\underline{y}}$, where e.g. $\mu_x = \underline{x}_* \mu^r$ is the pushforward of μ^r on G^r under the map

$$\underline{x}: (g_1, \ldots, g_r) \mapsto x_1g_1 + \cdots + x_rg_r.$$

6. Further open questions

Our discussion above leads to a possible alternative approach to Conjectures 1.9 and 1.10. This consists of the following program:

- I: Resolve Question 1.11, i.e. show that the elements of $ext[\mathcal{P}_1(\mathbf{F})^{Aut(\mathbf{F})}]$ separate $Aut(\mathbf{F})$ -orbits.
- II: Prove that the elements of $ext[\mathcal{P}_1(\mathbf{F})^{\operatorname{Aut}(\mathbf{F})}]$ can be approximated in a suitable way by elements arising from finite or compact groups via the construction given in Example 1.4.

⁶Although [Bur91, Prop. 9] states the result for $SL_r(\mathbf{Z})$, it also holds for $GL_r(\mathbf{Z})$.

Whether or not step II above can be accomplished is of independent interest. The following question is enticing:

Question 6.1. Is it possible to classify the elements of $ext[\mathcal{P}_1(\mathbf{F})^{Aut(\mathbf{F})}]$ in a way that generalizes Proposition 5.1?

As mentioned above, Question 6.1 may be very hard or impossible. It would be nice to reduce Question 6.1 to a question about the classification of $\operatorname{Aut}(\mathbf{F})$ -invariant ergodic measures as in Proposition 5.1. The problem with this is that the measure on $\operatorname{ext}[\mathcal{P}_1(\mathbf{F})]$ that represents an element of $\operatorname{ext}[\mathcal{P}_1(\mathbf{F})]$, given by Theorem 4.2, may not be unique; however we do not know whether this is the case in practice. Therefore one has the technical question:

Question 6.2. Is there some $\tau \in \text{ext}[\mathcal{P}_1(\mathbf{F})^{\text{Aut}(\mathbf{F})}]$ that is not represented by a unique regular Borel probability measure ν_{τ} supported on $\text{ext}[\mathcal{P}_1(\mathbf{F})]$?

Setting aside the technical issue presented in Question 6.2, one can still ask about the classification of $Aut(\mathbf{F})$ -invariant ergodic measures.

Question 6.3. Classify the Borel probability measures supported on $ext[\mathcal{P}_1(\mathbf{F})]$ that are invariant and ergodic for the action of $Aut(\mathbf{F})$.

One specific instance of Question 6.3 that is much more approachable is the following.

Question 6.4. Let G be a compact topological group. For simplicity, one might like to assume that G is a connected compact semisimple Lie group. What are the $Aut(\mathbf{F})$ -invariant and ergodic Borel measures on G^r ?

Note that Theorem 4.4 classifies, under certain hypotheses, the $Aut(\mathbf{F})$ -invariant and ergodic Borel measures on G^r that are absolutely continuous with respect to the Haar measure, and Question 6.4 removes this assumption.

Short of classification results, one may hope for other statements that would accomplish step II above. For example,

Question 6.5. Is it possible that the weak-* closure of the functions $\tilde{\tau}_{G,\pi}$ (cf. Examples 1.4, 3.4, 3.10) contains $\exp[\mathcal{P}_1(\mathbf{F})^{\operatorname{Aut}(\mathbf{F})}]$?

Again, Question 6.5 may be very difficult. However, considering Question 6.5 leads us to realize that we do not even know very basic things about $\operatorname{ext}[\mathcal{P}_1(\mathbf{F})^{\operatorname{Aut}(\mathbf{F})}]$. Note that by (2.1), all the examples of elements $\tau \in \operatorname{ext}[\mathcal{P}_1(\mathbf{F})^{\operatorname{Aut}(\mathbf{F})}]$ given in this paper, other than $\tau_{\operatorname{triv}}$, have the property that $\tau(x_1) = 0$. This invites the following basic and intriguing question.

Question 6.6. Is there $a \ \tau \in \text{ext}[\mathcal{P}_1(\mathbf{F})^{\text{Aut}(\mathbf{F})}]$ with $\tau \neq \tau_{\text{triv}}$ such that $\tau(x_1) \neq 0$?

Also with Question 6.5 in mind, if τ is a weak-* limit of functions $\tilde{\tau}_{G_i,\pi_i}$ with dim $(\pi_i) \to \infty$ as $i \to \infty$, then by Theorem 2.2, $\tau([x_1, x_2]) = 0$. This suggests that it might be helpful to ask the converse.

Question 6.7. If $r \ge 2$ and $\tau \in \text{ext}[\mathcal{P}_1(\mathbf{F})^{\text{Aut}(\mathbf{F})}]$ with $\tau([x_1, x_2]) = 0$, is τ a weak-* limit of the functions $\tilde{\tau}_{G,\pi}$?

Finally, turning to Question 1.11 in view of step I above, we propose the following.

Question 6.8. Find new constructions of $Aut(\mathbf{F})$ -invariant positive definite functions on \mathbf{F} .

APPENDIX A. PROOFS OF BACKGROUND RESULTS

In some of our proofs we use the following simple fact.

Lemma A.1. If G is a compact topological group with probability Haar measure μ , (π, V) is an irreducible unitary representation of G, and $A \in \text{End}(V)$, then

$$\int_G \pi(g) A \pi(g)^{-1} d\mu(g) = \frac{\operatorname{tr}(A)}{\dim V} \operatorname{Id}_V.$$

Proof. The left hand side is invariant under conjugation by elements $\pi(g)$ with $g \in G$, so by Schur's Lemma is a scalar multiple of the identity. The trace of the matrices inside the integral is constant and equal to $\operatorname{tr}(A)$, and so the result of the integral is a scalar multiple of the identity with trace $\operatorname{tr}(A)$.

Proof of Lemma 1.5. It is enough to show that μ^r is invariant under the Nielsen generators given in (1.1), (1.2), (1.3). The measure μ^r is determined by the formula, for any continuous $f: G^r \to \mathbf{C}$,

$$\int_{G^r} f(\mathbf{g}) d\mu^r(\mathbf{g}) = \int_G \dots \int_G f(g_1, \dots, g_r) d\mu(g_1) \dots d\mu(g_r).$$

For $\sigma \in S_r$ we have

$$\int_{G^r} f(\alpha_{\sigma}(\mathbf{g})) d\mu^r(\mathbf{g}) = \int_G \dots \int_G f(g_{\sigma(1)}, \dots, g_{\sigma(r)}) d\mu(g_1) \dots d\mu(g_r)$$
$$= \int_G \dots \int_G f(g_1, \dots, g_r) d\mu(g_1) \dots d\mu(g_r)$$
$$= \int_{G^r} f(\mathbf{g}) d\mu^r(\mathbf{g})$$

by Fubini's Theorem. We have

$$\int_{G^r} f(\iota(\mathbf{g})) d\mu^r(\mathbf{g}) = \int_G \dots \int_G f(g_1^{-1}, \dots, g_r) d\mu(g_1) \dots d\mu(g_r)$$
$$= \int_G \dots \int_G f(g_1, \dots, g_r) d\mu(g_1) \dots d\mu(g_r)$$
$$= \int_{G^r} f(\mathbf{g}) d\mu^r(\mathbf{g})$$

since μ is invariant under pushforward by $g \mapsto g^{-1}$ (that is a result of the bi-invariance and uniqueness of Haar measure). Finally, we have

$$\int_{G^r} f(\gamma(\mathbf{g})) d\mu^r = \int_G \dots \int_G f(g_1 g_2, \dots, g_r) d\mu(g_1) \dots d\mu(g_r)$$
$$= \int_G \dots \int_G f(g_1, \dots, g_r) d\mu(g_1) \dots d\mu(g_r)$$
$$= \int_{G^r} f(\mathbf{g}) d\mu^r(\mathbf{g})$$

by the right-invariance of Haar measure.

Proof of Lemma 1.12. Let C(G) denote the Banach space of continuous complex valued functions on G with supremum norm. Since G^r and G are compact and Hausdorff, and $w: G^r \to G$ is continuous, μ^r is a regular Borel probability measure, and so too is the pushforward measure $\mu_w = w_*\mu^r$. Hence by the Riesz-Markov Theorem μ_w is uniquely determined by the formula

$$\int_{g \in G} f(g) d\mu_w(g) = \int_{(g_1, \dots, g_r) \in G^r} f(w(g_1, \dots, g_r)) d\mu^r(g_1, \dots, g_r), \quad \forall f \in C(G).$$

Since the linear span of matrix coefficients of irreducible unitary representations is dense in C(G) by the Peter-Weyl Theorem, it follows that μ_w is determined by the integrals

$$\int_{(g_1,\ldots,g_r)\in G^r} \langle \pi(w(g_1,\ldots,g_r))v_1,v_2\rangle d\mu^r(g_1,\ldots,g_r).$$

where $\pi : G \to U(V)$ is an irreducible unitary representation of G and $v_1, v_2 \in V$. On the other hand, we have

$$\begin{split} &\int_{(g_1,\dots,g_r)\in G^r} \langle \pi(w(g_1,\dots,g_r))v_1,v_2\rangle \, d\mu^r(g_1,\dots,g_r) \\ &= \int_{h\in G} \int_{(g_1,\dots,g_r)\in G^r} \langle \pi(w(hg_1h^{-1},\dots,hg_rh^{-1}))v_1,v_2\rangle d\mu^r(g_1,\dots,g_r)d\mu(h) \\ &= \int_{h\in G} \int_{(g_1,\dots,g_r)\in G^r} \langle \pi(h)\pi(w(g_1,\dots,g_r))\pi(h)^{-1}v_1,v_2\rangle d\mu^r(g_1,\dots,g_r)d\mu(h) \\ &= \int_{(g_1,\dots,g_r)\in G^r} \langle \left(\int_{h\in G} \pi(h)\pi(w(g_1,\dots,g_r))\pi(h)^{-1}d\mu(h)\right)v_1,v_2\rangle d\mu^r(g_1,\dots,g_r) \\ &= \frac{\langle v_1,v_2\rangle}{\dim V} \int_{(g_1,\dots,g_r)\in G^r} \operatorname{tr}(\pi(w(g_1,\dots,g_r)))d\mu^r(g_1,\dots,g_r) \\ &= \frac{\langle v_1,v_2\rangle}{\dim V} \tau_{G,\pi}(w), \end{split}$$

where the third equality used Fubini's Theorem and the fourth equality used Lemma A.1. This shows that μ_w is determined by the values $\tau_{G,\pi}(w)$ with π irreducible.

Proof of Lemma 2.4. Suppose for simplicity that w_1 is generated by x_1, \ldots, x_s and w_2 is generated by x_{s+1}, \ldots, x_r . Let (w_1, w_2) be the map that takes $G^r \to G \times G$, $(w_1, w_2)(g_1, \ldots, g_r) =$

 $(w_1(g_1,\ldots,g_s), w_2(g_{s+1},\ldots,g_r))$. Let ν be the pushforward of μ^r under (w_1,w_2) . By Fubini's Theorem, the pushforward of a product measure under a product of two continuous maps is the product of the pushforward measures of the two maps. Since μ^r is the product measure of μ^s and μ^{r-s} on $G^r = G^s \times G^{r-s}$, we obtain $\nu = \mu_{w_1} \times \mu_{w_2}$. Furthermore, the word map w is obtained by the composition

$$G^r \xrightarrow{(w_1, w_2)} G \times G \xrightarrow{\text{mult}} G$$

where $\text{mult}(g_1, g_2) = g_1 g_2$. This shows that $\mu_w = \text{mult}_*[\nu] = \text{mult}_*[\mu_{w_1} \times \mu_{w_2}] = \mu_{w_1} * \mu_{w_2}$.

If μ_1 and μ_2 are two conjugation invariant measures on G and (π, V) is an irreducible representation of G then

$$\begin{split} \mu_1 * \mu_2[\operatorname{tr}(\pi)] &= \int_{g_2 \in G} \int_{g_1 \in G} \operatorname{tr}(\pi(g_1 g_2)) d\mu_1(g_1) d\mu_2(g_2) \\ &= \int_{h \in G} \int_{g_2 \in G} \int_{g_1 \in G} \operatorname{tr}(\pi(hg_1 h^{-1}) \pi(g_2)) d\mu_1(g_1) d\mu_2(g_2) d\mu(h) \\ &= \int_{g_2 \in G} \int_{g_1 \in G} \operatorname{tr}\left(\left(\int_{h \in G} \pi(h) \pi(g_1) \pi(h)^{-1} d\mu(h)\right) \pi(g_2)\right) d\mu_1(g_1) d\mu_2(g_2) \\ &= \frac{1}{\dim V} \int_{g_2 \in G} \int_{g_1 \in G} \operatorname{tr}(\pi(g_1)) \operatorname{tr}(\pi(g_2)) d\mu_1(g_1) d\mu_2(g_2) \\ &= \frac{1}{\dim V} \mu_1[\operatorname{tr}(\pi)] \mu_2[\operatorname{tr}(\pi)], \end{split}$$

where the second last equality used Lemma A.1. Here we use the notation $\mu[f]$ for the integral of a function f with respect to a measure μ . The stated formula for $\tau_{G,\pi}(w)$ now follows from $\mu_w = \mu_{w_1} * \mu_{w_2}$ and the fact that μ_{w_1} and μ_{w_2} are conjugation invariant.

Proof of Proposition 3.6. Let Λ_1 and Λ_2 be the characteristic subgroups of \mathbf{F} generated by $\operatorname{Aut}(\mathbf{F}).w_1$ and $\operatorname{Aut}(\mathbf{F}).w_2$ respectively. Suppose $\Lambda_1 \neq \Lambda_2$. Then at most one of the intersections

 $\operatorname{Aut}(\mathbf{F}).w_2 \cap \Lambda_1, \quad \operatorname{Aut}(\mathbf{F}).w_1 \cap \Lambda_2$

is non-empty. Indeed if $\operatorname{Aut}(\mathbf{F}).w_i \cap \Lambda_j \neq \emptyset$ for $i \neq j$ then since Λ_j is characteristic, this implies $\operatorname{Aut}(\mathbf{F}).w_i \subset \Lambda_j$ and so $\Lambda_i \subset \Lambda_j$. So suppose without loss of generality that $\operatorname{Aut}(\mathbf{F}).w_2 \cap \Lambda_1 = \emptyset$. Then (recalling the notation from Example 3.5) $\tau_{\Lambda_1}(w_2) = 0$ but $\tau_{\Lambda_1}(w_1) = 1$ showing **PosDef** $w_1 \not\sim w_2$.

Proof of Lemma 3.9. Consider a finite sequence of elements $\{(\gamma_i, \alpha_i)\}_{i=1}^N \subset \Gamma \rtimes \operatorname{Aut}(\Gamma)$. We need to prove that the matrix A with

$$A_{ij} \stackrel{\text{def}}{=} \tau^+((\gamma_i, \alpha_i)(\gamma_j, \alpha_j)^{-1})$$

is positive semidefinite. To this end,

$$A_{ij} = \tau^{+}((\gamma_{i}, \alpha_{i})(\gamma_{j}, \alpha_{j})^{-1})$$

= $\tau^{+}((\gamma_{i}, \alpha_{i})(\alpha_{j}^{-1}(\gamma_{j}^{-1}), \alpha_{j}^{-1}))$
= $\tau^{+}((\gamma_{i}[\alpha_{i}\alpha_{j}^{-1}](\gamma_{j}^{-1}), \alpha_{i}\alpha_{j}^{-1}))$
= $\tau(\gamma_{i}[\alpha_{i}\alpha_{j}^{-1}](\gamma_{j}^{-1}))$
= $\tau(\alpha_{i}^{-1}(\gamma_{i})\alpha_{j}^{-1}(\gamma_{j}^{-1})) = \tau(\alpha_{i}^{-1}(\gamma_{i})\alpha_{j}^{-1}(\gamma_{j})^{-1}).$

In other words, A_{ij} is the matrix associated to τ and the sequence $\{\alpha_i^{-1}(\gamma_i)\}_{i=1}^N$ and so is positive semidefinite, since τ is positive definite.

Proof of Theorem 4.3. We use the notation from Example 3.10. Suppose first that the action of Aut(**F**) on $G^r \cong \text{Hom}(\mathbf{F}, G)$ is not ergodic, so that there exists a Borel set $E \subset G^r$ such that $\alpha(E) = E$ for all $\alpha \in \text{Aut}(\mathbf{F})$ and $0 < \mu(E) < 1$. Then letting

$$\tau_1(w) = \frac{1}{\mu(E)\dim V} \int_{\mathbf{g}\in G^r} \operatorname{tr}(\pi(w(\mathbf{g})))\mathbf{1}_E(\mathbf{g})d\mu^r(\mathbf{g}),$$

$$\tau_2(w) = \frac{1}{(1-\mu(E))\dim V} \int_{\mathbf{g}\in G^r} \operatorname{tr}(\pi(w(\mathbf{g})))(1-\mathbf{1}_E(\mathbf{g}))d\mu^r(\mathbf{g}),$$

we have that τ_1 and τ_2 are in $\mathcal{P}_1(\mathbf{F})^{\operatorname{Aut}(\mathbf{F})}$, as the measure $\mathbf{1}_E(\mathbf{g})d\mu^r(\mathbf{g})$ is $\operatorname{Aut}(\mathbf{F})$ -invariant. On the other hand

$$\tilde{\tau}_{G,\pi} = \frac{\mu(E)}{2}\tau_1 + \frac{1-\mu(E)}{2}\tau_2,$$

so in this case, $\tilde{\tau}_{G,\pi}$ is not extremal in $\mathcal{P}_1(\mathbf{F})^{\operatorname{Aut}(\mathbf{F})}$.

Now, for the other direction, suppose that π is irreducible and that the action of Aut(**F**) on G^r is ergodic, but for the sake of a contradiction, suppose that $\tilde{\tau}_{G,\pi} = t\tau_1 + (1-t)\tau_2$ with $t \in (0,1)$ and $\tau_1, \tau_2 \in \mathcal{P}_1(\mathbf{F})^{\operatorname{Aut}(\mathbf{F})}$, with τ_1 not a positive multiple of $\tau_{G,\pi}$. Under our assumptions we have

$$\tilde{\tau}^+_{G,\pi} = t\tau^+_1 + (1-t)\tau^+_2$$

with $\tau_1^+, \tau_2^+ \in \mathcal{P}_1(\mathbf{F} \rtimes \operatorname{Aut}(\mathbf{F}))$, and τ_1^+ not a multiple of $\tilde{\tau}_{G,\pi}^+$. By standard facts [BdlHV08, Prop. C.5.1], this means that $\Pi_{G,\pi}^+$ is <u>reducible</u> as a unitary representation of $\mathbf{F} \rtimes \operatorname{Aut}(\mathbf{F})$. Therefore (see [BdlHV08, Proof of Theorem C.5.2]) there is some projection P that commutes with all the elements $\Pi_{G,\pi}^+(w,\alpha), P\xi_{G,\pi}^+ \neq 0$, and

$$\tau_3^+(w,\alpha) = \left\langle \Pi_{G,\pi}^+(w,\alpha) \frac{P\xi_{G,\pi}^+}{\|P\xi_{G,\pi}^+\|}, \frac{P\xi_{G,\pi}^+}{\|P\xi_{G,\pi}^+\|} \right\rangle$$

is in $\mathcal{P}_1(\mathbf{F} \rtimes \operatorname{Aut}(\mathbf{F}))$ with $\tau_3^+ \neq \tilde{\tau}_{G,\pi}^+$ (i.e. $\frac{P\xi_{G,\pi}^+}{\|P\xi_{G,\pi}^+\|} \neq \xi_{G,\pi}^+$). It follows that $P\xi_{G,\pi}^+$ is an invariant vector for $\operatorname{Aut}(\mathbf{F})$ under Π_0 . However, when restricted to $\operatorname{Aut}(\mathbf{F})$, the representation Π_0 is simply the representation of $\operatorname{Aut}(\mathbf{F})$ on the $\operatorname{End}(V)$ -valued L^2 functions on G^r acting by

permutations of G^r . Since Aut(**F**) acts ergodically on G^r , we must have

$$\frac{P\xi_{G,\pi}^+}{\|P\xi_{G,\pi}^+\|} = \int_{G^r}^{\oplus} Bd\mu^r(\mathbf{g}),$$

where $B \in \text{End}(V)$ is a constant with $\text{tr}(BB^*) = 1$. But this means in turn, using the invariance of Haar measure under conjugation,

$$\begin{aligned} \tau_3^+(w,\alpha) &= \tau_3^+(w,e) = \int_{G^r} \operatorname{tr}(\pi(w(\mathbf{g}))BB^*)d\mu^r(\mathbf{g}) \\ &= \int_{(g_1,\dots,g_r)\in G^r} \left(\int_{h\in G} \operatorname{tr}\left(\pi(w(hg_1h^{-1},\dots,hg_rh^{-1}))BB^*\right)d\mu(h)\right) d\mu^r(g_1,\dots,g_r) \\ &= \int_{(g_1,\dots,g_r)\in G^r} \left(\int_{h\in G} \operatorname{tr}\left(\pi(h)\pi(w(g_1,\dots,g_r))\pi(h)^{-1}BB^*\right)d\mu(h)\right) d\mu^r(g_1,\dots,g_r) \\ &= \frac{1}{\dim V} \int_{(g_1,\dots,g_r)\in G^r} \operatorname{tr}(\pi(w(\mathbf{g})))\operatorname{tr}(BB^*)d\mu^r(\mathbf{g}) \\ &= \frac{1}{\dim V} \int_{(g_1,\dots,g_r)\in G^r} \operatorname{tr}(\pi(w(\mathbf{g})))d\mu^r(\mathbf{g}) = \tilde{\tau}^+_{G,\pi}(w,\alpha). \end{aligned}$$

The second last equality used Lemma A.1. This is a contradiction.

Proof of Theorem 5.2. If $\underline{x} \in \operatorname{GL}_r(\mathbf{Z}).\underline{y}$ then it is easy to check that $\mu_{\underline{x}} = \mu_{\underline{y}}$ on any finite abelian group.

The other direction is the more interesting one. Assume that $\underline{x} \notin \operatorname{GL}_r(\mathbf{Z}).\underline{y}$. The orbit of $\underline{x} = (x_1, \ldots, x_r)$ is parametrized by the modulus of the greatest common divisor of the x_i (which we take to be ∞ if $\underline{x} = \underline{0}$), and similarly for y.

Thus our assumptions entail, by switching \underline{x} and \underline{y} if necessary, that there is a prime pand an exponent f such that $\underline{x} \equiv 0 \mod p^f$ and $\underline{y} \neq 0 \mod p^f$. This means that for any $\mathbf{g} = (g_1, \ldots, g_r) \in (\mathbf{Z}/p^f \mathbf{Z})^r$, $x_1g_1 + \cdots + x_rg_r = \underline{0}$, so the \underline{x} -measure on $\mathbf{Z}/p^f \mathbf{Z}$ is an atom at $\underline{0}$. On the other hand, $\underline{y} \neq 0 \mod p^f$ implies there is some $\mathbf{g} = (g_1, \ldots, g_r) \in (\mathbf{Z}/p^f \mathbf{Z})^r$ such that $y_1g_1 + \cdots + y_rg_r \neq \underline{0}$, so the \underline{y} -measure on $\mathbf{Z}/p^f \mathbf{Z}$ is not supported at $\underline{0} \in \mathbf{Z}/p^f \mathbf{Z}$. This proves the \underline{x} - and y-measures on $\mathbf{Z}/p^f \mathbf{Z}$ are distinct.

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