

UNEXTENDIBLE PRODUCT BASES OF PAULI EIGENSTATES: AN ORTHOGONALITY LAYER OVER TOTAL DOMINATION IN

$$K_q^{\times n}$$

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ABSTRACT. Call a set $S \subseteq [q]^n$ of words *unextendible* if every word of $[q]^n$ disagrees with some member of S in every coordinate. The minimum size of such a set carries two names in two literatures that do not cite each other: it is the minimum skirting set $f(n, q)$ of Adriaensen, Ihringer, Martin and Villagrán, and it is the total domination number $\gamma_t(K_q^{\times n})$ of the direct power of a complete graph, studied since Mekiš through Defant–Iyer and Vemuri. Reading the six letters of [6] as the six single-qubit Pauli eigenstates turns a word into a stabilizer product state, and a *pairwise orthogonal* unextendible set into an unextendible product basis. Neither literature imposes orthogonality, and the unextendible-product-basis literature never fixes the local alphabet; this paper works at that intersection. We prove that the minimum size $s_{\text{stab}}(5)$ of a Pauli-eigenstate unextendible product basis on five qubits is exactly 6, attained by an explicit six-state example in which every one of the six letters occurs exactly once at every coordinate — it is the GenShifts basis of DiVincenzo, Mor, Shor, Smolin and Terhal with its two free local bases taken to be the X - and Y -eigenbases, and five is the largest number of qubits at which that specialisation is available — and we prove $9 \leq \gamma_t(K_6^{\times 6}) \leq 10$, whose upper half improves the published bound $f(q, q) \leq 2q - 1$ at $q = 6$. Along the way we record, with their sources, the covering bounds that are already in print, give a short self-contained proof of $\gamma_t(K_q^{\times n}) \geq n + 3$ for $4 \leq q \leq n$ (a bound implied by two published theorems), and separate $s_{\text{stab}}(n)$ from the unrestricted qubit minimum $f(n)$ for every $n \geq 6$ not divisible by 4. Every combinatorial statement below is machine-checked in Lean 4.

1. INTRODUCTION

One parameter, two names. Fix an alphabet $[q] = \{0, 1, \dots, q-1\}$ and a length n , and call a finite set $S \subseteq [q]^n$ *unextendible* when

- (1) for every $\ell \in [q]^n$ there is $s \in S$ with $s_i \neq \ell_i$ for every coordinate i .

Write $\gamma_t(K_q^{\times n})$ for the least size of such a set. The notation is the second of two names this quantity already has.

In the direct (categorical, tensor, Kronecker) power $K_q^{\times n}$ two words are adjacent exactly when they differ in every coordinate, so (1) says precisely that every vertex has a neighbour in S : an unextendible set is a *total dominating set*, and the minimum size is the total domination number. Lower bounds for domination and total domination in direct products of complete graphs have been studied since Mekiš [11]; the two results this paper leans on are Defant and Iyer’s [4, Thm. 2.6], $\gamma(\prod_{i=1}^t K_{n_i}) \geq t + 1 + \lfloor (t-1)/(n_1-1) \rfloor$ whenever $2 \leq n_1 \leq \dots \leq n_t$, $t \geq 4$

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and $n_2 \geq 3$, and Vemuri's [15, Thm. 1.5], which characterises, under the same hypotheses, when $\gamma = t + 2$.

Independently, Adriaensen, Ihringer, Martin and Villagr  n [1] call a set satisfying (1) a *skirting set* in $\mathbb{Z}_q^n$ and write $f(n, q)$ for the minimum size. They identify the two objects in one sentence — “a skirting set S in $\mathbb{Z}_q^n$ is exactly the same thing as a total dominating set in $G(n, q)$ ” — and prove, among other things, $f(n, q) = n + 1$ for $n < q$ [1, Lem. 2], the volume bound $f(n, q) \geq (q/(q-1))^n$ [1, Prop. 3], sub-multiplicativity $f(n+m, q) \leq f(n, q)f(m, q)$ [1, Thm. 1], and $f(q, q) \leq 2q - 1$ for $q \geq 3$ [1, Lem. 4]. Their tables cover $q = 3$ and $q = 4$. For $q = 3$ the same question is a problem of Imre Leader, treated by Kuang and Wang [10], who write the identification as $f(n, q) = \gamma_t(K_q^{\times n})$.

Remark 1.1. The two literatures do not cite each other, and the cost is measurable. At $q = n = 6$ the skirting-set vocabulary alone gives $7 \leq f(6, 6) \leq 11$ — the lower bound from the monotonicity of [1, Lem. 6] and $f(5, 6) = 6$, the upper from [1, Lem. 4] — while the domination chain already forces $\gamma_t(K_6^{\times 6}) \geq 9$ (Section 4). A verdict of “open” reached inside one vocabulary is evidence about the vocabulary. The non-citation is checkable: the bibliography of [1] has exactly three entries — a paper on the hat guessing number, the *Handbook of Combinatorial Designs*, and a table of covering array numbers — and no domination paper among them. The traffic runs the other way only in [10], which cites both sides.

The layer neither literature has. Now take $q = 6$ and read the six letters as the six single-qubit Pauli eigenstates

$$(2) \quad 0 = |0\rangle, \quad 1 = |1\rangle, \quad 2 = |+\rangle, \quad 3 = |-\rangle, \quad 4 = |+i\rangle, \quad 5 = |-i\rangle,$$

so that a word $w \in [6]^n$ names the n -qubit stabilizer product state $|w\rangle = |w_1\rangle \otimes \cdots \otimes |w_n\rangle$. Two of the six letters are orthogonal exactly when they are antipodal on the Bloch sphere, i.e. related by the fixed-point-free involution

$$(3) \quad \alpha = (0\ 1)(2\ 3)(4\ 5),$$

and a product state $|w\rangle$ is orthogonal to $|w'\rangle$ exactly when $w_i = \alpha(w'_i)$ for some i . A set of pairwise orthogonal product states spanning a proper subspace, to which no further product state is orthogonal, is an *unextendible product basis* (UPB), and — as we recall in Section 2 — for a set of Pauli-eigenstate product states the unextendibility requirement is exactly (1), because a single-qubit state that is not one of the six letters is orthogonal to none of them. So the object of this paper is

$$s_{\text{stab}}(n) = \min\{|S| : S \subseteq [6]^n \text{ unextendible and pairwise orthogonal}\},$$

the minimum size of an n -qubit UPB every one of whose tensor factors is a Pauli eigenstate. Neither the skirting-set papers nor the domination chain ever restricts to pairwise orthogonal sets, and the UPB literature never restricts the local states to a fixed six-letter alphabet. Trivially

$$s_{\text{stab}}(n) \geq \max(f(n), \gamma_t(K_6^{\times n})),$$

where $f(n)$ is Johnston's unrestricted qubit minimum [8, Thm. 1]: $f(n) = n + 1$ for odd n ; $f(n) = n + 2$ for $n = 4$ and $n \equiv 2 \pmod{4}$; $f(8) = 11$; $f(n) = n + 4$ otherwise. The question is when that inequality is strict, i.e. what the Pauli restriction costs.

Results.

- $s_{\text{stab}}(5) = 6$ (Theorem 5.4). Five qubits admit a six-state UPB every tensor factor of which is a Pauli eigenstate; six is also the unrestricted minimum $f(5)$ and the covering minimum $\gamma_t(K_6^{\times 5})$, so at five qubits orthogonality is free. The witness uses each of the six letters exactly once at every coordinate, which meets the block bound with equality and is why five is the last length at which six states can do it. The upper bound is not new as a construction: the witness *is* the GenShifts UPB of DiVincenzo, Mor, Shor, Smolin and Terhal [5], with its two free local bases taken to be $\{|+\rangle, |-\rangle\}$ and $\{|+i\rangle, |-i\rangle\}$ (Remark 5.6). What Theorem 5.4 adds is the value together with its matching lower bound inside the combinatorial model, and the observation that five qubits is the last odd length at which GenShifts admits a Pauli-eigenstate specialisation at all.
- $9 \leq \gamma_t(K_6^{\times 6}) \leq 10$ (Theorem 6.1). In the skirting-set notation, $9 \leq f(6, 6) \leq 10$. The upper half is an explicit ten-word set and improves the published $f(q, q) \leq 2q - 1$ [1, Lem. 4] at $q = 6$, where it reads $f(6, 6) \leq 11$; the lower half is the $n + 3$ bound of Section 4, which is implied by [4, Thm. 2.6] together with [15, Thm. 1.5].

Both cells sit in the table below; boldface marks the entries settled or bracketed here.

n	1	2	3	4	5	6	7
$f(n)$ (unrestricted, [8])	2	4	4	6	6	8	8
$\gamma_t(K_6^{\times n})$	2	3	4	5	6	[9, 10]	≥ 10
$s_{\text{stab}}(n)$	2	—	4	6	6	[9, 12]	≥ 10

The entries $\gamma_t(K_6^{\times n}) = n + 1$ for $n \leq 5$ are [1, Lem. 2]. The dash at $n = 2$ records that $\mathbb{C}^2 \otimes \mathbb{C}^2$ admits no UPB at all: the combinatorial conditions are satisfiable there, but only by complete bases. The two $n = 1$ entries are the complete one-qubit basis $|0\rangle, |1\rangle$ and are listed under the convention of [8], which does not ask a UPB to span a proper subspace. Every set considered below at $n \geq 3$ has fewer than 2^n elements and therefore does span a proper subspace, as a UPB must under the convention in force here (Remark 2.2).

Two readings of the table are worth isolating. At four qubits orthogonality *strictly costs a state*: five words cover $[6]^4$, so $\gamma_t(K_6^{\times 4}) = 5$, while $s_{\text{stab}}(4) = 6$ (Theorem 5.3). At five qubits it is free (Theorem 5.4). From six qubits on, the covering bound alone gives $s_{\text{stab}}(n) \geq n + 3$, which separates s_{stab} from f for every $n \geq 6$ not divisible by 4 (Theorem 5.8); at $n = 8$ it ties $f(8) = 11$ and for $n \equiv 0 \pmod{4}$, $n \geq 12$, it falls one short of $f(n) = n + 4$, so no separation is claimed there.

What is not new. The covering bounds of Section 3 are recalled with their sources and are not offered as results: the trivial bound $\gamma_t \geq n + 1$ is the first half of [1, Lem. 2] with the same argument, and is also the combinatorial form of the classical UPB bound $1 + \sum_i (d_i - 1)$; the block bound $qn \leq (q - 1)|S|$ is [4, Thm. 2.6] specialised to equal factor sizes, where it reads $\lceil qn/(q - 1) \rceil = n + 1 + \lfloor (n - 1)/(q - 1) \rfloor$; the volume bound and sub-multiplicativity are [1, Prop. 3] and [1, Thm. 1], the latter a special case of $\gamma_t(G \times H) \leq \gamma_t(G)\gamma_t(H)$ [13, Thm. 3]. The bound $\gamma_t(K_q^{\times n}) \geq n + 3$ for $4 \leq q \leq n$ (Section 4) is implied by [4, Thm. 2.6] together with [15, Thm. 1.5], whose three cases for $\gamma = t + 2$ are each contradictory when

all factors have the same size $q \leq t$; what Section 4 contributes is a short direct proof, for γ_t and with no classification theorem behind it. The value $s_{\text{stab}}(3) = 4$ is attained by the Shifts UPB of Bennett, DiVincenzo, Mor, Shor, Smolin and Terhal [3], and matches $f(3) = 4$. For $s_{\text{stab}}(4) = 6$ both halves are in print separately: $s_{\text{stab}}(4) \geq f(4) = 6$ is [8, Thm. 1(b)], and substituting Pauli eigenstates for the free local bases in the four-qubit example U_8 of [2, Table I] produces a six-state Pauli-eigenstate UPB. Only the comparison with $\gamma_t(K_6^{\times 4}) = 5$ is new there. Likewise the parity lemma of Section 5 has a conclusion already implied by $s_{\text{stab}} \geq f$; what it buys is a proof inside the combinatorial model, which is what makes $s_{\text{stab}}(4) = 6$ a self-contained statement here rather than a quotation. The six-state witness at five qubits is in print too, in a different language: it is the GenShifts UPB of DiVincenzo, Mor, Shor, Smolin and Terhal [5] with its free local bases specialised to Pauli eigenbases, as Remark 5.6 spells out. What is left for Theorem 5.4 is the value $s_{\text{stab}}(5) = 6$ with a lower bound proved inside the combinatorial model, and the fact that five qubits is where that specialisation runs out.

Grounds for the novelty claims. The one wholly new statement is $\gamma_t(K_6^{\times 6}) \leq 10$; that s_{stab} is a parameter nobody has defined or tabulated is a separate, negative claim, and both searches deserve to be stated. For s_{stab} : the quantity was not found as a defined parameter or a sequence in preprint metadata (nine query combinations of “unextendible product bas*” against *stabilizer*, *Pauli*, *Clifford* and *graph state*, all returning nothing behind positive controls returning 43, 73 and 435 items), nor in the OEIS, which holds Johnston’s unrestricted sequence [9] but no stabilizer-restricted one, nor in a local full-text preprint corpus, where 439 occurrences of “unextend[ai]ble product bas” across about 126 papers yielded 38 hits near *stabilizer*/*Pauli*/*Clifford*, all coincidental on inspection. The corpus does not contain the quantum-physics category, so that last negative is weak and the metadata channels carry the weight. The nearest recent work, Frembs [6] (“stabiliser”, in the British spelling that American-spelled queries miss), studies unextendibility *by* stabiliser states, a different object; its four-qubit Pauli-product example has eight elements, and the minimality it establishes is in the number of qubits, not in the size of the set. The bases-per-site and weak-UPB literature that does contain a Pauli-eigenstate example [2, 14] classifies four qubits only. These channels look for names, and the five-qubit witness marks their limit: it is a named object nowhere, yet it is an instance of one (Remark 5.6), and no metadata query would have surfaced that. For $\gamma_t(K_6^{\times 6}) \leq 10$: no table, formula or witness for $f(6, 6)$ was found in preprint metadata, the OEIS (which holds no sequence for this parameter at all) or the corpus; [1] is the state of the art and stops at $q = 4$.

2. PRELIMINARIES

Words, boxes and blocks. Throughout, $n, q \geq 1$, coordinates are indexed by $\{1, \dots, n\}$, and S is a finite subset of $[q]^n$. We say $\ell \in [q]^n$ *escapes* S if every $s \in S$ agrees with ℓ in at least one coordinate; S is *unextendible* iff nothing escapes it, which is (1). Equivalently, the *boxes* $\prod_i ([q] \setminus \{s_i\})$, $s \in S$, cover $[q]^n$. The *block* of S at coordinate i carrying letter a is

$$B(S, i, a) = \{s \in S : s_i = a\};$$

for fixed i the nonempty blocks partition S , and there are at most q of them. A block with exactly two elements is a *doubleton*.

The quantum reading. Under (2) a word $w \in [6]^n$ names a product state $|w\rangle$ of n qubits, and α of (3) sends each letter to the unique letter orthogonal to it. Since $\langle w | w' \rangle = \prod_i \langle w_i | w'_i \rangle$ and no two non-antipodal letters are orthogonal,

$$(4) \quad |w\rangle \perp |w'\rangle \iff w_i = \alpha(w'_i) \text{ for some } i.$$

We write $\text{Orth}(w, w')$ for the right-hand side and call $S \subseteq [6]^n$ a *stabilizer UPB* when it is unextendible and pairwise Orth.

The next proposition is why that combinatorial definition is the right one; it is quoted, not proved here.

Proposition 2.1 (Sainz et al. [14]). *For local dimension $d = 2$, every weak UPB is a UPB. Concretely, if $S \subseteq [6]^n$ is pairwise orthogonal and unextendible in the sense of (1), then no product state of $(\mathbb{C}^2)^{\otimes n}$ at all, Pauli-eigenstate or otherwise, is orthogonal to $|s\rangle$ for every $s \in S$.*

The mechanism is worth recording because it is what makes the problem finite. Suppose $|u\rangle = |u_1\rangle \otimes \cdots \otimes |u_n\rangle$ is orthogonal to every $|s\rangle$, $s \in S$. For each s some factor must vanish, say $\langle u_i | s_i \rangle = 0$; but the only single-qubit state orthogonal to the letter s_i is the letter $\alpha(s_i)$, so u_i is itself a letter — of a local vector belonging to none of the chosen bases, [14] says that “it cannot be orthogonal to any local component of any vector in S ”. Defining $\ell_i = \alpha(u_i)$ where u_i is a letter and arbitrarily elsewhere produces a word that escapes S . Hence restricting the extending state to the six letters is no restriction at all, and unextendibility becomes the finite condition (1).

Remark 2.2 (the properness clause, and two conventions). A UPB is also required to span a proper subspace: Bennett et al. [3] define a product basis to be “a set S of pure orthogonal product states spanning a proper subspace $\mathcal{H}_S$ of $\mathcal{H}$ ”, and a UPB to be one whose complementary subspace contains no product state. A pairwise orthogonal $S \subseteq [6]^n$ spans a subspace of dimension $|S|$, so the requirement is automatic as soon as $|S| < 2^n$, which holds for every set considered below at $n \geq 3$ ($|S| \leq 12$). At $n \leq 2$ it is not automatic, and there it bites: every orthogonal product set in $\mathbb{C}^2 \otimes \mathbb{C}^d$ is completable to a full product basis [5], so “in $\mathbb{C}^2 \otimes \mathbb{C}^d$ there are no UPBs for any d ” [2]. That is why $s_{\text{stab}}(2)$ is left undefined in the table of Section 1: the combinatorial conditions (1) and (4) are satisfiable at $n = 2$ — by 00, 01, 10, 11, say — but only by sets that span all of $\mathbb{C}^2 \otimes \mathbb{C}^2$.

The neighbouring entry $f(2) = 4$ of the same table obeys the other convention. Johnston [8] defines a UPB to be “an orthonormal set $\mathcal{S} \subseteq (\mathbb{C}^2)^{\otimes p}$ of product states such that there is no product state orthogonal to every member of $\mathcal{S}$ ”, with no properness clause, so a complete product basis qualifies; the OEIS entry for f , which is Johnston’s own, records the same reading — “ $a(2) = 4$ because there is no nontrivial UPB on two qubits” [9]. The two conventions differ only where the minimum reaches 2^n , i.e. at $n \leq 2$; from $n = 3$ on every value in the table is the same under either.

Nothing in the formal development mentions a quantum state: it works with (1) and (4) as definitions, and Proposition 2.1 is the bridge, cited from [14].

3. THE COVERING THEORY, AND WHERE IT IS ALREADY IN PRINT

All of this section is about unextendibility alone, so every bound is a bound on $\gamma_t(K_q^{\times n}) = f(n, q)$ and a fortiori on $s_{\text{stab}}(n)$ at $q = 6$. The engine is the following

lemma, of which the published bounds are the instances $|K| = 0, 1$ and which we will need at $|K| = 2$ in Section 4.

Lemma 3.1 (the catch lemma). *Let $S \subseteq [q]^n$ be unextendible. For every set K of coordinates and every $c \in [q]^n$,*

$$|\{s \in S : s_i \neq c_i \text{ for all } i \in K\}| > n - |K|.$$

Proof sketch. Contrapositive. If the words avoiding c on all of K number at most $n - |K|$, assign them injectively to coordinates outside K , let ℓ take at each such coordinate the value its assigned word has there, and let $\ell = c$ on K . Every word of S then agrees with ℓ somewhere — the caught ones on K , the uncaught ones at their assigned coordinate — so ℓ escapes S . The formal proof runs an induction that spends one free coordinate on one word, which avoids constructing the injection explicitly. $\square$

Proposition 3.2 (the trivial bound; [1, Lem. 2]). *An unextendible $S \subseteq [q]^n$ has $|S| > n$; that is, $\gamma_t(K_q^{\times n}) \geq n + 1$.*

Proof. Lemma 3.1 with $K = \emptyset$. $\square$

This is the first half of [1, Lem. 2], proved there by the same argument (“If S is a set of n vertices in $\mathbb{Z}_q^n$, say $x_1, \dots, x_n$, then we can make a vector y with $y(i) = x_i(i)$, which is clearly not skirted by any vector of S ”), and it is the combinatorial shadow of the classical UPB bound $1 + \sum_i (d_i - 1)$. The second half of [1, Lem. 2] is that $n + 1$ is attained when $n < q$, so $\gamma_t(K_6^{\times n}) = n + 1$ for $n \leq 5$.

Proposition 3.3 (blocks and the block bound; [4, Thm. 2.6]). *Let $S \subseteq [q]^n$ be unextendible. Then*

- (1) $|B(S, i, a)| + n \leq |S|$ for every coordinate i and letter a ;
- (2) $qn \leq (q - 1)|S|$, i.e. $\gamma_t(K_q^{\times n}) \geq \lceil qn/(q - 1) \rceil$;
- (3) if $|S| = n + 1$ then the letters used at any one coordinate are pairwise distinct, and consequently $n + 1 \leq q$ — so no set of size $n + 1$ is unextendible once $n \geq q$.

Proof. (i) is Lemma 3.1 at $K = \{i\}$, $c_i = a$. For (ii), the at most q blocks at one coordinate partition S and each has at most $|S| - n$ elements, so $|S| \leq q(|S| - n)$, which rearranges to $qn \leq (q - 1)|S|$. For (iii), at $|S| = n + 1$ (i) gives blocks of size at most 1, so $s \mapsto s_i$ is injective on S and $n + 1 = |S| \leq q$. $\square$

Part (ii) is exactly Defant and Iyer’s [4, Thm. 2.6] specialised to equal factor sizes: their bound $\gamma \geq t + 1 + \lfloor (t - 1)/(n_1 - 1) \rfloor$ becomes, at $n_i = q$ and $t = n$, the identity $n + 1 + \lfloor (n - 1)/(q - 1) \rfloor = \lceil qn/(q - 1) \rceil$, which we verified by cases on $n \bmod (q - 1)$. Their parameter is the domination number γ and $\gamma_t \geq \gamma$, so the bound transfers. It does not appear on the skirting-set side, whose own linear lower bound is the monotonicity of [1, Lem. 6].

Proposition 3.4 (volume bound and sub-multiplicativity; [1, Prop. 3 and Thm. 1]). *Let $S \subseteq [q]^n$ and $T \subseteq [q]^m$ be unextendible. Then $q^n \leq |S|(q - 1)^n$, and the concatenation $S * T = \{st : s \in S, t \in T\} \subseteq [q]^{n+m}$ is unextendible with $|S * T| \leq |S||T|$. Hence $\gamma_t(K_q^{\times(n+m)}) \leq \gamma_t(K_q^{\times n})\gamma_t(K_q^{\times m})$ and the limit $\lim_n \gamma_t(K_q^{\times n})^{1/n}$ exists.*

Proof. The boxes cover $[q]^n$ and each has $(q-1)^n$ elements, which is the volume bound. For the concatenation, given $\ell \in [q]^{n+m}$ pick $s \in S$ disagreeing with the first n coordinates of ℓ everywhere and $t \in T$ disagreeing with the last m likewise; then st disagrees with ℓ everywhere. The cardinality bound is immediate. $\square$

Both statements are in [1] verbatim, the first inside the proof of Proposition 3 (“if S is a skirting set in $G(n, q)$, then $|S|(q-1)^n \geq q^n$, from which $f(n, q) \geq (q/(q-1))^n$ ”), the second inside the proof of Theorem 1 (“It readily follows that $f(n+m, q) \leq f(n, q)f(m, q)$ ”). In graph-theoretic generality the sub-multiplicativity is [13, Thm. 3]: “If G and H have no isolated vertices, then $\gamma_t(G \times H) \leq \gamma_t(G)\gamma_t(H)$ ”, a statement Rall credits to the observation of Nowakowski and himself in [12] that the set product of two total dominating sets is a total dominating set of the product.

4. PAST $n+2$: THE BOUND $\gamma_t(K_q^{\times n}) \geq n+3$

Proposition 3.3(iii) kills the value $n+1$ once $n \geq q$. The next theorem kills $n+2$ as well, provided the alphabet is not too small. Its conclusion is not new: it follows from [4, Thm. 2.6], which gives $\gamma \geq n+2$ when $q \leq n$, together with [15, Thm. 1.5], whose three cases characterising $\gamma = t+2$ are each contradictory when all factors have the same size $q \leq t$; with $\gamma_t \geq \gamma$ that is exactly $n+3$. We give the proof because it is short, because it treats γ_t directly, and because it needs no classification theorem.

Theorem 4.1. *Let $4 \leq q \leq n$ and let $S \subseteq [q]^n$ be unextendible. Then $|S| \neq n+2$, and hence $|S| \geq n+3$; that is, $\gamma_t(K_q^{\times n}) \geq n+3$ whenever $4 \leq q \leq n$.*

Proof. Suppose $|S| = n+2$. By Proposition 3.3(i) every block has at most 2 elements, and by Lemma 3.1 at $K = \{i, j\}$ with $i \neq j$,

$$(5) \quad |B(S, i, a) \cup B(S, j, b)| \leq |S| - n + 1 = 3.$$

Two doubletons at *different* coordinates therefore meet, having 4 elements between them and at most 3 in their union; two doubletons at the *same* coordinate are disjoint. Since a two-element set cannot meet three pairwise disjoint sets, no coordinate carries three doubletons as soon as some other coordinate carries one. Counting at a coordinate i , the at most q blocks partition $n+2$ elements into parts of size at most 2, so the number a_i of doubletons at i satisfies $a_i \geq n+2-q \geq 2$ (using $q \leq n$). Hence every coordinate carries a doubleton, every $a_i \leq 2$, and so $n+2-q \leq 2$, forcing $n=q$ and $a_i = 2$ for every i .

Fix the first coordinate, with its two doubletons B, B' , necessarily disjoint, and fix $b' \in B'$. Let i be any other coordinate and C one of its two doubletons. Then C meets both B and B' and has only two elements, so $C = \{x, y\}$ with $x \in B$, $y \in B'$. The two doubletons at i are disjoint, so their B' -parts are distinct and together exhaust the two-element set B' ; exactly one of them therefore contains b' , say $\{x_i, b'\}$ with $x_i \in B$.

Finally, one doubleton cannot occur at two different coordinates: if F is a doubleton at both i and j with $i \neq j$, take the other doubleton G at j ; then F and G are disjoint, being doubletons at the same coordinate j , yet F is a doubleton at $i \neq j$ and G one at j , so they must meet. Since $n=q \geq 4$ there are at least three coordinates besides the first; their partners x_i all lie in the two-element set B , so two coincide, and the corresponding doubletons $\{x_i, b'\}$ are one and the same set occurring at two different coordinates. Contradiction.

With Proposition 3.2 and Proposition 3.3(iii) this leaves $|S| \geq n + 3$. $\square$

Both hypotheses are load-bearing and both are refuted in Section 7. The bound is sharp at the smallest instance its hypotheses allow.

Proposition 4.2. $\gamma_t(K_4^{\times 4}) = 7$.

Proof. The lower bound is Theorem 4.1 at $q = n = 4$. For the upper bound, the seven words

0000, 1111, 0211, 1221, 2122, 3333, 1210

form an unextendible subset of $[4]^4$; this is verified by evaluating (1) at all $4^4 = 256$ words. The value also appears as $f(4, 4) = 7$ in the table of [1], computed there by integer programming. $\square$

Remark 4.3. Outside the formal development we reproduced the value by exhaustive search: a depth-first search with minimum-remaining-values branching and arc consistency visited 3 530 369 206 nodes without finding a six-word unextendible subset of $[4]^4$, and found seven-word ones in seconds. The same programs reproduce $f(n, 3) = 3, 5, 8$ and $f(n, 4) = 3, 4, 7$ for $n = 2, 3, 4$, matching the tables of [1], which begin at $n = 2$; they also give the trivial $f(1, 3) = f(1, 4) = 2$.

5. THE ORTHOGONALITY LAYER

We now impose (4). The first lemma is where orthogonality does work that covering cannot do; its conclusion is implied by $s_{\text{stab}} \geq f$ and [8, Thm. 1(b,c,d)], and what it adds is a proof inside the combinatorial model.

Theorem 5.1. *Let n be even and positive. No stabilizer UPB in $[6]^n$ has exactly $n + 1$ elements.*

Proof. Let S be one, with $|S| = n + 1$. By Proposition 3.3(iii) the map $s \mapsto s_i$ is injective for each i , so the set $L_i = \{s_i : s \in S\}$ of letters used at coordinate i has $n + 1$ elements. Let

$$M_i = \{(s, t) \in S \times S : s_i = \alpha(t_i)\}$$

be the ordered pairs orthogonal at i . The map $(s, t) \mapsto s_i$ is injective on M_i : s_i determines s by injectivity, and $t_i = \alpha(s_i)$ determines t . Its image lies in $\{a \in L_i : \alpha(a) \in L_i\}$, a subset closed under α and hence, α being a fixed-point-free involution, of even cardinality. That cardinality is at most $|L_i| = n + 1$, and being even with n even it is at most n ; so $|M_i| \leq n$. Pairwise orthogonality puts every one of the $(n + 1)n$ ordered pairs of distinct elements of S into some M_i , whence $(n + 1)n \leq \sum_{i=1}^n |M_i| \leq n \cdot n$, which is false. $\square$

The parity step — every α -closed subset of the six letters has even size — is also verified directly in the formal development, by evaluating it at all $2^6 = 64$ subsets.

Theorem 5.2. $s_{\text{stab}}(3) = 4$, attained by the Shifts UPB

$$|0, 1, -\rangle, \quad |1, -, 0\rangle, \quad |-, 0, 1\rangle, \quad |+, +, +\rangle,$$

which uses only the four real letters $|0\rangle, |1\rangle, |+\rangle, |-\rangle$.

Proof. The lower bound is Proposition 3.2 at $n = 3$. For the upper bound, the four words 013, 130, 301, 222 are pairwise orthogonal (six pairs) and unextendible; the covering condition is verified at all $6^3 = 216$ words. Both checks are exhaustive evaluations. $\square$

The set is the Shifts UPB of [3], displayed there as

$$|0, 1, +\rangle, \quad |1, +, 0\rangle, \quad |+, 0, 1\rangle, \quad |-, -, -\rangle;$$

the form in the theorem is that one conjugated by $Z^{\otimes 3}$, which exchanges $|+\rangle$ and $|-\rangle$. It is also what the tile construction of [7, Thm. 1] produces from the five-tile decomposition of $\mathbb{Z}_2^3$, and it is the case $k = 2$ of the GenShifts family of [5]. The value 4 equals $f(3)$.

Theorem 5.3. $s_{\text{stab}}(4) = 6$, while $\gamma_t(K_6^{\times 4}) = 5$. At four qubits the orthogonality requirement strictly costs one state over the covering minimum.

Proof. Lower bound: Proposition 3.2 gives $|S| \geq 5$ and Theorem 5.1 excludes $5 = n + 1$. Upper bound: the six words

$$0000, 2221, 0431, 3512, 1343, 2150,$$

that is $|0, 0, 0, 0\rangle, |+, +, +, 1\rangle, |0, +i, -, 1\rangle, |- , -i, 1, +\rangle, |1, -, +i, -\rangle, |+, 1, -i, 0\rangle$, are pairwise orthogonal (15 pairs) and unextendible, the latter verified at all $6^4 = 1296$ words. For $\gamma_t(K_6^{\times 4}) = 5$: the lower bound is [1, Lem. 2] ($n = 4 < q = 6$), and the five constant words 0000, 1111, 2222, 3333, 4444 are unextendible, since any word of $[6]^4$ uses at most four distinct letters and so one of the five disagrees with it everywhere. $\square$

The witness above uses the Y basis: some coordinate of some word is $|+i\rangle$ or $|-i\rangle$, and this is not an accident of the search — over the real (i.e. X/Z) four-letter alphabet the minimum at four qubits is 8, not 6 (Remark 5.7). Neither half of Theorem 5.3 is new: $s_{\text{stab}}(4) \geq f(4) = 6$ is [8, Thm. 1(b)], and the six-element set

$$U_8 = \{|0000\rangle, |e1e\bar{e}\rangle, |1e\bar{e}f\rangle, |\bar{e}\bar{e}f1\rangle, |e01\bar{f}\rangle, |01fe\rangle\}$$

of [2, Table I] becomes a six-state Pauli-eigenstate UPB on substituting $|e\rangle = |+\rangle$ and $|f\rangle = |+i\rangle$. Here $\{|0\rangle, |1\rangle\}$, $\{|e\rangle, |\bar{e}\rangle\}$ and $\{|f\rangle, |\bar{f}\rangle\}$ are the three independent local bases of that table, (2, 2, 3, 3) of them per site, and the bar is that paper's own notation: $|\bar{e}\rangle$ “stands for the unit vector orthogonal to $|e\rangle$ (unique up to phase)”. Under the substitution the six states read 0000, 2123, 1234, 3351, 2015, 0142 in the alphabet (2), and we checked pairwise orthogonality and unextendibility for them independently of our own witness. What is new is only the comparison with the covering minimum.

Five qubits. The next theorem settles the five-qubit cell.

Theorem 5.4. $s_{\text{stab}}(5) = 6$. A six-state Pauli-eigenstate UPB on five qubits is

$$\begin{aligned} &|0, 0, 0, 0, 0\rangle, \quad |1, +, +i, -i, -\rangle, \quad |-, 1, +, +i, -i\rangle, \\ &|-i, -, 1, +, +i\rangle, \quad |+i, -i, -, 1, +\rangle, \quad |+, +i, -i, -, 1\rangle, \end{aligned}$$

in letters

$$00000, \quad 12453, \quad 31245, \quad 53124, \quad 45312, \quad 24531,$$

and every coordinate of it carries each of the six letters exactly once.

Proof. Lower bound: the block bound of Proposition 3.3(ii) at $q = 6$, $n = 5$ reads $30 \leq 5|S|$, so $|S| \geq 6$ — with no orthogonality used, so $\gamma_t(K_6^{\times 5}) = 6$ as well, in agreement with [1, Lem. 2]. Upper bound: the displayed set is pairwise orthogonal (15 pairs, each verified by exhibiting a coordinate carrying an antipodal pair) and unextendible; unextendibility is the assertion that each of the $6^5 = 7776$ words of

$[6]^5$ disagrees with one of the six in every coordinate, and is discharged by exhaustive evaluation. That each coordinate carries all six letters is likewise checked directly; it also follows from the equality case of the block bound, since $|S| - n = 1$ forces every block to be a singleton. $\square$

Remark 5.5. The witness was produced by exhaustive depth-first search over $[6]^5$ with an orthogonality constraint, and was then re-verified from scratch three ways before being written down: combinatorially, by an independently written re-verifier, and numerically, by building the actual vectors in $(\mathbb{C}^2)^{\otimes 5}$ and checking that every cross inner product vanishes to machine precision and that dropping any one state destroys unextendibility. These re-verifications are outside the formal development; the statements of Theorem 5.4 are inside it.

The lower bound is known twice over ([8, Thm. 1(a)] gives $f(5) = 6$ and [1, Lem. 2] gives $\gamma_t(K_6^{\times 5}) = 6$). The witness, it turns out, is known as well, and the next remark says exactly how.

Remark 5.6 (the witness is GenShifts). Case (a) of [8, Thm. 1] is, in that paper’s words, “demonstrated by the ‘GenShifts’ UPB constructed in” [5]. GenShifts is defined there on $2k - 1$ qubits with $2k$ members: the first state is $|0, \dots, 0, 0\rangle$, the second is

$$|1, \psi_1, \psi_2, \dots, \psi_{k-1}, \psi_{k-1}^\perp, \dots, \psi_2^\perp, \psi_1^\perp\rangle,$$

and the rest are its cyclic right shifts, where the only conditions on the local states are that $|\psi_i\rangle$ and $|\psi_j\rangle$ for $i \neq j$ be “neither orthogonal nor identical” and that each $|\psi_i\rangle$ be neither orthogonal nor identical to $|0\rangle$. Nothing there asks the $|\psi_i\rangle$ to be real. Taking $k = 3$, $|\psi_1\rangle = |+\rangle$ and $|\psi_2\rangle = |+i\rangle$ satisfies every condition, and the resulting six states are, word for word, the witness of Theorem 5.4. So the upper bound of Theorem 5.4 is a specialisation of a published construction, not a new one.

Five qubits is where that specialisation stops. In a GenShifts instance every local state is one of $|0\rangle, |1\rangle, |\psi_i\rangle, |\psi_i^\perp\rangle$, and α carries letters to letters, so the instance consists of Pauli eigenstates exactly when every $|\psi_i\rangle$ is one. Being neither orthogonal nor identical to $|0\rangle$ rules out $|0\rangle$ and $|1\rangle$, so $|\psi_i\rangle \in \{|+\rangle, |-\rangle, |+i\rangle, |-i\rangle\}$; and being pairwise non-orthogonal and pairwise distinct allows at most one from each of the two antipodal pairs there. Hence $k - 1 \leq 2$, so $2k - 1 \leq 5$. What Theorem 5.4 adds to the literature is therefore the value $s_{\text{stab}}(5) = 6$ together with a lower bound proved inside the combinatorial model, and this last observation.

Remark 5.7. Restricting further, to the four real letters $|0\rangle, |1\rangle, |+\rangle, |-\rangle$, changes the answer. Outside the formal development we computed by exhaustive search that the minimum real stabilizer UPB on four qubits has 8 states, none existing at size ≤ 7 (379 245 nodes) — consistent with [14], which states for two bases per party that “the UPBs obtained in this way have only 8, 9, 10 or 12 elements”. Against $f(4) = 6$ and $\gamma_t(K_6^{\times 4}) = 5$ this shows that a restricted local alphabet can cost more than one state.

The separation from the unrestricted minimum.

Theorem 5.8. $s_{\text{stab}}(n) \geq n + 3$ for every $n \geq 6$. Consequently $s_{\text{stab}}(n) > f(n)$ for every $n \geq 6$ that is not divisible by 4.

Proof. The first claim is Theorem 4.1 at $q = 6 \leq n$, and uses no orthogonality. For the second, compare with [8, Thm. 1]: for odd n , $f(n) = n + 1 < n + 3$; for $n \equiv 2 \pmod{4}$, $f(n) = n + 2 < n + 3$. Together these are exactly the $n \geq 6$ not divisible by 4. $\square$

The scope is the whole of the statement. At $n = 8$ the bound ties, $f(8) = 11 = n + 3$, and for $n \equiv 0 \pmod{4}$ with $n \geq 12$ it falls one short of $f(n) = n + 4$; in those cases we claim no separation. The smallest separated case is $n = 6$, where $s_{\text{stab}}(6) \geq 9 > 8 = f(6)$.

6. SIX LETTERS, SIX COORDINATES

At $q = n = 6$ the alphabet and the length agree, and this is the first length at which Theorem 4.1 says anything about the six-letter alphabet. The cell is out of reach of the tables of [1], which stop at $q = 4$.

Theorem 6.1. $9 \leq \gamma_t(K_6^{\times 6}) \leq 10$; equivalently $9 \leq f(6, 6) \leq 10$. The upper bound is attained by the ten words

001255 041453 124144 230532 303415
353020 412321 452010 545203 555400

Proof. The lower bound is Theorem 4.1 at $q = n = 6$. The upper bound is the assertion that the displayed set is unextendible, i.e. that each of the $6^6 = 46\,656$ words of $[6]^6$ disagrees with one of the ten in every coordinate. This is an exhaustive check of 46 656 words against ten, about 2.8 million letter comparisons; in the formal development it is discharged by compiled evaluation rather than by kernel reduction (Section 8), which is the one place in this paper where that distinction matters. The set is not pairwise orthogonal — the first two displayed words carry no antipodal pair at any coordinate — so it is a total dominating set and not a stabilizer UPB. $\square$

The published state of this cell is $f(6, 6) \leq 2q - 1 = 11$ [1, Lem. 4] on the skirting side, with $f(6, 6) \geq 7$ from the monotonicity of [1, Lem. 6] and $f(5, 6) = 6$; the tables of [1] stop at $q = 4$. So Theorem 6.1 improves the published upper bound at $q = 6$ by one, to $2q - 2$, and combines it with the lower bound the domination literature supplies. We do not know whether $f(q, q) \leq 2q - 2$ holds in general.

Remark 6.2. The ten-word set was found by simulated annealing and re-verified from scratch against all 46 656 words before being used, with every one of the ten shown to be load-bearing. A heuristic *failure* would be worthless evidence here, and we record why: the same repair heuristic reproduces the known optima at $q = 3$ (5 at $n = 3$, 8 at $n = 4$, and correctly fails at 7) and yet fails to find the highly structured six-word optimum of Theorem 5.4 at $q = 6$, $n = 5$. Its failures at sizes 9 to 12 for $n = 6$ are therefore no evidence at all about the true value. Deciding $\gamma_t(K_6^{\times 6}) \in \{9, 10\}$ calls for the instrument [1] used at $q = 3, 4$, an integer program over 46 656 binary variables and 46 656 constraints; we did not run it.

Theorem 6.3. Concatenation preserves pairwise orthogonality as well as unextendibility, so $s_{\text{stab}}(a + b) \leq s_{\text{stab}}(a)s_{\text{stab}}(b)$. In particular $9 \leq s_{\text{stab}}(6) \leq 12$.

Proof. For unextendibility this is Proposition 3.4. For orthogonality, two distinct concatenations st and $s't'$ differ in the first block or in the second; in either case the block where they differ contains a coordinate carrying an antipodal pair, which

serves the concatenation. Now the two one-letter words $0, 1$ of $[6]^1$ are unextendible and orthogonal, and $s_{\text{stab}}(5) = 6$ by Theorem 5.4, giving $|S| \leq 12$ for the concatenation and hence $s_{\text{stab}}(6) \leq 12$ — the twelve words span a subspace of dimension $12 < 2^6$, so the properness clause of Remark 2.2 is met even though it is not at $n = 1$. The lower bound 9 is Theorem 4.1 at $q = n = 6$, which needs no orthogonality. The twelve concatenated words are recorded explicitly in the formal development, and their two defining properties are verified there by exhaustive evaluation over $[6]^6$. $\square$

So $s_{\text{stab}}(6) > 8 = f(6)$: six qubits is where the Pauli restriction first provably bites. The cell $s_{\text{stab}}(6) \in [9, 12]$ is open. An exhaustive search is out of reach without symmetry reduction: the unrestricted search at $n = 6$ needs a 272 MB neighbourhood bitmap and about 3.4×10^7 population counts per node, and the residual symmetry group after fixing one word, of order $8^6 \cdot 6!$, is entirely unexploited.

7. NEGATIVE CONTROLS

A development in which every hypothesis is decorative would prove all of the above and mean none of it. The following are verified against the same definitions as the positive results.

- Proposition 7.1.** (1) $\gamma_t(K_6^{\times 5}) = 6 = n + 1$, so Theorem 4.1 is false without the hypothesis $q \leq n$.
- (2) $\gamma_t(K_3^{\times 3}) = 5 = n + 2$, witnessed by *000, 111, 221, 122, 212*, so Theorem 4.1 is false without the hypothesis $4 \leq q$. (The block bound gives ≥ 5 here, so the value is exact.)
- (3) The five constant words *0000, ..., 4444* are unextendible in $[6]^4$ and are not pairwise orthogonal. So the value $s_{\text{stab}}(4) = 6$ is not a covering fact: its lower bound fails once orthogonality is dropped, and the orthogonality hypothesis of Theorem 5.3 is therefore not vacuous.
- (4) Deleting the state $|+, +, +\rangle$ from the Shifts UPB destroys unextendibility, so the value $s_{\text{stab}}(3) = 4$ is not attained one state lower by that candidate.
- (5) The pair $|0, 0, 0, 0\rangle, |1, 1, 1, 1\rangle$ is orthogonal and extendible, so the covering clause is not implied by pairwise orthogonality.
- (6) Proposition 4.2: $\gamma_t(K_4^{\times 4}) = 7$ exactly, so Theorem 4.1 is sharp at the smallest instance its hypotheses allow.

8. VERIFICATION

Every combinatorial statement in this paper is machine-checked in Lean 4, in a development of seven modules and 31 statements built on Mathlib; repository reference to be added at submission. The development defines (1) and (4) directly and proves the general theory — Lemma 3.1, Propositions 3.2, 3.3 and 3.4, Theorems 4.1, 5.1, 5.8 and the concatenation half of Theorem 6.3 — with no appeal to any finite computation, and discharges the explicit witnesses by evaluation: kernel reduction (**decide +kernel**) for the witnesses at $n = 3, 4, 5$ and for $\gamma_t(K_4^{\times 4}) = 7$, where the largest single check walks all $6^5 = 7776$ words of $[6]^5$, and compiled evaluation (**native_decide**) for the two covering checks at $n = 6$, whose 46 656 words are twelve times that and past the memory budget of kernel reduction. An audit of the axiom set of all 31 statements found no incomplete proof anywhere: exactly

three statements carry a compiled-evaluation axiom — the two $n = 6$ covering checks and the results consuming them, that is the upper halves of Theorems 6.1 and 6.3 — and every other statement, including both $n = 6$ *lower* bounds, uses only propositional extensionality, quotient soundness and choice. No statement of the formal development mentions a quantum state: Proposition 2.1, which bridges (1) to unextendibility among arbitrary product states, is cited from [14] and not re-proved, as are Johnston’s values $f(n)$ [8] and every attribution in Sections 3 and 4. For the same reason Remarks 2.2 and 5.6 are outside the formal development: both argue about quantum states, the first from the cited absence of UPBs in $\mathbb{C}^2 \otimes \mathbb{C}^d$ and the second from the conditions [5] places on the free local states of GenShifts. The searches reported in Remarks 4.3, 5.5, 5.7 and 6.2 were run by two independently written programs sharing no code, each calibrated against published values — the tables $f(n, 3)$ and $f(n, 4)$ of [1], the minimum UPB size on three qubits, and the four-qubit real spectrum of [14] — and are outside the formal development; every object they produced was re-verified inside it.

9. OPEN QUESTIONS

- (1) *Is $\gamma_t(K_6^{\times 6}) = 9$ or 10?* A nine-word skirting set would give $f(q, q) \leq 2q - 3$ at $q = 6$; the natural instrument is the integer program of Remark 6.2.
- (2) *Is $s_{\text{stab}}(6) = 9$?* The cell is open on [9, 12]. Orthogonality prunes hard — at four qubits the orthogonal exhaustion closed size ≤ 5 in 955 093 nodes against 3.5×10^9 for the unrestricted search at $q = 4$ — so a symmetry-reduced search is the right instrument.
- (3) *Is $s_{\text{stab}}(n) = \max(f(n), \gamma_t(K_6^{\times n}))$ always?* It holds at $n = 3, 4, 5$. Remark 5.7 shows that the analogous identity fails for the real four-letter alphabet at $n = 4$, so there is no general reason to expect it.
- (4) *Does the exponent $\lim_n s_{\text{stab}}(n)^{1/n}$ exceed $\lim_n \gamma_t(K_6^{\times n})^{1/n}$?* Both limits exist by Proposition 3.4 and Theorem 6.3; the covering one lies in $[6/5, 6^{1/5}]$ by the volume bound and $\gamma_t(K_6^{\times 5}) = 6$. Nothing is known about the gap.
- (5) *Can the argument of Theorem 4.1 be pushed to $n + 4$?* The analysis of doubletons at $|S| = n + 2$ is what gives $n + 3$; the catch lemma at $|S| = n + 3$ gives blocks of size at most 3 and a three-coordinate constraint, and whether that closes $n + 3$ at $q = n$ is unexamined.

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