Atomic Latin Squares of Order Eleven

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Abstract: A Latin square is *pan-Hamiltonian* if the permutation which defines row i relative to row j consists of a single cycle for every $i \neq j$. A Latin square is *atomic* if all of its conjugates are pan-Hamiltonian. We give a complete enumeration of atomic squares for order 11, the smallest order for which there are examples distinct from the cyclic group. We find that there are seven main classes, including the three that were previously known. A *perfect* 1-*factorization* of a graph is a decomposition of that graph into matchings such that the union of any two matchings is a Hamiltonian cycle. Each pan-Hamiltonian Latin square of order n describes a perfect 1-*factorization* of $K_{n,n}$, and vice versa. Perfect 1-factorizations of $K_{n,n}$ can be constructed from a perfect 1-factorization of K_{n+1}. Six of the seven main classes of atomic squares of order 11 can be obtained in this way. For each atomic square of order 11, we find the largest set of Mutually Orthogonal Latin Squares (MOLS) involving that square. We discuss algorithms for counting orthogonal mates, and discover the number of orthogonal mates possessed by the cyclic squares of orders up to 11 and by Parker's famous turn-square. We find that the number of atomic orthogonal mates possessed by a Latin square is not a main class invariant. We also define a new sort of Latin square, called a pairing square, which is mapped to its transpose by an involution acting on the symbols. We show that pairing squares are often orthogonal mates for symmetric Latin squares. Finally, we discover connections between our atomic squares and Franklin's diagonally cyclic self-orthogonal squares, and we correct a theorem of Longyear which uses tactical representations to identify self-orthogonal Latin squares in the same main class as a given Latin square. © 2003 Wiley Periodicals, Inc. J Combin Designs 12: 12–34, 2004

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1. INTRODUCTION

A *Latin square* is a matrix of order n in which each row and column is a permutation of some (fixed) symbol set of size n. It is also sometimes convenient to think of a Latin square of order n as a set of n^2 triples of the form (row, column, symbol). The Latin property means that distinct triples never agree in more than one coordinate. For each Latin square there are six conjugate squares obtained by uniformly permuting the coordinates of each triple. These conjugates can be labelled by a permutation giving the new order of the coordinates, relative to the former order of $(1, 2, 3)$. Hence, the $(1, 2, 3)$-conjugate is the square itself and the $(2, 1, 3)$-conjugate is its transpose. The $(1, 3, 2)$-conjugate, also known as the row-inverse [20], is found by interchanging columns and symbols, which is another way of saying that each row, when thought of as a permutation, is replaced by its inverse. Throughout this paper, we will use L^T and L^* to denote the transpose and row-inverse, respectively, of a given Latin square L. A square is said to be *symmetric* if it is equal to its transpose and *totally symmetric* if it is equal to all six of its conjugates. To check that L is totally-symmetric it is sufficient to establish that $L = L^T = L^*$. In several places in this paper, we use L_{ij} to denote the symbol in row i, column j of the Latin square L.

A *Latin rectangle* is a matrix in which each row is a permutation of the same symbols and no symbol occurs more than once in any column. An *isotopy* of a Latin rectangle R is a permutation of its rows, permutation of its columns and relabelling of its symbols. The resulting rectangle is said to be *isotopic* to R. An isotopy which maps R to itself is called an *autotopy* of R.

The combination of an isotopy with the taking of a conjugate is called a *paratopy*. The set of Latin squares paratopic to a given Latin square L is called the *main class* of L. A paratopy which maps L to itself is an *autoparatopy* of L. These notions can be extended to Latin rectangles as well, with the understanding that the identity and row-inverse are the only two conjugates that it makes sense to use.

If R is a $2 \times n$ Latin subrectangle of some Latin square L, and R is minimal in that it contains no $2 \times n'$ Latin subrectangle for $2 \leq n' < n$, then we say that R is a *row cycle* of length n. Row cycles correspond to cycles in the permutation which defines one row relative to another. Column cycles and symbol cycles are defined similarly, and the operations of conjugacy on L interchange these objects. Row cycles, column cycles and symbol cycles will collectively be known as *cycles*.

A Latin square of order n is *pan-Hamiltonian* if every row cycle has length n. A square is pan-Hamiltonian if and only if its row-inverse is pan-Hamiltonian. A Latin square is *atomic* if all of its conjugates are pan-Hamiltonian. In other words, an atomic square is a Latin square in which all of the cycles have length equal to the order of the square. This terminology comes from [20], in which both pan-Hamiltonian and atomic squares are investigated in some detail. In that paper it is shown that for orders up to 10, the only main classes of atomic squares are based on the cyclic group tables of prime orders. There is one additional main class containing a pan-Hamiltonian Latin square of order 7 and 37 main classes containing pan-Hamiltonian Latin squares of order 9. Note that pan-Hamiltonian Latin squares (and hence also atomic squares) of order n can exist only if n is odd or $n = 2$.

Pan-Hamiltonicity is an isotopy invariant and the atomic property is a main class invariant. The original interest in pan-Hamiltonian Latin squares arose from the fact that they contain no non-trivial Latin subsquares. In fact, they contain no non-trivial

Latin subrectangles. Latin squares with no non-trivial Latin subsquares are called N_∞ squares. For more information on N_∞ squares, consult [3].

A 1-*factorization* of a graph is a decomposition of that graph into 1-factors (perfect matchings). A 1-factorization is *perfect* if the union of any two of its 1-factors is a Hamiltonian cycle. For background on these concepts, consult [17] and [19]. There is a close relationship between Latin squares and 1-factorizations of complete bipartite graphs, in which each row of a square L corresponds to a 1-factor. The two vertex sets of the bipartite graph correspond to the columns and the symbols of L, respectively. The Latin property of L means that the edges corresponding to the (column, symbol) pairs within a row are a 1-factor, and the 1-factors corresponding to different rows are disjoint. Hence a Latin square L of order n neatly encodes a 1-factorization F of $K_{n,n}$. Taking the union of two 1-factors from F, we get cycles in the graph which correspond exactly to row cycles of L. In fact, it is easy to see that F is perfect if and only if L is pan-Hamiltonian.

Theorem 1.1. *A pan-Hamiltonian Latin square of order n encodes a perfect* 1-*factorization of* $K_{n,n}$, *and vice versa.*

There is also an important connection with perfect 1-factorizations of complete graphs, which has been observed by Laufer [8] and others.

Theorem 1.2. *If there is a perfect* 1-*factorization of* K_{n+1} *then* $K_{n,n}$ *also has a perfect* 1-*factorization.*

We now describe the construction behind this result. From a perfect 1-factorization F of K_{n+1}, construct a pan-Hamiltonian Latin square $\mathcal{L}(F)$ of order n, with rows, columns and symbols labelled from 1 to n, as follows. First choose one vertex of K_{n+1} to be ∞, the "point at infinity", and label the other vertices $1, 2, \ldots, n$. For each 1-factor

$$\{(\infty, i), (a_1, b_1), (a_2, b_2), \ldots, (a_{(n-1)/2}, b_{(n-1)/2})\}$$

in F, create a row of $\mathcal{L}(F)$ by putting i in the ith column, a_j in the b_jth column and b_j in the a_jth column, for each $j = 1, 2, \ldots, (n-1)/2$. Note that by Theorem 1.1, a perfect 1-factorization of $K_{n,n}$ is described by $\mathcal{L}(F)$.

There are a number of important things to note about this construction. Firstly, non-isomorphic factorizations of $K_{n,n}$ can result from different choices of the point at infinity. Examples can be found in Section 3. Secondly, $\mathcal{L}(F) = \mathcal{L}(F)^*$. Thirdly, not all perfect 1-factorizations of $K_{n,n}$ are isomorphic to a 1-factorization which is derived in this way. Those that are have a Latin square representation which is isotopic to a pan-Hamiltonian Latin square L satisfying $L = L^*$. This seems to be a strong restriction, as attested to by the observation in [20] that only one of the 37 non-isomorphic perfect 1-factorizations of $K_{9,9}$ is related by the above construction to a perfect 1-factorization of K_{10}.

The only known infinite families of perfect 1-factorizations of complete graphs are for K_{p+1} and K_{2p}, where p is an odd prime. Hence, we immediately get perfect 1-factorizations for $K_{p,p}$ and $K_{2p-1,2p-1}$ by Theorem 1.2. A third infinite family of perfect 1-factorizations of complete bipartite graphs was recently described in [1]. Unlike the first two families, it does not correspond to a family of factorizations of complete graphs. It is generated in terms of pan-Hamiltonian Latin squares, and covers all orders of the form p^2, where p is an odd prime. The construction of the require pan-Hamiltonian Latin square starts with the addition table of the direct product $\mathbb{Z}_p \oplus \mathbb{Z}_p$ and then slightly perturbs it to destroy the short cycles.

The present paper deals with the atomic squares of order 11. In the next section, we describe an algorithm which was used to enumerate them. In Section 3, we give the results of the enumeration and we show how these relate to perfect 1-factorizations of K_{12}. The remainder of the paper considers sets of mutually orthogonal Latin squares which contain an atomic square. In Section 4, we cover the theory of orthogonal squares, in Section 5, we discuss some algorithms for finding orthogonal mates and in Section 6, we examine the results of those algorithms.

The results of a number of computations are reported in this paper. All computations were performed at least twice to effectively eliminate the possibility of random clerical or hardware errors. All times quoted are for a 700 MHz PC or equivalent.

2. GENERATION OF ATOMIC SQUARES

In this section, we describe an algorithm that was used to generate all the atomic squares of order 11. Since we are only interested in obtaining a representative of each main class of atomic squares, we can use isotopy and conjugacy to drastically cut the number of possibilities we need to consider. By reordering the rows, we may assume that the first column is in natural order. Then, because we know that the second row must be a full cycle permutation relative to the first row, we can reorder the columns and then relabel the symbols in such a way that the first two rows are:

$$\begin{pmatrix} 1 & 2 & 3 & \cdots & n-1 & n \\ 2 & 3 & 4 & \cdots & n & 1 \end{pmatrix} \tag{1}$$

where n is the order of the square.

While the first two rows can be fixed, there are many possibilities for the third row. Our algorithm works by trying to make this third row lexicographically least amongst all the possible third rows. By applying isotopies (described below), we can get the first column in natural order and the first two rows matching (1), but with a variety of different third rows.

For each choice of an ordered pair (i,j) of distinct rows and of a column k of an atomic square A, we define a canonical relabelling of A as follows:

(a) Permute the rows so that row i is first, followed by row j.
(b) Permute the columns so that column k becomes the first column.
(c) Permute the remaining columns so that, using the new row and column indices, $A_{1m} = A_{2,m-1}$ for each $m = 2, 3, \ldots, n$.
(d) Relabel the symbols so that the first two rows match (1).
(e) Reorder the remaining rows so that the first column is in natural order.

In other words, we choose two entries A_{ik} and A_{jk} from distinct rows of the same column, move them up to the top left of the square and the relabelling follows naturally from there. For each i, j, k, the canonical labelling will give us a new third row r_3', which we can compare to the original third row r_3. We make the following definition.

Definition 2.1. *An atomic square is minimal if its first two rows match* (1) *and its third row is lexicographically least among all the third rows which can be produced by the above canonical labelling for some* i, j, k, *and also among the third rows produced by taking the row-inverse of the square and then finding any canonical labelling*.

It should be clear that every main class of atomic squares contains at least one minimal square, and hence our enumeration can safely concentrate on building minimal squares. The enumeration uses backtracking to build the Latin square one entry at a time, deciding all the entries in one row before beginning the next. Each new entry is screened to reject any which complete a row, column or symbol cycle of length less than n. In addition, there is a check for minimality whenever a new row is completed. If the partial square A is provably *not* extendable to a minimal square then it is rejected. This test involves four steps being carried out when we complete row j. For each choice of a column k and a row $i < j$, we:

(a) Consider having row i as the first row, row j as the second row and column k as the first column. If the row that would come third has yet to be built (that is, the symbol that gets relabelled as 3 has not yet been used in column k), this part of the test for these values of i, j, k is inconclusive and we continue. If we have built the row, the canonical labelling gives a new third row r_3' and we compare this to the existing third row r_3. If $r_3' < r_3$ in the lexicographic order, then we know that A can never be extended to a minimal square, so we discard it. Otherwise we continue.

(b) As for (a), but interchange row i and row j.

(c) Consider having row j as the third row, row i as the second row and column k as the first column. This determines which row must go in first place as follows. Let s_1 and s_2 be respectively the symbols in row i and row j of column k. We simply find the column c in which s_2 occurs in row i and then, if it exists, the row r_1' in which s_1 occurs in column c. If we have not yet built r_1' then the test is inconclusive. Otherwise we make r_1' the first row. With row i as the second row and column k as the first column, this will force row j to be the third row. The canonical relabelling of row j gives r_3' and we compare this to the original r_3 in A, rejecting A if $r_3' < r_3$ as before.

(d) Repeat steps (a) to (c) operating on A^*. The benchmark remains the original row r_3, being the third row of A not of A^*.

In this way we ensure that we only build minimal atomic squares. Note that our algorithm will still produce duplication in the sense that we can get more than one representative of a main class from it. There are two reasons why this might happen:

(a) The definition of minimality only requires us to check the square and its row-inverse, which means that some other conjugate of a minimal square M may have a canonical labelling as a minimal square distinct from M. We could have defined minimality differently to allow for the other four conjugates. However, in the early stages of building a square we would rarely have enough information for testing of the other conjugates to be decisive, so screening is of dubious value. The point is that we build A row by row, which breaks the usually symmetry between rows, columns and symbols.

(b) During the test, we may find situations in which $r_3 = r'_3$ in which case, as it stands, we accept A. It would be possible to use the fourth and subsequent rows to break these ties. However the ties are rare and there would be a cost, both in programming and execution time, in order to deal with them. So we chose instead to accept the occasional duplication from, say, two minimal atomic squares in the same main class which differ only after the third row.

In practice, duplication arose for both the above reasons. However the number of duplicates was quite small, and easily eliminated by a subsequent paratopy test, for which we used McKay's *nauty* program [10]. The algorithm took nearly a week to compile an initial list of 36 atomic squares of order 11. When *nauty* was applied to this list, it established that there are seven main classes of atomic squares of order 11.

We attempted to compile a complete catalogue of atomic squares of order 13 by the same method, but found that the search space was too large. The level of difficulty of the problem can be gauged by counting the number of $r \times n$ Latin rectangles which the algorithm generates. Table I shows the number of atomic rectangles that pass the minimality test, and hence need to be developed if a complete list of minimal atomic squares is to be compiled. The computation of the number of 4×13 Latin rectangles required approximately 1000 hours. For $n = 13$ and $r > 4$, our code was incapable of determining these numbers.

It is worth mentioning that we originally enumerated the atomic squares of order 11 by a different method. Instead of using the idea of minimality, we used *nauty* to screen for paratopic Latin rectangles each time we completed a row (at least for the early rows). This method was substantially slower and also required the storage of representatives of each main class of Latin rectangles, whereas the algorithm outlined above requires basically no storage. The advantages of canonical labelling over isomorphism testing (in our case, paratopy testing) are documented in [11]. However, since only a small amount of code was reused in our second approach, the original computation at least provides an almost independent validation of our results.

TABLE I. Number of Minimal $r \times n$ Atomic Latin Rectangles

r	$n = 7$	$n = 9$	$n = 11$	$n = 13$
2	1	1	1	1
3	5	76	3612	346212
4	4	1300	3734893	35570076348
5	1	1183	281291604	
6	1	15	395189650	
7	1	0	2064530	
8		0	46	
9		0	36	
10			36	
11			36	

3. ATOMIC SQUARES OF ORDER ELEVEN

From [20] we know that eleven is the smallest order for which there are atomic squares outside the main classes of cyclic squares of prime order. In the previous section, we described how we established that there are exactly seven different main classes of atomic squares of this order. Table II lists the seven main classes, together with some information on their symmetries and relationship to perfect 1-factorizations. The second column of the table gives the number of conjugates which are isotopic to any given member of the main class. The third column says how many autotopies each square possesses. Hence the size of the autoparatopy group is the product of the numbers in columns two and three.

The first three main classes were previously known. $\mathcal{A}_{11}^1$ is the main class of the cyclic group of order 11. $\mathcal{A}_{11}^2$ and $\mathcal{A}_{11}^3$ contain the atomic squares from the infinite families given respectively by Owens and Preece [12] and Wanless [20]. Representatives of each of the non-cyclic main classes are given in Figure 1.

In order to describe the representative squares in Figure 1, a few extra definitions are required. A *diagonally cyclic* Latin square L of order n based on the symbols 1 to n is generated from its first row by applying the rule that the triple (i,j,L_{ij}) implies the triple $(i+1,j+1,L_{ij}+1)$, where all additions are performed modulo n. This can be thought of as developing each diagonal cyclically from the entry in the first row. A *bordered diagonally-cyclic* Latin square L of order n based on the symbols 1 to n is generated cyclically from its first row by applying the following rules in which all additions are reduced modulo $n-1$ to lie in the range $1,\ldots,n-1$:

(a) the triple (i,j,L_{ij}) with $n \notin \{i,j,L_{ij}\}$ implies the triple $(i+1,j+1,L_{ij}+1)$;
(b) the triple (i,j,n) with $n \notin \{i,j\}$ implies the triple $(i+1,j+1,n)$;
(c) the values of x and y in the triples (i,n,x) and (n,j,y) are whichever symbols are needed to satisfy the Latin property.

Thus the submatrix formed by deleting the last row and column of L has a very similar structure to a diagonally cyclic Latin square except that there is one constant diagonal.

These two types of squares were studied by Franklin [6,7]. Note that we have given a slightly narrower definition of a bordered diagonally cyclic square than Franklin. A survey of results on (bordered) diagonally cyclic squares can be found in [21].

TABLE II. The Main Classes of Atomic Squares of Order 11

	Isotopic conjugates	Autotopies	Factorization of K_{12}: Choice of ∞
$\mathcal{A}_{11}^1$	6	1210	E : 9
$\mathcal{A}_{11}^2$	6	10	C : 11
$\mathcal{A}_{11}^3$	2	10	E : 1–8,10–12
$\mathcal{A}_{11}^4$	2	10	C : 1
$\mathcal{A}_{11}^5$	2	1	C : 2–10,12
$\mathcal{A}_{11}^6$	2	55	D : 9
$\mathcal{A}_{11}^7$	2	5	None

$$\begin{pmatrix} 3 & 5 & 1 & 10 & 2 & 11 & 8 & 7 & 9 & 4 & 6 \\ 5 & 4 & 6 & 2 & 1 & 3 & 11 & 9 & 8 & 10 & 7 \\ 1 & 6 & 5 & 7 & 3 & 2 & 4 & 11 & 10 & 9 & 8 \\ 10 & 2 & 7 & 6 & 8 & 4 & 3 & 5 & 11 & 1 & 9 \\ 2 & 1 & 3 & 8 & 7 & 9 & 5 & 4 & 6 & 11 & 10 \\ 11 & 3 & 2 & 4 & 9 & 8 & 10 & 6 & 5 & 7 & 1 \\ 8 & 11 & 4 & 3 & 5 & 10 & 9 & 1 & 7 & 6 & 2 \\ 7 & 9 & 11 & 5 & 4 & 6 & 1 & 10 & 2 & 8 & 3 \\ 9 & 8 & 10 & 11 & 6 & 5 & 7 & 2 & 1 & 3 & 4 \\ 4 & 10 & 9 & 1 & 11 & 7 & 6 & 8 & 3 & 2 & 5 \\ 6 & 7 & 8 & 9 & 10 & 1 & 2 & 3 & 4 & 5 & 11 \end{pmatrix}$$
$\mathcal{A}_{11}^2$

$$\begin{pmatrix} 6 & 5 & 3 & 10 & 2 & 11 & 8 & 7 & 1 & 4 & 9 \\ 5 & 7 & 6 & 4 & 1 & 3 & 11 & 9 & 8 & 2 & 10 \\ 3 & 6 & 8 & 7 & 5 & 2 & 4 & 11 & 10 & 9 & 1 \\ 10 & 4 & 7 & 9 & 8 & 6 & 3 & 5 & 11 & 1 & 2 \\ 2 & 1 & 5 & 8 & 10 & 9 & 7 & 4 & 6 & 11 & 3 \\ 11 & 3 & 2 & 6 & 9 & 1 & 10 & 8 & 5 & 7 & 4 \\ 8 & 11 & 4 & 3 & 7 & 10 & 2 & 1 & 9 & 6 & 5 \\ 7 & 9 & 11 & 5 & 4 & 8 & 1 & 3 & 2 & 10 & 6 \\ 1 & 8 & 10 & 11 & 6 & 5 & 9 & 2 & 4 & 3 & 7 \\ 4 & 2 & 9 & 1 & 11 & 7 & 6 & 10 & 3 & 5 & 8 \\ 9 & 10 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 11 \end{pmatrix}$$
$\mathcal{A}_{11}^3$

$$\begin{pmatrix} 6 & 5 & 1 & 10 & 2 & 11 & 8 & 7 & 9 & 4 & 3 \\ 5 & 7 & 6 & 2 & 1 & 3 & 11 & 9 & 8 & 10 & 4 \\ 1 & 6 & 8 & 7 & 3 & 2 & 4 & 11 & 10 & 9 & 5 \\ 10 & 2 & 7 & 9 & 8 & 4 & 3 & 5 & 11 & 1 & 6 \\ 2 & 1 & 3 & 8 & 10 & 9 & 5 & 4 & 6 & 11 & 7 \\ 11 & 3 & 2 & 4 & 9 & 1 & 10 & 6 & 5 & 7 & 8 \\ 8 & 11 & 4 & 3 & 5 & 10 & 2 & 1 & 7 & 6 & 9 \\ 7 & 9 & 11 & 5 & 4 & 6 & 1 & 3 & 2 & 8 & 10 \\ 9 & 8 & 10 & 11 & 6 & 5 & 7 & 2 & 4 & 3 & 1 \\ 4 & 10 & 9 & 1 & 11 & 7 & 6 & 8 & 3 & 5 & 2 \\ 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 1 & 2 & 11 \end{pmatrix}$$
$\mathcal{A}_{11}^4$

$$\begin{pmatrix} 1 & 4 & 8 & 2 & 10 & 11 & 9 & 3 & 7 & 5 & 6 \\ 3 & 2 & 1 & 10 & 9 & 8 & 11 & 6 & 5 & 4 & 7 \\ 10 & 6 & 3 & 9 & 7 & 2 & 5 & 11 & 4 & 1 & 8 \\ 11 & 8 & 5 & 4 & 3 & 9 & 10 & 2 & 6 & 7 & 1 \\ 8 & 10 & 9 & 11 & 5 & 7 & 6 & 1 & 3 & 2 & 4 \\ 7 & 11 & 10 & 5 & 4 & 6 & 1 & 9 & 8 & 3 & 2 \\ 5 & 9 & 6 & 8 & 1 & 3 & 7 & 4 & 2 & 11 & 10 \\ 4 & 5 & 7 & 1 & 2 & 10 & 3 & 8 & 11 & 6 & 9 \\ 6 & 3 & 2 & 7 & 11 & 1 & 4 & 10 & 9 & 8 & 5 \\ 9 & 7 & 11 & 6 & 8 & 4 & 2 & 5 & 1 & 10 & 3 \\ 2 & 1 & 4 & 3 & 6 & 5 & 8 & 7 & 10 & 9 & 11 \end{pmatrix}$$
$\mathcal{A}_{11}^5$

$$\begin{pmatrix} 1 & 4 & 8 & 10 & 2 & 5 & 11 & 9 & 7 & 6 & 3 \\ 4 & 2 & 5 & 9 & 11 & 3 & 6 & 1 & 10 & 8 & 7 \\ 8 & 5 & 3 & 6 & 10 & 1 & 4 & 7 & 2 & 11 & 9 \\ 10 & 9 & 6 & 4 & 7 & 11 & 2 & 5 & 8 & 3 & 1 \\ 2 & 11 & 10 & 7 & 5 & 8 & 1 & 3 & 6 & 9 & 4 \\ 5 & 3 & 1 & 11 & 8 & 6 & 9 & 2 & 4 & 7 & 10 \\ 11 & 6 & 4 & 2 & 1 & 9 & 7 & 10 & 3 & 5 & 8 \\ 9 & 1 & 7 & 5 & 3 & 2 & 10 & 8 & 11 & 4 & 6 \\ 7 & 10 & 2 & 8 & 6 & 4 & 3 & 11 & 9 & 1 & 5 \\ 6 & 8 & 11 & 3 & 9 & 7 & 5 & 4 & 1 & 10 & 2 \\ 3 & 7 & 9 & 1 & 4 & 10 & 8 & 6 & 5 & 2 & 11 \end{pmatrix}$$
$\mathcal{A}_{11}^6$

$$\begin{pmatrix} 6 & 4 & 10 & 2 & 9 & 1 & 11 & 8 & 5 & 3 & 7 \\ 10 & 6 & 5 & 11 & 3 & 2 & 8 & 7 & 9 & 1 & 4 \\ 4 & 11 & 6 & 1 & 7 & 3 & 5 & 9 & 8 & 10 & 2 \\ 8 & 5 & 7 & 6 & 2 & 4 & 3 & 1 & 10 & 9 & 11 \\ 3 & 9 & 1 & 8 & 6 & 5 & 7 & 4 & 2 & 11 & 10 \\ 7 & 8 & 9 & 10 & 11 & 6 & 4 & 5 & 1 & 2 & 3 \\ 5 & 2 & 11 & 9 & 1 & 10 & 6 & 3 & 7 & 4 & 8 \\ 2 & 1 & 3 & 7 & 10 & 11 & 9 & 6 & 4 & 8 & 5 \\ 11 & 3 & 2 & 4 & 8 & 7 & 1 & 10 & 6 & 5 & 9 \\ 9 & 7 & 4 & 3 & 5 & 8 & 10 & 2 & 11 & 6 & 1 \\ 1 & 10 & 8 & 5 & 4 & 9 & 2 & 11 & 3 & 7 & 6 \end{pmatrix}$$
$\mathcal{A}_{11}^7$

FIGURE 1. Representatives of the non-cyclic main classes of atomic squares.

We define a *pairing* Latin square L to be a Latin square of odd order for which the symbol set can be partitioned into a single symbol, called the *unpaired symbol*, and a collection of unordered pairs such that the following conditions are satisfied. The unpaired symbol must occur in every position on the main diagonal. Off the main diagonal, if a symbol x occurs in row i, column j then the symbol paired with x must occur in row j, column i. Thus L must be isotopic to L^T, with the isotopy being to simply interchange the symbols within each pair. There is a connection between pairing squares and bordered diagonally cyclic squares. The following theorem is proved in [21].

Theorem 3.1. *Each symmetric bordered diagonally cyclic Latin square of odd order is isotopic to a bordered diagonally cyclic pairing Latin square.*

As indicated in the final column of Table II, six of the seven main classes can be constructed from perfect 1-factorizations of K_{12}. The five perfect 1-factorizations of K_{12} were first catalogued by Petrenyuk and Petrenyuk [16], who labelled them A, B, C, D and E. The last three of these give rise to atomic squares. Note that the relationship between factorizations and atomic squares is not one-to-one because of the choice of the point at infinity (see the comments following Theorem 1.2). Factorisation C generates three different main classes of atomic square, depending on the choice of ∞. Using the vertex labelling from [16], $\mathcal{A}_{11}^2$ is obtained when vertex 11 is chosen as ∞, $\mathcal{A}_{11}^4$ is obtained from a choice of vertex 1 as ∞ and any other choice of ∞ yields $\mathcal{A}_{11}^5$. Factorisation D gives rise to both atomic squares (when vertex 9 is chosen as ∞) and squares which are pan-Hamiltonian but not atomic (when any other vertex is chosen as ∞). Factorisation E generates two different main classes of atomic square; $\mathcal{A}_{11}^1$ is obtained when vertex 9 is chosen as ∞ and any other choice of ∞ yields $\mathcal{A}_{11}^3$.

It turns out that every atomic square of order 11 is isotopic to at least one of its conjugates other than itself. In the six cases which are derived from perfect 1-factorizations of K_{12}, it is known a priori that this will be true, since the construction produces a square which equals its row-inverse. $\mathcal{A}_{11}^7$ is the only main class which does not contain any square for which two conjugates are equal. However, it still has an isotopy between conjugates, as the example given in Figure 1 shows. This square is a pairing square in which 6 is the unpaired symbol and the other symbols are in pairs (x, y) obeying the rule $|x - y| = 6$.

Squares in $\mathcal{A}_{11}^5$ have the least symmetry of all. The example from $\mathcal{A}_{11}^5$ given in Figure 1 has been constructed directly from factorization C with the choice of vertex 12 as the point at infinity. Hence it is equal to its row-inverse, but this is its only non-trivial autoparatopy. In contrast, $\mathcal{A}_{11}^2$ has some very nice symmetry. The example given in Figure 1 exhibits the symmetry of the main class nicely, as it is totally symmetric and bordered diagonally cyclic. Note that Owens and Preece [12] construct their square in $\mathcal{A}_{11}^2$ by slightly perturbing a square in $\mathcal{A}_{11}^1$, and that $\mathcal{A}_{11}^1$ also contains a totally symmetric bordered diagonally cyclic square. Indeed, let L_1, L_2, L_3 and L_4 be the bordered diagonally cyclic squares with the respective first rows:

$$\begin{array}{l} [9\ \ 5\ \ 3\ \ 10\ \ 2\ \ 11\ \ 8\ \ 7\ \ 1\ \ 4\ \ 6], \\ [3\ \ 5\ \ 1\ \ 10\ \ 2\ \ 11\ \ 8\ \ 7\ \ 9\ \ 4\ \ 6], \\ [6\ \ 5\ \ 3\ \ 10\ \ 2\ \ 11\ \ 8\ \ 7\ \ 1\ \ 4\ \ 9], \\ [6\ \ 5\ \ 1\ \ 10\ \ 2\ \ 11\ \ 8\ \ 7\ \ 9\ \ 4\ \ 3]. \end{array} \tag{2}$$

Then each L_i is a representative of $\mathcal{A}_{11}^i$ and in fact L_2, L_3 and L_4 appear in Figure 1 in that role. Moreover, all four squares are symmetric and both L_1 and L_2 are totally symmetric. So the first four main classes of atomic squares of order 11 have strikingly similar bordered diagonally cyclic forms. This pattern will be studied and generalised in a subsequent paper, and will also be revisited in Section 6.

A bordered diagonally cyclic square of order n necessarily possesses an autotopy of order $n-1$, while a diagonally cyclic square of order n has an autotopy of order n [21]. By looking at the orders of the autotopy groups as given in Table II, we see immediately that only the first four main classes may contain bordered diagonally cyclic squares and only A_{11}^1 and $\mathcal{A}_{11}^6$ may contain diagonally cyclic squares. All of these possibilities are realised, as is shown by (2) and the next two observations. $\mathcal{A}_{11}^1$ has a diagonally cyclic representative generated from a first row in which the ith entry equals $2i$ modulo 11. The representative of $\mathcal{A}_{11}^6$ given in Figure 1 is symmetric and diagonally cyclic. It also has some nice orthogonality properties, which will be examined in Section 6.

4. ORTHOGONALITY—THE THEORY

Atomic squares (and to a lesser degree pan-Hamiltonian Latin squares) share some structural similarity with the cyclic squares of prime order. As such, it might be hoped that they could be useful in some of the same ways. One well-known use for cyclic Latin squares is in the construction of projective planes of prime order, using sets of *mutually orthogonal Latin squares* (MOLS) as defined below. It would be interesting to know if there are large sets of MOLS based on other atomic squares. To this end, the remainder of this paper is devoted to the study of the orthogonality properties of the atomic squares of order 11. In this section, we cover the theory; in the next we outline the algorithms and then in Section 6 we give the results of those algorithms.

Two Latin squares A and B of the same order are said to be *orthogonal* if the ordered pairs (A_{ij}, B_{ij}) are all distinct as i and j vary. A set of MOLS is a set of Latin squares in which each pair is orthogonal. A Latin square is said to be *self-orthogonal* if it is orthogonal to its transpose. Orthogonality is closely tied to the concept of transversals. A *transversal* of a Latin square is a subset of the entries which includes exactly one representative from each row, column and symbol. For more information on these concepts see, for example, [3].

Let S be a set of cardinality s, and let O be a $k \times s^2$ array of symbols chosen from S. If, for any pair of rows of O, the ordered pairs in $S \times S$ each occur exactly once among the columns in the chosen rows then O is an example of what is called an *orthogonal array* of strength 2 and index 1. Throughout this paper, the term "orthogonal array" will mean an orthogonal array of this type. From a set $\{L_1, L_2, \ldots, L_k\}$ of MOLS of order n, it is possible to build a $(k+2) \times n^2$ orthogonal array where for each row r and column c there is one column of the array equal to

$$\begin{pmatrix} r \\ c \\ L_1[r,c] \\ L_2[r,c] \\ \vdots \\ L_k[r,c] \end{pmatrix}$$

where $L_i[r,c]$ is the symbol in row r, column c of the square L_i. Moreover this process is reversible, so that any $(k+2) \times n^2$ orthogonal array can be interpreted as a set of k MOLS of order n. See [2], for example, for more details and background on orthogonal arrays. The interpretation of MOLS in terms of orthogonal arrays is useful for proving the following well-known result.

Theorem 4.1. *Let k be any fixed positive integer and L be a Latin square chosen from a main class M. The number of sets of k MOLS including L is a main class invariant, that is, it is independent of the choice of $L \in M$.*

Let P be a set of MOLS containing k squares, the first of which is L. The definition of orthogonality is such that if an isotopy is applied uniformly to the squares in P then orthogonality is preserved. The same is true when taking the transpose, but other conjugations can destroy orthogonality. Since transposition and taking row-inverses generate the six conjugates of a square, to prove Theorem 4.1 it suffices to find a bijective map between sets of MOLS including L and sets of MOLS including L^*. This is easy if we think in terms of orthogonal arrays, where taking conjugates corresponds to reordering the rows of the orthogonal array. The bijection we want is obtained simply by writing P as an orthogonal array, interchanging the second and third rows, and then reinterpreting the result as a set of MOLS, P'. The first square in P' will be L^*, as required, and the process is reversible by applying the same operation a second time, so it must be a bijection.

An important caveat is that this bijection does not preserve the main classes of all the elements of P, only of the pivotal element L. An example of order 7 is presented below. This is the smallest possible order for this illustration, since no smaller order has two main classes each containing squares with orthogonal mates.

$$A = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 7 & 3 & 1 & 6 & 4 & 2 & 5 \\ 4 & 7 & 5 & 3 & 2 & 1 & 6 \\ 3 & 6 & 2 & 5 & 7 & 4 & 1 \\ 6 & 5 & 4 & 1 & 3 & 7 & 2 \\ 2 & 4 & 6 & 7 & 1 & 5 & 3 \\ 5 & 1 & 7 & 2 & 6 & 3 & 4 \end{pmatrix} \qquad B = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 5 & 4 & 2 & 7 & 3 & 1 & 6 \\ 2 & 6 & 7 & 1 & 4 & 3 & 5 \\ 6 & 3 & 5 & 2 & 1 & 7 & 4 \\ 4 & 1 & 6 & 5 & 7 & 2 & 3 \\ 7 & 5 & 1 & 3 & 6 & 4 & 2 \\ 3 & 7 & 4 & 6 & 2 & 5 & 1 \end{pmatrix} \tag{3}$$

Consider the pair (A, B) of orthogonal squares of order 7 shown in (3). The corresponding orthogonal array is

$$\begin{pmatrix} 1111111222222233333334444444555555566666667777777 \\ 1234567123456712345671234567123456712345671234567 \\ 1234567731642547532163625741654137224671535172634 \\ 1234567542731626714356352174416572375136423746251 \end{pmatrix}$$

If we swap the second and third rows and reinterpret this as a set of MOLS we get,

$$A' = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 3 & 6 & 2 & 5 & 7 & 4 & 1 \\ 6 & 5 & 4 & 1 & 3 & 7 & 2 \\ 7 & 3 & 1 & 6 & 4 & 2 & 5 \\ 4 & 7 & 5 & 3 & 2 & 1 & 6 \\ 5 & 1 & 7 & 2 & 6 & 3 & 4 \\ 2 & 4 & 6 & 7 & 1 & 5 & 3 \end{pmatrix} \qquad B' = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 2 & 1 & 4 & 3 & 6 & 7 & 5 \\ 3 & 4 & 1 & 2 & 7 & 5 & 6 \\ 4 & 5 & 6 & 7 & 2 & 3 & 1 \\ 5 & 3 & 7 & 6 & 1 & 4 & 2 \\ 6 & 7 & 2 & 5 & 4 & 1 & 3 \\ 7 & 6 & 5 & 1 & 3 & 2 & 4 \end{pmatrix} \tag{4}$$

Of course, $A' = A^*$ and B' is orthogonal to A'. However it is a simple matter to check that B and B' are from different main classes. In fact A, B and A' are all from the main class containing the cyclic group table, as can be quickly confirmed using standard techniques [18]. To see that B' does not belong to this class, it suffices to note the intercalate (subsquare of order 2) in the top left corner. In particular, this means that B' is not atomic, whereas A, B and A' are. It should not be surprising then, to learn that despite Theorem 4.1 the number of atomic orthogonal mates is not a main class invariant. An example that proves this will be discussed in Section 6.

This phenomenon of main classes varying among related sets of MOLS has been observed by Owens and Preece [13], who studied the sets of MOLS which define the affine planes of order 9. They found that even for these sets of MOLS which are geometrically equivalent, the main classes involved vary from set to set. For the purposes of this paper, we define two sets of MOLS to be *equivalent* if they define the same orthogonal array up to permutation of the rows and columns of the array and of the symbols within each row of the array. We next rephrase this definition in the terminology of Longyear [9].

Suppose that M is a set of t MOLS of order n, and that O is the associated $(t+2) \times n^2$ orthogonal array. The *tactical representation* $\mathrm{TR}(M)$ of M is an undirected graph defined by Longyear [9]. We shall define it in terms of O. There are three sets X, Y and Z of vertices, of respective cardinalities $t+2, n(t+2)$ and n^2. They correspond respectively to the rows, symbols and columns of O, where symbols are distinguished according to their row. Each row in X is joined to the n symbols in Y which are used in that row. Similarly, each column in Z is joined to the $t+2$ symbols in Y which are used in that column. There are no other edges in the graph. The degrees of the vertices in X, Y and Z are respectively $n, n+1$ and $t+2$, with vertices in Y having a unique neighbour in X and n neighbours in Z. This information is sufficient to establish that any graph automorphism of $\mathrm{TR}(M)$ preserves membership of the sets X, Y and Z. It then follows that equivalent MOLS are precisely those which have isomorphic tactical representations. Such a characterisation allows a simple test for equivalence using *nauty* [10].

Longyear's tactical representations are very useful in this setting, but unfortunately her paper [9] contains some incorrect results. Her Theorem 1 is tantamount to the following.

Claim 4.1. *Let P be a pair of orthogonal Latin squares. Then there exists a self-orthogonal Latin square S such that P is equivalent to $\{S, S^T\}$ if and only if* $\mathrm{TR}(P)$ *has an automorphism which when restricted to the set X (as defined above) acts as a pair of disjoint transpositions.*

A counterexample to Claim 4.1 will be cited in Section 6. The claimed proof in [9] seems to assume that the automorphism acts as an involution on Y as well as X. In fact, the "only if" direction of the proof shows that the automorphism will be an involution on the whole graph. We therefore offer this corrected statement, the proof of which is Longyear's original proof.

Theorem 4.2. *Let P be a pair of orthogonal Latin squares. Then there exists a self-orthogonal Latin square S such that P is equivalent to $\{S, S^T\}$ if and only if the automorphism group of* $\mathrm{TR}(P)$ *contains an involution which fixes no point in X.*

Longyear's second theorem, which relies on the first theorem, is also in need of correction. The test in Theorem 4.2 can easily be performed using *nauty* [10] to compute the automorphism group of $\mathrm{TR}(P)$. Alternatively, the following result can be used.

Theorem 4.3. *Let L be a Latin square. To check whether L is isotopic to a self-orthogonal square it suffices to identify the transversals of L, and for each transversal t, permute the rows of L so that the cells of t occupy the main diagonal. If any of the squares so produced turn out to be self-orthogonal then clearly the answer is resolved in the affirmative. Otherwise the answer is negative.*

Proof. Suppose that there is an isotopy I that maps L to a self-orthogonal square S. Since symbol permutations do not affect orthogonality properties, we can assume that I only permutes rows and columns. Also, if the same permutation is applied simultaneously to the rows and columns, this does not affect which pairs of entries lie in symmetrically placed positions, and hence whether or not a square is self-orthogonal. It follows that we can assume without loss of generality that I only permutes rows. Finally, we note that it is well known (and obvious) that the main diagonal of a self-orthogonal square must be a transversal, and that for any given transversal t there is a unique permutation of the rows which places t on the main diagonal. □

We close this section with a result which shows that pairing squares, as defined in Section 3, are of interest in the study of pairs of orthogonal Latin squares.

Theorem 4.4. *Let $\mathcal{C}$ be any class of Latin squares which is closed under transposition, and suppose that L is a symmetric Latin square of odd order. If $\mathcal{C}$ contains a unique (up to permutation of the symbols) orthogonal mate of L then that orthogonal mate is a pairing square.*

Proof. Suppose that M is the unique mate of L in $\mathcal{C}$. Since $\{L, M\}$ is an orthogonal set, it follows that $\{L^T, M^T\}$ is also. But $L = L^T$ so the uniqueness of M implies that M must be related to M^T by some symbol permutation σ. Now σ must be an involution because tranposition is its own inverse. Moreover, σ cannot fix any symbol which occurs off the main diagonal of M because M is orthogonal to the symmetric square L and hence has no two symmetrically placed copies of the same symbol. It follows that σ has at most one fixed point and therefore the 2-cycles of σ yield the required pairing. □

In Section 6, we shall apply Theorem 4.4 using $\mathcal{C}$ to be the class of atomic squares. Other examples of classes to which it could be applied are all Latin squares, diagonally cyclic squares, bordered diagonally cyclic squares or self-orthogonal squares.

5. ORTHOGONALITY ALGORITHMS

The three basic steps below can be used to count the number of Latin squares orthogonal to a particular Latin square L of order n. Since permuting the symbols in a Latin square has no effect on its orthogonality properties, we adopt the convention that whenever we refer to the number of orthogonal mates (or more generally to the number of sets of MOLS including L), we consider only those orthogonal mates in which the first row is in natural order.

(a) Use backtracking to generate and store all transversals of L.
(b) Build a graph G_L in which the vertices are the transversals found in step (a) and two vertices are adjacent if and only if the corresponding transversals contain no entries in common.
(c) Find all cliques of size n in G_L. Such cliques are in one-to-one correspondence with the orthogonal mates of L (given our counting convention).

For step (c) it helps to think of G_L as an n-partite graph, by grouping the transversals into sets $T_1, T_2, \ldots, T_n$ according to which column they use in the first row. Each clique must involve exactly one vertex from each of the T_i, an observation which significantly speeds up the search.

Thus in practice we performed the following task for each $t \in T_1$, in turn. Working exclusively with the transversals adjacent to t, we built a graph as defined above. For each vertex of this graph in T_i, we compiled a list of its neighbours in T_{i+1}. Then we built cliques by choosing a vertex from T_i at the ith stage for $i = 2, 3, \ldots, n$ and backtracking where necessary. To choose the ith vertex, we need only consider vertices on the list of neighbours of the $(i-1)$th vertex.

The above algorithm was used to write a program to find the orthogonal mates of each atomic square of order 11, which will be referred to as program A. It turns out that our approach is quite similar to that of Parker [14], who noted that a small saving could be made by ignoring T_n, since $n-1$ disjoint transversals necessarily leave a transversal uncovered. However, we wanted to test the orthogonal squares for certain properties, not just count them, so we did not adopt Parker's shortcut.

There were two properties for which we screened the orthogonal mates as they were discovered. The results of these tests will be reported in Section 6.

Firstly, for each Latin square L' orthogonal to L we tested whether the set $\{L, L'\}$ could be extended to a larger set of MOLS. In order to do this quickly, in practice we actually tested the necessary condition that through each entry in the first row, L and L' have a shared transversal. Any squares passing this test were output for later analysis. As it happened, for the squares which we tested, our necessary condition turned out to be sufficient, although presumably there are examples for which this is not the case.

Secondly, we tested each orthogonal mate to decide whether it was itself an atomic square, in which case we called it an *atomic mate*. Some care is needed in interpreting this test, on account of the difficulties mentioned in Section 4. Suppose that L is a representative of a main class M, and that L has m atomic mates. Then any square isotopic to L or to L^T will also have m atomic mates, since isotopies and transposition preserve both orthogonality and the atomic property. However, other representatives of M may have different numbers of atomic mates. To cover all possibilities it would be necessary in general to test three representatives of M, one from each of the three pairs of conjugates which are related by transposition. In the present case though, there are isotopies between conjugates which cut down our workload. For main classes $\mathcal{A}_{11}^1$ and $\mathcal{A}_{11}^2$ which contain totally symmetric squares, it is clear that all representatives of the main class will have the same number of atomic mates. The other five main classes detailed in Section 3 contain a square L which is isotopic to L^T. It follows that the $(1,3,2)$ and $(2,3,1)$-conjugates of L are isotopic. Hence the six conjugates of L partition into two classes as follows:

$$\begin{aligned} C_1 &= \{(1,2,3),\ (2,1,3)\} \text{ and} \\ C_2 &= \{(1,3,2),\ (2,3,1),\ (3,1,2),\ (3,2,1)\}. \end{aligned} \tag{5}$$

The conjugates within a class necessarily have the same number of atomic mates because they are related by transposition and/or isotopy. However, as we shall see in Section 6, it is possible for squares from different classes to have different numbers of atomic mates. The very possibility meant that we needed to test one square from each of C_1 and C_2, and hence had to run the whole process twice for each of the five main classes concerned.

Program A was sufficient for our needs in all cases except for the cyclic square of order 11. This square has vastly more orthogonal mates than other atomic squares of the same order, but it also has a much larger autoparatopy group. A specialist program, called program B, was written to take account of these facts.

Program B dealt exclusively with cyclic squares of odd order n (in reality, we only care about the case $n = 11$). All calculations in the subsequent discussion will be performed modulo n. The square L was written with rows, columns and symbols indexed from 0 to $n-1$ according to the rule $L_{ij} = -i - j$. Thus L is the cyclic square in totally symmetric form. It has autoparatopies that perform the following actions, modulo a permutation of the symbols:

- A1: Cyclically permute the columns.
- A2: Cyclically permute the rows.
- A3: For any k relatively prime to n move every entry from its original position in, say, row r of column c to row kr of column kc.
- A4: Take any conjugate of the square.

It is clear that these autoparatopies generate a group G, of order $|G| = 6n^2\phi(n)$ where ϕ is the Euler ϕ function (in the case of prime n, of course, $\phi(n) = n - 1$). Note that G maps transversals to transversals. In fact, G has an induced action on the orthogonal mates of L, found by considering the images of the transversals which define each orthogonal mate.

Now L has the same number of transversals through each of its entries (c.f. Corollary 2 on page 22 of [3]). In the case $n = 11$, this number is 3441. Consider the set T of transversals of L which include the entry with row, column and symbol all zero. Every transversal of L can be converted into an element of T by using a paratopy of type A1, and we always think of the transversals outside T in this way. For each $t \in T$ we assign a distinct *index* $i(t)$, chosen from the natural numbers. Then for each transversal t we calculate $\mu(t)$, which is the lowest index of a transversal in T which gets mapped to t by some autoparatopy of L. We also determine $\lambda(t)$, which is defined to be the number of autoparatopies in G which map t to the transversal in T with index $\mu(t)$. The definitions of μ and λ extend naturally to transversals outside T, so it suffices to calculate them for $t \in T$.

Squares orthogonal to L are in one-to-one correspondence with $\mathcal{D}$, the set of decompositions of L into n mutually disjoint transversals. Ideally, we would like to choose one canonical representative of each orbit under the action of G on $\mathcal{D}$. We could then count $\mathcal{D}$ by enumerating the canonical representatives and calculating their orbit sizes. However, we found the enumeration and recognition of canonical representatives simpler if we allowed the possibility of more than one representative from each orbit. Hence, in practice we chose the following definition.

Let $S = [t_0, t_1, \ldots, t_{n-1}] \in \mathcal{D}$ be a list in which each transversal t_i hits column i in row 0. We say that S is a *canonical list* if $i(t_0) \le \mu(t_i)$ for each $i = 0, 1, \ldots, n-1$. The benefit of this definition is that it allows a single rapid test of the suitability of all transversals to be in a canonical list starting with a given t_0. The cost is that there may be more than one canonical list in some orbits. Crucially though, there is at least one canonical list in each orbit, as we now argue. For any $S = [t_0, t_1, \ldots, t_{n-1}] \in \mathcal{D}$ we can choose t_i to minimize $\mu(t_i)$. For this t_i, there is some $g \in G$ which maps t_i to $t \in T$ satisfying $i(t) = \mu(t_i)$. Applying the autoparatopy g to S produces a canonical list which begins with t.

Suppose that we have identified a canonical $S = [t_0, t_1, \ldots, t_{n-1}] \in \mathcal{D}$. The set of autoparatopies of L which fix S will be some subgroup of G of order, say, h. The orbit size of S under the action of G will be $|G|/h$. Suppose that this orbit includes exactly c canonical lists. Then to avoid overcounting we need to count a contribution of $|G|/(ch)$ from S. The denominator ch is the number of autoparatopies in G which map S to (not necessarily distinct) canonical lists. This number can be found by considering which transversal gets mapped to the first transversal in the image. If $\mu(t_i) = i(t_0)$ then there are $\lambda(t_i)$ autoparatopies in G which map t_i to the first transversal in a canonical list, whereas if $\mu(t_i) > i(t_0)$ then no autoparatopy can achieve this. We conclude that the contribution that we want to count from a canonical set S of transversals is

$$\frac{|G|}{ch} = \frac{6n^2\phi(n)}{\sum \lambda(t)} \tag{6}$$

where the sum is over those $t \in S$ for which $\mu(t) = i(t_0)$. Note that for canonical sets $\mu(t_0) = i(t_0)$, so this sum is positive.

The generation of canonical lists by program B was similar in spirit to the finding of cliques by program A, with some important differences. As already mentioned, only the transversals in T were built, and all other transversals were thought of as translates of these (using a paratopy of type A1). The "graph" was then built by computing, for each ordered pair (t, t') of transversals in T, a single integer whose bits denoted which translates of t intersected with t'. Once t_0 was chosen, any transversal t such that $\mu(t) < i(t_0)$ was immediately ruled out of contention because it could not be part of a canonical list starting with t_0. Once t_0, t_1 and t_2 had been chosen, a record was compiled for each $i \ge 3$ of the choices for t_i which were compatible with the first three transversals chosen. These records were what were examined at each later stage for extending the canonical list. When a canonical list was identified, its contribution according to (6) was added to the total.

At the end of approximately 2 years of computation, program B as just outlined arrived at the (rather large!) number in the top line of Table III. The significant amount of book-keeping, together with the size of the computation, mean that there is no good way to confirm this number short of an independent researcher confirming it.

However, the soundness of the method can be tested by running programs A and B on cyclic squares of smaller orders. Both programs agreed that the cyclic squares of orders 3, 5, 7 and 9 have respectively 1, 3, 635 and 2049219 orthogonal mates. Another check is that program B determined that only eleven different choices for t_0 need to be considered and these transversals correspond neatly with the eleven different types of orthomorphisms of $\mathbb{Z}_{11}$ listed by Evans [4, p 83].

As an additional test for program A, we computed the number of squares which are orthogonal to Parker's famed turn-square of order ten. This square has 5504 transversals, an unusually high number for squares of order ten, and arose during Parker's attempts to find a triple of MOLS of that order. Extrapolating from a partial enumeration, he reported in [14] that it "has one million orthogonal mates (probably a conservative estimate; likely correct within a factor of ten)." This estimate has since become ingrained in the literature; for example, [2, p 105], [3, p 15] and [15]. Our code found that the exact number of orthogonal mates is 12 265 168 and this has been independently confirmed by B. D. McKay. So Parker's estimate was conservative by an order of magnitude. We also confirmed Parker's finding that his turn-square is not part of a mutually orthogonal triple.

6. ORTHOGONALITY RESULTS

Using the algorithms in the previous section, we discovered the results summarised in Table III. For a representative, R, of each of the seven main classes of atomic square of order 11, the table shows

(a) the number of transversals in R;
(b) the number of orthogonal mates for R;
(c) the cardinality of the largest set of MOLS including R.

It is clear from Theorem 4.1 and the definition of transversals that these three quantities are main class invariants, so the choice of the representative R is irrelevant. We reiterate that in part (b), only squares with their first row in natural order were counted.

TABLE III. Orthogonality Properties of Atomic Squares of Order 11

	Transversals	Mates	MOLS
$\mathcal{A}_{11}^1$	37851	7372235460687	10
$\mathcal{A}_{11}^2$	6291	957771	4
$\mathcal{A}_{11}^3$	5511	135076	2
$\mathcal{A}_{11}^4$	4051	10262	2
$\mathcal{A}_{11}^5$	3509	962	2
$\mathcal{A}_{11}^6$	3597	1868	4
$\mathcal{A}_{11}^7$	3981	9684	2

From Table III we see that three of the main classes contain squares which can be involved in at least a triple of MOLS. The first of these, unsurprisingly, is the main class of the cyclic squares, the second is the Owens-Preece class $\mathcal{A}_{11}^2$ and the third is the main class $\mathcal{A}_{11}^6$.

There is a set of four mutually orthogonal, bordered diagonally cyclic Latin squares, in which the first rows are respectively:

$$\begin{array}{lcccccccccc} [3 & 5 & 1 & 10 & 2 & 11 & 8 & 7 & 9 & 4 & 6], \\ [11 & 1 & 9 & 4 & 7 & 10 & 8 & 6 & 2 & 5 & 3], \\ [1 & 9 & 11 & 7 & 3 & 5 & 8 & 10 & 4 & 6 & 2], \\ [1 & 7 & 6 & 3 & 2 & 10 & 9 & 4 & 11 & 8 & 5]. \end{array} \tag{7}$$

The first of these squares is L_2, the representative of $\mathcal{A}_{11}^2$ given in Figure 1. Note that L_2 is totally symmetric. The second, third and fourth squares are not atomic. The second square is a pairing square in which 11 is the unpaired symbol and the other symbols are in pairs (x, y) obeying the rule $|x - y| = 5$. The third and fourth squares are transposes of each other, so in particular they are self-orthogonal.

Up to a relabelling of the symbols within the squares, (7) is the unique set of four MOLS containing L_2. Indeed, the only triples of MOLS containing L_2 are subsets of this set. Every set of MOLS which is equivalent, as defined in Section 4, to (7), is composed of squares from the three main classes represented in (7), but the exact composition varies. An exhaustive list of the possibilities is easy to compile because we only need to consider permutations of the six rows of the relevant orthogonal array. Permutation of the symbols within a row of the array corresponds to taking an isotopy of the squares and hence cannot alter the main classes involved. If M and N denote respectively the main classes of the second and third squares in (7), then the possible combinations of main classes which occur in equivalent sets of MOLS are:

- $\mathcal{A}_{11}^2, M, N, N$;
- M, M, N, N;
- N, N, N, N.

We will next turn our attention to the sets of MOLS involving the representative L_6 of $\mathcal{A}_{11}^6$ given in Figure 1. In order to describe the sets, we need some further definitions. For any Latin square L of order 11, we use $I(L)$ to denote the square obtained from L by applying the isotopy which permutes the rows, columns and symbols by the permutation $(2, 11)(3, 10)(4, 9)(5, 8)(6, 7)$. Let F denote the $(3, 1, 2)$-conjugate of $I(L_6)$. Note that F belongs to $\mathcal{A}_{11}^6$.

We need to define three more squares. Firstly, let C be the square with constant diagonals defined by $C_{ij} \equiv j - i \bmod 11$. Thus C is in $\mathcal{A}_{11}^1$ and is orthogonal to every diagonally cyclic Latin square. Secondly, let D be the diagonally cyclic square generated from the first row $[1, 6, 11, 5, 10, 4, 9, 3, 8, 2, 7]$. The square D also belongs to $\mathcal{A}_{11}^1$ since each entry exceeds its predecessor in the same row by 5, modulo 11. Thirdly, let E be the diagonally cyclic square generated from the first row $[1, 3, 2, 7, 9, 11, 4, 10, 5, 8, 6]$. Although E is not atomic, four of its six conjugates are pan-Hamiltonian. Note that E is equal to its row-inverse and orthogonal to the four of its conjugates to which it is not equal. The self-orthogonality of E was identified by Franklin [7] during an investigation into quadruples of MOLS which consist of a self-orthogonal diagonally cyclic square and its transpose, a symmetric diagonally cyclic square and C. Many of the quadruples we describe below fit this pattern.

Every triple of MOLS including L_6 is extendable to a set of four MOLS, and no such set of four can be extended further. There are twelve different quadruples of MOLS which include L_6. However, all twelve sets contain three diagonally-cyclic squares and C. The twelve sets can be found by extending $\{L_6, C\}$ by the following pairs of orthogonal squares:

$$\{E, E^T\},\ \{F, F^T\},\ \{D, I(E^T)\},\ \{D^T, I(E)\}, \tag{8}$$

$$\{F, I(E^T)\},\ \{F^T, I(E)\},\ \{D^T, E\},\ \{D, E^T\}, \tag{9}$$

$$\{D, D^T\},\ \{E^T, F\},\ \{E, F^T\}, \tag{10}$$

$$\{I(E),\ I(E^T)\}. \tag{11}$$

By forming the orthogonal array corresponding, say, to the set of MOLS $\{L_6, C, E, E^T\}$ and permuting its rows, and also by applying the isotopy I, it can be shown that the four quadruples of MOLS derived from (8) are equivalent. Similarly, we can show that the four quadruples from (9) are equivalent to each other, as are the three quadruples from (10). However, two sets of MOLS chosen from different lines are not equivalent. We can establish this by noting the main classes involved in equivalent sets, as we did for the MOLS based on $\mathcal{A}_{11}^2$. Sets of MOLS equivalent to those in (8) can have the following combinations of main classes

- $\mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1$;
- $\mathcal{A}_{11}^1,\ \mathcal{A}_{11}^6,\ \mathcal{A}_{11}^6,\ \mathcal{A}_{11}^6$;
- $\mathcal{A}_{11}^1,\ A_{11}^1,\ \mathcal{A}_{11}^6,\quad \mathcal{E}$;
- $\mathcal{A}_{11}^1,\ \mathcal{A}_{11}^6,\quad \mathcal{E},\quad \mathcal{E}$;

where $\mathcal{E}$ is the main class of E. Those equivalent to (9) have the combinations:

- $\mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1$;
- $\mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1,\ \mathcal{A}_{11}^6,\quad \mathcal{E}$;
- $\mathcal{A}_{11}^1,\ \mathcal{A}_{11}^6,\ \mathcal{A}_{11}^6,\quad \mathcal{E}$;
- $\mathcal{A}_{11}^1,\quad \mathcal{E},\quad \mathcal{E},\quad \mathcal{E}$;

whereas sets of MOLS equivalent to (10) combine:

- $\mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1$;
- $\mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1,\ \mathcal{A}_{11}^6$;
- $\mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1,\quad \mathcal{E}$;
- $\mathcal{A}_{11}^1,\ \mathcal{A}_{11}^6,\ \mathcal{A}_{11}^6,\quad \mathcal{E}$;
- $\mathcal{A}_{11}^1,\ \mathcal{A}_{11}^6,\quad \mathcal{E},\quad \mathcal{E}$.

Finally, the set of MOLS given by (11) is equivalent to sets of MOLS which combine:

- $\mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1,\ \mathcal{A}_{11}^1$;
- $\mathcal{A}_{11}^1,\ \mathcal{A}_{11}^6,\ \mathcal{A}_{11}^6,\ \ \mathcal{E}$;
- $\mathcal{A}_{11}^1,\ \mathcal{A}_{11}^6,\ \ \mathcal{E},\ \ \mathcal{E}$.

Since the set of combinations is different in each case, we conclude that (8), (9), (10) and (11) describe four distinct equivalence classes of MOLS involving L_6. This conclusion was independently confirmed by using *nauty* [10] on Longyear's tactical representations [9] of the MOLS. By the same means, we confirmed that the maximal set of four MOLS of order 11 constructed by Evans [5] is equivalent to those in (10).

Interestingly, each of the equivalence classes contains quadruples of MOLS fitting Franklin's pattern described above. This is obvious for (8), (10) and (11) because E, D and $I(E)$ are clearly self-orthogonal and we know that L_6 is symmetric. For (9) it is less obvious, but there is a set of MOLS equivalent to (9) involving C, E, E^T and the $(2, 3, 1)$-conjugate of E, which is symmetric.

Another property shared by the four equivalence classes is that they contain quadruples of MOLS, each of which comes from $\mathcal{A}_{11}^1$. This property can be explained by a theorem proved in [21] which states that any set of MOLS consisting solely of a square with constant diagonals and some diagonally cyclic squares is equivalent to a set of MOLS in which every square is isotopic to the cyclic group table. Note, however, that in the cases above the sets of MOLS from $\mathcal{A}_{11}^1$ are not extendable to complete sets of MOLS, because maximality of a set of MOLS is preserved under equivalence. Among the vast number of orthogonal mates of squares in $\mathcal{A}_{11}^1$, there is the possibility of many interesting structures of MOLS. Unfortunately, we were not able to investigate this structure in depth because program B lacked the analysis of orthogonal mates performed by program A and to rectify this deficit would have rendered program B too slow.

We now report the results of the second test performed on the orthogonal mates found by program A, which was to screen for atomic squares. As described in Section 5, this test was carried out on one representative of $\mathcal{A}_{11}^2$ and two representatives of each of $\mathcal{A}_{11}^3, \mathcal{A}_{11}^4, \mathcal{A}_{11}^5, \mathcal{A}_{11}^6$ and $\mathcal{A}_{11}^7$. Among other things, it helped us to detect self-orthogonal Latin squares in our atomic main classes. For example, no square in main classes $\mathcal{A}_{11}^5$ or $\mathcal{A}_{11}^7$ has an atomic mate, so we know immediately that these classes contain no self-orthogonal squares. The main classes $\mathcal{A}_{11}^2, \mathcal{A}_{11}^3$ and $\mathcal{A}_{11}^4$ do not contain self-orthogonal squares either, as we show below.

Let L_1, L_2, L_3 and L_4 be as defined by (2). Program A reported that L_2, L_3 and L_4 have a unique atomic mate. It follows from Theorem 4.4 that these mates must be pairing squares. In fact, they are the pairing squares of Theorem 3.1, which happen to be the bordered diagonally cyclic pairing squares P_1, P_2, P_3 and P_4 with the respective first rows:

$$\begin{array}{l}[11\ \ 8\ \ 7\ \ 1\ \ 4\ \ 9\ \ 5\ \ 3\ \ 10\ \ 2\ \ 6],\\ [11\ \ 8\ \ 7\ \ 9\ \ 4\ \ 3\ \ 5\ \ 1\ \ 10\ \ 2\ \ 6],\\ [11\ \ 8\ \ 7\ \ 1\ \ 4\ \ 6\ \ 5\ \ 3\ \ 10\ \ 2\ \ 9],\\ [11\ \ 8\ \ 7\ \ 9\ \ 4\ \ 6\ \ 5\ \ 1\ \ 10\ \ 2\ \ 3].\end{array} \tag{12}$$

The isotopy that produces P_i from L_i is to permute the columns according to the permutation $(1,6)(2,7)(3,8)(4,9)(5,10)$.

Now, suppose that L_2 is isotopic to a self-orthogonal square S. The only option is that the same isotopy maps P_2 to a square equivalent to S^T up to relabelling of its symbols, since we know that P_2 is the unique atomic mate of L_2. However, we can use Theorem 4.2 to check that $\{L_2, P_2\}$ is not equivalent to $\{S, S^T\}$ for any S. We conclude that no square in $\mathcal{A}_{11}^2$ is orthogonal to its transpose. Despite this, the bordered diagonally cyclic square with first row $[2,4,9,8,10,11,6,5,7,3,1]$ is in $\mathcal{A}_{11}^2$. This square is symmetric and is orthogonal to the four conjugates to which it is not equal.

We can use Theorem 4.2 in the same way to show that neither L_3 nor L_4 is isotopic to a self-orthogonal square, although in each case it is crucial to use our corrected version of the theorem, not the one published in [9]. To see this, observe that the tactical representation of $\{L_3, P_3\}$ has an automorphism θ which, when restricted to the four row vertices $X = \{R_1, R_2, R_3, R_4\}$, acts as two disjoint transpositions

$$(R_1R_2)\ (R_3R_4). \tag{13}$$

Meanwhile, on the 44 symbol vertices Y which we label as the symbols $1, 2, \ldots, 11$ with a subscript indicating the row from which each symbol is drawn, θ acts as follows:

$$\begin{array}{l}(1_1 1_2 6_1 6_2)\ (2_1 2_2 7_1 7_2)\ (3_1 3_2 8_1 8_2)\ (4_1 4_2 9_1 9_2)\ (5_1 5_2 10_1 10_2)\ (11_1 11_2)\\ (1_3 6_4 6_3 1_4)\ (2_3 7_4 7_3 2_4)\ (3_3 8_4 8_3 3_4)\ (4_3 9_4 9_3 4_4)\ (5_3 10_4 10_3 5_4)\ (11_3 11_4).\end{array} \tag{14}$$

The action of θ on the column vertices Z can be reconstructed from (14). The important point is that according to Longyear's claim, $\{L_3, P_3\}$ should be equivalent to $\{S, S^T\}$ for a self-orthogonal square S because of (13). However, it is simple enough to check that this is not the case, by using Theorem 4.3 to establish that no conjugate of L_3 or P_3 is isotopic to a self-orthogonal square. Note that for L_3^*, program A reported a unique atomic mate, M, which is also from $\mathcal{A}_{11}^3$. The pair $\{L_3^*, M\}$ is equivalent to $\{L_3, P_3\}$. Since P_3 is isotopic to L_3, it follows that we need only establish that L_3 itself is not isotopic to a self-orthogonal square. Despite the lack of a self-orthogonal form, the bordered diagonally cyclic square with first row $[11,1,6,4,3,8,2,9,5,7,10]$ belongs to $\mathcal{A}_{11}^3$ and is orthogonal to its own $(3,1,2)$-conjugate.

It is easy enough to establish that the tactical representations of $\{L_2, P_2\}$ and $\{L_4, P_4\}$ have an automorphism θ as given by (13) and (14) and that they provide further counterexamples to Longyear's theorem as it was published. There is one very important distinction between L_4 and the other squares given in (2) though, which is that L_4^* has no atomic mate. Referring to (5), we see that the same is true for the four conjugates of L_4 which differ from L_4. However L_4 itself is orthogonal to P_4 as we have seen, which demonstrates that the number of atomic mates is not a main class invariant.

We know from results earlier in this section that there are five atomic squares orthogonal to L_6, namely C, D, D^T, F and F^T, and this turns out to be the full complement. Similarly, L_6^* has five atomic mates, which are $(L_6^*)^T, I(L_6), D^*, (D^T)^*$

and C. In particular, this reveals that L_6^* is a self-orthogonal square in $\mathcal{A}_{11}^6$. Also D is a self-orthogonal square in $\mathcal{A}_{11}^1$; in fact all six conjugates of D are mutually orthogonal. So we have established that $\mathcal{A}_{11}^1$ and $\mathcal{A}_{11}^6$ both contain diagonally cyclic self-orthogonal squares. No other atomic main class contains diagonally-cyclic *or* self-orthogonal Latin squares. Interestingly, we have also seen that $\mathcal{A}_{11}^1$ and $\mathcal{A}_{11}^6$ are the only atomic main classes involved in a pair of orthogonal atomic squares which originate from different main classes. Indeed, we seem to have reinforced Franklin's original assessment that diagonally cyclic squares are worth studying for the richness of their orthogonality structure.

7. CONCLUDING REMARKS

In this paper we have reported the results of a complete enumeration of the atomic Latin squares of order 11, the smallest order for which there are ‘‘interesting’’ examples. There are seven main classes, three of which were previously known. Our method is not powerful enough for an exhaustive enumeration of main classes for higher orders. We have investigated some orthogonality properties of the atomic squares of order 11 and also their relationship to the perfect 1-factorizations of K_{12}. In a subsequent paper, we plan to study the structure of these atomic squares further, and thereby find atomic squares of larger orders.

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