Linear-Algebraic Results Associated with

Antiferromagnetic Heisenberg Chains*

by

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Abstract. This paper analyses the $3^N \times 3^N$ self-adjoint matrix $H_N = \sum_{j=1}^{N-1} S_x^{(j)} S_x^{(j+1)} + S_y^{(j)} S_y^{(j+1)} + S_z^{(j)} S_z^{(j+1)}$, the Hamiltonian of a spin-1, one-dimensional, Heisenberg antiferromagnet. Various results are obtained, including alternative representations of H_N, families of operators commuting with H_N, a complete description of the spin-0 subspace (which includes all one- and two-dimensional eigenspaces of H_N), and a proof that H_N must have an eigenvalue smaller than $-\frac{4}{3}(N-1)$.

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1. Introduction.

There are several interesting, important and difficult problems concerning the eigenvalues and eigenvectors of a certain sequence of Hermitian matrices that arise in the quantum-mechanical study of antiferromagnetic Heisenberg chains.

Let $\mathcal{V}$ be the three-dimensional inner-product space $\mathbf{C}^3$. The "spin-1 operators" (see, e.g. [8]) are the operators on $\mathcal{V}$ defined by

$$S_x \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S_y \;=\; \frac{i}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \quad S_z \;=\; \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

with respect to an orthonormal basis which we denote by $\{v_{-1}, v_0, v_1\}$. The choice of subscripts on the v_j is such that $S_z(v_j) = j\, v_j$, for $j = -1, 0, 1$. (Physicists write v_{-1} as $|-1\rangle$, v_0 as $|0\rangle$, and v_1 as $|1\rangle$.)

For each positive integer N, denote the N-fold tensor product of $\mathcal{V}$ with itself by $\mathcal{V}^{\otimes N}$. For each linear operator $F : \mathcal{V} \to \mathcal{V}$, let $F^{(j)} : \mathcal{V}^{\otimes N} \to \mathcal{V}^{\otimes N}$ be the operator

$$F^{(j)} \;=\; F_1 \otimes F_2 \otimes \cdots \otimes F_N$$

with $F_j = F$ and $F_k = I$ for $k \neq j$.

The operator we are concerned with is defined on $\mathcal{V}^{\otimes N}$ (for $N \geq 2$) by

$$H_N \;=\; \sum_{j=1}^{N-1} S_x^{(j)} S_x^{(j+1)} + S_y^{(j)} S_y^{(j+1)} + S_z^{(j)} S_z^{(j+1)} .$$

The operator H_N is the Hamiltonian of the spin-1, antiferromagnetic, Heisenberg (= isotropic), one-dimensional (= linear) spin chain with N sites. This Hamiltonian is of great importance in interpretting certain results in expermental physics (see [5], [12]). Physically, such a Hamiltonian describes a crystal lattice of atoms of spin 1, in which all interactions take place along a preferred direction, and are given by the dot-product of the spin vectors of all nearest-neighbour pairs.

The operator H_N has been widely studied by solid state physicists (see [1], [3], [7], and references therein). There have also been numerical ([4], [11]) and experimental ([5], [12]) investigations of the eigenvalues and eigenvectors of H_N. Much of the recent work has been motivated by a conjecture of Haldane ([9], [10]). Let λ_N^0 and λ_N^1 be the smallest and the second smallest eigenvalues of H_N. Haldane's conjecture may be stated as saying that $\lim_{N\to\infty} (\lambda_N^1 - \lambda_N^0) > 0$. While numerical and experimental work appears to support this statement, the conjecture remains unproven. Even the precise mathematical formulation of the conjecture is controversial; in [1] it is argued that the conjecture should be studied in an (inequivalent) "infinite chain" context.

We study H_N by direct, linear-algebraic methods in the present paper. We obtain a number of results that may provide insight into its underlying structure. Results presented here include alternative representations of H_N (Corollary 2.2 and Proposition 2.4), families of operators commuting with H_N (Theorems 3.3 and 3.5), properties of the "spin-0" subspace (Propositions 4.3 and 4.5), a complete description of this subspace (Theorems 5.4 and 5.8), and a new proof that H_N must have an eigenvalue smaller that $-\frac{4}{3}(N-1)$ for all N (Theorem 6.7). The value $-\frac{4}{3}(N-1)$ is reasonably close to the estimate of $-1.40(N-1)$ for the smallest eigenvalue of H_N, which has been extrapolated from certain numerical approximations [11]. The spin-0 subspace is important in relation to Haldane's conjecture since it contains all one-dimensional (and two- dimensional) eigenspaces of H_N (see Corollary 4.2 and Proposition 6.8 below), and since it is shown in [1] that the eigenspace of H_N corresponding to λ_N^0 is one-dimensional for even N. This paper also includes simple, direct proofs of certain well-known facts about H_N, to make the presentation self-contained.

One way that physicists have varied the problem is by replacing H_N by the "periodic

Hamiltonian"

$$P_N \;=\; H_N + S_x^{(N)} S_x^{(1)} + S_y^{(N)} S_y^{(1)} + S_z^{(N)} S_z^{(1)} \;.$$

It is expected, on physical grounds, that the Haldane conjectures should be decided in the same way for P_N as for H_N. There are, however, no definitive results concerning P_N either. We consider below both P_N and H_N. We often find it more natural (see section 2) to study operators K_N and Q_N which are equal to the negatives of H_N and P_N, respectively.

This paper is organized as follows. In section 2, we derive several representations of H_N and P_N. In section 3, we list a number of operators on $\mathcal{V}^{\otimes N}$ which commute with H_N and P_N. In section 4, we use some of these operators to present the standard decomposition of H_N and P_N into direct sums, and in section 5 we investigate in detail the spin- 0 subspace of $\mathcal{V}^{\otimes N}$. Some bounds on the eigenvalues of H_N and P_N are obtained in section 6. In section 7, we describe the corresponding problems for spins other than 1, and state the more general Haldane conjecture, which remains one of most important open mathematical problems in solid state physics.

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2. Other representations of the operators.

The following leads to new representations of H_N and P_N that we have found useful.

Theorem 2.1. *There exists an orthonormal basis $\{e_1, e_2, e_3\}$ of $\mathcal{V}$ with respect to which the triple (S_x, S_y, S_z) has matrix representation (iR, iS, iT), where*

$$R = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad T = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} .$$

Proof. Define the basis $\{e_1, e_2, e_3\}$ by

$$\begin{aligned} e_1 &= \frac{i}{\sqrt{2}}(v_{-1} - v_1) \\ e_2 &= \frac{-1}{\sqrt{2}}(v_{-1} + v_1) \\ e_3 &= i\, v_0 \ . \end{aligned}$$

Then the stated matrix representations are easily checked. •

Corollary 2.2. *The operators H_N and P_N are equal, respectively, to the negatives of the operators K_N and Q_N defined (in the basis of $\mathcal{V}^{\otimes N}$ induced by $\{e_1, e_2, e_3\}$) by*

$$K_N = \sum_{j=1}^{N} R^{(j)} R^{(j+1)} + S^{(j)} S^{(j+1)} + T^{(j)} T^{(j+1)}$$

and

$$Q_N = K_N + R^{(N)} R^{(1)} + S^{(N)} S^{(1)} + T^{(N)} T^{(1)} \ .$$

Proof. This follows immediately from the preceeding theorem. •

The representations given in the corollary above will be used throughout the rest of this paper. It should be observed that R, S, and T are skew-symmetric matrices, with $RS - SR = T$, $ST - TS = R$, $TR - RT = S$, and $R^2 + S^2 + T^2 = -2I$. Also, it is clear that the triple (R, S, T) is simultaneously unitarily equivalent to the triples (S, T, R) and

(T, R, S). A possible interpretation of the matrices R, S, and T is suggested by the fact that for $v \in \mathbf{R}^3$, $Rv = e_1 \times v$, $Sv = e_2 \times v$, and $Tv = e_3 \times v$, where $\times$ indicates the ordinary cross-product (vector-product) on $\mathbf{R}^3$. We also have the following uniqueness property of the matrices R, S, and T.

Proposition 2.3. *Let A, B, and C be three skew- Hermetian operators on $\mathbf{R}^3$, with $AB - BA = C$, $BC - CB = A$, and $CA - AC = B$. Then either $A = B = C = 0$, or there is an orthonormal basis $\{f_1, f_2, f_3\}$ of $\mathbf{R}^3$ such that in this basis A, B, and C have the matrix representations of R, S, and T above.*

Proof. Since $\det A = \det A^* = -\det A$, there is a vector $f_1 \in \mathbf{R}^3$ with $\|f_1\| = 1$ and $Af_1 = 0$. If $Cf_1 = 0$, then $Bf_1 = (CA - AC)f_1 = 0$, so with respect to any orthonormal basis containing f_1, each of A, B, and C are of the form

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -k \\ 0 & k & 0 \end{pmatrix} .$$

Hence, A, B and C all commute, and thus are all zero. If $Cf_1 \neq 0$, then write $Cf_1 = cf_2$, with $\|f_2\| = 1$ and $c > 0$. Since

$$\langle Cf_1, f_1 \rangle = \langle f_1, C^* f_1 \rangle = \langle f_1, -Cf_1 \rangle = -\langle Cf_1, f_1 \rangle ,$$

we have $f_1 \perp f_2$. Extend $\{f_1, f_2\}$ to an orthonormal basis $\{f_1, f_2, f_3\}$ of $\mathbf{R}^3$. With respect to this basis, we have

$$A = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -a \\ 0 & a & 0 \end{pmatrix} , \quad B = \begin{pmatrix} 0 & * & * \\ * & 0 & * \\ * & * & 0 \end{pmatrix} , \quad C = \begin{pmatrix} 0 & -c & 0 \\ c & 0 & * \\ 0 & * & 0 \end{pmatrix} ,$$

for some $a \in \mathbf{R}$. Direct computation then shows that

$$A = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -a \\ 0 & a & 0 \end{pmatrix} , \quad B = \begin{pmatrix} 0 & 0 & b \\ 0 & 0 & 0 \\ -b & 0 & 0 \end{pmatrix} , \quad C = \begin{pmatrix} 0 & -c & 0 \\ c & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} ,$$

for some $b \in \mathbf{R}$, with $ab = c$, $bc = a$, and $ca = b$. Replacing f_3 by $-f_3$ if necessary, we may assume $a > 0$. It then follows that $a = b = c = 1$, completing the proof. •

An interesting representation of the operator $K_2 = R \otimes R + S \otimes S + T \otimes T$ can be obtained by considering the space $M_3(\mathbf{C})$ of 3×3 complex matrices with inner product $\langle A, B \rangle = \text{trace } AB^*$. We identify $e_i \otimes e_j$ with the matrix unit E_{ij}, where $\{e_1, e_2, e_3\}$ is the orthonormal basis of Theorem 2.1; this induces a unitary equivalence of $\mathcal{V}^{\otimes 2}$ with $M_3(\mathbf{C})$. Under this equivalence, an operator on $\mathcal{V}^{\otimes 2}$ of the form $F \otimes G$ corresponds to the operator on $M_3(\mathbf{C})$ given by $A \mapsto FAG^t$, where F and G are written as matrices in the basis $\{e_1, e_2, e_3\}$.

Proposition 2.4. *Under the above unitary equivalence of $\mathcal{V}^{\otimes 2}$ with $M_3(\mathbf{C})$, the operator K_2 corresponds to the operator Γ defined on $M_3(\mathbf{C})$ by*

$$\Gamma(A) \ = \ -A^t + (\operatorname{tr} A)I \ ,$$

where A^t is the transpose of A, $\operatorname{tr} A$ is the trace of A, and I is the identity matrix.

Proof. We have

$$\Gamma(E_{ij}) \ = -E_{ji} + \delta_{ij} I = \ -E_{ji} + \delta_{ij}(E_{11} + E_{22} + E_{33})$$

where δ is the Kronecker delta. On the other hand,

$$\begin{aligned} K_2(E_{ij}) &= RE_{ij}R^t + SE_{ij}S^t + TEijT^t \\ &= (E_{32} - E_{23})E_{ij}(E_{23} - E_{32}) + (E_{13} - E_{31})E_{ij}(E_{31} - E_{13}) \\ &\qquad + (E_{21} - E_{12})E_{ij}(E_{12} - E_{21}) \ , \end{aligned}$$

and the two expressions are easily seen to be equal. •

The spectrum of K_2 is very well-known. It is not hard to compute this spectrum in any representation, but the proposition above makes it particularly easy.

Corollary 2.5. *The eigenvalues of K_2 are $2, 1$ and -1 with multiplicities $1, 3$, and 5 respectively. The corresponding eigenspaces of Γ are the subspaces respectively spanned by the identity matrix, the skew-symmetric matrices, and the symmetric matrices with trace 0.*

Proof. This follows immediately from the observation that $\Gamma(I) = 2I$, $\Gamma(A) = A$ if $A = -A^t$, and $\Gamma(A) = -A$ if $A = A^t$ and $\operatorname{tr} A = 0$. •

3. Operators commuting with the Hamiltonian.

As mentioned in the introduction, it is shown in [1] that the eigenspaces of H_N and P_N corresponding to the smallest eigenvalue λ_N^0 have dimension 1 for N even. It is therefore important to study one-dimensional eigenspaces of H_N and P_N or, equivalently, of K_N and Q_N. Clearly, any such eigenspace is invariant under all operators commuting with K_N or Q_N. Hence, each operator A communting with H_N or P_N puts a constraint on any eigenvector w of H_N or P_N corresponding to an eigenvalue of multiplicity 1, namely that Aw must be a scalar multiple of w. This section describes two families of such operators. These families include operators which are known to physicists.

Lemma 3.1. *Let F be a linear operator on $\mathcal{V}$. Then $F \otimes F$ commutes with K_2 if and only if, in the basis $\{e_1, e_2, e_3\}$ of Theorem 2.1, $FF^t = F^tF = \lambda I$, for some complex number λ, where I is the 3×3 identity matrix.*

Proof. We use Proposition 2.4. Under the equivalence given there, the operator $F \otimes F$ corresponds to multiplying an element of $M_3(\mathbf{C})$ on the left by F and on the right by F^t, where F is written as a matrix in the basis $\{e_1, e_2, e_3\}$. Hence $F \otimes F$ commutes with K_2

if and only if, for each $J \in M_3(\mathbf{C})$,

$$\Gamma(FJF^t) = F\,\Gamma(J)F^t,$$

i.e.,

$$-FJ^tF^t + \mathrm{tr}(FJF^t)\ I = F\,(-J^t + \mathrm{tr}(J)\ I)\,F^t,$$

which is true if and only if

$$(\dagger) \qquad \mathrm{tr}(FJF^t)\ I = \mathrm{tr}(J)\ FF^t.$$

If $FF^t = F^tF = \lambda I$, then (†) clearly holds. Conversely, if (†) holds, then setting $J = I$ shows that $FF^t = \frac{1}{3}\,\mathrm{tr}(FF^t)\ I$, a multiple of the identity. If $FF^t \neq 0$, we clearly have $F^tF = FF^t$. If $FF^t = 0$, then setting $J = (F^tF)^*$ in (†) shows that $\langle F^tF, F^tF\rangle = \mathrm{tr}\ (F^tFJ) = \mathrm{tr}\ (FJF^t) = 0$, so that $F^tF = 0$. •

Remark. The condition $FF^t = F^tF = \lambda I$ is not unitarily invariant, since in general $F^t \neq F^*$.

Lemma 3.2. *Let F be a linear operator on $\mathcal{V}$. Let $\Theta_N^{(ij)} = R^{(i)}R^{(j)} + S^{(i)}S^{(j)} + T^{(i)}T^{(j)}$, where $i, j \in \{1, 2, \ldots, N\}$, $i \neq j$. Let $F^{\otimes N}$ denote the N-fold tensor product of F with itself. Then $F^{\otimes N}$ commutes with $\Theta_N^{(ij)}$ if and only if, in the basis $\{e_1, e_2, e_3\}$ of Theorem 2.1, $FF^t = F^tF = \lambda I$, for some complex number λ. .*

Proof. Let Z be the operator on $\mathcal{V}^{\otimes N}$ defined by

$$Z(v_1 \otimes v_2 \otimes \cdots \otimes v_N) = v_{\sigma(1)} \otimes v_{\sigma(2)} \otimes \cdots \otimes v_{\sigma(N)},$$

extended by linearity, where σ is any fixed element of S_N (the symmetric group on N letters) with $\sigma(i) = 1$ and $\sigma(j) = 2$. Then Z clearly commutes with $F^{\otimes N}$, and $\Theta_N^{(ij)} = Z^{-1}\Theta_N^{(12)}Z$. Hence, $F^{\otimes N}$ commutes with $\Theta_N^{(ij)}$ if and only if it commutes with $\Theta_N^{(12)}$.

We can write $\Theta_N^{(12)} = K_2 \otimes I \otimes I \otimes \cdots \otimes I$. The lemma now follows easily from Lemma 3.1, by noting that $[F^{\otimes N}, \Theta_N^{(12)}] = [F \otimes F, K_2] \otimes F^{\otimes N-2}$. •

Theorem 3.3. *Let $F^{\otimes N}$ be a linear operator on $\mathcal{V}$. Then $F^{\otimes N}$ commutes with K_N and with Q_N (and hence also with H_N and P_N) if and only if, in the basis $\{e_1, e_2, e_3\}$, $FF^t = F^tF = \lambda I$, for some complex number λ.*

Proof. Since each of K_N and Q_N are sums of $\Theta_N^{(ij)}$'s, it follows immediately from Lemma 3.2 that K_N and Q_N commute with operators of the given form.

For the converse, let F be any operator on $\mathcal{V}$ such that $F^{\otimes N}$ commutes with K_N or Q_N. We shall show that $F^{\otimes N}$ must commute with $\Theta_N^{(1,2)}$; the result will then follow from the previous lemma.

Write the commutator of $F^{\otimes N}$ and $\Theta_N^{(12)}$ as

$$[F^{\otimes N}, \Theta_N^{(12)}] \ = \ \sum_j A_j \otimes B_j \otimes I^{\otimes N-2}$$

for some finite collection of operators A_j and B_j on $\mathcal{V}$. (In fact, it is easily seen that we only need 3 of each.) Now, recalling the definitions of K_N and Q_N, the only way we could possibly have

$$[F^{\otimes N}, K_N] \ = \ 0 \qquad \text{or} \qquad [F^{\otimes N}, Q_N] \ = \ 0$$

would be if for each j, either $A_j = I$ or $B_j = I$, and if furthermore $\sum_j B_j = -\sum_j A_j$. This would imply that

$$[F^{\otimes N}, \Theta_N^{(12)}] \ = \ (I \otimes C - C \otimes I) \otimes I^{\otimes N-2}$$

for some operator C on $\mathcal{V}$. But by symmetry, we must also have

$$[F^{\otimes N}, \Theta_N^{(12)}] \ = \ (C \otimes I - I \otimes C) \otimes I^{\otimes N-2} \ .$$

It follows that $C = 0$, so that $F^{\otimes N}$ commutes with $\Theta_N^{(12)}$. The theorem follows. •

Lemma 3.4. *Let F be a linear operator on $\mathcal{V}$. Then $F \otimes I + I \otimes F$ commutes with K_2 if and only if, in the basis $\{e_1, e_2, e_3\}$, $F + F^t = \lambda I$, for some complex number λ.*

Proof. We again use Proposition 2.4. We have that

$$\begin{aligned}(F \otimes I + I \otimes F)\Gamma(A) &= -FA^t - A^t F^t + (\text{tr } A)F + (\text{tr } A)F^t \\ &= -FA^t - A^t F^t + (\text{tr } A)(F + F^t) \ ,\end{aligned}$$

and that

$$\begin{aligned}\Gamma\,(F \otimes I + I \otimes F)(A) &= -FA^t - A^t F^t + (\text{tr } FA)I + (\text{tr } AF^t)I \\ &= -FA^t - A^t F^t + (\text{tr } A(F + F^t)\,)I \ .\end{aligned}$$

The two operators commute if and only if the above two expressions are equal for every matrix A, and this is easily seen to be true if and only if $F + F^t$ is a multiple of the identity matrix. •

Theorem 3.5. *Let F be a linear operator on $\mathcal{V}$. Then $\sum_{j=1}^{N} F^{(j)}$ commutes with K_N and with Q_N if and only if, in the basis $\{e_1, e_2, e_3\}$, $F + F^t = \lambda I$ for some complex number λ.*

Proof. This follows easily from the lemma above, by techniques very similar to the proof of Lemma 3.2 and Theorem 3.3. •

Two other operators, both well-known to physicists, deserve mention. Another operator in the commutant of K_N and of Q_N is the "left-right symmetry" L, of order 2, defined by

$$L(v_1 \otimes v_2 \otimes \cdots \otimes v_{N-1} \otimes v_N) \ = \ v_N \otimes v_{N-1} \otimes \cdots \otimes v_2 \otimes v_1 \ ,$$

extended by linearity. The commutant of Q_N also contains the "rotation" operator Π, of order N, defined by

$$\Pi(v_1 \otimes v_2 \otimes \cdots \otimes v_{N-1} \otimes v_N) \;=\; v_N \otimes v_1 \otimes v_2 \otimes \cdots \otimes v_{N-1}\ ,$$

extended by linearity. Since K_N and Q_N, and also Π and L, are real in the basis $\{e_1, e_2, e_3\}$, an element w of an eigenspace of K_N or Q_N of dimension one must satisfy $L(w) = \pm w$, and in the case of Q_N must also satisfy $\Pi(w) = \pm w$.

4. A decomposition of K_N and Q_N.

Let k be an integer with $-N \leq k \leq N$. Let $\mathcal{M}_k^z$ be the eigenspace of $\sum_{j=1}^{N} S_z^{(j)}$ corresponding to the eigenvalue k. Similarly, let $\mathcal{M}_k^x$ and $\mathcal{M}_k^y$ be the eigenspaces of $\sum_{j=1}^{N} S_x^{(j)}$ and $\sum_{j=1}^{N} S_y^{(j)}$, respectively, corresponding to the eigenvalue k. Recall that in the basis $\{e_1, e_2, e_3\}$, the operators S_x, S_y, S_z have matrix representations iR, iS, iT, respectively.

Using the orthonormal basis $\{v_{-1}, v_0, v_1\}$ of $\mathcal{V}$, note that

$$S_z^{(j)}(v_{r_1} \otimes \ldots \otimes v_{r_N}) \;=\; r_j(v_{r_1} \otimes \ldots \otimes v_{r_N}),$$

so that $\mathcal{M}_k^z$ is the span of

$$\Big\{ v_{r_1} \otimes v_{r_2} \otimes \ldots \otimes v_{r_N} \;\Big|\; r_1, \ldots, r_N \in \{-1, 0, 1\},\ r_1 + r_2 + \ldots + r_N = k \Big\}\ .$$

This shows that $\mathcal{V}^{\otimes N} \;=\; \bigoplus_{k=-N}^{N} \mathcal{M}_k^z$, and by symmetry we have that $\mathcal{V}^{\otimes N} \;=\; \bigoplus_{k=-N}^{N} \mathcal{M}_k^x$ and $\mathcal{V}^{\otimes N} \;=\; \bigoplus_{k=-N}^{N} \mathcal{M}_k^y$.

The following theorem and its corollary are well-known to physicists.

Proposition 4.1. *Let q be one of x, y, or z. Then each $\mathcal{M}_k^q$ is invariant under K_N and under Q_N. Furthermore, every one-dimensional eigenspace of K_N or of Q_N is contained in $\mathcal{M}_0^q$.*

Proof. By symmetry, it suffices to consider the case $q = x$. The invariance of the $\mathcal{M}_k^x$ follows from the fact that $\sum_{j=1}^{N} R^{(j)}$ commutes with K_N and with Q_N, by Theorem 3.5. For the second statement, note that if $\mathcal{E}$ is a one-dimensional eigenspace, then since K_N and Q_N are real in the basis generated by $\{e_1, e_2, e_3\}$, we can choose $w \in \mathcal{E}$ with $w \neq 0$ and with w real in this basis. Suppose $w \in \mathcal{M}_k^x$. Then w is an eigenvector of $\sum_{j=1}^{N} R^{(j)}$ with eigenvalue $-ik$. But since $\sum_{j=1}^{N} R^{(j)}$ and w are real in the same basis, the eigenvalue must be real, so we must have $k = 0$. $\bullet$

Corollary 4.2. *Any eigenspace of K_N or Q_N of dimension 1 is contained in the subspace $\mathcal{M}_0$ defined by*

$$\mathcal{M}_0 \;=\; \mathcal{M}_0^x \cap \mathcal{M}_0^y \cap \mathcal{M}_0^z \; .$$

Furthermore, $\mathcal{M}_0$ is invariant under K_N and Q_N.

Physically, $\mathcal{M}_0$ corresponds to the subspace of $\mathcal{V}^{\otimes N}$ with spin 0. If we had $\mathcal{M}_0 = \{0\}$, then K_N and Q_N would have no eigenspaces of multiplicity 1, contradicting [1]. However, it is known (see, e.g. [7]) that $\mathcal{M}_0$ is in fact fairly large. In the next section we describe $\mathcal{M}_0$ precisely. We first present alternative characterizations of some of the subspaces considered in this section.

Proposition 4.3. *The subspace $\mathcal{M}_0$ is equal to the intersection of the kernels of all operators on $\mathcal{V}^{\otimes N}$ of the form $\sum_{j=1}^{N} F^{(j)}$ where F is a linear operator on $\mathcal{V}$ with $F^t = -F$ in the basis $\{e_1, e_2, e_3\}$.*

Proof. Since each of the matrices R, S, and T of Theorem 2.1 are skew-symmetric, it is clear that $\mathcal{M}_0$ contains the given intersection. On the other hand, since every skew-symmetric matrix F is a linear combination of R, S, and T, it follows that $\sum_{j=1}^{N} F^{(j)}$ for such an F must annihilate every element in the kernels of each of $\sum_{j=1}^{N} R^{(j)}$, $\sum_{j=1}^{N} S^{(j)}$, and $\sum_{j=1}^{N} T^{(j)}$, and hence the given intersection must contain $\mathcal{M}_0$. •

Proposition 4.4. *The subspaces* $\mathcal{M}_0^x$, $\mathcal{M}_0^y$, *and* $\mathcal{M}_0^z$ *are equal to the set of vectors in* $\mathcal{V}^{\otimes N}$ *left fixed by all operators of the form* $F^{\otimes N}$, *where* F *is a linear operator on* $\mathcal{V}$ *corresponding to a rotation about the* e_1*-axis, the* e_2*-axis, and the* e_3*-axis, respectively.*

Proof. We prove only the $\mathcal{M}_0^z$ part; the other statements then follow by permuting the roles of the e_i's. It is easily checked that a rotation through an angle θ about the e_3- axis has eigenvectors v_{-1}, v_0, and v_1, with eigenvalues $e^{-i\theta}$, 1, and $e^{i\theta}$, respectively. Hence, any element of $\mathcal{M}_0^z$ is fixed by any N-fold tensor product of such a rotation.

Conversely, if a vector w is left invariant by all such N-fold products of rotations, choose any θ with θ/π irrational. Then the only way w can be fixed by the N-fold product of a rotation about the e_3-axis through that θ is if, in the basis generated by $\{v_{-1}, v_0, v_1\}$, each non-zero term in the expression for w has an equal number of v_{-1}'s and v_1's. Hence $w \in \mathcal{M}_0^z$. •

Proposition 4.5. *The subspace* $\mathcal{M}_0$ *is equal to the set of vectors in* $\mathcal{V}^{\otimes N}$ *which are left fixed by all operators of the form* $F^{\otimes N}$, *where* F *is a linear operator on* $\mathcal{V}$ *with* $F^t F = I$ *in the basis* $\{e_1, e_2, e_3\}$, *and with* $\det F = 1$.

Proof. If an element of $\mathcal{V}^{\otimes N}$ is left fixed by all such $F^{\otimes N}$, then by the above proposition it must be in each of $\mathcal{M}_0^x$, $\mathcal{M}_0^y$, and $\mathcal{M}_0^z$, and hence in $\mathcal{M}_0$.

For the converse, note that it follows by direct computation (by writing $F = A + iB$

and using the polar decomposition of A) that, in the basis $\{e_1, e_2, e_3\}$, we must have

$$F = O_1 \begin{pmatrix} \sqrt{1+b^2} & ib & 0 \\ -ib & \sqrt{1+b^2} & 0 \\ 0 & 0 & 1 \end{pmatrix} O_2,$$

for some real number b and some real, orthogonal matrices O_1 and O_2. Furthermore, since $\det F = 1$, we can assume (by multiplying O_1 and O_2 by -1 if necessary) that $\det O_1 = \det O_2 = 1$. Now, every real, orthogonal matrix of determinant 1 can be written as a product of rotations about the e_1-axis and e_2-axis, so by Proposition 4.4 every element of $\mathcal{M}_0$ is fixed by every such matrix. As for the matrix

$$\begin{pmatrix} \sqrt{1+b^2} & ib & 0 \\ -ib & \sqrt{1+b^2} & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

it has eigenvectors v_{-1}, v_0, and v_1, with eigenvalues γ, 1, and γ^{-1}, respectively, where $\gamma = \sqrt{1+b^2} - b$, so it clearly fixes every element of $\mathcal{M}_0^z$. •

Remarks.

1. The proof above also shows that in fact $\mathcal{M}_0 = \mathcal{M}_0^x \cap \mathcal{M}_0^y$, etc. In other words, we can omit any one of the three sets being intersected in the definition of $\mathcal{M}_0$. However, we do not make use of this fact here.

2. Part of the theorem above can be generalized to the statement that if $FF^t = F^tF = \lambda I$, then $F^{\otimes N}$ multiplies each element of $\mathcal{M}_0$ by $(\det F)^N$. For $\lambda \neq 0$ this follows immediately by considering $F \,/\, (\det F)$. For $\lambda = 0$, direct computation shows that up to real orthogonal matrices

$$F = \begin{pmatrix} 1 & i & 0 \\ -i & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

so that $F(v_{-1}) = 2v_{-1}$ and $F(v_0) = F(v_1) = 0$, from which it follows that $F^{\otimes N}$ annihilates each element of $\mathcal{M}_0^z$.

5. The structure of $\mathcal{M}_0$.

In this section, we examine the subspaces $\mathcal{M}_0^x$, $\mathcal{M}_0^y$, $\mathcal{M}_0^z$ and $\mathcal{M}_0$ described above. Our main result (Theorems 5.4 and 5.8) is an explicit description of $\mathcal{M}_0$. Other, alternative descriptions of $\mathcal{M}_0$ have been obtained in [7] by the "valence-bond basis" approach.

We require some notation. For $\sigma \in S_N$ (the symmetric group on N letters), we define the linear operator Ω_σ on $\mathcal{V}^{\otimes N}$ by

$$\Omega_\sigma(u_1 \otimes \cdots \otimes u_N) \;=\; u_{\sigma(1)} \otimes \cdots \otimes u_{\sigma(N)} \;,$$

extended by linearity.

Definition. Given a set $Y \subseteq \mathcal{V}^{\otimes N}$, the *permutation set* of Y is $P(Y) = \{\Omega_\sigma(y) \mid \sigma \in S_N, y \in Y\}$, and the *permutation-span* of Y, written P-sp(Y), is the linear span of $P(Y)$.

In this notation, we may write $\mathcal{M}_0^z$ as

$$\mathcal{M}_0^z = P\text{-sp}\Big\{(v_{-1} \otimes v_1)^{\otimes a} \otimes v_0^{\otimes b} \;\mid\; 2a+b=N\Big\},$$

where, given a vector u, $u^{\otimes k}$ denotes the k-fold tensor product of u with itself.

In the basis $\{e_1, e_2, e_3\}$ of Theorem 2.1, this becomes

$$\mathcal{M}_0^z = P\text{-sp}\Big\{\big((-ie_1 - e_2) \otimes (ie_1 - e_2)\big)^{\otimes a} \otimes e_3^{\otimes b} \;\mid\; 2a+b=N\Big\} \;.$$

Now note that this is the same as

$$P\text{-sp}\Big\{\big((ie_1 - e_2) \otimes (-ie_1 - e_2)\big) \otimes \big((-ie_1 - e_2) \otimes (ie_1 - e_2)\big)^{\otimes a-1} \otimes e_3^{\otimes b} \;\mid\; 2a+b=N\Big\} \;.$$

By taking sums and differences of corresponding vectors in these two expressions, we obtain the "real" and "imaginary" parts of two tensor positions of these vectors (in the basis $\{e_{j_1} \otimes \cdots \otimes e_{j_N} \mid j_i \in \{1,2,3\}\}$), so we conclude that

$$\begin{aligned}\mathcal{M}_0^z =\, & P\text{-sp}\Big(\big\{(e_1 \otimes e_1 + e_2 \otimes e_2) \otimes \big((-ie_1 - e_2) \otimes (ie_1 - e_2)\big)^{\otimes a-1} \otimes e_3^{\otimes b} \mid 2a+b=N\big\} \\ & \cup \big\{(e_1 \otimes e_2 - e_2 \otimes e_1) \otimes \big((-ie_1 - e_2) \otimes (ie_1 - e_2)\big)^{\otimes a-1} \otimes e_3^{\otimes b} \;\mid\; 2a+b=N\big\}\Big) \;.\end{aligned}$$

Continuing in this way, we obtain, finally, that

$$(\dagger\dagger) \qquad \mathcal{M}_0^z \;=\; P\text{-sp}\Big\{\psi^{\otimes a}\otimes\chi^{\otimes b}\otimes e_3^{\otimes c} \;\;\Big|\;\; 2a+2b+c=N\Big\}\ ,$$

where $\psi = e_1\otimes e_2 - e_2\otimes e_1$ and $\chi = e_1\otimes e_1 + e_2\otimes e_2$.

Now, note that $\psi\otimes\psi = \Omega_{\sigma_1}(\chi\otimes\chi)-\Omega_{\sigma_2}(\chi\otimes\chi)$, where σ_1 and σ_2 are the transpositions $\sigma_1 = (2\ 3)$ and $\sigma_2 = (2\ 4)$ (this can be checked simply by expanding both sides). This implies that we may assume in $(\dagger\dagger)$ that $a = 0$ or 1. Also, we can clearly replace χ by

$$\phi \;=\; \chi + e_3\otimes e_3 \;=\; e_1\otimes e_1 + e_2\otimes e_2 + e_3\otimes e_3\ ,$$

so we have

$$(*)\quad \mathcal{M}_0^z \;=\; P\text{-sp}\Big(\big\{\phi^{\otimes a}\otimes e_3^{\otimes b} \;\big|\; 2a+b=N\big\}\cup\big\{\psi\otimes\phi^{\otimes a}\otimes e_3^{\otimes b} \;\big|\; 2+2a+b=N\big\}\Big)\ .$$

Let $R, S,$ and T be as in Theorem 2.1. We can obtain $-S$ from T by interchanging the vectors e_2 and e_3 in the basis $\{e_1, e_2, e_3\}$. Similarly, we obtain $-R$ from T by interchanging e_1 and e_3. Since $\mathcal{M}_0^z = \ker\left(\sum_{j=1}^N T^{(j)}\right)$, $\mathcal{M}_0^x = \ker\left(\sum_{j=1}^N R^{(j)}\right)$, and $\mathcal{M}_0^y = \ker\left(\sum_{j=1}^N S^{(j)}\right)$, we have immediately from $(*)$ that

$$(**)\qquad \begin{aligned}\mathcal{M}_0^x \;=\; P\text{-sp}\Big(&\big\{\phi^{\otimes a}\otimes e_1^{\otimes b} \;\big|\; 2a+b=N\big\}\\ &\cup\big\{(e_2\otimes e_3 - e_3\otimes e_2)\otimes\phi^{\otimes a}\otimes e_1^{\otimes b} \;\big|\; 2+2a+b=N\big\}\Big)\end{aligned}$$

and

$$(***)\qquad \begin{aligned}\mathcal{M}_0^y = P\text{-sp}\Big(&\big\{\phi^{\otimes a}\otimes e_2^{\otimes b} \;\big|\; 2a+b=N\big\}\\ &\cup\big\{(e_3\otimes e_1 - e_1\otimes e_3)\otimes\phi^{\otimes a}\otimes e_2^{\otimes b} \;\big|\; 2+2a+b=N\big\}\Big)\ .\end{aligned}$$

Since the vector ϕ will be important in what follows, we pause to note that ϕ will be seen to be the unique (up to scalar multiple) element of $\mathcal{M}_0$ for $N = 2$, and that $K_2\phi = 2\phi$.

Having derived these expressions for $\mathcal{M}_0^x$, $\mathcal{M}_0^y$, and $\mathcal{M}_0^z$, we now consider their intersection, $\mathcal{M}_0$. We sometimes write $\mathcal{M}_{0,N}^x$ for $\mathcal{M}_0^x$, $\mathcal{M}_{0,N}^y$ for $\mathcal{M}_0^y$, $\mathcal{M}_{0,N}^z$ for $\mathcal{M}_0^z$, and $\mathcal{M}_{0,N}$ for $\mathcal{M}_0$, to emphasize the value of N under consideration.

Lemma 5.1.

(1) *Let q be one of x, y, and z. Let $u_1 \in \mathcal{M}^q_{0,N_1}$, and $u_2 \in \mathcal{M}^q_{0,N_2}$. Then $u_1 \otimes u_2 \in \mathcal{M}^q_{0,N_1+N_2}$. The same result holds if we replace $\mathcal{M}^q_0$ by $\mathcal{M}_0$.*

(2) *Let $w \in \mathcal{M}_{0,N}$. Then $P\text{-sp}\{w\} \subseteq \mathcal{M}_{0,N}$.*

Proof. For (1), we have

$$\sum_{j=1}^{N_1+N_2} S_q^{(j)}(u_1 \otimes u_2) \quad = \quad \sum_{j=1}^{N_1} S_q^{(j)}(u_1 \otimes u_2) \quad + \quad \sum_{j=N_1+1}^{N_1+N_2} S_q^{(j)}(u_1 \otimes u_2) \ .$$

Since $u_1 \in \mathcal{M}^q_{0,N_1}$, the first of these two sums is zero. Since $u_2 \in \mathcal{M}^q_{0,N_2}$, the second is also zero. Hence $u_1 \otimes u_2 \ \in \ \ker\left(\sum_{i=1}^{N_1+N_2} S_q^{(i)}\right) \ = \ \mathcal{M}^q_{0,N_1+N_2}$. The statement for $\mathcal{M}_0$ follows immediately. (2) is obvious. •

Lemma 5.2. *Let $N \geq 2$ be even. Then*

$$\mathcal{M}_{0,N} \ = P\text{-sp}\big\{\phi^{\otimes a} \otimes e_1^{\otimes b} \ \big| \ 2a+b=N\big\} \ \cap \ P\text{-sp}\big\{\phi^{\otimes a} \otimes e_2^{\otimes b} \ \big| \ 2a+b=N\big\}$$
$$\cap \ P\text{-sp}\big\{\phi^{\otimes a} \otimes e_3^{\otimes b} \ \big| \ 2a+b=N\big\} \ .$$

Proof. We use equations $(*)$, $(**)$, and $(***)$. Equation $(*)$ shows that

$$\mathcal{M}^z_{0,N} \subseteq \ \text{span}\{e_{j_1} \otimes \cdots \otimes e_{j_N} \ \big| \ e_3 \text{ appears in an even number of positions}\} \ .$$

Combining this with equations $(**)$ and $(***)$ shows that

$$\mathcal{M}_{0,N} \subseteq \ \text{span}\{e_{j_1} \otimes \cdots \otimes e_{j_N} \ \big| \ \text{each of } e_1, e_2, \text{ and } e_3 \text{ appears in an even number of positions}\} \ .$$

Now, an examination of equation $(*)$ shows that the only elements of $\mathcal{M}^z_{0,N}$ in this span are those in

$$P\text{-sp}\big\{\phi^{\otimes a} \otimes e_3^{\otimes b} \ \big| \ 2a+b=N\big\} \ .$$

Similarly, the only elements of $\mathcal{M}^x_{0,N}$ and $\mathcal{M}^y_{0,N}$ in this span are, respectively, those in

$$P\text{-sp}\{\phi^{\otimes a} \otimes e_1^{\otimes b} \mid 2a + b = N\}$$

and in

$$P\text{-sp}\{\phi^{\otimes a} \otimes e_2^{\otimes b} \mid 2a + b = N\}\ .$$

Since $\mathcal{M}_{0,N} = \mathcal{M}^x_{0,N} \cap \mathcal{M}^y_{0,N} \cap \mathcal{M}^z_{0,N}$, this completes the proof. •

Corollary 5.3. *Let $N \geq 2$ be even and let F be a linear operator on $\mathcal{V}$ which permutes the basis $\{e_1, e_2, e_3\}$. Then $F^{\otimes N}$ fixes $\mathcal{M}_{0,N}$.*

Proof. Since every element of $P\text{-sp}\{\phi^{\otimes a} \otimes e_3^{\otimes b} \mid 2a + b = N\}$ is unchanged upon interchanging e_1 and e_2, the theorem is true when F arises from the transposition (1 2). Similarly, the theorem is true when F arises from the transposition (2 3). Since (1 2) and (2 3) generate S_3, we are done. (This corollary also follows from Proposition 4.5.) •

Theorem 5.4. *Let $N \geq 2$ be even, and let $\phi = e_1 \otimes e_1 + e_2 \otimes e_2 + e_3 \otimes e_3$. Then*

$$\mathcal{M}_{0,N} = P\text{-sp}\{\phi^{\otimes N/2}\}\ .$$

Proof. Equations $(*)$, $(**)$, and $(***)$ show $\mathcal{M}_{0,N} \supseteq P\text{-sp}\{\phi^{\otimes N/2}\}$. Conversely, given $w \in \mathcal{M}_{0,N}$, we proceed to show that $w \in P\text{-sp}\{\phi^{\otimes N/2}\}$.

By Lemma 5.2,

$$w \in P\text{-sp}\{\phi^{\otimes a} \otimes e_3^{\otimes b} \mid 2a + b = N\},$$

so we can write

$$w = \sum_{\substack{b=0 \\ b \text{ even}}}^{N/2} \sum_{\sigma \in S_N} \alpha_{b,\sigma}\, \Omega_\sigma \left(\phi^{\otimes (N-b)/2} \otimes e_3^{\otimes b}\right),$$

where the coefficients $\alpha_{b,\sigma}$ are complex numbers. Let b_{max} be the largest value of b for which some $\alpha_{b,\sigma} \neq 0$, and let us suppose our expression for w is such that b_{max} is as small as possible. We wish to show that this minimal b_{max} is 0, for then $w \in$ P-sp$\{\phi^{\otimes N/2}\}$, as desired.

Suppose $b_{max} > 0$, so $b_{max} \geq 2$. By Corollary 5.3, w is invariant upon interchanging e_1 and e_3, so we have

$$(\diamond) \qquad w = \sum_{\substack{b=0 \\ b \text{ even}}}^{N} \sum_{\sigma \in S_N} \alpha_{b,\sigma} \, \Omega_\sigma \left(\phi^{\otimes (N-b)/2} \otimes e_1^{\otimes b} \right).$$

Define the operator Φ_N on $\mathcal{V}^{\otimes N}$ to be the orthogonal projection onto $\mathcal{M}^z_{0,N}$. Thinking in the basis $\{v_{-1}, v_0, v_1\}$ and using Lemma 5.1 (1), it is clear that if $w_1 \in \mathcal{M}^z_{0,N_1}$, and if $w_2 \in \mathcal{V}^{\otimes N_2}$, then $\Phi_{N_1+N_2}(w_1 \otimes w_2) = w_1 \otimes \Phi_{N_2}(w_2)$. Now, $\Phi_N(w) = w$, so we have

$$\begin{aligned}
w &= \Phi_N \left(\sum_{\substack{b=0 \\ b \text{ even}}}^{N} \sum_{\sigma \in S_N} \alpha_{b,\sigma} \, \Omega_\sigma \left(\phi^{\otimes (N-b)/2} \otimes e_1^{\otimes b} \right) \right) \\
&= \sum_{\substack{b=0 \\ b \text{ even}}}^{N} \sum_{\sigma \in S_N} \alpha_{b,\sigma} \, \Phi_N \left(\, \Omega_\sigma \left(\phi^{\otimes (N-b)/2} \otimes e_1^{\otimes b} \right) \right) \\
&= \sum_{\substack{b=0 \\ b \text{ even}}}^{N} \sum_{\sigma \in S_N} \alpha_{b,\sigma} \, \Omega_\sigma \left(\, \Phi_N \left(\phi^{\otimes (N-b)/2} \otimes e_1^{\otimes b} \right) \right) \\
&= \sum_{\substack{b=0 \\ b \text{ even}}}^{N} \sum_{\sigma \in S_N} \alpha_{b,\sigma} \, \Omega_\sigma \left(\phi^{\otimes (N-b)/2} \otimes \Phi_b \left(e_1^{\otimes b} \right) \right),
\end{aligned}$$

the last equality following from the fact that $\phi^{\otimes (N-b)/2} \in \mathcal{M}^z_{0,N-b}$. Now,

$$
\begin{aligned}
\Phi_b\left(e_1^{\otimes b}\right) &= \Phi_b\left(\left(\frac{i}{\sqrt{2}}\,(v_{-1}-v_1)\right)^{\otimes b}\right)\\
&= (-\frac{1}{2})^{b/2}\,\frac{1}{\left(\frac{b}{2}!\right)^2}\sum_{\sigma\in S_b}\Omega_\sigma\left((-v_{-1}\otimes v_1)^{\otimes b/2}\right)\\
&= (\frac{1}{2})^{b/2}\,\frac{1}{\left(\frac{b}{2}!\right)^2}\sum_{\sigma\in S_b}\Omega_\sigma\left((v_{-1}\otimes v_1)^{\otimes b/2}\right)\\
&= (\frac{1}{2})^{b/2}\,\frac{1}{\left(\frac{b}{2}!\right)^2}\sum_{\sigma\in S_b}(\frac{1}{2})^{b/2}\,\Omega_\sigma\left((v_{-1}\otimes v_1\ +v_1\otimes v_{-1})^{\otimes b/2}\right)\\
&= \frac{1}{2^b}\,\frac{1}{\left(\frac{b}{2}!\right)^2}\sum_{\sigma\in S_b}\Omega_\sigma\left((\phi-e_3\otimes e_3)^{\otimes b/2}\right)\\
&= \frac{(-1)^{b/2}\,b!}{2^b\,\left(\frac{b}{2}!\right)^2}\,e_3^{\otimes b}\ +\ \ldots\ ,
\end{aligned}
$$

where the "…" indicates terms involving at least one ϕ, and hence no more than $b-2$ e_3's. Hence,

$$
w = \sum_{\substack{b=0\\ b\ \text{even}}}^{N}\ \sum_{\sigma\in S_N}\alpha_{b,\sigma}\,\Omega_\sigma\left(\phi^{\otimes(N-b)/2}\otimes\left(\beta_b\,e_3^{\otimes b}+\ldots\right)\right),
$$

where $\beta_b = \frac{(-1)^{b/2}\,b!}{2^b\,\left(\frac{b}{2}!\right)^2}$. Note that for any $b\geq 2$, β_b is not 1. Subtracting this expression for w from $\beta_{b_{max}}$ times ($\diamond$) yields

$$
(\beta_{b_{max}}-1)\,w = \sum_{\substack{b=0\\ b\ \text{even}}}^{N}\ \sum_{\sigma\in S_N}\alpha_{b,\sigma}\,\Omega_\sigma\left(\phi^{\otimes(N-b)/2}\otimes\left((\beta_{b_{max}}-\beta_b)\,e_3^{\otimes b}+\ldots\right)\right)\ .
$$

Dividing this last expression by $(\beta_{b_{max}}-1)$ yields an expression for w which has terms corresponding only to values of b strictly less than b_{max}. This contradicts the assumption that our b_{max} in ($\diamond$) was minimal. Hence, it must have been that the true minimal b_{max} was 0, and therefore that $w\in\ P\text{-sp}\{\phi^{\otimes N/2}\}$. •

Remark. Note that the vector $\Omega_\sigma\left(\phi^{\otimes N/2}\right)$ depends on σ only through the unordered, indistinguishable pairs $\{\sigma(1),\sigma(2)\},\{\sigma(3),\sigma(4)\},\ldots,\{\sigma(N-1),\sigma(N)\}$. Hence, when considering a vector of the form $\Omega_\sigma\left(\phi^{\otimes N/2}\right)$, we can assume without loss of generality that σ is *canonical* in the sense that $\sigma(2j-1)<\sigma(2j)$ for $1\le j\le N/2$, and that $\sigma(2)<\sigma(4)<\ldots<\sigma(N)$.

To determine the structure of $\mathcal{M}_{0,N}$ for N odd, we require two additional linear operators. For $N\ge 1$, for any $w\in\mathcal{V}^{\otimes N-1}$, and (i,j,k) any cyclic permutation of $(1,2,3)$, we define $\Psi : \mathcal{V}^{\otimes N}\to\mathcal{V}^{\otimes N+1}$ by

$$\Psi(w\otimes e_i)=\frac{1}{2}\left(w\otimes(e_j\otimes e_k-e_k\otimes e_j)\right) ,$$

and define $\Lambda : \mathcal{V}^{\otimes N+1}\to\mathcal{V}^{\otimes N}$ by

$$\begin{aligned} \Lambda(w\otimes e_i\otimes e_i) &= 0 , \\ \Lambda(w\otimes e_i\otimes e_j) &= w\otimes e_k , \\ \text{and}\quad \Lambda(w\otimes e_j\otimes e_i) &= -w\otimes e_k . \end{aligned}$$

We extend Ψ and Λ by linearity.

Lemma 5.5.

(1) $\Lambda\circ\Psi$ *is the identity on* $\mathcal{V}^{\otimes N}$.

(2) $\Psi\left(\mathcal{M}_{0,N}\right)\subseteq\mathcal{M}_{0,N+1}$.

(3) $\Lambda\left(\mathcal{M}_{0,N+1}\right)\subseteq\mathcal{M}_{0,N}$.

Proof. (1) is obvious. For (2), note that it suffices to show that

$$\left(\sum_{j=1}^{N+1}X^{(j)}\right)\Psi \;=\; \Psi\left(\sum_{j=1}^{N}X^{(j)}\right) ,$$

where $X = R$, S, and T, as defined in Theorem 2.1. By symmetry, it suffices to consider the case $X = R$, and clearly we need only show

$$\left(R^{(N)} + R^{(N+1)}\right) \Psi \;=\; \Psi \, R^{(N)} \ .$$

This follows by direct computation on elements of the form $w \otimes e_i$, where $i = 1, 2, 3$. Similarly, for (3), it suffices to show

$$R^{(N)} \Lambda \;=\; \Lambda \left(R^{(N)} + R^{(N+1)}\right) \ ,$$

and this follows by direct computation on elements of the form $w \otimes e_i \otimes e_j$, where $i, j = 1, 2, 3$. •

Proposition 5.6. *For any $N \geq 2$,*

$$\mathcal{M}_{0,N} = \Lambda \left(\mathcal{M}_{0,N+1}\right) \ .$$

Proof. By (3) of the previous lemma, it suffices to show $\Lambda \left(\mathcal{M}_{0,N+1}\right) \supseteq \mathcal{M}_{0,N}$. Using (2) and (1) of the previous lemma, we have

$$\Lambda \left(\mathcal{M}_{0,N+1}\right) \supseteq \Lambda \left(\Psi \left(\mathcal{M}_{0,N}\right)\right) = \mathcal{M}_{0,N} \ ,$$

completing the proof. •

Lemma 5.7. *Let $\Delta = \sum\limits_{\sigma \in S_3} (\mathrm{sgn}\ \sigma) \, e_{\sigma(1)} \otimes e_{\sigma(2)} \otimes e_{\sigma(3)}$, where S_3 is the symmetric group on three letters, and* sgn σ *is the sign of the permutation σ. Then $\Delta \in \mathcal{M}_{0,3}$.*

Proof. We first show that $\left(\sum\limits_{j=1}^{3} R^{(j)}\right)(\Delta) = 0$. Note that

$$\begin{aligned} \left(R^{(1)} + R^{(2)} + R^{(3)}\right)(e_1 \otimes e_2 \otimes e_3) \;&=\; 0 \;+\; e_1 \otimes e_3 \otimes e_3 \;-\; e_1 \otimes e_2 \otimes e_2 \\ &=\; \left(R^{(1)} + R^{(3)} + R^{(2)}\right)(e_1 \otimes e_3 \otimes e_2) \ . \end{aligned}$$

Hence, $\left(\sum_{j=1}^{3} R^{(j)}\right)(e_1 \otimes e_2 \otimes e_3 - e_1 \otimes e_3 \otimes e_2) = 0$. The other terms in $\left(\sum_{j=1}^{3} R^{(j)}\right)(\Delta)$ cancel similarly. Hence, $\Delta \in \mathcal{M}_0^x$. Similarly, $\Delta \in \mathcal{M}_0^y$ and $\Delta \in \mathcal{M}_0^z$. •

Theorem 5.8. *Let $N \geq 3$ be odd. Then*

$$\mathcal{M}_{0,N} \;=\; P\text{-sp}\left\{\phi^{\otimes(N-3)/2} \otimes \Delta\right\} \;,$$

with $\Delta = \sum_{\sigma \in S_3} (\operatorname{sgn} \sigma)\, e_{\sigma(1)} \otimes e_{\sigma(2)} \otimes e_{\sigma(3)}$.

Proof. Theorem 5.4 and Lemmas 5.1 and 5.7 show

$$\mathcal{M}_{0,N} \;\supseteq\; P\text{-sp}\left\{\phi^{\otimes(N-3)/2} \otimes \Delta\right\} \;.$$

Conversely, Proposition 5.6 and Theorem 5.4 show that

$$\begin{aligned} \mathcal{M}_{0,N} \;&=\; \Lambda\left(\mathcal{M}_{0,N+1}\right) \\ &=\; \Lambda\left(P\text{-sp}\left\{\phi^{\otimes(N+1)/2}\right\}\right) \;, \end{aligned}$$

so it suffices to show

$$\Lambda\left(\Omega_\sigma\left(\phi^{\otimes(N+1)/2}\right)\right) \;\in\; P\text{-sp}\left\{\phi^{\otimes(N-3)/2} \otimes \Delta\right\} \;,$$

for any $\sigma \in S_{N+1}$. By the remark following Theorem 5.4, we can assume σ is "canonical", and in particular that $\sigma(N+1) = N+1$, and either $\sigma(N) = N$ or $\sigma(N-1) = N$. In the first case, $\Lambda\left(\Omega_\sigma\left(\phi^{\otimes(N+1)/2}\right)\right)$ is zero, while in the second case

$$\Lambda\left(\Omega_\sigma\left(\phi^{\otimes(N+1)/2}\right)\right) \;=\; \Omega_\tau\left\{\phi^{\otimes(N-3)/2} \otimes \Delta\right\} \;,$$

where τ equals σ restricted to $\{1, 2, \ldots, N\}$. This completes the proof. •

Remark. The proof above actually shows that

$$P\text{-sp}\left\{\phi^{\otimes(N-3)/2} \otimes \Delta\right\} = \text{span}\;\left\{\Omega_\sigma\left(\phi^{\otimes(N-3)/2} \otimes \Delta\right)\;\middle|\; \sigma \in S_N,\; \sigma(N-1) = N\right\}.$$

In other words, we need only consider those σ with $\sigma(N-1) = N$. Since Δ is skew-symmetric upon interchanging its last two tensor positions, we may instead assume $\sigma(N) = N$. Combining this with reasoning as in the remark following Theorem 5.4, we see that we can assume σ is *canonical* in the sense that $\sigma(N) = N$, $\sigma(2j-1) < \sigma(2j)$ for $1 \leq j \leq (N-1)/2$, and $\sigma(2) < \sigma(4) < \ldots \sigma(N-3)$. (Note that we cannot assume $\sigma(N-3) < \sigma(N-1)$, since the unordered pair $\{\sigma(N-2), \sigma(N-1)\}$ is special and must be allowed to occur anywhere.)

We now turn our attention to the dimension of $\mathcal{M}_{0,N}$. By Proposition 5.6, this dimension is an increasing function of N. It is shown in [6] (see [7]) that for N even,

$$\dim \mathcal{M}_{0,N} \;=\; \sum_{m=0}^{N/2} \frac{N!}{(m!)^2\,(N-2m)!} \;-\; \sum_{m=0}^{(N/2)-1} \frac{N!}{m!(m+1)!(N-2m-1)!}\;.$$

This expression, while exact, is difficult to work with. Furthermore, it holds for even N only.

We present here some upper bounds on $\dim \mathcal{M}_{0,N}$ in closed form, which follow directly from the results of this section.

Proposition 5.9. *Let $N \geq 4$ be even. Then*

$$\dim \mathcal{M}_{0,N} \leq (N-1) \dim \mathcal{M}_{0,N-2}\,.$$

Proof. Recall that

$$\mathcal{M}_{0,N} \;=\; \operatorname{span}\left\{\Omega_\sigma\left(\phi^{\otimes N/2}\right)\right\}\,.$$

Furthermore, by the remark following Theorem 5.4, we need only consider "canonical" σ, so that $\sigma(N) = N$. There are then $(N-1)$ possible values of $\sigma(N-1)$. If we "delete" tensor positions N and $\sigma(N-1)$, we are left with an element of $\mathcal{M}_{0,N-2}$, so that

$$\dim\ \operatorname{span}\left\{\Omega_\sigma\left(\phi^{\otimes N/2}\right) \mid \sigma(N) = N, \sigma(N-1) = j\right\} = \dim \mathcal{M}_{0,N-2}$$

for $j = 1, 2, \ldots, N-1$. The result follows. $\bullet$

Corollary 5.10. *Let $N \geq 2$ be even. Then*

$$\dim \mathcal{M}_{0,N} \leq (N-1)(N-3)\ldots \cdot 3 \cdot 1 = \frac{N!}{\left(\frac{N}{2}\right)!\, 2^N}\,.$$

Furthermore, equality holds for $N = 2$, 4, or 6.

Proof. For $N = 2$, clearly $\dim \mathcal{M}_{0,2} = \dim \{\phi\} = 1$. The inequality now follows from the previous proposition by induction. For $N = 6$, to show equality it suffices to show the set

$$\left\{ \Omega_\sigma \left(\phi^{\otimes 3}\right) \,\middle|\, \sigma \in S_6,\ \sigma \text{ canonical}\right\}$$

is linearly independent. This follows from the observation that for σ_1 and σ_2 canonical,

$$\left\langle\ \Omega_{\sigma_1}\left(\phi^{\otimes 3}\right)\ ,\ \Omega_{\sigma_2}\left(e_1 \otimes e_1 \otimes e_2 \otimes e_2 \otimes e_3 \otimes e_3\right)\ \right\rangle$$

is 1 or 0 as $\sigma_1 = \sigma_2$ or $\sigma_1 \neq \sigma_2$. The proof of equality for $N = 4$ is similar, involving $e_1 \otimes e_1 \otimes e_2 \otimes e_2$ in place of $e_1 \otimes e_1 \otimes e_2 \otimes e_2 \otimes e_3 \otimes e_3$. $\bullet$

Proposition 5.11. *Let $N \geq 3$ be odd. Then*

$$\dim \mathcal{M}_{0,N} \leq \left(\frac{N-1}{2}\right)(N-2)(N-4)\ldots \cdot 3 \cdot 1\,.$$

Furthermore, equality holds for $N = 3$ and $N = 5$.

Proof. The inequality follows immediately from the fact that the number of "canonical" elements of S_N, in the sense of the remark following Theorem 5.8, is precisely $\left(\frac{N-1}{2}\right)(N-2)(N-4)\ldots \cdot 3 \cdot 1$. For $N = 3$, clearly $\dim \mathcal{M}_{0,3} = \dim \{\Delta\} = 1$. For equality when $N = 5$, note that if σ_1 and σ_2 are two canonical elements of S_5, then

$$\left\langle\ \Omega_{\sigma_1}\left(\phi \otimes \Delta\right)\ ,\ \Omega_{\sigma_2}\left(e_1 \otimes e_1 \otimes e_2 \otimes e_3 \otimes e_1\right)\ \right\rangle$$

is 1 or 0 as $\sigma_1 = \sigma_2$ or $\sigma_1 \neq \sigma_2$. Hence, the set

$$\left\{ \Omega_\sigma \left(\phi \otimes \Delta\right) \,\middle|\, \sigma \in S_5,\ \sigma \text{ canonical}\right\}$$

is linearly independent. •

6. Some special vectors; bounds on eigenvalues of K_N and Q_N.

As mentioned in the Introduction, Haldane's conjecture ([9], [10]) involves the lowest eigenvalues of H_N and P_N, or equivalently the highest eigenvalues of $K_N = -H_N$ and $Q_N = -P_N$. Numerical work by physicists (see, e.g., [11]) suggests that for large N the lowest eigenvalues of P_N are approximately $-1.4015\,N$, with a difference (or "gap") of about 0.41 between the two lowest ones, and it is believed the the corresponding values for H_N are similar. In this section, we present a few bounds on eigenvalues of K_N and Q_N, and show (Theorem 6.7) that H_N and P_N have eigenvalues lower than $-\frac{4}{3}(N-1)$ and about $-\frac{4}{3}N$, respectively.

A similar result to this is obtained by a "valence bond approach" in [2]. There, vectors $\Omega_{\alpha\beta}$ $(\alpha, \beta \in \{1,2\})$ are constructed, and the expected values of H_N are considered. (The vectors $\Omega_{\alpha\beta}$ are defined more explicitly in [3].) Our approach will be somewhat similar, in that we will construct vectors $\omega_{j,N}$ and consider expressions like $\langle H_N(\omega_{j,N}),\ \omega_{j,N}\rangle$. Our vectors $\omega_{j,N}$ are different than the vectors $\Omega_{\alpha\beta}$, and are defined in a quite different way. However, there are certain strong connections. For example, the identity $\Omega_{12}+(-1)^N\Omega_{21} = 2\,\omega_{0,N}$ appears to hold in general.

We begin with an obvious bound.

Proposition 6.1. *The spectrum of K_N is contained in $[-(N-1), 2(N-1)]$, and that of Q_N is contained in $[-N, 2N]$.*

Proof. Recall from Corollary 2.5 that the spectrum of K_2 is $\{-1, 1, 2\}$. This is clearly the same as the spectrum of $\Theta_N^{(ij)}$ as defined in Lemma 3.2. The proposition follows from the fact that K_N is the sum of $N-1$ operators of the form $\Theta_N^{(ij)}$, and Q_N is the sum of N operators of the form $\Theta_N^{(ij)}$. •

The smallest eigenvalues above are not relevant to Haldane's conjecture, but they are important in the study of ferromagnets, where the Hamiltonian is the negative of the operator H_N presented here. To examine these, we require the following definitions, also to be used elsewhere in this section.

Definitions. A vector $u \in \mathcal{V}^{\otimes N}$ is

(a) *symmetric,*

(b) *skew-symmetric,*

(c) *scalar,* or

(d) *of trace 0,*

in tensor positions 1 and 2, if

(a) $\Omega_{(12)}(u) = u$,

(b) $\Omega_{(12)}(u) = -u$,

(c) $u = \phi \otimes u_0$, for some $u_0 \in \mathcal{V}^{\otimes N-2}$, where $\phi = e_1 \otimes e_1 + e_2 \otimes e_2 + e_3 \otimes e_3$, or

(d) $u = \sum_{ij} e_i \otimes e_j \otimes u_{ij}$, with $u_{11} + u_{22} + u_{33} = 0$.

(Here Ω permutes the tensor positions, and is defined in the beginning of section 5.) The vector u has one of the above properties in tensor positions k and l $(k < l)$ if $\Omega_{(2l)(1k)}(u)$ has the corresponding property in tensor positions 1 and 2. We say u is *scalar plus skew-symmetric* in tensor positions k and l if $u + \Omega_{(kl)}(u)$ is scalar in tensor positions k and l, or equivalently if $u = u_1 + u_2$ with u_1 scalar and u_2 skew-symmetric in tensor positions k

and l.

By Corollary 2.5, u is scalar in tensor positions k and l if and only if $\Theta_N^{(kl)}(u) = 2u$, u is skew-symmetric in tensor positions k and l if and only if $\Theta_N^{(kl)}(u) = u$, and u is symmetric and of trace 0 in tensor positions k and l if and only if $\Theta_N^{(kl)}(u) = -u$.

The following proposition, important in the study of ferromagnets, is well-known to physicists.

Proposition 6.2. *The eigenspace of K_N corresponding to the eigenvalue $-(N-1)$ is the same as the eigenspace of Q_N corresponding to the eigenvalue $-N$. This common eigenspace has dimension $2N+1$.*

Proof. For a vector $w \in \mathcal{V}^{\otimes N}$ to be in the eigenspace for K_N, it must be that $\Theta_N^{(i,i+1)}(w) = -w$, for all adjacent positions i and $i+1$. ¿From the above, this happens precisely when w is symmetric and of trace 0 in each two adjacent positions. This condition translates into the following. If we write

$$w = \sum_h \alpha_h \, e_{h(1)} \otimes e_{h(2)} \otimes \dots e_{h(N)} \ ,$$

where the sum is taken over all functions $h : \{1, 2, \dots, N\} \to \{1, 2, 3\}$ and the coefficients α_h are complex numbers, then we must have

(A) $\alpha_{h_1} = \alpha_{h_2}$ whenever $h_1 = h_2 \circ \tau$ for some $\tau = (i \ i{+}1) \in S_N$, and

(B) $\alpha_{h_1} + \alpha_{h_2} + \alpha_{h_3} = 0$ whenever for some i, $h_1(i) = h_1(i{+}1) = 1, \ h_2(i) = h_2(i{+}1) = 2, \ h_3(i) = h_3(i+1) = 3$, and $h_1(k) = h_2(k) = h_3(k)$ for $k \neq i, i+1$.

In the case of Q_N, we require the same conditions, but must also allow the pair $(N, 1)$ in place of $(i, i+1)$. In either case, conditions (A) and (B) are easily seen to be equivalent to

(A') $\alpha_{h_1} = \alpha_{h_2}$ whenever $h_1 = h_2 \circ \tau$ for any $\tau \in S_N$, and

(B') $\alpha_{h_1} + \alpha_{h_2} + \alpha_{h_3} = 0$ whenever for some $i \neq j$, $h_1(i) = h_1(j) = 1,\ h_2(i) = h_2(j) = 2,\ h_3(i) = h_3(j) = 3$, and $h_1(k) = h_2(k) = h_3(k)$ for $k \neq i, j$.

Conditions (A') and (B') make it clear that we can choose arbitrarily the coefficients α_h for "primitive" functions h, i.e. functions h with at most one element in $h^{-1}\{3\}$, and with $h(1) \leq h(2) \leq \ldots \leq h(N)$. The coefficients α_h with at most one element in $h^{-1}\{3\}$, but with arbitrary ordering, are then forced by condition (A'). The coefficients α_h with h having more and more elements in $h^{-1}\{3\}$ are then forced in turn by condition (B'). Under such a procedure, condition (A') is satisfied automatically. Since there are $2N+1$ "primitive" functions h, this is the dimension in question. •

As a simple example of vectors in the eigenspace described above, note that if $u = v_{-1}$ or v_1, then $K_2(u \otimes u) = -u \otimes u$, so $K_N\big(u^{\otimes N}\big) = -(N-1)u^{\otimes N}$ and $Q_N\big(u^{\otimes N}\big) = -Nu^{\otimes N}$.

To investigate the largest eigenvalues of K_N and Q_N, we make the following definitions. For even N, let

$$\begin{aligned}
\mathcal{J}_{0,N} = \mathrm{span}\Big\{ e_{j_1} \otimes e_{j_2} \otimes \ldots \otimes e_{j_N} \ \Big|\ & \text{each of } e_1, e_2, \text{ and } e_3 \text{ appears in an} \\
& \text{even number of positions} \Big\}, \\
\mathcal{J}_{1,N} = \mathrm{span}\Big\{ e_{j_1} \otimes e_{j_2} \otimes \ldots \otimes e_{j_N} \ \Big|\ & \text{each of } e_2 \text{ and } e_3 \text{ appears in an} \\
& \text{odd number of positions, and } e_1 \text{ appears in an} \\
& \text{even number of positions} \Big\}, \\
\mathcal{J}_{2,N} = \mathrm{span}\Big\{ e_{j_1} \otimes e_{j_2} \otimes \ldots \otimes e_{j_N} \ \Big|\ & \text{each of } e_1 \text{ and } e_3 \text{ appears in an} \\
& \text{odd number of positions, and } e_2 \text{ appears in an} \\
& \text{even number of positions} \Big\}, \\
\mathcal{J}_{3,N} = \mathrm{span}\Big\{ e_{j_1} \otimes e_{j_2} \otimes \ldots \otimes e_{j_N} \ \Big|\ & \text{each of } e_1 \text{ and } e_2 \text{ appears in an} \\
& \text{odd number of positions, and } e_3 \text{ appears in an} \\
& \text{even number of positions} \Big\}.
\end{aligned}$$

For odd N, make the same definitions, except write “odd” for “even” and “even” for “odd”.

Clearly, $\mathcal{V}^{\otimes N} = \mathcal{J}_{0,N} \oplus \mathcal{J}_{1,N} \oplus \mathcal{J}_{2,N} \oplus \mathcal{J}_{3,N}$. Each of these four subspaces is easily seen to be invariant under an operator of the form $X^{(i)}X^{(j)}$, where X is one of R, S, and T, and hence to be invariant under K_N and Q_N. Furthermore, by Theorems 5.4 and 5.8, we have $\mathcal{M}_{0,N} \subseteq \mathcal{J}_{0,N}$.

For a function $h : \{1, 2, \ldots, N\} \to \{1, 2, 3\}$, define

$$e_h \equiv e_{h(1)} \otimes e_{h(2)} \otimes \ldots \otimes e_{h(N)} \ \in \ \mathcal{V}^{\otimes N} \ ,$$

and

$$(-1)^h \equiv (-1)^{\#(h)},$$

where

$$\#(h) \equiv \text{ number of pairs } (i,j) \text{ with } i<j \text{ and } h(i)>h(j)\,.$$

Define $\omega_{j,N} \in \mathcal{J}_{j,N}$, for $j = 0,1,2,3$, by

$$\omega_{j,N} = \sum_{\substack{h \\ e_h \in \mathcal{J}_{j,N}}} (-1)^h \, e_h \ ,$$

where the sum is taken over all functions $h : \{1,2,\dots,N\} \to \{1,2,3\}$ with e_h in the given subspace.

It is easily seen that $\Pi(\omega_{0,N}) = \omega_{0,N}$, where Π is the "rotation" operator defined at the end of section 3. Furthermore, $\omega_{0,1} = 0$, $\omega_{0,2} = \phi$, and $\omega_{0,3} = \Delta$,

$$\omega_{0,N} \ = \ \omega_{1,N-1} \otimes e_1 \ + \ (-1)^N \, \omega_{2,N-1} \otimes e_2 \ + \ \omega_{3,N-1} \otimes e_3 \ ,$$

and

$$\omega_{0,N} \ = \ \omega_{0,N-2} \otimes \phi \ + \ (-1)^{N-1} \, \Psi\left(\omega_{0,N-1}\right) \ .$$

It follows immediately that with Λ and Ψ as defined in section 5,

$$\Lambda\left(\omega_{0,N}\right) \ = \ (-1)^{N-1} \, \omega_{0,N-1}$$

and

$$\omega_{0,N} \ = \ \omega_{0,N-2} \otimes \phi \ + \ (-1)^{N-1} \, \Psi\left(\omega_{0,N-1}\right) \ ;$$

this second equation shows $\omega_{0,N} \in \mathcal{M}_{0,N}$ for all N. More generally, it follows by similar reasoning that for $j = 0,1,2,3$,

$$\Lambda\left(\omega_{j,N}\right) \ = \ (-1)^{j+N-1} \, \omega_{j,N-1}$$

and

$$\omega_{j,N} \ = \ \omega_{j,N-2} \otimes \phi \ + \ (-1)^{j+N-1} \, \Psi\left(\omega_{j,N-1}\right) \ .$$

It is easily seen from the definitions that each of $\omega_{0,N}$, $\omega_{1,N}$, $\omega_{2,N}$, and $\omega_{3,N}$ is "scalar plus skew-symmetric" in each two adjacent tensor positions. It follows immediately that $\langle \Theta^{(k,k+1)}(\omega_{j,N}), \omega_{j,N}\rangle \geq \langle \omega_{j,N}, \omega_{j,N}\rangle$ for any k and for $j = 0,1,2,3$. We improve this result in Lemma 6.6 below.

The vector $\omega_{0,N}$ has the following uniqueness property.

Lemma 6.3. *Let $N \geq 2$ be even. Let $y \in \mathcal{J}_{0,N}$ be scalar plus skew-symmetric in each two adjacent tensor positions. Then y is a scalar multiple of $\omega_{0,N}$.*

Proof. Note that $\langle \omega_{0,N}, e_1^{\otimes N}\rangle = 1$, so there is a complex number λ such that if $z = y + \lambda\,\omega_{0,N}$, then $\langle z, e_1^{\otimes N}\rangle = 0$. We wish to show that $z = 0$. We proceed by induction on even N, the induction hypothesis being that if $z \in \mathcal{J}_{0,N}$ is such that z satisfies the hypothesis of y in the statement of the lemma, and if furthermore z is perpendicular to $e_1^{\otimes N}$, then $z = 0$. For $N = 2$, the hypothesis is clearly true. Assuming it is true for $N-2$, with $N \geq 4$, write

$$z = \phi \otimes u_0 \;+\; (e_1 \otimes e_2 - e_2 \otimes e_1) \otimes u_3 \;+\; (e_2 \otimes e_3 - e_3 \otimes e_2) \otimes u_1 \;+\; (e_3 \otimes e_1 - e_1 \otimes e_3) \otimes u_2\,,$$

for some vectors $u_0, u_1, u_2, u_3 \in \mathcal{V}^{\otimes N-2}$. Note that u_0 satisfies the same properties as does z, so by the induction hypothesis $u_0 = 0$. This means that z is skew-symmetric in tensor positions 1 and 2. Similarly, z is skew-symmetric in tensor positions k and $k+1$ for each k. Since $N \geq 4$, and z must be built out of only the 3 vectors e_1, e_2, and e_3, this implies that $z = 0$. This completes the induction step, and proves the lemma. •

Proposition 6.4. *Let N be even. Then*

$$\omega_{0,N} \;=\; \sum_{\substack{\sigma \in S_N \\ \sigma \text{ canonical}}} (\operatorname{sgn} \sigma)\, \Omega_\sigma \left(\phi^{\otimes N/2}\right)\,,$$

with "canonical" as in the remark following Theorem 5.4. Hence, $\omega_{0,N} \in \mathcal{M}_{0,N}$.

Proof. Let

$$y = \sum_{\substack{\sigma \in S_N \\ \sigma \text{ canonical}}} (\text{sgn } \sigma)\, \Omega_\sigma \left(\phi^{\otimes N/2}\right) .$$

Then y satisfies the hypothesis of the previous lemma, so y is a scalar multiple of $\omega_{0,N}$. To show the scalar is 1, note that $\langle \omega_{0,N}, e_1^{\otimes N} \rangle = 1$, while

$$\langle y, e_1^{\otimes N} \rangle = \sum_{\substack{\sigma \in S_N \\ \sigma \text{ canonical}}} (\text{sgn } \sigma) ,$$

and this last expression is easily seen to be 1 by induction. •

Remarks.

1. The analogous statements to Lemma 6.3 for $\omega_{j,N}$, for $j = 0, 1, 2, 3$, and for N even or odd, are also true.

2. In addition to Proposition 6.4, we also have the following. For odd N,

$$\omega_{0,N} \;=\; \sum_{\substack{\sigma \in S_N \\ \sigma \text{ canonical}}} (\text{sgn } \sigma)\, \Omega_\sigma \left(\phi^{\otimes (N-3)/2} \otimes \Delta\right) ,$$

with "canonical" as in the remark following Theorem 5.8. Also, for $j = 1, 2, 3$,

$$\omega_{j,N} \;= \sum_{\sigma} (\text{sgn } \sigma)\, \Omega_\sigma \left(\phi^{\otimes (N-1)/2} \otimes e_j\right) ,$$

with the sum taken over all $\sigma \in S_N$ with $\sigma(2i-1) < \sigma(2i)$ for $i = 1, 2, \ldots, (N-1)/2$, and with $\sigma(2) < \sigma(4) < \ldots < \sigma(N-1)$. For even N, and for $j = 1, 2, 3$,

$$\omega_{j,N} \;= \sum_{\sigma} (\text{sgn } \sigma)\, \Omega_\sigma \left(\phi^{\otimes (N-2)/2} \otimes (e_k \otimes e_l \;-\; e_l \otimes e_k)\right) ,$$

where $k < l$ and $\{j, k, l\} = \{1, 2, 3\}$ as sets, and with the sum taken over all $\sigma \in S_N$ with $\sigma(2i-1) < \sigma(2i)$ for $i = 1, 2, \ldots, N/2$, and with $\sigma(2) < \sigma(4) < \ldots < \sigma(N-2)$.

Lemma 6.5. *For even N, $\|\omega_{0,N}\|^2 = \frac{1}{4}\left(3^N + 3\right)$, and $\|\omega_{1,N}\|^2 = \|\omega_{2,N}\|^2 = \|\omega_{3,N}\|^2 = \frac{1}{4}\left(3^N - 1\right)$. For odd N, $\|\omega_{0,N}\|^2 = \frac{1}{4}\left(3^N - 3\right)$, and $\|\omega_{1,N}\|^2 = \|\omega_{2,N}\|^2 = \|\omega_{3,N}\|^2 = \frac{1}{4}\left(3^N + 1\right)$.*

Proof. Let N be even. We have that

$$\|\omega_{0,N}\|^2 \ = \ \sum_{\substack{h \\ e_h \in \mathcal{J}_{0,N}}} 1 \ .$$

To evaluate this number, note that it is equal to the number of ways of partitioning the integers $\{1, 2, \ldots, N\}$ into three disjoint subsets, each of which has even cardinality. Hence,

$$\|\omega_{0,N}\|^2 \ = \sum_{\substack{N_1+N_2 \leq N \\ N_1, N_2 \ \text{even}}} \binom{N}{N_1} \binom{N-N_1}{N_2} \ .$$

This last expression is simply the sum of the coefficients of all terms in the expansion of the polynomial $(a+b+c)^N$ corresponding to even powers of each of a, b, and c, and is thus equal to

$$\frac{1}{4}\Big((1+1+1)^N + (-1+1+1)^N + (1-1+1)^N + (1+1-1)^N\Big) \ = \ \frac{1}{4}\left(3^N+3\right) \ .$$

The other norms may be similarly evaluated. •

Lemma 6.6. *For even N,*

$$\frac{\langle K_N(\omega_{0,N}), \ \omega_{0,N}\rangle}{\langle \omega_{0,N}, \omega_{0,N}\rangle} \ = \ (N-1)\left(\frac{4}{3} \ + \ \frac{8}{3^N+3}\right) \ ,$$

$$\frac{\langle Q_N(\omega_{0,N}), \ \omega_{0,N}\rangle}{\langle \omega_{0,N}, \omega_{0,N}\rangle} \ = \ N\left(\frac{4}{3} \ + \ \frac{8}{3^N+3}\right) \ ,$$

and

$$\frac{\langle K_N(\omega_{1,N}), \ \omega_{1,N}\rangle}{\langle \omega_{1,N}, \omega_{1,N}\rangle} \ = \ \frac{\langle K_N(\omega_{2,N}), \ \omega_{2,N}\rangle}{\langle \omega_{2,N}, \omega_{2,N}\rangle} \ = \ \frac{\langle K_N(\omega_{3,N}), \ \omega_{3,N}\rangle}{\langle \omega_{3,N}, \omega_{3,N}\rangle}$$
$$= \ (N-1)\left(\frac{4}{3} \ - \ \frac{8}{3^{N+1}-3}\right) \ ,$$

while for odd N,

$$\frac{\langle K_N(\omega_{0,N}), \ \omega_{0,N}\rangle}{\langle \omega_{0,N}, \omega_{0,N}\rangle} \ = \ (N-1)\left(\frac{4}{3} \ - \ \frac{8}{3^N-3}\right) \ ,$$

$$\frac{\langle Q_N(\omega_{0,N}),\ \omega_{0,N}\rangle}{\langle \omega_{0,N}, \omega_{0,N}\rangle} \ = \ N\left(\frac{4}{3} \ - \ \frac{8}{3^N - 3}\right) \ ,$$

and

$$\frac{\langle K_N(\omega_{1,N}),\ \omega_{1,N}\rangle}{\langle \omega_{1,N}, \omega_{1,N}\rangle} \ = \ \frac{\langle K_N(\omega_{2,N}),\ \omega_{2,N}\rangle}{\langle \omega_{2,N}, \omega_{2,N}\rangle} \ = \ \frac{\langle K_N(\omega_{3,N}),\ \omega_{3,N}\rangle}{\langle \omega_{3,N}, \omega_{3,N}\rangle}$$
$$= \ (N-1)\left(\frac{4}{3} \ + \ \frac{8}{3^{N+1} + 3}\right) \ .$$

Proof. Recall that

$$\omega_{0,N} \ = \ \omega_{0,N-2} \otimes \phi \ + \ (-1)^{N-1}\, \Psi\left(\omega_{0,N-1}\right) \ .$$

Now, $\omega_{0,N-2} \otimes \phi$ is symmetric in tensor positions $N-1$ and N, while $(-1)^{N-1}\, \Psi\left(\omega_{0,N-1}\right)$ is skew-symmetric in these tensor positions. Hence, $\Theta_N^{(N-1,N)}\left(\omega_{0,N}\right) \ = \ 2\, \omega_{0,N-2} \otimes \phi \ + \ (-1)^{N-1}\, \Psi\left(\omega_{0,N-1}\right) \ = \ \omega_{0,N} \ + \ \omega_{0,N-2} \otimes \phi$. It follows that

$$\begin{aligned}
\langle \Theta_N^{(1,2)}(\omega_{0,N}),\, \omega_{0,N}\rangle \ &= \ \|\omega_{0,N}\|^2 \ + \ \langle \omega_{0,N},\, \omega_{0,N-2} \otimes \phi\rangle \\
&= \ \|\omega_{0,N}\|^2 \ + \ \|\omega_{0,N-2}\|^2 \|\phi\|^2 \\
&= \ \|\omega_{0,N}\|^2 \ + \ 3\, \|\omega_{0,N-2}\|^2 \ .
\end{aligned}$$

By symmetry, the same result holds when $(N-1,\, N)$ is replaced by $(k, k+1)$, so

$$\langle K_N(\omega_{0,N}), \omega_{0,N}\rangle \ = \ (N-1)\left(\|\omega_{0,N}\|^2 + 3\|\omega_{0,N-2}\|^2\right) \ .$$

The results for $K_N(\omega_{0,N})$ now follow from Lemma 6.5 and simple algebraic manipulation. The results for $Q_N(\omega_{0,N})$ follow similarly, using the fact that $\Pi(\omega_{0,N}) = \omega_{0,N}$. The results for $\omega_{1,N}$, $\omega_{2,N}$, and $\omega_{3,N}$ are proved similarly. •

Theorem 6.7. *The operators $K_N|_{\mathcal{M}_{0,N}}$, $Q_N|_{\mathcal{M}_{0,N}}$, $K_N|_{\mathcal{J}_{1,N}}$, $K_N|_{\mathcal{J}_{2,N}}$, and $K_N|_{\mathcal{J}_{3,N}}$ have eigenvalues at least as large as the values, respectively, of $\frac{\langle K_N(\omega_{0,N}),\ \omega_{0,N}\rangle}{\langle \omega_{0,N}, \omega_{0,N}\rangle}$, $\frac{\langle Q_N(\omega_{0,N}),\ \omega_{0,N}\rangle}{\langle \omega_{0,N}, \omega_{0,N}\rangle}$, $\frac{\langle K_N(\omega_{1,N}),\ \omega_{1,N}\rangle}{\langle \omega_{1,N}, \omega_{1,N}\rangle}$, $\frac{\langle K_N(\omega_{2,N}),\ \omega_{2,N}\rangle}{\langle \omega_{2,N}, \omega_{2,N}\rangle}$, and $\frac{\langle K_N(\omega_{3,N}),\ \omega_{3,N}\rangle}{\langle \omega_{3,N}, \omega_{3,N}\rangle}$ as given in the previous lemma. In particular, for any N, K_N has an eigenvalue larger than $\frac{4}{3}(N-1)$, and has at least 4 eigenvalues (counting multiplicity) asymptotically larger than or equal to $\frac{4}{3}N$. Also Q_N has an eigenvalue asymptotically larger than or equal to $\frac{4}{3}N$.*

Proof. Since the operators K_N and Q_N are Hermetian, this is immediate. •

The methods of this section also allow us to prove the following generalization of Corollary 4.2. It is previously known, and in fact follows from the representation theory of $SU(2)$.

Proposition 6.8. *The subspace $\mathcal{M}_{0,N}$ contains all eigenspaces of H_N and P_N of dimension 1 or 2.*

Proof. Let $\mathcal{E}$ be an eigenspace of H_N or P_N not contained in $\mathcal{M}_{0,N}$. Then by the decomposition of Section 4, there is a non- zero vector $w \in \mathcal{E} \cap \mathcal{M}_k^q$ for some $k \neq 0$ and $q = x$, y, or z. Now, it is easily seen that for any $k \neq 0$, $\mathcal{M}_k^q$ does not intersect $\mathcal{J}_{0,N}$. Indeed, $S_q^{(i)}(\mathcal{J}_{0,N})$ is orthogonal to $\mathcal{J}_{0,N}$, for each i, so no element of $\mathcal{J}_{0,N}$ can be an eigenvector of $\sum_{i=1}^{N} S_q^{(i)}$ corresponding to a non-zero eigenvalue. Hence, $w \notin \mathcal{J}_{0,N}$. But this means that w has a non-zero projection onto some $\mathcal{J}_{j,N}$, $j > 0$. Since the $\mathcal{J}_{j,N}$ are invariant subspaces of H_N and P_N, this projection is an element of $\mathcal{E}$. Then permuting the basis $\{e_1, e_2, e_3\}$ yields a non-zero element of $\mathcal{E}$ in *each* $\mathcal{J}_{j,N}$, $j = 1, 2, 3$. Since the $\mathcal{J}_{j,N}$ are orthogonal, we must have $\dim \mathcal{E} \geq 3$, completing the proof. •

7. Other spin values.

The vector space $\mathcal{V}$ and spin operators S_x, S_y, and S_z discussed in this paper correspond to atoms with spin 1. In general, spin values may be any element of $\{\frac{1}{2}, 1, \frac{3}{2}, 2, \ldots\}$. In this section, we discuss the spin operators for all spin values (see, e.g. [8]), and Haldane's more general conjecture ([9], [10]).

For spin $s \in \{\frac{1}{2}, 1, \frac{3}{2}, 2, \ldots\}$, the vector space required is $\mathcal{V}_s = \mathbf{C}^{2s+1}$ with orthonormal basis $\{v_{-s}, v_{-s+1}, \ldots, v_{s-1}, v_s\}$. The operator S_z on $\mathcal{V}_s$ is defined by $S_z(v_j) = jv_j$, extended by linearity. The operators S_x and S_y are defined, for $m, n \in \{-s, -s+1, \ldots, s\}$, by the relations

$$\langle v_m, S_x v_n \rangle \;=\; \frac{1}{2}\Big[\sqrt{s(s+1) - n(n+1)}\,\delta_{m,n+1} + \sqrt{s(s+1) - m(m+1)}\,\delta_{m+1,n}\Big]$$

and

$$\langle v_m, S_y v_n \rangle \;=\; \frac{1}{2i}\Big[\sqrt{s(s+1) - n(n+1)}\,\delta_{m,n+1} - \sqrt{s(s+1) - m(m+1)}\,\delta_{m+1,n}\Big]$$

extended by linearity, where δ is the Kronecker delta.

Once we have specified $s, \mathcal{V}_s, S_x, S_y$, and S_z, we may define the operators H_N and P_N on $\mathcal{V}_s^{\otimes N}$ exactly as before. These operators may be decomposed into operators on $\mathcal{M}_k^z$, $k \in \{-sN, -sN+1, \ldots, sN\}$, by exact analogy with section 4 of this paper (invariance can be easily checked directly).

We may now state the general form of Haldane's conjecture ([9], [10]). Let $\lambda_N^{0(s)}$ and $\lambda_N^{1(s)}$ be the smallest and second-smallest eigenvalues, respectively, of H_N (or P_N) with spin value s. Then Haldane's conjecture may be stated as saying that $\lim\limits_{N\to\infty}\big(\lambda_N^{1(s)} - \lambda_N^{0(s)}\big) > 0$ if and only if s is an integer. (Again, there are other, inequivalent, mathematical formulations of the conjecture; see [1].) The mathematical proof or disproof of this conjecture would be of extreme interest in solid state physics. See [1] for a proof of the non-integer s statement, at least for P_N. The integer s statement, however, is considered to be more surprising, and remains unproven.

The following proposition is known, and follows from the representation theory of $SU(2)$.

Proposition 7.1. *If $s \in \{\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots\}$, and if N is odd, then each eigenspace of H_N and P_N has even dimension.*

Proof. As mentioned above, we decompose the space $\mathcal{V}_s^{\otimes N}$ into spaces $\mathcal{M}_k^z$, for $k = -sN, -sN+1, \ldots, sN$. Note that each of these values of k differs by $\frac{1}{2}$ from an integer, and in particular that k is never 0. It is easily checked that the mapping $v_m \mapsto v_{-m}$ induces a unitarily equivalence of $H_N|_{\mathcal{M}_k^z}$ with $H_N|_{\mathcal{M}_{-k}^z}$, and of $P_N|_{\mathcal{M}_k^z}$ with $P_N|_{\mathcal{M}_{-k}^z}$. Let $\mathcal{M}^+ = \bigcup_{k>0} \mathcal{M}_k^z$, and let $\mathcal{M}^- = \bigcup_{k<0} \mathcal{M}_k^z$. Then $\mathcal{V}_s^{\otimes N} = \mathcal{M}^+ \oplus \mathcal{M}^-$, and we have $H_N = H_N^+ \oplus H_N^-$ and $P_N = P_N^+ \oplus P_N^-$, where $H_N^+ = H_N|_{\mathcal{M}^+}$, etc. The result now follows from the observation that H_N^+ is unitarily equivalent to H_N^-, and P_N^+ is unitarily equivalent to P_N^-. •

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