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Regular fractal structure of the energy matrix in 1D Heisenberg open spin-$\frac{1}{2}$ chains

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Abstract. A permutation group approach to a one-dimensional Heisenberg open spin chain with nearest neighbor interactions is studied. Regular fractal structures appear matrices of the Hamiltonian constructed under the outer-product basis of the permutation group, which enables one to solve the eigenvalue problem in a systematic manner.

The one-dimensional Heisenberg quantum spin-$\frac{1}{2}$ chain with nearest neighbor interactions is a basic model of physics. Solutions of this simple but important model have been studied extensively since the pioneering work of Bethe [1]. Besides semiclassical treatments [2]-[3], a lot of work has been focused on the Bethe ansatz [4]-[7]. The Bethe ansatz is certainly very useful in understanding the large $N$ limit, where $N$ is the number of sites, and has been developed into a powerful self-consistent method in dealing with a large number of quantum many-body problems. However, the Bethe ansatz solution is a formal expression, one that is neither easy nor straightforward to use because it requires the solution of a set of highly non-linear algebraic equations. Numerical algorithms for systematically solving such non-linear equations are generally not available. Since a limitation (numerical and computational) exists, a long-standing argument as to whether the Bethe ansatz solutions are complete or not remains unresolved [6, 8].

The Hamiltonian can be written as

$$\hat{H} = 2J \sum_{i=1}^{N-1} \left( \hat{s}_i \cdot \hat{s}_{i+1} + \frac{1}{4} \right),$$

where the extra constant $\frac{1}{4}$ simplifies expressions that enter in a permutation group approach to the solution. It is well-known that (1) can be rewritten as

$$\hat{H} = J \sum_{i=1}^{N-1} g_i,$$

where $g_i = 2 \left( \hat{s}_i \cdot \hat{s}_{i+1} + \frac{1}{4} \right)$, with $i = 1, 2, \ldots, N - 1$, are generators of the spin-compon permutation group $S_N$. Let $c_{i\sigma}$ be the creation operator of an electron at the $i$-th site with the $\sigma$ component of spin $\sigma$, and $|0\rangle$ be the vacuum state. Then, $c_{1\sigma_1}^d c_{2\sigma_2}^d \cdots c_{k\sigma_k}^d |0\rangle$ are basis vectors of the $k$-electron tensor product space $V^{(1)} \otimes V^{(2)} \otimes \cdots \otimes V^{(k)}$, where each space $V^{(i)}$ is $t$ dimensional. The action of $g_i$ ($i \leq k$) on the $k$-electron basis vector is given by

$$g_i \left( c_{1\sigma_1}^d c_{2\sigma_2}^d \cdots c_{i\sigma_i}^d c_{i+1\sigma_{i+1}}^d \cdots c_{k\sigma_k}^d \right) |0\rangle = c_{1\sigma_1}^d c_{2\sigma_2}^d \cdots c_{i\sigma_i}^d c_{i+1\sigma_{i+1}}^d \cdots c_{k\sigma_k}^d |0\rangle.$$

The generators $g_i$ ($i = 1, 2, \ldots, N - 1$) satisfy the following well-known relations
\[ g_{i+1} - g_i = g_i - g_{i+1}, \quad g_i g_j = g_j g_i \quad \text{for} \quad |i - j| \geq 2, \quad g_i^2 = 1. \quad (4) \]

Let \( Y_{m}^{(\lambda)} \) be a standard Young tableau, and \( |Y_{m}^{(\lambda)}\rangle \) the corresponding orthogonal basis vector, \( \langle Y_{m}^{(\lambda)}|Y_{m'}^{(\lambda)}\rangle = \delta_{mm'} \). Here \( \lambda = [\lambda_1, \lambda_2, \ldots, \lambda_N] \), with \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N \) and \( \sum_{i=1}^{N} \lambda_i = N \), stands for a standard Young diagram with \( N \) boxes \([9, 10] \), and \( m \) denotes a component of an irreducible representation (irrep) of \( S_{N} \) in the standard basis. Also, by construction, the \( \{|Y_{m}^{(\lambda)}\rangle\} \) form a Yamanouchi basis relative to operations on the indices \( (1, \ldots, N) \), where \( m \) can be understood either as a Yamanouchi symbol or the indice of the basis components in so-called decreasing page order of a Yamanouchi symbol \([10] \). Let \( g_i |Y_{m}^{(\lambda)}\rangle \) be the Young tableau obtained by interchanging the numbers \( i \) and \( i+1 \) in \( Y_{m}^{(\lambda)} \). It is understood that if the resultant tableau is not a standard one the corresponding basis vector \( |g_i Y_{m}^{(\lambda)}\rangle \) is set to zero. The irreducible representation of \( S_{N} \) in the standard basis, i.e. a basis adapted to the group chain \( S_{N} \supset S_{N-1} \supset \cdots \supset S_{2} \), is given by

\[ g_i |Y_{m}^{(\lambda)}\rangle = \frac{1}{d_i} |Y_{m}^{(\lambda)}\rangle + \left( \frac{(d_i + 1)(d_i - 1)}{d_i^2} \right)^{\frac{1}{2}} |g_i Y_{m}^{(\lambda)}\rangle, \quad (5) \]

where \( d_i \) is the axial distance from the box \( i \) to the box \( i+1 \) in the Young tableau \( Y_{m}^{(\lambda)} \) with movement upward and to the right being counted as positive.

It should be clear that Hamiltonian \((2)\) is diagonalizable within a given irrep \( \lambda \) of \( S_{N} \). Furthermore, it can easily be proven that Hamiltonian \((2)\) is invariant under \( U(2) \) transformations that are generated by the total spin operators \( \hat{S}_{\mu} \) \((\mu = 0, +, -)\) and the total electron number operator \( \hat{N} \) with

\[ \hat{S}_{+} = \sum_{i=1}^{N} c_{i}^{\dagger} c_{i+1}, \quad \hat{S}_{-} = \sum_{i=1}^{N} c_{i}^{\dagger} c_{i+1}, \quad \hat{S}_{0} = \frac{1}{2} \sum_{i=1}^{N} \left( c_{i+1}^{\dagger} c_{i} - c_{i+1} c_{i}^{\dagger} \right), \quad \hat{N} = \sum_{i=1}^{N} \sum_{\sigma} c_{i}^{\dagger} c_{i \sigma}. \quad (6) \]

Therefore, Hamiltonian \((2)\) should also be diagonalizable under an irrep \( \lambda \) of \( U(2) \). Due to the Schur-Weyl duality relation between the permutation group \( S_{N} \) and \( U(2) \) in this case, any irrep \( \lambda \) of \( U(2) \) with exactly \( N \) boxes is simultaneously the same irrep of \( S_{N} \). According to the Schur-Weyl duality relation, Hamiltonian \((2)\) for \( N \) electrons on an \( N \)-site lattice with total spin \( S = \frac{1}{2} (N - 2n) \) can be diagonalized in the irrep \([N-n, n]\) of \( S_{\mu} \) with basis vectors \( |Y_{m}^{(N-n,n)}\rangle; S = \frac{1}{2} (N - 2n); \) \( S_{0} = S \) which are simultaneously basis vectors of \( U(2) \). Nevertheless, there are two drawbacks in this direct diagonalization process. Firstly, there is no regularity in the structure to the energy matrix for \( n \geq 2 \) due to the nature of the matrix elements that enter in \((5)\). Therefore, one can only construct the energy matrix on a case-by-case basis for \( n \geq 2 \), which with increasing values of \( N \) and \( n \) very quickly becomes an intractable task. Secondly, the basis vectors \( |Y_{m}^{(N-n,n)}\rangle; S = \frac{1}{2} (N - 2n); \) \( S_{0} = S \) should be expanded in terms of products of single electron states, of which the expansion coefficients should be evaluated separately according to representation theory of the permutation group. Evaluation of these expansion coefficients is of the same level of complexity as diagonalization of Hamiltonian \((2)\) within basis vectors of the \([N-n, n]\) irrep of \( S_{N} \).

In the following, we will deal with this problem in an alternative way to avoid these drawbacks. It can be proven that eigenstates of \((2)\) with \( S_{0} = \frac{1}{2} (N - 2n) \) can be written as

\[ |\zeta, [N-n, n]; S = \frac{1}{2} (N - 2\nu), S_{0} = \frac{1}{2} (N - 2n)\rangle = \sum_{\omega} \alpha_{\omega}^{(\zeta)} Q_{\omega} |[n] \downarrow; (\omega_{0}^{\downarrow}) \rangle \{[N-n] \uparrow; (\omega_{0}^{\uparrow}) \}, \quad (7) \]
where \( \nu = 0, 1, 2, \ldots, n \), \((\omega_0^\nu) = (12 \cdots n)\), \((\omega_1^\nu) = (n+1 \cdots 2n)\), \(\zeta\) is an additional quantum number needed to distinguish different eigenstates with the same total spin and its third component, \(\alpha_w^{(\zeta)}\) expansion coefficients to be determined by the corresponding eigenequation \((\omega)\) is the so-called normal-ordering sequences, \((\omega) = (\omega_1, \omega_2, \ldots, \omega_n)\), and \((\omega_2) = (a_n+1, a_n+2, \ldots, a_N)\) with \(a_1 < a_2 < \cdots < a_n, a_{n+1} < a_{n+2} < \cdots < a_N\). General wavefunction with any allowed \(S_0\) value can be obtained by applying the lowering \(\hat{S}_-\) or raising \(\hat{S}_+\) operators onto (7). Equation (7) is constructed according to the Littlewood rules of the outer-product \([n!][N-n!][N-n, \nu, \nu]\) of the permutation group \(S_n \times S_{n-n} \otimes [N-n, \nu, \nu] \) as long as \(N \geq 2n\). In our construction we always choose \(n\) to satisfy condition \(N \geq 2n\). \(Q_\omega\) with \(Q_\omega(\omega^\nu) = (\omega)\) in (7) is the left coset representative in the decomposition \(S_n \times S_{n-n} \downarrow S_N, S_N = \sum_{\nu=0}^{n} Q_\omega (S_n \times S_{N-n})\). It should be noted that the number \(N(\omega)\) of the left coset representatives \(Q_\omega\) is equal to the sum of the dimensions of the irreps of \(S_N\) occurring in the outer-product, namely \(N(\omega) = \sum_{\nu=0}^{n} \dim([N-n, \nu, \nu])\) with \(\dim([N-n, \nu, \nu]) = N!(N-2n+1)/n!(N-n+1)!\). The uncoupled basis vectors on the right-hand-side of (7) can be expressed in terms of the electron creation operators as

\[
\begin{align*}
[|n\rangle \downarrow; (a_1, a_2, \ldots, a_n)] &= c_{a_1}^\dagger c_{a_2}^\dagger \cdots c_{a_n}^\dagger |0\rangle, \\
|[N-n\rangle \uparrow; (a_{n+1}, a_{n+2}, \ldots, a_N)] &= c_{a_{n+1}}^\dagger c_{a_{n+2}}^\dagger \cdots c_{a_N}^\dagger |0\rangle.
\end{align*}
\]

(8)

One also needs to first arrange the ordering of the basis vectors \(\{Q_\omega, |n\rangle \downarrow; (\omega^\nu)\}|[N-n\rangle \uparrow; (\omega^\nu)\} = \{(\omega_1, \omega_2)\}\). The ordering of the sequences \((\omega_1, \omega_2)\) is specified in the following way. The \((\omega_1)\) part of \((\omega_1, \omega_2)\) is regarded as a vector of dimension \(n\). If the last non-zero component of the vector \((\omega_1) - (\omega_2)\) is less than zero, we arrange that \((\omega_1, \omega_2)\) precede \((\omega_1', \omega_2')\). For example, if \(n = 2\) and \(N = 4\), the ordering of the basis vectors is \{([12), (34)], ([13), (24)], ([23), (14)]; ([14), (23)], ([24), (13)], ([34), (12)]\}. After diagonalizing the energy matrix \(h(N, n)\), with matrix elements given by

\[
\langle (\omega_1), (\omega_2) | \hat{H} | (\omega_1'), (\omega_2') \rangle,
\]

(9)

one simultaneously obtains eigenenergies and the corresponding expansion coefficients \(\alpha_w^{(\zeta)}\) for all irreps \([N-n, \nu, \nu]\) of \(S_N\) with \(\nu = 0, 1, 2, \ldots, n\). Direct calculation shows that the energy matrix \(h(N, n)\) has the following simple structure:

\[
h(N, n) = \begin{pmatrix}
M_0^N(n) & I_{M_0^N(n)} & \ldots & I_{M_{N-n-2}^N(n)} & I_{M_{N-n-1}^N(n)} \\
I_{M_0^N(n)} & M_1^N(n) & \ldots & I_{M_{N-n-2}^N(n)} & I_{M_{N-n-1}^N(n)} \\
I_{M_1^N(n)} & M_2^N(n) & \ldots & I_{M_{N-n-2}^N(n)} & I_{M_{N-n-1}^N(n)} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
I_{M_{N-n-2}^N(n)} & I_{M_{N-n-1}^N(n)} & \ldots & I_{M_{N-n-2}^N(n)} & I_{M_{N-n-1}^N(n)} \\
I_{M_{N-n-1}^N(n)} & I_{M_{N-n-1}^N(n)} & \ldots & I_{M_{N-n-1}^N(n)} & I_{M_{N-n-1}^N(n)} \\
\end{pmatrix}
\]

(10)

where \(M_{\mu}^N(n)\) (\(\mu = 0, 1, \ldots, N-n\)) is the energy sub-matrix formed under the subspace spanned by \{([\omega) \equiv Q_\omega[|n\rangle \downarrow; (\omega^\nu)\]|[N-n\rangle \uparrow; (\omega^\nu)\} with \((\omega) = (a_1, a_2, \ldots, a_{n-1}, n+\mu)\) and \(a_1 < a_2 < \cdot \cdot \cdot < a_{n-1}\) are different indices less than \(n+\mu\). \(I_{M_{\mu-1}^N(n)}\) is a \(\dim(M_{\mu-1}^N(n))\) \(\dim(M_{\mu}^N(n))\) matrix that is formed by adding \(\dim(M_{\mu}^N(n)) - \dim(M_{\mu-1}^N(n))\) rows with entries to the bottom of the \(\dim(M_{\mu-1}^N(n)) \times \dim(M_{\mu-1}^N(n))\) identity matrix.
\[ I_{M_{\mu-1}} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \cdots & 1 \\ 0 & \cdots & \cdots & 0 \end{pmatrix} \] (11)

Other entries not written explicitly in (10) are all zero. \( \tilde{I}_{M_{\mu}} \) in (10) is the transposition of \( I_{M_{\mu}} \). Similarly to the tridiagonal case, the energy matrix (10) is called quasi-tridiagonal. The dimension of \( M_{\mu}^N (n) \) is \((n + \mu - 1)!/\mu!(n-1)!\). It is important to note that the energy sub-matrix \( M_{\mu}^N (n) \) has the following recurring structure:

\[ M_{\mu}^N (n) = \begin{pmatrix} M_{\mu}^N (n-1) - 2 + \delta_{N \mu+n} & I_{M_{\mu}^N (n-1)} & \cdots & I_{M_{\mu}^N (n-1)} \\ I_{M_{\mu}^N (n-1)} & M_{\mu}^N (n-1) - 2 + \delta_{N \mu+n} & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ I_{M_{\mu}^N (n-1)} & \cdots & \cdots & M_{\mu}^N (n-1) - 2 + \delta_{N \mu+n} \end{pmatrix} \] (12)

for \( \mu = 0, 1, 2, \cdots, N - n \), starting with

\[ M_{\mu}^N (1) = N - 2 + \delta_{N1}, \quad M_{\mu}^N (1) = N - 3 + \delta_{N1}, \quad \cdots \]

\[ M_{N-2}^N (1) = N - 3 + \delta_{N1}, \quad M_{N-1}^N (1) = N - 2 + \delta_{N1}. \] (13)

Clearly, the energy matrix has self-similarity for different \( n \) values. Such a regular fractal structure of the energy matrix can be used to construct the energy matrix for any \( N \) and \( \mu \) values easily.

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