PERMUTATION GROUP APPROACH TO THE ONE-DIMENSIONAL XXX HEISENBERG OPEN SPIN-1/2 CHAINS

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Permutation group approach to the one-dimensional XXX Heisenberg open spin-1/2 chain with nearest neighbor interaction is proposed, which is formulated not only for half-filling excitations, but also for general case. Regularity of energy matrices and the corresponding wavefunctions are made up by using an induction method, which makes it possible to study the eigenvalue problem systematically. A Mathematica package for generating the energy matrices is implemented according to this procedure.

Keywords: Spin chain; excitation spectrum; permutation group approach.

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1. Introduction

The one-dimensional XXX Heisenberg quantum spin-1/2 chain is one of the fundamental models in physics. Solutions of this simple but important model have been studied extensively since the pioneering work of Bethe.1 Besides studies based on semiclassical treatments,2,3 a lot of work has been focused on algebraic,4–8 or analytic9,10 Bethe ansatz, and various approaches including coordinate Bethe ansatz,11 especially, the Bethe ansatz method for open spin chains.12–14 Needless to say, Bethe ansatz method is very much useful in understanding the large N limit situations, and has been developed into a powerful self-consistent method in dealing with a great number of quantum many-body problems. However, Bethe ansatz solution is a formal expression, which is not always easy and straightforward to be used due to a set of highly nonlinear equations involved. Furthermore, as noticed by Bethe himself that the Bethe ansatz solutions for the model in some cases are incomplete, in which one of the variables must be infinite.1 The incompleteness of
the Bethe ansatz solutions for the XXZ model is more complicated, and has been studied extensively by many authors.8,15–18

Therefore, in many cases numerical algorithms in diagonalizing the Hamiltonian for small number of sites are adopted for either open19,20 or closed21,22 chain cases. In fact, there is an abundance of work on numerical diagonalizations of the Heisenberg chains. References 19–22 are only a few examples. Generally, a well-known direct diagonalization procedure in the SU(2) tensor product space is adopted in these numerical diagonalization procedures, which is referred to as the M-scheme for similar problems in nuclear physics.23 In this direct diagonalization procedure, one needs to arrange ordering of the basis vectors of the SU(2) tensor product space beforehand, and then to evaluate entries of the energy matrix according to the ordering of the basis vectors. Such procedure is not difficult when the number of sites and the number of electrons are small. However, for cases with large dimension, one can only do so, case by case, since there is no systematic way in arranging the ordering of the basis vectors. Accordingly, entries of the energy matrix will also be totally different in different arrangements of the ordering of the basis vectors. With increasing dimension, one will soon find it intractable to construct the energy matrix in such direct diagonalization scheme. In addition, it is obvious that there must be a systematic way in arranging the basis vectors, and a special ordering of the basis vectors under which the structure of the energy matrix is much simpler than that in other cases. However, it is difficult to find a systematic way and such a special ordering of the basis vectors without the knowledge of permutation groups.

Actually, there is a close inter-relation between the permutation group $S_f$ and tensor product space of SU($m$), where $m = 2$, in one-dimensional XXX Heisenberg open spin-1/2 chain model, called Schur–Weyl duality relation.24–26 It is the Schur–Weyl duality relation that reveals the permutation symmetry of the model, which also makes it possible to study the problem in the permutation group space. Thus, our objectives of this paper are the following: (1) It will be shown that the ordering of the basis vectors of the model can systematically be arranged using the induction method of the permutation group. It will be shown that the procedure consistently applies to the half-filling case and the symmetric case for any configuration; (2) and most importantly, in such ordering of the tensor product basis of SU(2), there is regularity in the energy matrix, which can be easily used to construct the energy matrix for these cases in any configuration. Therefore, the permutation group approach will provide a practical and efficient way in arranging the ordering of the basis vectors in the model and systematically in constructing the energy matrix in the above mentioned cases for any configuration. The procedure will easily be programmable according to the regularity of the energy matrix, which can then be used to generate the energy matrix for any configuration. Therefore, this new approach is extremely useful for cases with large dimension, and avoids case by case construction of the energy matrix. Hence, the permutation group approach will make it possible to systematically study the model. Furthermore, the method can easily be extended to XXX SU($m$) chains with $m \geq 3$. It should be pointed
out that Refs. 19 and 20 were the first attempt to use permutation group theory to study the Heisenberg spin-1/2 open chain model though only some simple cases were studied and no systematic procedure for the construction of the energy matrix and the corresponding eigenstates were given.

In Sec. 2, we will outline a permutation group approach to the solutions of the one-dimensional XXX Heisenberg open spin-1/2 chain with nearest neighbor interaction, which provides a systematic way for arranging the ordering of the basis vectors in the corresponding SU(2) tensor product space. In Sec. 3, it will be shown that the energy matrix can be constructed easily according to the regularity of the energy matrix structure under the basis constructed by using the permutation group approach. Some examples of the solutions will be given in Sec. 4. A Mathemtica package for generating the energy matrices is given in the Appendix.

2. Permutation Group Approach

The Hamiltonian of the one-dimensional XXX Heisenberg open spin-1/2 chain with nearest neighbor interaction can be written as

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

(1)

It will be seen that the extra constant 1/4 in Eq. (1) simplifies the expression in the permutation group approach. It is well-known that Eq. (1) can be rewritten as

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

(2)

where

\[ g_i = 2 \left( \hat{s}_i \cdot \hat{s}_{i+1} + \frac{1}{4} \right), \]  

(3)

for \( i = 1, 2, \ldots, N - 1 \), are generators of the spin-component permutation group \( S_N \). Let \( c_{i \sigma}^\dagger \) be the creation operator of an electron at the \( i \)th site with the third component of spin \( \sigma \), and \( |0 \rangle \) be the vacuum state. Then

\[ c_{1 \sigma_1}^\dagger c_{2 \sigma_2}^\dagger \cdots c_{k \sigma_k}^\dagger |0 \rangle \]  

(4)

forms basis vectors of \( k \)-electron tensor product space \( V^{(1)} \otimes V^{(2)} \otimes \cdots \otimes V^{(k)} \), where each space \( V^{(i)} \) is two-dimensional. The action of \( g_i \) \( (i < k) \) on Eq. (4) is given by

\[ g_i(c_{i \sigma_1}^\dagger c_{i+1 \sigma_{i+1}}^\dagger \cdots c_{k \sigma_k}^\dagger |0 \rangle = c_{i \sigma_1}^\dagger c_{i+1 \sigma_{i+1}}^\dagger \cdots c_{k \sigma_k}^\dagger |0 \rangle. \]  

(5)

Using the above correspondence, one can establish a permutation group approach for diagonalizing the Hamiltonian Eq. (1).

The generators of \( S_N \), \( g_i \) \( (i = 1, 2, \ldots, N - 1) \) satisfy the following well-known relations

\[ g_i g_{i+1} g_i = g_{i+1} g_i g_{i+1}, \]  

(6a)
\[ g_i g_j = g_j g_i \text{ for } |i - j| \geq 2, \quad (6b) \]
\[ g_i^2 = 1. \quad (6c) \]

Irreducible representations of \( S_N \) will be briefly reviewed in the following.\(^{27,28}\)
Let \( Y^{[\lambda]}_m \) be a standard Young tableau, and \( |Y^{[\lambda]}_m\rangle \) be the orthogonal basis vector, i.e., the basis vectors \( |Y^{[\lambda]}_m\rangle \) satisfy \( \langle Y^{[\lambda]}_m | Y^{[\lambda]}_{m'} \rangle = \delta_{m m'}, \) where \( \lambda \equiv [\lambda_1, \lambda_2, \ldots, \lambda_N] \) with \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N \) and \( \sum_{i=1}^{N} \lambda_i = N, \) which stands for a standard Young diagram with \( N \) boxes. A Young tableau \( Y^{[\lambda]}_m \) is an arrangement of the numbers \( 1, 2, \ldots, N \) in a Young diagram \( [\lambda] \) in which the numbers increase as one moves to the right and one goes down, where \( m \) is the index of the Young tableau. The numbers filled in a Young diagram in this way is consistent with the branching rule occurring in the chain \( S_N \supset S_{N-1} \supset \cdots \supset S_2. \) Thus, a component of an irreducible representation (irrep) of \( S_N \) in the standard basis, or called Young–Yamanouchi basis, which is the basis adapted to the chain \( S_N \supset S_{N-1} \supset \cdots \supset S_2, \) is denoted by the Young tableau \( Y^{[\lambda]}_m \). Let \( g_i Y^{[\lambda]}_m \) be the Young tableau obtained by interchanging the numbers \( i \) and \( i + 1 \) in \( Y^{[\lambda]}_m \). It is understood that if the resultant tableau is not a standard one, the corresponding basis vector \( |g_i Y^{[\lambda]}_m\rangle \) 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
\[ g_i |Y^{[\lambda]}_m\rangle = \frac{1}{d_i} |Y^{[\lambda]}_m\rangle + \left( \frac{(d_i + 1)(d_i - 1)}{d_i^2} \right)^{1/2} |g_i Y^{[\lambda]}_m\rangle, \quad (7) \]
where \( d_i \) is axial distance from box \( i \) to box \( i + 1 \) in the Young tableau \( Y^{[\lambda]}_m \) with the upward or to the right being counted as positive.\(^{27}\) The axial distance from \( i \) to \( i + 1 \) in a Young tableau \( Y^{[\lambda]}_m \) is defined as follows: starting from the position of \( i \) in the Young tableau \( Y^{[\lambda]}_m \), we proceed by any rectangular route, one box at a time, until we reach the position of \( i + 1 \). Counting plus one for each step made upwards or to the right, and minus one for each step made downwards or to the left, the resulting number of steps made will be the axial distance from \( i \) to \( i + 1 \) in \( Y^{[\lambda]}_m \).

Because the open spin chain Hamiltonian (2) is a sum of all generators of \( S_N \), it should be diagonalizable in a given irrep \([\lambda]\) of \( S_N \). Furthermore, it can easily be proved that the total spin of the system is conserved, namely total spin operators \( \hat{S}_\mu (\mu = 0, +, -) \) with
\[ \hat{S}_+ = \sum_{i=1}^{N} c_{i}^\dagger c_{i+1}, \quad \hat{S}_- = \sum_{i=1}^{N} c_{i+1}^\dagger c_{i}, \quad \hat{S}_0 = \frac{1}{2} \sum_{i=1}^{N} (c_{i+1}^\dagger c_{i+1} - c_{i}^\dagger c_{i}), \quad (8) \]
commute with the Hamiltonian (2),
\[ [\hat{H}, \hat{S}_\mu] = 0 \text{ for } \mu = 0, +, - . \quad (9) \]
In addition, the total number of electrons
\[ \hat{k} = \sum_{i=1}^{N} \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} \quad (10) \]
is also conserved, $[\hat{k}, \hat{H}] = 0$. Therefore, the Hamiltonian (2) should be diagonalizable under an irrep $[\lambda]$ of $U(2)$, which is generated by $\{\hat{S}_+, \hat{S}_-, \hat{S}_0, \hat{k}\}$.

Let $V^{(i)} (i = 1, 2, \ldots, N)$ denote $N$ copies of irreducible representation of $U(m)$ corresponding to the fundamental weight, and let $S_N$ be the permutation group, of which an element $(i, j)$ of $S_N$ exchanges the component of $V^{(i)}$ with that of $V^{(j)}$. Then, an irreducible representation of $[\lambda]$ of $S_N$ occurs in the $N$-time outer-products $\{1\} \otimes \{1\} \otimes \cdots \otimes \{1\}$ of $S_1 \otimes S_1 \otimes \cdots \otimes S_1 \downarrow S_N$ is the same as the irrep of $U(m)$ occurs in the $N$-times tensor product $\{1\} \otimes \{1\} \otimes \cdots \otimes \{1\}$ of $U(m) \otimes U(m) \otimes \cdots \otimes U(m) \downarrow U(m)$. This is the so-called Schur–Weyl duality relation\textsuperscript{24–26} between the permutation group $S_N$ and $U(m)$. In the present case, $m = 2$. Due to the Schur–Weyl duality relation between the permutation group $S_N$ and $U(2)$, any irrep $[\lambda]$ of $U(2)$ with exactly $N$ boxes is simultaneously the same irrep of $S_N$.

It can be proved that the operations $p \in S_N$ and $q \in U(2)$ are commutative with each other, where $p \in S_N$ is any spin-component permutation defined by (5) among spin components in different spin space $V^{(i)} (i = 1, 2, \ldots, N)$, while $q \in U(2)$ is any unitary transformation of the basis vectors of $U(2)$,

$$ q \cdot (c_{1_{\sigma_1}}^L c_{2_{\sigma_2}}^L \cdots c_{N_{\sigma_N}}^L)|0\rangle = \sum_{\sigma_i^L} (q)_{\sigma_1^L \sigma_1', \sigma_2^L \sigma_2', \ldots, \sigma_N^L \sigma_N'} c_{i_{\sigma_i^L}}^L c_{i_{\sigma_i'}^L}^L \cdots c_{N_{\sigma_N}^L}^L |0\rangle. \quad (11) $$

Then,

$$ [p, q] = 0 \forall p \in S_N, \quad q \in U(2). \quad (12) $$

A complete proof of Eq. (12) can be found in Ref. 26, which manifests the Schur–Weyl duality relation. Hence, one can study the $N$-time tensor products of fundamental irrep of $U(2)$ in the corresponding $S_N$ space.

For $k$-electron excitation on a $k$-site lattice, the diagonalization of the Hamiltonian Eq. (2) can be denoted as

$$ |Y_m^{[k-n,n]}; S = 1/2(k-2n), S_0\rangle, \quad (13) $$

which is simultaneously basis vector of $S_k$ in the standard basis and that of $U(2)$ with $k$ electrons, where $S$ and $S_0$ denote quantum numbers of the total spin and its third component of the system.

For convenience, one can construct the basis vector $|Y_m^{[k-n,n]}; S = 1/2(k-2n), S_0 = S\rangle$ by using the following induction method. First, assign electrons at the first $k-n$ sites spin up, and the electrons at rest $n$ sites spin down, which can be used to construct the so-called primitive basis vector $|\{k - n\} \uparrow; (\omega_1^0) \downarrow; (\omega_2^0)\rangle$, where $(\omega_1^0) = (1, 2, \ldots, k-n)$, $(\omega_2^0) = (k - n + 1, k - n + 2, \ldots, k)$, which can easily be expressed by the electron creation operators as

$$ |\{k - n\} \uparrow; (1, 2, \ldots, n)\rangle = c_{1+}^L c_{2+}^L \cdots c_{k-n+1}^L |0\rangle, \quad (14) $$

$$ |\{k - n\} \downarrow; (k - n + 1, k - n + 2, \ldots, k)\rangle = c_{k-n+1}^L c_{k-n+2}^L \cdots c_{k}^L |0\rangle. $$
It is obvious that the basis vectors given in Eq. (14) are all symmetric with respect to any spin component permutations defined by Eq. (5). Then, one can construct the desired basis vector as

\[
\begin{align*}
Y_m^{[k-n,n]}; S &= \frac{1}{2}(k-2n), S_0 = S \\
&= \sum_{\omega} C_{\omega}^{m} Q_\omega ([k-n] \uparrow; \omega) [n] \downarrow; \omega_2) ,
\end{align*}
\]

where \((\omega)\) is the so-called normal-order sequences, \((\omega) = (\omega_1, \omega_2), (\omega_1) = (a_1, a_2, \ldots, a_{k-n}), (\omega_2) = (a_{k-n+1}, a_{k-n+2}, \ldots, a_{k})\) with \(a_1 < a_2 < \ldots < a_{k-n}\), \(a_{k-n+1} < a_{k-n+2} < \ldots < a_{k}\), \(Q_\omega\) is the left coset representative in the decomposition of \(S_k \downarrow S_{k-n} \times S_n\),

\[
S_k = \sum_{\omega} Q_\omega (S_{k-n} \times S_n)
\]

with \(Q_\omega (\omega^0) = (\omega)\), and \(C_{\omega}^{m}\) is called the \([k-n] \otimes [n] \uparrow [k-n, n]\) induction coefficient.\(^{27}\) Because the basis vector \(Y_m^{[k-n,n]}\) of \(S_k\) in Eq. (13) is induced from basis vectors of \(S_{k-n} \otimes S_n\) shown in Eq. (15), the procedure is thus called induction method.

Eigenstates of Eq. (2) can then be expressed in terms of Eq. (13) as

\[
\begin{align*}
\zeta; k, S &= \frac{1}{2}(k-2n), S_0 = S \\
&= \sum_m \alpha_m^{(\zeta)} Y_m^{[k-n,n]}; S = \frac{1}{2}(k-2n), S_0 = S ,
\end{align*}
\]

where \(\zeta\) is an additional quantum number needed in distinguishing from different eigenstates with the same total spin and its third component, \(\alpha_m^{(\zeta)}\), is the expansion coefficients to be determined by the corresponding eigenequation. Finally, the general wavefunctions with \(S \neq S_0\) can be obtained from those with \(S = S_0\) by applying \(S - S_0\) times the lowering operator \(S_-\) to Eq. (17). Thus, we have

\[
\begin{align*}
\zeta; k, S &= \frac{1}{2}(k-2n), S_0 \\
&= \left( \frac{(S + S_0)!}{(2S)! (S - S_0)!} \right)^{1/2} \left( S_- \right)^{S-S_0} \zeta; k, S = \frac{1}{2}(k-2n), S_0 = S
\end{align*}
\]

In previous discussions on the XXX spin-1/2 chain with nearest neighbor interaction, only half-filling case was studied, in which the total number of electrons is equal to the number of sites. Though the half-filling case is of importance, there are more general cases that can be studied by using the permutation group approach. Generally, for an \(N\)-site chain, there may be \(k\)-electron excitation states with \(k = 0, 1, 2, \ldots, N\). Eigenstate with \(k = 0\) trivially corresponds to the vacuum state, while \(k \neq 0\) cases are all nontrivial. Such a generalization including hopping terms related to the \(t-J\) model with supersymmetry has been intensively studied.\(^{20}\)

In these nontrivial cases, one can use creation operators of \(k \leq N\) electrons with total spin \(S = (1/2)(k - 2n)\), and \(S_0 = S\) to construct the primitive state
\[ |Y_m^{k-n, n}(\omega^0), S = (1/2)(k-2n), S_0 = S \rangle = \sum_{\alpha} \alpha_{m\omega}^{(\zeta)} Q_{\omega} Y_m^{k-n, n}(\omega^0), S = \frac{1}{2}(k-2n), S_0 = S \rangle, \] (19)

where \( Q_{\omega} \) is the left coset representative in the decomposition \( S_N \downarrow S_{N-k} \times S_k \) with \( Q_{\omega}(\omega^0) = (\omega) \), \( \alpha_{m\omega}^{(\zeta)} \) is the corresponding expansion coefficient that should be determined by the corresponding eigenequation, \( \zeta \) is an additional quantum number needed in distinguishing from different eigenstates with other quantum numbers being the same. Similar to Eq. (18), general wavefunctions with \( S \neq S_0 \) can be obtained from those given in Eq. (19) with \( S = S_0 \) by applying \( S - S_0 \) times the lowering operator \( \hat{S}_- \). The \( k = N \) case corresponds to the half-filling situation, of which some special cases were discussed in Refs. 19 and 20.

3. Structures of the Energy Matrix

3.1. Symmetric case

When \( k \)-electron states are symmetric with respect to spin component permutation, eigenstate of Eq. (2) can be written as

\[ \zeta; k, S = \frac{k}{2}, S_0 = S \rangle = \sum_{\omega} \alpha_{\omega}^{(\zeta)} Q_{\omega}[k] \uparrow; (\omega^0). \] (20)

In order to use Eq. (20) to diagonalize the Hamiltonian (2), one first needs to arrange the ordering of the basis vectors \( \{ Q_{\omega}[k] \uparrow; (\omega^0) \} \equiv \{|(\omega)\}\}. The ordering of the sequences (\( \omega \)) is specified in the following way. (\( \omega \)) is regarded as a vector of dimension \( k \). If the last nonzero component of the vector (\( \omega \)) is less than zero, we arrange that (\( \omega \)) precedes (\( \omega' \)). For example, if \( k = 2 \) and \( N = 4 \), the ordering of the basis vectors is \( \{|(12)\},|(13)\},|(23)\},|(14)\},|(24)\},|(34)\} \}. The energy matrix is the matrix of the Hamiltonian (2) under the basis vectors (\( |(\omega)\}\)), of which the elements are defined by \( \langle (\omega)|H/J|(\omega') \rangle \). Once the energy matrix is constructed, eigenvalues of excitation energy and the corresponding eigenstates can be obtained by diagonalizing the energy matrix. Matrix elements of the energy matrix can be calculated by using the following results:

\[ g_k(|(\omega)\rangle) = \begin{cases} 
|(|(\omega')\rangle) & \text{if } i \in (\omega) \text{ and } i + 1 \notin (\omega), \\
|(|(\omega'')\rangle) & \text{if } i + 1 \in (\omega) \text{ and } i \notin (\omega), \\
|(|(\omega)\rangle) & \text{if } i, i + 1 \in (\omega), \text{ or } i, i + 1 \notin (\omega),
\end{cases} \] (21)
\[ |Y_m^{[k-n,n]}(\omega^0), S = (1/2)(k-2n), S_0 = S \rangle = \sum_{m=0}^{k} \alpha_m \left. Q_\omega |Y_m^{[k-n,n]}(\omega^0), S = \frac{1}{2}(k-2n), S_0 = S \rangle \right., \]

where \( Q_\omega \) is the left coset representative in the decomposition \( S_N / S_{N-k} \times S_k \) with \( Q_\omega(\omega^0) = (\omega) \), \( \alpha_m \) is the corresponding expansion coefficient that should be determined by the corresponding eigenequation, \( \zeta \) is an additional quantum number needed in distinguishing from different eigenstates with other quantum numbers being the same. Similar to Eq. (18), general wavefunctions with \( S \neq S_0 \) can be obtained from those given in Eq. (19) with \( S = S_0 \) by applying \( S - S_0 \) times the lowering operator \( \tilde{S}_- \). k = N case corresponds to the half-filling situation, of which some special cases were discussed in Refs. 19 and 20.

3. Structures of the Energy Matrix

3.1. Symmetric case

When \( k \)-electron states are symmetric with respect to spin component permutation, eigenstate of Eq. (2) can be written as

\[ |\zeta; k, S = \frac{k}{2}, S_0 = S \rangle = \sum_{\omega} \alpha_{\omega} |Q_\omega |k\rangle |\omega^0\rangle. \]

In order to use Eq. (20) to diagonalize the Hamiltonian (2), one first needs to arrange the ordering of the basis vectors \( \{Q_\omega |k\rangle |\omega\rangle\} \). The ordering of the sequences \( (\omega) \) is specified in the following way. \( \omega \) is regarded as a vector of dimension \( k \). If the last nonzero component of the vector \( (\omega) - (\omega') \) is less than zero, we arrange that \( (\omega) \) precedes \( (\omega') \). For example, if \( k = 2 \) and \( N = 4 \), the ordering of the basis vectors is \( \{(12); (13); (23); (14); (24); (34)\} \). The energy matrix is the matrix of the Hamiltonian (2) under the basis vectors \( |(\omega)\rangle \), of which the elements are defined by \( \langle (\omega)|\tilde{H}|(\omega')\rangle \). Once the energy matrix is constructed, eigenvalues of excitation energy and the corresponding eigenstates can be obtained by diagonalizing the energy matrix. Matrix elements of the energy matrix can be calculated by using the following formula:

\[ g_{i|}(\omega) = \begin{cases} 
|\omega'\rangle & \text{if } i \in (\omega) \text{ and } i + 1 \notin (\omega), \\
|\omega''\rangle & \text{if } i + 1 \in (\omega) \text{ and } i \notin (\omega), \\
|\omega\rangle & \text{if } i, i + 1 \in (\omega), \text{ or } i, i + 1 \notin (\omega), 
\end{cases} \]
where \((\omega')\) is obtained by replacing \(i\) by \(i + 1\) in \((\omega)\), and \((\omega'')\) is obtained by replacing \(i + 1\) by \(i\) in \((\omega)\). Since the basis vectors \(\{|(\omega)\}\) is orthogonal, the energy matrix, i.e., the matrix of \(\hat{H}/J = \sum_{i=1}^{N-1} g_i\), can be derived by using the rules given in Eq. (21). Direct calculation shows that the energy matrix under the basis \(\{|(\omega)\}\) has the following simple structure:

\[
\begin{pmatrix}
M_0 & \tilde{I}_{M_0} \\
I_{M_0} & M_1 & \tilde{I}_{M_1} \\
I_{M_1} & M_2 & \tilde{I}_{M_2} & \ddots \\
I_{M_{N-1}} & \vdots & \ddots & \ddots \\
I_{M_{N-k-1}} & M_{N-1-k} & \ldots & \tilde{I}_{M_{N-k-1}} \\
I_{M_{N-k-1}} & \vdots & \ldots & M_{N-k}
\end{pmatrix},
\]

where \(M_\mu (\mu = 0, 1, \ldots, N - k)\) is the energy sub-matrix formed under the subspace spanned by \(\{|(\omega)\}\) with \((\omega) = (a_1, a_2, \ldots, a_{k-1}, k + \mu), a_1 < a_2 < \cdots < a_{k-1}\), are different indices less than \(k + \mu\). Dimension of \(M_\mu\) is given by

\[
\text{dim}(M_\mu) = \frac{(k + \mu - 1)!}{(k - 1)!\mu!}.
\]

\(I_{M_{\mu-1}}\) in Eq. (22) is a \(\text{dim}(M_{\mu-1}) \times \text{dim}(M_\mu)\) matrix, which is formed by adding \(\text{dim}(M_\mu) - \text{dim}(M_{\mu-1})\) rows with 0 entries to the bottom of \(\text{dim}(M_{\mu-1}) \times \text{dim}(M_{\mu-1})\) identity matrix,

\[
I_{M_{\mu-1}} = \begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
\vdots & \ddots & \ddots \\
0 & 1 & 0 \\
0 & \ldots & \ldots & 0 \\
\vdots \\
0 & \ldots & \ldots & \ldots & 0
\end{pmatrix}.
\]

Other entries not written explicitly in Eq. (22) are all zero. \(\tilde{I}_{M_\mu}\) in Eq. (22) is the transposition of \(I_{M_\mu}\). Similar to tridiagonal case, the energy matrix Eq. (22) is called quasi-tridiagonal. Such quasi-tridiagonal structure enables one to inductively calculate the energy matrix.

### 3.2. Nonsymmetric case

When permutations of spin components of \(k\) electrons are nonsymmetric, the sub-label \(m\) of an irrep \([k - n, n]\) of \(S_k\) appears in the summation in Eq. (19) with \(n = 1, 2, \ldots, [k/2]\), where the symbol \([x]\) denotes the integer part of \(x\). Similar to the symmetric case, we need to arrange the ordering of the basis vectors
\{ |Y_m^{[k-n,n]}(\omega); S = (1/2)(k - 2n), S_0 = S \equiv |Y_m^{[k-n,n]}(\omega)\}\). In this case, we first arrange \(\omega\) in the orders assigned previously, and then arrange the label \(m\) in the order the same as that in the representation theory \(^{20}\) of \(S_k\). For example, when \(k = 3\) and \(N = 4\) for irrep \(^{21}\) the ordering of the basis vectors is \(|Y_1^{[21]}(123)), |Y_2^{[21]}(123)), |Y_1^{[21]}(124)), |Y_2^{[21]}(124)), |Y_1^{[21]}(134)), |Y_2^{[21]}(134)), |Y_1^{[21]}(234)), |Y_2^{[21]}(234))\}. The actions of the generators \(g_i\) on the basis vector \(|Y_m^{[k-n,n]}(\omega)\) are given by

\[
g_i |Y_m^{[k-n,n]}(\omega)\rangle = \begin{cases} 
|Y_m^{[k-n,n]}(\omega')\rangle & \text{if } i \in (\omega) \text{ and } i + 1 \notin (\omega), \\
Y_m^{[k-n,n]}(\omega'') & \text{if } i + 1 \in (\omega) \text{ and } i \notin (\omega), \\
\frac{1}{d_i} |Y_m^{[k-n,n]}(\omega)\rangle + \left(\frac{(d_i + 1)(d_i - 1)}{d_i^2}\right)^{1/2} |g_i Y_m^{[k-n,n]}(\omega)\rangle & \text{if } i \text{ and } i + 1 \in (\omega), \\
|Y_m^{[k-n,n]}(\omega)\rangle & \text{if } i, i + 1 \notin (\omega), 
\end{cases}
\]

(25)

where \((\omega')\) is obtained by replacing \(i\) by \(i+1\) in \((\omega)\), and \((\omega'')\) is obtained by replacing \(i+1\) by \(i\) in \((\omega)\). In this case, the energy matrices are still quasi-tridiagonal, which can be written as

\[
(\hat{h}) = \begin{pmatrix}
M_0^{[k-n,n]} & \tilde{I}_{M_0^{[k-n,n]}} \\
I_{M_0^{[k-n,n]}} & M_1^{[k-n,n]} & \tilde{I}_{M_1^{[k-n,n]}} \\
I_{M_1^{[k-n,n]}} & M_2^{[k-n,n]} & \tilde{I}_{M_2^{[k-n,n]}} \\
& \ddots & \ddots & \ddots \\
& & I_{M_N^{[k-n,n]}} & M_N^{[k-n,n]} & \tilde{I}_{M_N^{[k-n,n]}} \\
& & I_{M_N^{[k-n,n]}} & M_{N-k}^{[k-n,n]} & \tilde{I}_{M_{N-k}^{[k-n,n]}} \\
& & I_{M_{N-k}^{[k-n,n]}} & M_{N-k-1}^{[k-n,n]} & \tilde{I}_{M_{N-k-1}^{[k-n,n]}} \\
\end{pmatrix}
\]

(26)

where \(M_\mu^{[k-n,n]} (\mu = 0, 1, \ldots, N - k)\) is the energy sub-matrix under the subspace spanned by \(|Y_m^{[k-n,n]}(\omega)\rangle\) with \((\omega) = (a_1, a_2, \ldots, a_{k-1}, k + \mu), a_1 < a_2 < \cdots < a_{k-1}\), are different indices less than \(k + \mu\). Since dimension of the irrep \([k - n, n]\) of \(S_k\) is

\[
\text{dim}([k - n, n]) = \frac{k!(k - 2n + 1)}{n!(k - n + 1)!},
\]

(27)
dimension of $M^{[k-n,n]}_{\mu}$ is given by

$$\dim(M^{[k-n,n]}_{\mu}) = \frac{k(k - 2n + 1)(k + \mu - 1)!}{n!(k - n + 1)!\mu!}.$$ (28)

Again, similar to Eq. (24), $I_{M_{\mu}^{-1}}$ in Eq. (27) is a $\dim(M^{[k-n,n]}_{\mu}) \times \dim(M^{[k-n,n]}_{\mu})$ matrix, which is formed by adding $\dim(M^{[k-n,n]}_{\mu}) - \dim(M^{[k-n,n]}_{\mu})$ rows with 0 entries to the bottom of the $\dim(M^{[k-n,n]}_{\mu}) \times \dim(M^{[k-n,n]}_{\mu})$ identity matrix.

Denote the energy matrix for $N$-site case as $(\hat{h})_N$ given by Eq. (22) or Eq. (26), then the energy matrix for $(N+1)$-site can be written as

$$(\hat{h})_{N+1} = \begin{pmatrix} (\hat{h})_{N \rightarrow N+1} & I_{M_{N-k}} \\ I_{M_{N-k}} & M^{[k-n,n]}_{N-k+1} \end{pmatrix},$$ (29)

where $(\hat{h})_{N \rightarrow N+1}$ means the expression of $(\hat{h})_N$ given by Eq. (22) or Eq. (26) with the replacement of $N$ in Eq. (22) or Eq. (26) by $N+1$.

### 3.3. The half-filling case

As has been mentioned in the previous section, the half-filling case with $N$ electrons on an $N$-site lattice can be diagonalized directly within a given irrep $[N-n,n]$ of $S_N$ with eigenstates given by Eq. (17), where the basis vectors of $S_N$ in the expansion of Eq. (17) should be constructed by induction method shown by Eq. (15). The advantage of this direct diagonalization within a given irrep $[N-n,n]$ of $S_N$ is that the dimension of a given irrep $[N-n,n]$ of $S_N$ is relatively small. Once the energy matrix is calculated according to Eq. (7), eigenvalues and the corresponding eigenstates can be obtained by directly diagonalizing the energy matrix. Nevertheless, there are two drawbacks in this direct diagonalization process. Firstly, there is no regularity in structure of the energy matrix for $n \geq 2$ due to matrix entries of $g_i$ given in Eq. (7) involved. Therefore, one can only construct the energy matrix case by case for $n \geq 2$, which will soon become an intractable task with increasing of $N$ and $n$. The same situation also occurs in the construction of energy sub-matrix $M^{[k-n,n]}_{\mu}$ for $k$ electrons on an $N$-site lattice for nonsymmetric case shown in Eq. (25), because the third case of the matrix entry of $g_i$ given in Eq. (25) is the same as that given in Eq. (7). Because the action of the generator $g_i$ will mix the basis vector $|Y^{[A]}_m\rangle$ with $|g_iY^{[A]}_m\rangle$, the energy matrix in such cases will become irregular, i.e., one cannot find a way to set the entries of the energy matrix as a function of $N$ and $n$. Therefore, one can only use this procedure to construct the energy matrix for specific $N$ and $n$ values at a time. But the dimension of the nonsymmetric case is always relatively smaller. Secondly, in order to obtain the eigenstates in this direct diagonalization process, the basis vectors of an irrep $[N-n,n]$ of $S_N$ should then be constructed by using the induction method shown in Eq. (15), in which the induction coefficients should be determined according to the representation theory of permutation groups separately. The evaluation of
the induction coefficients appearing in Eq. (15) is of the same complexity as the diagonalization of Eq. (2) under the basis vectors shown in Eq. (17).

As has been stated previously, our objective is to find a systematic way to construct the energy matrix. Unlike other direct diagonalization scheme, in which the energy matrix is constructed for specific number of sites and electrons, our procedure should work for any number of sites and electrons, i.e., the procedure will be used to generate the energy matrix for any configuration, and not just for a specific case. Therefore, we will deal with this problem alternatively.

By combining Eqs. (15) and (17), eigenstates of Eq. (2) for the half-filling case can be written as

\[
\left| \zeta, [N - \nu, \nu]; S = \frac{1}{2}(N - 2\nu), S_0 = \frac{1}{2}(N - 2n) \right> = \sum_{\omega} \alpha_{\omega}^{(\zeta),[N - \nu, \nu]} Q_\omega [n] \downarrow; (\omega_1^0)] [N - n] \uparrow; (\omega_2^0)),
\]

(30)

where \(\nu = 0, 1, 2, \ldots, n\). Equation (30) is constructed according to the Littlewood rules of the outer-product \([n] \times [N - n] \downarrow [N - \nu, \nu]\) of the permutation group \(S_n \times S_{N-n}\),

\[
[n] \otimes [N - n] = \sum_{\nu=0}^{n} \oplus [N - \nu, \nu]
\]

(31)
as long as \(N \geq 2n\). In our construction, we always choose \(n\) to keep the condition \(N \geq 2n\) being satisfied. \(Q_\omega\) in Eq. (30) is the left coset representative in the decomposition \(S_n \times S_{N-n} \downarrow S_N\),

\[
S_N = \sum_{\omega} Q_\omega (S_n \times S_{N-n}).
\]

(32)

It should be noted that the number of the left coset representatives \(Q_\omega, N(\omega)\), is equal to the sum of dimensions of the irreps of \(S_N\) occurring in the outer-product Eq. (31), namely

\[
N(\omega) = \sum_{\nu=0}^{n} \dim([N - \nu, \nu]).
\]

(33)

Therefore, after diagonalizing the energy matrix, of which matrix elements are given by \(\langle\omega_1, (\omega_2) | h | \omega_1', (\omega_2')\rangle\), where \(\langle\omega_1, (\omega_2) \equiv Q_\omega [n] \downarrow; (\omega_1^0)][N - n] \uparrow; (\omega_2^0)\rangle\), one simultaneously obtains eigenenergies and the corresponding eigenstates for all irreps \([N - \nu, \nu]\) of \(S_N\) with \(\nu = 0, 1, 2, \ldots, n\). Though it is not easy to distinguish these eigenvalues from different irreps of \(S_N\), one can obtain results of different irreps inductively. More precisely, if one wants to calculate eigenenergies and the eigenstates for irrep \([N - n, n]\), one can first diagonalize the energy matrix \(h(n-1)\) under the basis vectors \([n - 1] \downarrow; (\omega_1)][N - n + 1] \uparrow; (\omega_2)\rangle\); then diagonalize the energy matrix \(h(n)\) under the basis vectors \([n] \downarrow; (\omega_1)][N - n] \uparrow; (\omega_2)\rangle\). There must be \(N!(N - 2n + 1)/n!(N - n + 1)\) more new eigenvalues of \(h(n)\) that \(h(n-1)\) does
not provide. These new eigenvalues and the corresponding eigenstates belong to the irrep \([N - n, n]\). In this case, though dimension of the energy matrix increases rapidly with the increasing of \(n\), it avoids evaluation of the induction coefficients involved in Eq. (17). More importantly, the energy matrix in this new scheme can easily be constructed inductively. Furthermore, similar to \(k\)-electron on an \(N\)-site lattice case with spin-component permutation symmetric, the energy matrix is also quasi-tridiagonal with structure precisely the same as that given by Eq. (22) if \([k]\) is replaced by \([n]\) in Eq. (20) in the construction of Eq. (22). Hence, we get the following theorem.

**Theorem.** Eigenenergies for the half-filling case with \(N\) electrons on an \(N\)-site lattice for all irreps \([N - \nu, \nu]\) of \(S_N\) and total spin \(S = (1/2)(N - 2\nu)\) with \(\nu = 0, 1, 2, \ldots, n\), are the same as those for \(n\) electrons on the \(N\)-site lattice with irrep \([n]\) of \(S_n\) and total spin \(S = n/2\).

Therefore, diagonalizing Eq. (22) provides eigenenergies and the corresponding expansion coefficients in eigenstates for both the half-filling and the symmetric cases. Similar to Eq. (18), general wavefunction with any allowed \(S_0\) value can be obtained by applying the lowering \(\hat{S}_-\) or raising \(\hat{S}_+\) operators onto Eq. (30).

**3.4. The energy matrices for both half-filling and symmetric cases**

Since the half-filling case is of importance, and the energy matrices for both the half-filling and the symmetric cases are the same, in this subsection, energy matrices for both cases will be presented.

For \(n\) electrons on an \(N\)-site lattice with irrep \([n]\) or the half-filling case with irreps \([N - \nu, \nu]\) \((\nu = 0, 1, 2, \ldots, n\)) denote the energy matrix explicitly as \((\hat{h})_N(n)\), which is given by

\[
(\hat{h})_N(n) = \\
\begin{pmatrix}
M_0^N(n) & \tilde{I}_M^N(n) \\
I_{M_0^N(n)} & M_1^N(n) & \tilde{I}_M^N(n) \\
I_{M_1^N(n)} & M_2^N(n) & \tilde{I}_M^N(n) \\
\vdots & \ddots & \ddots \\
I_{M_{N-n-2}^N(n)} & M_{N-n-1}^N(n) & \tilde{I}_{M_{N-n-1}^N(n)} \\
I_{M_{N-n-1}^N(n)} & M_{N-n}^N(n) & \tilde{I}_{M_{N-n}^N(n)}
\end{pmatrix}
\]

(34)

where \(M_\mu^N(n) \ (\mu = 0, 1, \ldots, N - n)\) is the energy sub-matrix formed under the subspace spanned by \(\{|(\omega)\} \equiv Q_\omega[n] \uparrow; (\omega^0)\}\) given in Eq. (20) for the symmetric.
case or by \( \{(\omega) = Q, [n] \uparrow; (\omega^0) \} \) \([N-n] \uparrow; (\omega^0)\) given in Eq. (30) for the half-filling case with \((\omega) = (a_1, a_2, \ldots, a_{n-1}, n + \mu), a_1 < a_2 < \cdots < a_{n-1},\) are different indices less than \(n + \mu, I_{M^N_{\mu-1}(n)}\) is a \(\dim(M^N_{\mu-1}(n)) \times \dim(M^N_{\mu}(n))\) matrix, which is formed by adding \(\dim(M^N_{\mu-1}(n)) - \dim(M^N_{\mu-1}(n))\) rows with 0 entries to the bottom of the \(\dim(M_{\mu-1}) \times \dim(M_{\mu-1})\) identity matrix shown by Eq. (24), and \(I_{M^N_{\mu}(n)}\) is the transposition of \(I_{M^N_{\mu}(n)}\). The dimension of \(M^N_{\mu}(n)\) is
\[
\dim(M^N_{\mu}(n)) = \frac{(n + \mu - 1)!}{\mu!(n - 1)!}. \tag{35}
\]
Noteworthily, the energy sub-matrix \(M^N_{\mu}(n)\) has the following recurrence structure:
\[
\begin{pmatrix}
M^N_0(n) = 1 & I_{M^N_0(n-1)} & I_{M^N_1(n-1)} & \cdots & I_{M^N_{N-1}(n-1)} \\
I_{M^N_0(n-1)} & M^N_1(n-1) - 2 + \delta_{N,n+1} & M^N_2(n-1) - 2 + \delta_{N,n+1} & \cdots & I_{M^N_{N-2}(n-1)} \\
I_{M^N_1(n-1)} & M^N_2(n-1) - 2 + \delta_{N,n+1} & M^N_3(n-1) - 2 + \delta_{N,n+1} & \cdots & I_{M^N_{N-3}(n-1)} \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
I_{M^N_{N-2}(n-1)} & I_{M^N_{N-3}(n-1)} & I_{M^N_{N-4}(n-1)} & \cdots & M^N_{N-1}(n-1) + \delta_{N,n+1}
\end{pmatrix}
\tag{36}
\]
for \(\mu = 0, 1, 2, \ldots, N - n\), starting with
\[
M^N_0(1) = N - 2 + \delta_{N,1}, \quad M^N_1(1) = N - 3 + \delta_{N,1}, \ldots,
\tag{37}
\]
\[
M^N_{N-2}(1) = N - 3 + \delta_{N,1}, \quad M^N_{N-1}(1) = N - 2 + \delta_{N,1}.
\]
Clearly, the energy matrix has a self-similarity. Such recurring structure of the energy matrix can easily be implemented in a computer code to construct the energy matrix not only for specific \(N\) and \(n\), but also for any \(N\) and \(n\) values, which, however, is impossible in other diagonalization scheme without taking the permutation group structure into account.

4. Some Examples

In this section, some examples of the energy matrices for both the half-filling and the symmetric cases will be presented. Energy eigenvalues and the corresponding set of expansion coefficients for eigenstates can be calculated by using any diagonalization algorithm.

4.1. \(n = 1\) case

This case corresponds to both one electron on an \(N\)-site lattice with spin \(1/2\) and half-filling case for irrep \([N]\) with total spin \((1/2)N\) and \([N - 1, 1]\) with total spin
The energy matrix is simply in tridiagonal form with

\[
\langle \hat{h} \rangle_N(1) = \begin{pmatrix}
N - 2 & 1 \\
1 & N - 3 & 1 \\
& 1 & N - 3 & 1 \\
& & \ddots & \ddots \\
& & & 1 & N - 3 & 1 \\
& & & & 1 & N - 2
\end{pmatrix}
\] (38)

for \( N > 2 \). Eigenenergies can be written as

\[
\frac{E^{(\zeta)}}{J} = N - 3 + 2 \cos \frac{\zeta \pi}{N}
\] (39)

with \( \zeta = 0, 1, 2 \ldots, N - 1 \). The corresponding eigenstates for one electron excitation are

\[
\left| \zeta; k = 1, S = \frac{1}{2}, S_0 = \frac{1}{2} \right\rangle = \sum_\omega \alpha^{(\zeta)}_\omega Q_\omega \left| S = (N - 2) \uparrow; 1 \uparrow \right\rangle,
\] (40a)

while the corresponding eigenstates for \([N - \nu, \nu]\) irreps with \( \nu = 0, 1 \) are

\[
\left| \zeta, [N - \nu, \nu]; S = \frac{1}{2}(N - 2 \nu), S_0 = \frac{1}{2}(N - 2) \right\rangle = \sum_\omega \alpha^{(\zeta), [N - \nu, \nu]}_\omega Q_\omega \left| [1 \uparrow; 1 \downarrow; (N - 1) \uparrow \downarrow; (2 \ldots N) \right\rangle,
\] (40b)

where \( \zeta = 0 \) for \( \nu = 0 \) and \( \zeta \neq 0 \) for \( \nu = 1 \). Up to a normalization constant, the expansion coefficients \( \alpha^{(\zeta)}_\omega \) for both \( \nu = 0 \) and 1 cases can be expressed as

\[
\alpha^{(\zeta)}_\mu = (-)^{\mu - 1} + 2 \sum_{\tau=0}^{\mu-1} (-)^\tau \cos \left( \frac{\mu - 1 - \tau}{N} \right) \zeta \pi 
\] for \( N - 1 \geq \mu \geq 1 \),

\[
\alpha^{(\zeta)}_N = \begin{cases} 
1 & \text{when } \zeta = \frac{N}{3}, \\
\frac{1}{2 \cos \left( \frac{\zeta \pi}{N} \right) - 1} \alpha^{(\zeta)}_{N-1} & \text{for other cases}.
\end{cases}
\] (41)

Therefore, \( n = 1 \) case is solved analytically. The excitation energies and a recurring relation for the expansion coefficients shown in Eq. (41) were also given in Ref. 19.

4.2. \( n \geq 2 \) case

When \( n \geq 2 \), one cannot solve the corresponding eigenvalue problem analytically. However, a simple Mathematica package has been compiled by using its Matrix Manipulation package according to the permutation group approach. By using the built-in functions, such as AppendColumns[], AppendRows[], ZeroMatrix[], IdentityMatrix[], etc., a simple routine for generating the energy matrix for both the half-filling and symmetric cases can be realized according to the results given
in Eqs. (34)–(37). This Mathematica package is given in the Appendix. With this simple package, one only needs to input the number of sites \( N \) and an integer \( n \). The output will be the corresponding energy matrix. While, as far as we know, other direct diagonalization procedures reported up to now have been designed only for specific \( N \) and \( n \) values, and one needs to compile a new code for other \( N \) and \( n \) values in order to generate the corresponding energy matrix.

In the following, we present an example of the energy matrix for \( n = 2 \) to show its structure. Suppose that there are \( N = 6 \) sites, the energy matrix for \( n = 2 \) can be written as

\[
(\hat{h})_6(2) = \begin{pmatrix}
M_0^6(2) & I_{M_0^6(2)} \\
I_{M_0^6(2)} & M_1^6(2) & I_{M_1^6(2)} \\
I_{M_1^6(2)} & M_2^6(2) & I_{M_2^6(2)} \\
I_{M_2^6(2)} & M_3^6(2) & I_{M_3^6(2)} \\
I_{M_3^6(2)} & M_4^6(2) & I_{M_4^6(2)}
\end{pmatrix},
\]

where, according to Eqs. (36) and (37),

\[
M_0^6(2) = M_0^6(1) = 4, \quad M_1^6(2) = \begin{pmatrix} M_0^6(1) - 2 & 1 \\ 1 & M_1^6(1) \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix},
\]

\[
M_2^6(2) = \begin{pmatrix} M_0^6(1) - 2 & 1 & 0 \\ 1 & M_1^6(1) - 2 & 1 \\ 0 & 1 & M_2^6(1) \end{pmatrix} = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 3 \end{pmatrix},
\]

\[
M_3^6(2) = \begin{pmatrix} M_0^6(1) - 2 & 1 & 0 & 0 \\ 1 & M_1^6(1) - 2 & 1 & 0 \\ 0 & 1 & M_2^6(1) - 2 & 1 \\ 0 & 0 & 1 & M_3^6(1) \end{pmatrix} = \begin{pmatrix} 2 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 3 \end{pmatrix},
\]

\[
M_4^6(2) = \begin{pmatrix} M_0^6(1) - 2 & 1 & 0 & 0 & 0 \\ 1 & M_1^6(1) - 2 & 1 & 0 & 0 \\ 0 & 1 & M_2^6(1) - 2 & 1 & 0 \\ 0 & 0 & 1 & M_3^6(1) - 2 & 1 \\ 0 & 0 & 0 & 1 & M_4^6(1) \end{pmatrix}
\]

\[
= \begin{pmatrix} 2 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 3 \end{pmatrix}.
\]
Therefore,

\[
I_{M_0^g(2)} = 1, \quad I_{M_1^g(2)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad I_{M_2^g(2)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix},
\]

\[
I_{M_3^g(2)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}.
\]

(43b)

Such energy matrices can easily be generated by our simple Mathematica package. The output of the Mathematica package for generating the energy matrix for any configuration can then be used as input of any code for diagonalizing the energy matrix numerically, which provides an easy routine for generating the energy matrix for any \( N \) and \( n \) values.

5. Conclusions

In this paper, permutation group approach to one-dimensional XXX Heisenberg open spin-1/2 chain with nearest neighbor interaction is proposed. The method can be used to generate the energy matrix of the problem with any number of sites and configuration for both the half-filling and symmetric cases. In the permutation group approach, the recurring structure of the energy matrices appears in the construction, which enables one to construct the energy matrix systematically. A simple Mathematica package is designed according to this approach, which can be used to generate the energy matrix for any \( N \) and \( n \) values easily. It is found that the energy matrix for the half-filling case with \( N \) electrons on an \( N \)-site lattice for all irreps \([N - \nu, \nu]\) of \( S_N \) and total spin \( S = (1/2)(N - 2\nu) \) with \( \nu = 0, 1, 2, \ldots, n \), are the same as that for \( n \) electrons on the \( N \)-site lattice with irrep \([n]\) of \( S_n \) and the total spin \( S = n/2 \). The \( n = 1 \) case is solved analytically. Though analytical solutions for \( n \geq 2 \) are still inaccessible, one can use this new approach to obtain the energy matrix with a simple Mathematica package. The output can then be used as input for any diagonalization program, which makes it possible to get solutions for any configuration without approximation. The results can thus be used to verify solutions obtained by other methods.

It is still not possible to generate the energy matrix of the model systematically for the nonsymmetric cases. Therefore, one can only construct the energy matrix for specific values of \( N \) and \( n \) in those cases. The model with infinite sites and translational symmetry also remains to be studied by using the permutation group approach.
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Appendix

The Mathematica package for generating the energy matrices for any number of electrons on any number of sites according to the permutation group approach.

<< LinearAlgebra'MatrixManipulation'

(** Define M[0, t], M[1, t], M[2, t] Matrices p = N is the number of sites, t = \[mu] in the text**) p = 8 (** input the number of sites **) M[2, 0] = \{\{p - 2+ KroneckerDelta[p, 2]\}\}; b[1] = p - 4+ KroneckerDelta[p, 3]; b[2] = p - 3+ KroneckerDelta[p, 3]; a[1] = 1; c[1] = 1; M[2, 1] = Table[Switch[i - j, -1, a[i], 0, b[i], 1, c[i - 1], 0, \{i, 2\}, \{i, 2\}, \{i, 2\}]; For[k = 1, k \leq p - 2, \{Do[a[[i]] = 1, \{i, k + 1\}], Do[b[2] = p - 5+ KroneckerDelta[p, k + 2], \{i, 2, k\}], b[1] = p - 4+ KroneckerDelta[p, k + 2], b[k + 1] = p - 3+ KroneckerDelta[p, k + 2], M[2, k] = Table[Switch[i - j, -1, a[i], 0, b[i], 1, c[i - 1], 0, \{i, k + 1\}, \{i, k + 1\}, \{i, k + 1\}], h[2, k] = AppendColumns[AppendRows[h[2, k - 1], Transpose[AppendRows[ZeroMatrix[k + 1, (k + 1)/2], AppendColumns[IdentityMatrix[k], ZeroMatrix[1, k]]]]], AppendRows[AppendRows[ZeroMatrix[k + 1, (k + 1)/2], AppendColumns[IdentityMatrix[k], ZeroMatrix[1, k]]], M[2, k]]], k++]; (**Define M[n, 1] matrix**) M[1, 0] = p - 2+ KroneckerDelta[p, 1]; M[1, p - 1] = M[1, 0]; Do[M[1, j] = p - 3+ KroneckerDelta[p, 1], \{j, 1, p - 2\}]; Do[M[n, 1] = M[n - 1, 0] + KroneckerDelta[p, n], \{n, 2, p\}]; Dim[n_, j_] := (n + j - 1)!(j!(n - 1)!) For[n = 2, n \leq p - 3, \{ A1 = AppendColumns[IdentityMatrix[1], ZeroMatrix[Dim[n - 1, 1] - Dim[n - 1, 0], 1]], A2 = AppendRows[\{\{M[n - 1, 0] - 2+ KroneckerDelta[p, n + 1]\}\}, Transpose[A1]] A3 = AppendRows[A1, M[n - 1, 1] + KroneckerDelta[p, n + 1]], M[n, 1] = AppendColumns[A2, A3]], n++]; (*Define M[n, t] matrix *) s = IntegerPart[p/2];
Do[{Do[d1 = TakeMatrix[M[n, t - 2], {1, 1}, {Dim[n, t - 3], Dim[n, t - 3]}],
    d2 = M[n - 1, t - 2] - 2 IdentityMatrix[Dim[n - 1, t - 2]],
    P1 = AppendColumns[IdentityMatrix[Dim[n - 1, t - 3]],
    ZeroMatrix[Dim[n - 1, t - 2] - Dim[n - 1, t - 3], Dim[n - 1, t - 3]],
    P2 = AppendRows[ZeroMatrix[Dim[n - 1, t - 2]],
    Dim[n, t - 3] - Dim[n - 1, t - 3]], P1],
    g1 = AppendRows[d1, Transpose[P2]], g2 = AppendRows[P2, d2],
    MM[n, t - 2] = AppendColumns[g1, g2].
If[t <= 2, a1 = M[n, t - 2] - (2 - KroneckerDelta[p, n + t]) IdentityMatrix[Dim[n, t - 2]],
    a1 = MM[n, t - 2] + KroneckerDelta[p, n + t] IdentityMatrix[Dim[n, t - 2]],
    a2 = M[n - 1, t - 1] - (2 - KroneckerDelta[p, n + t]) IdentityMatrix[Dim[n - 1, t - 1]],
    a3 = M[n - 1, t] + KroneckerDelta[p, n + t] IdentityMatrix[Dim[n - 1, t]],
    I0 = AppendColumns[IdentityMatrix[Dim[n - 1, t - 2]],
    ZeroMatrix[Dim[n - 1, t - 1] - Dim[n - 1, t - 2], Dim[n - 1, t - 1]],
    I1 = AppendRows[ZeroMatrix[Dim[n - 1, t - 1], Dim[n, t - 2] - Dim[n - 1, t - 2]], I0],
    a0 = ZeroMatrix[Dim[n - 1, t], Dimensions[I1][[2]],
    I2 = AppendColumns[IdentityMatrix[Dim[n - 1, t - 1]], ZeroMatrix[Dim[n - 1, t] - Dim[n - 1, t - 1]],
    Dim[n - 1, t - 1]], b1 = AppendRows[a1, Transpose[I1]], b2 = AppendRows[I1, a2],
    h3 = AppendRows[AppendRows[a0, I2], a3],
    h2 = AppendRows[b2, Transpose[I2]], h1 = AppendRows[b1, Transpose[a0]],
    M[n, t] = AppendColumns[AppendColumns[h1, h2], h3], {t, 2, p - n}], {n, 3, s}];

(**Generating energy matricies hh[n,p-n] which is h[n] in the text, where n is
the number of electrons**)  
Do[{a[i] = 1, {i, 1, p}}; Do[c[i] = 1, {i, 1, p}]; Do[b[i] = p - 3, {i, 2, p - 1}];
    b[1] = p - 2; b[p] = p - 2;
    hh[1, p - 1] = Table[Switch[i - j, -1, a[i], 0, b[i], 1, c[i - 1], -1, 0], {i, p}, {j, p}];
    Do[{hh[n, 0] = M[n, 0]}],
    Do[{L1 = AppendColumns[IdentityMatrix[Dim[n, k - 1]],
    ZeroMatrix[Dim[n, k] - Dim[n, k - 1], Dim[n, k - 1]],
    L2 = AppendRows[ZeroMatrix[Dim[n, k], Dimensions[hh[n, k - 1]][[1]] -
    Dimensions[L1][[2]], L1],
    hh1 = AppendRows[hh[n, k - 1], Transpose[L2]], hh2 = AppendRows[L2, M[n, k]],
    hh[n, k] = AppendColumns[hh1, hh2], {k, 1, p - n}], {n, 2, s}];

References
15. R. Siddharthan, cond-mat/9804210.