Symmetry Considerations in the Exact Diagonalization of Heisenberg Spin Chains

^{1*}Ehika S., ¹Ataman O. J. and ²Idiodi J.O.A.

¹Department of physics, Ambrose Alli University, Ekpoma, Edo State, Nigeria. ²Department of Physics, University of Benin, Benin City, Nigeria.

Abstract

This paper presents a more practical approach, with no reference to group theory terminology on the use of symmetries in the exact diagonalization of Heisenberg spin systems. From the knowledge of these symmetries, a simplified version of the Heisenberg model is obtained. This simplification helps to solve the problem of applying the Heisenberg model to all the basis states in a finite system. Here, one dimensional lattices are considered.

1.0 Introduction

The size of Hilbert space of many body systems is known to increase exponentially with system size. With current memory limitations of present day computers, it becomes difficult to carry out full exact diagonalization of finite size clusters. Theorists are therefore confronted with the formidable task of developing mathematical tools or techniques that can drastically reduce the size of the Hilbert space. Several methods like Lanczos technique, quantum Monte Carlo numerical simulations, variational approach, perturbation etc have been developed over the past years to tackle this problem [1-4]. These methods are still confronted with the problems of diagonalizing large matrices, slow convergence to the ground state and sign problems. More so, for these aforementioned methods to be effective in solving quantum many body problems, they must first utilize the symmetry properties of the systems.

Symmetry can be understood as similarity, correspondence, or balance among systems or parts of a system. Symmetry generally conveys two primary meanings. The first is an imprecise sense of harmonious or aesthetically pleasing proportionality and balance such that it reflects beauty or perfection [5, 6, 7]. The second meaning is a precise and welldefined concept of balance or "patterned self-similarity". In physics, symmetry is conceived as an aspect of a physical system that remains unchanged under certain transformations according to a particular observation. The symmetry properties of a physical system are intimately related to the conservation laws characterizing that system. Noether theorem gives a precise description of this relation [8]. The theorem states that each continuous symmetry of a physical system implies that some physical property of that system is conserved. Conversely, each conserved quantity has a corresponding symmetry. For example, the isometry of space gives rise to conservation of linear momentum, and <u>isometry</u> of time gives rise to conservation of energy [9-13]. The aim of the current presentation is to utilize the symmetries of Heisenberg systems in reducing the size of its Hilbert space. This was demonstrated on four, six and eight Heisenberg spin chains using conserved eventum number. S^{z}

quantum number S_{tot}^{z} , spin inversion and translational symmetries.

The paper is structured as follows. In Sec. 2, we present the Heisenberg Hamiltonian. Sec. 3 presents the various symmetries and conservation laws for quantum spin systems. Application of these symmetries to some finite systems is examined in Sec. 4. Discussion of results is presented in Sec. 5. Sec. 6 concludes the presentation.

2.0 The Isotropic Heisenberg Spin Hamiltonian

The Heisenberg Hamiltonian is a quantum mechanical analogue of the Ising model [14]. This model is a variant of the Hubbard model at half filling and large onsite Coulomb repulsion U, which enforces the constraint of singly occupied site. The model, describing the pairwise interactions between localized spins, is one of the most fundamental models of

^{*}Corresponding author: Ehika S., E-mail: -, Tel. +234 8074478911

Journal of the Nigerian Association of Mathematical Physics Volume 22 (November, 2012), 9 – 20

Symmetry Considerations in the Exact Diagonalization... *Ehika, Ataman and Idiodi J of NAMP* correlated quantum matter. In spite of its simple mathematical form, it has an unimaginable richness, arising from dimensionality and geometrical constraints, competing exchange interaction, the type of spin degrees of freedom, and additional interactions with external magnetic fields or other degrees of freedom such as phonons. This model simply reads

$$H = J \sum_{i} \left[S_{i}^{z} S_{i+1}^{z} + \frac{1}{2} \left(S_{i}^{+} S_{i+1}^{-} + S_{i}^{-} S_{i+1}^{+} \right) \right], \tag{1}$$

where J is the superexchange coupling parameter between spins on site i and j which decays rapidly with the distance between these sites. S_i^Z and S_i^x are the spin operator in the z- and x- direction. The spin raising (S_i^+) and lowering (S_i^-) operators help to preserve the antiferromagnetic ground state. These operators act in the reduced Hilbert space of no doubly occupied sites. There are various version of the Heisenberg Hamiltonian, but this presentation shall be concerned with the study of isotropic Heisenberg model. In the isotropic case, the coupling constant J is taken to be the same in all directions.

3.0 Symmetries and Conservation Laws for Quantum Spin Systems

For electronic one-band models, the size of the S^z –bases set grows exponentially with the system size. For the Heisenberg model for example, the size of the Hilbert space is 2^N which gives approximately 10^6 states for N=20. Such memory requirements are beyond the reach of the present day computers. In practice, this problem can be considerably alleviated by the use of symmetries of the Hamiltonian or the geometry of the system that reduces the matrix to a block-diagonal form. The following symmetries will be employed for the exact diagonalization of Heisenberg spin chains.

I. Conservation Of Quantum Numbers

- NUMBER OF PARTICLES: This is the most obvious symmetry in quantum many body systems in which the number of particles in a system is usually conserved at least for a fermionic problem.
- TOTAL PROJECTION OF SPIN (S_{tot}^z) : This is the simplest example of magnetization (m_z) conservation. The magnetization of a given state is given by

$$m_z = \sum_{i=1}^N S_i^z \tag{2}$$

This conservation of total S^z makes it possible to work within a given S^z sector. It gives rise to a blockdiagonalized matrix, with each block corresponding to a given m_z . The number of states in the largest block ($m_z = 0$) for the Heisenberg model is given by

$$N_{s} = \frac{N!}{\left[\left(N/2\right)!\right]^{2}} \tag{3}$$

• TOTAL MOMENTUM (K): The total momentum K of the system is also conserved. This symmetry, as illustrated in Fig.1 can be used to further split the blocks, introducing a reduction of ~ 1/N in the number of states. Here, momentum states are constructed using translational invariance of the system under study.



Fig.1. Reduction of system size by S_{tot}^z and k. (a) Unblocked Hamiltonian matrix. (b) Blocked matrix after application of S_{tot}^z . (c) Further splitting of blocks after application of total momentum K.

II. Translational Symmetries

These spatial symmetries are represented by transformations of the form $\vec{r} \rightarrow \vec{r} + \vec{a}$ and describe those situations where a property of the system does not change with a continuous change in location. Translational symmetries are *Journal of the Nigerian Association of Mathematical Physics Volume* 22 (November, 2012), 9 – 20

found in translational invariant systems. Translational invariance exits in systems with periodic boundary conditions, for example a 4-site chain with periodic boundary conditions. The eigenstates of translational invariant systems are eigenstates of the translational operator T, i.e.

$$T|\psi\rangle = e^{-iK}|\psi\rangle,\tag{4}$$

where the momentum quantum number K is given by

$$K = \frac{2\pi m}{N}, \ m = 0, 1, \cdots, N - 1$$
 (5)

N is the number of lattice sites and *m* is an integer number labelling the quantization state. This gives us a recipe to construct translationally invariant basis states which have momentum *K* as a good quantum number. For a Hamiltonian *H* and a spin basis state $|S_1^z, S_2^z, \dots, S_N^z\rangle$, the operator *T* has the following properties:

$$T \left| S_1^z, S_2^z, \cdots, S_N^z \right\rangle = \left| S_N^z, S_1^z, \cdots, S_{N-1}^z \right\rangle$$
(6)
$$\begin{bmatrix} T & H \end{bmatrix} \quad 0 \quad (7)$$

$$[T,H] = 0 \tag{7}$$

Eq. (7) implies that T commutes with H, giving rise to momentum blocks of H. A momentum state can therefore be constructed from any representative state by using the eigenstates of T with given K. This momentum state is given by

$$\left|a(K)\right\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-iKr} T^r \left|a\right\rangle,\tag{8}$$

where $|a\rangle = |S_1^z, S_2^z, \dots, S_N^z\rangle$ is the representative of a given class and N_a is the number of basis states in a given class. The factor $1/\sqrt{N_a}$ ensures that a given class is normalized. If $|a\rangle$ and $|b\rangle$ are representative of two classes, then

$$T^{r}|a\rangle \neq |b\rangle \quad r \in \{1,...,N-1\}$$
(9)

In general, the total weight of the basis states produced by a translation operator T^r is given by

$$1 + e^{-iKr} + e^{-i2Kr} + \dots + e^{-iK(N-r)}$$
(10)

This weight will vanish unless $Kr = N2\pi$. The total weight of a given class is then N_a/r . Normalization of state $|a(K)\rangle$ with periodicity R_a gives

$$\langle a(k) | a(k) \rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \longrightarrow N_a = \frac{N^2}{R_a}$$
 (11)

The basic construction is to find all allowed representatives $(a_1, a_2, ..., a_M)$ and their periodicities $(R_1, R_2, ..., R_M)$. The block size M is initially not known, but is approximately 1/N of fixed m_z block. It also depends on the periodicity constraint for a given K.

III. Spin- Inversion Symmetry

These are represented by transformations of the form $\vec{r} \rightarrow -\vec{r}$ and indicate an invariance property of a system when the coordinates are 'inverted'. The spin inversion operator Z on a basis state is defined as

$$Z \left| S_1^z, S_2^z, \cdots, S_N^z \right\rangle = \left| -S_1^z, -S_2^z, \cdots, -S_N^z \right\rangle$$
(13)

In the magnetization block $m_z = 0$, the eigenstates of the operator Z can be used. An eigenstate of Z can be defined as

$$\left|a^{\sigma}(k,p,z)\right\rangle = \frac{1}{\sqrt{N_{a}^{\sigma}}} \sum_{r=0}^{N-1} C_{k}^{\sigma}(r)(1+pP)(1+zZ)T^{r} \left|a\right\rangle.$$
(14)

$$Z \left| a^{\sigma}(k, p, z) \right\rangle = z \left| a^{\sigma}(k, p, z) \right\rangle, \quad z = \pm 1$$
(15)

In the block $m_z = 0$, both reflection and spin inversion symmetry have the same effect.

Symmetry Considerations in the Exact Diagonalization... *Ehika, Ataman and Idiodi J of NAMP* 4.0 Application of Symmetries to Finite Heisenberg Chains

In this section, the various symmetries of the Heisenberg chains will be combined simultaneously to bring about a drastic reduction in the size of the Hilbert space.

I. Four-Site Heisenberg Chain

A four sites Heisenberg chain cluster is shown below. Periodic boundary conditions (PBC) is imposed on the spins system so that $S_{N+1}^z = S_1^z$. Thus, the topology of the spin space is that of a circle as shown in Fig. 2.



Fig. 2. A four-site Heisenberg chain. The topology of this system with periodic boundary conditions is that of a circle.

The Hilbert space of this system is of size $2^4=16$. Application of the Quantum number S_{tot}^z to the above system will generate five subspaces characterized by the quantum numbers: $S_{tot}^z = +2$, $S_{tot}^z = -2$, $S_{tot}^z = +1$, $S_{tot}^z = -1$ and $S_{tot}^z = 0$. The Hamiltonian is therefore block-diagonal with respect to the quantum numbers S_{tot}^z . Since emphasis is on the ground state properties of the system, calculations will be restricted to the subspace of $S_{tot}^z = 0$ which contains the ground state energy and wave function. The number of states N_s in this subspace is given by

$$N_s = \frac{N!}{\left[\left(N/2 \right)! \right]^2} = \frac{4!}{\left(2! \right)^2} = 6$$
(16)

The basis states in this subspace of $S_{tot}^{z} = 0$ are shown below.

$$|1\rangle = |1100\rangle , |2\rangle = |0110\rangle , |3\rangle = |0011\rangle , |4\rangle = |1001\rangle , |5\rangle = |1010\rangle , |6\rangle = |0101\rangle ,$$

where 1 denotes an up spin and 0 denotes a down spin. The Hamiltonian of this system is given by

$$H = \frac{J}{2} \left(S_1^+ S_2^- + S_1^- S_2^+ + S_2^+ S_3^- + S_2^- S_3^+ + S_3^+ S_4^- + S_3^- S_4^+ + S_4^+ S_1^- + S_1^- S_4^+ \right)$$

$$-J \left(S_1^z S_2^z + S_2^z S_3^z + S_3^z S_4^z + S_4^z S_1^z \right)$$
(17)
Exists in order to correction the beauty of summatry, it will be worthwhile to attempt a direction of summatry.

First, in order to appreciate the beauty of symmetry, it will be worthwhile to attempt a direct analytical diagonalization of the above Hamiltonian in the subspace of $S_{tot}^z = 0$ without making use of symmetries or conservation laws. The action of H on each of the basis states gives the following results

$$\begin{aligned} H|1\rangle &= H|1100\rangle = \frac{J}{2}|1010\rangle + \frac{J}{2}|0101\rangle = \frac{J}{2}|5\rangle + \frac{J}{2}|6\rangle \\ H|2\rangle &= H|0110\rangle = \frac{J}{2}|1010\rangle + \frac{J}{2}|0101\rangle == \frac{J}{2}|5\rangle + \frac{J}{2}|6\rangle \\ H|3\rangle &= H|0011\rangle = \frac{J}{2}|1010\rangle + \frac{J}{2}|0101\rangle == \frac{J}{2}|5\rangle + \frac{J}{2}|6\rangle \\ H|4\rangle &= H|0110\rangle = \frac{J}{2}|1010\rangle + \frac{J}{2}|0101\rangle == \frac{J}{2}|5\rangle + \frac{J}{2}|6\rangle \\ H|5\rangle &= H|1010\rangle = -J|1010\rangle + \frac{J}{2}|1100\rangle + \frac{J}{2}|0110\rangle + \frac{J}{2}|0011\rangle + \frac{J}{2}|1001\rangle \end{aligned}$$

Symmetry Considerations in the Exact Diagonalization... *Ehika, Ataman and Idiodi J of NAMP*

$$\therefore H|5\rangle = -J|5\rangle + \frac{J}{2}|1\rangle + \frac{J}{2}|2\rangle + \frac{J}{2}|3\rangle + \frac{J}{2}|4\rangle$$

$$H|6\rangle = H|0101\rangle = -J|0101\rangle + \frac{J}{2}|1100\rangle + \frac{J}{2}|0110\rangle + \frac{J}{2}|0011\rangle + \frac{J}{2}|1001\rangle$$

$$\therefore H|6\rangle = -J|6\rangle + \frac{J}{2}|1\rangle + \frac{J}{2}|2\rangle + \frac{J}{2}|3\rangle + \frac{J}{2}|4\rangle$$

The resulting Hamiltonian matrix from these operations is shown below

$$H = \begin{bmatrix} 0 & 0 & 0 & 0 & J/2 & J/2 \\ 0 & 0 & 0 & 0 & J/2 & J/2 \\ 0 & 0 & 0 & 0 & J/2 & J/2 \\ 0 & 0 & 0 & 0 & J/2 & J/2 \\ J/2 & J/2 & J/2 & J/2 & -J & 0 \\ J/2 & J/2 & J/2 & J/2 & 0 & -J \end{bmatrix}$$
(18)

The eigenvalues of this matrix are:

 $\lambda_1 = 0, \ \lambda_2 = 0, \ \lambda_3 = 0, \ \lambda_4 = -2J, \ \lambda_5 = -J, \ \lambda_6 = J,$

where $\lambda_4 = -2J$ is the ground state energy.

The size of the above matrix can further be reduced either by using translational or spin inversion symmetry. First, the translational symmetry is considered. Now, the periodicity of the system implies that the eigenstates of this cluster are eigenstates of the translational operator T, define by

$$T^{r} |\psi\rangle = \exp(i\vec{k}\cdot\vec{r})|\psi\rangle \tag{19}$$

This provides a recipe to construct translational invariant basis states with an additional fixed quantum $K = 2\pi n/N$, where n=0, 1, 2 ...N. The class of a given K generated by the action of the operator T on a given representative of a class is given by

$$\left|\psi_{k}\right\rangle = \frac{1}{\sqrt{N_{a}}} \sum_{r=0}^{N-1} e^{-iKr} T^{r} \left|\psi_{0}\right\rangle,\tag{20}$$

where N is the number of sites, N_a is the number of basis states or periodicity in the class $|\psi_K\rangle$, and $|\psi_0\rangle$ is the representative of that class. Working in the subspaces of K = 0, $K = \pi$, and $K = \pi/2$ as provided by n = 0, n = 1 and n = 2 respectively, the following reductions are obtained.

$$\begin{split} \left|\psi_{k=0}\right\rangle' &= \frac{1}{\sqrt{4}} \sum_{r=0}^{3} e^{-i \ 0 \ r} T^{r} \left|1100\right\rangle = \frac{1}{2} \left[\left|1100\right\rangle + \left|0110\right\rangle + \left|0011\right\rangle + \left|1001\right\rangle\right] \\ \left|\psi_{k=0}\right\rangle'' &= \frac{1}{\sqrt{2}} \sum_{r=0}^{3} e^{-i \ 0 \ r} T^{r} \left|1010\right\rangle = \frac{1}{\sqrt{2}} \left[\left|1010\right\rangle + \left|0101\right\rangle\right] \\ \left|\psi_{k=\pi}\right\rangle' &= \frac{1}{\sqrt{4}} \sum_{r=0}^{3} e^{-i \ \pi \ r} T^{r} \left|1100\right\rangle = \frac{1}{2} \left[\left|1100\right\rangle - \left|0110\right\rangle + \left|0011\right\rangle - \left|1001\right\rangle\right] \\ \left|\psi_{k=\pi}\right\rangle'' &= \frac{1}{\sqrt{2}} \sum_{r=0}^{3} e^{-i \ \pi \ r} T^{r} \left|1010\right\rangle = \frac{1}{\sqrt{2}} \left[\left|1010\right\rangle - \left|0101\right\rangle\right] \\ \left|\psi_{k=\pi/2}\right\rangle'' &= \frac{1}{\sqrt{4}} \sum_{r=0}^{3} e^{\frac{i \ \pi \ r}{2}} T^{r} \left|1100\right\rangle = \frac{1}{2} \left[\left|1100\right\rangle - i\left|0110\right\rangle - \left|0011\right\rangle - i\left|1001\right\rangle\right] \\ \left|\psi_{k=\pi/2}\right\rangle'' &= \frac{1}{\sqrt{4}} \sum_{r=0}^{3} e^{\frac{i \ \pi \ r}{2}} T^{r} \left|1100\right\rangle = \frac{1}{2} \left[\left|1100\right\rangle - i\left|0110\right\rangle - \left|0011\right\rangle + i\left|1001\right\rangle\right] \end{split}$$

.,

The action of H on each of these classes gives

$$H|\psi_{k=0}\rangle'' = J\sqrt{2}|\psi_{k=0}\rangle''$$

$$H|\psi_{k=0}\rangle'' = J\sqrt{2}|\psi_{k=0}\rangle' - J|\psi_{k=0}\rangle''$$

$$H|\psi_{k=\pi}\rangle'' = 0$$

$$H|\psi_{k=\pi}\rangle'' = -J|\psi_{k=\pi}\rangle''$$

$$H|\psi_{k=\pi/2}\rangle' = 0$$

$$H|\psi_{k=\pi/2}\rangle'' = 0$$

This gives rise to a block-diagonalized matrix in the subspaces of K = 0, $K = \pi$, and $K = \pi/2$ as shown in Eqs. (21), (22) and (23) respectively.

$$H_{K=0} = \begin{bmatrix} 0 & J\sqrt{2} \\ J\sqrt{2} & -J \end{bmatrix}$$
(21)

with eigenvalues -2J and J

$$H_{K=\pi} = \begin{bmatrix} 0 & 0\\ 0 & -J \end{bmatrix}$$
(22)

with eigenvalues 0 and -J

$$H_{K=\pi/2} = \begin{bmatrix} 0 & 0\\ 0 & 0 \end{bmatrix}$$
(23)

with eigenvalues 0.

Application of the spin inversion symmetry discuss in the section 3(III) gives the following reduction

$$\frac{1}{2} \left[|0011\rangle \pm |1100\rangle \right]$$

$$|\phi_2\rangle = \frac{1}{2} \left[|0101\rangle \pm |1010\rangle \right]$$

$$|\phi_2\rangle = \frac{1}{2} \left[|0110\rangle \pm |1001\rangle \right]$$
and state is contained in the '+' block. Thus,

The Hamiltonian for the ground state is contained in the '+' block. Thus,

$$H_{+} = \begin{bmatrix} 0 & J & 0 \\ J & -J & J \\ 0 & J & 0 \end{bmatrix}$$
(24)

with eigenvalues -2J, 0 and J. The four sites system also possesses reflection symmetry whose effect is the same with that of inversion symmetry in this subspace. In subsequent chains, the combined effect of these operators will be utilized in reducing the size of the system.

II. Six- Site Heisenberg Chain

The Hilbert space of this system is of size 2^6 =64. Application of the Quantum number S_{tot}^z to the above system will generate seven subspaces according to the quantum numbers:

$$S_{tot}^{z} = +3, \ S_{tot}^{z} = -3, \ S_{tot}^{z} = +2, \ S_{tot}^{z} = -2, \ S_{tot}^{z} = +1, \ S_{tot}^{z} = -1, \ S_{tot}^{z} = 0$$

The Hamiltonian is therefore block-diagonal with respect to the quantum numbers S_{tot}^z . For the subspace of $S_{tot}^z = 0$, which contains the ground state, the number of states N_s is given by

$$N_s = \frac{N!}{\left[\left(N/2 \right)! \right]^2} = \frac{6!}{\left(3! \right)^2} = 20$$
⁽²⁵⁾

The basis states in this subspace of the Hilbert space are

$$|1\rangle = ||000111\rangle, |2\rangle = ||100011\rangle, |3\rangle = ||110001\rangle, |4\rangle = ||111000\rangle, |5\rangle = ||011100\rangle$$
$$|6\rangle = ||001110\rangle, |7\rangle = ||001011\rangle, |8\rangle = ||100101\rangle, |9\rangle = ||110010\rangle, |10\rangle = ||011001\rangle$$
$$|11\rangle = ||101100\rangle, |12\rangle = ||010110\rangle, |13\rangle = ||100110\rangle, |14\rangle = ||010011\rangle, |15\rangle = ||101001\rangle$$
$$|16\rangle = ||110100\rangle, |17\rangle = ||011010\rangle, |18\rangle = ||001101\rangle, |19\rangle = ||101010\rangle, |20\rangle = ||010101\rangle$$

Since the system is translationally invariant, it is possible to construct translationally invariant basis states with fixed quantum number K. By making use of the translational operator discussed in section 3(II) in momentum space of K=0 in conjunction with spin inversion symmetry, the following reductions are obtained.

$$\begin{split} \left|\phi_{0}\right\rangle &= \frac{1}{\sqrt{6}} \left[\left|1\right\rangle + \left|2\right\rangle + \left|3\right\rangle + \left|4\right\rangle + \left|5\right\rangle + \left|6\right\rangle\right] \\ \left|\phi_{1}\right\rangle &= \frac{1}{\sqrt{12}} \left[\left|7\right\rangle + \left|8\right\rangle + \left|9\right\rangle + \left|10\right\rangle + \left|11\right\rangle + \left|12\right\rangle + \left|13\right\rangle + \left|14\right\rangle + \left|15\right\rangle + \left|16\right\rangle + \left|17\right\rangle + \left|18\right\rangle\right] \\ \left|\phi_{3}\right\rangle &= \frac{1}{\sqrt{2}} \left[\left|19\right\rangle + \left|20\right\rangle\right] \end{split}$$

The Hamiltonian of this system is given by

$$H = \frac{J}{2} \Big[S_1^+ S_2^- + S_1^- S_2^+ + S_2^+ S_3^- + S_2^- S_3^+ + S_3^+ S_4^- + S_3^- S_4^+ + S_4^+ S_5^- + S_4^- S_5^+ + S_5^+ S_6^- \Big] + \frac{J}{2} \Big[S_5^- S_6^+ + S_6^+ S_1^- + S_6^- S_1^+ \Big] + J \Big[S_1^Z S_2^Z + S_2^Z S_3^Z + S_3^Z S_4^Z + S_4^Z S_5^Z + S_5^Z S_6^Z + S_6^Z S_1^Z \Big]$$
(26)

On account of these symmetry operations, the action of the spin flip term of the Heisenberg Hamiltonian on any of the classes can be written as

$$H_{f}\left|\phi_{i}\right\rangle = \frac{J}{2}\sum_{j}\chi_{\phi_{j}}\left|\phi_{j}\right\rangle,\tag{27}$$

where χ_{ϕ_j} is the numerical electronic weight of $|\phi_j\rangle$ which arises from the action of the spin fluctuation term in the Heisenberg Hamiltonian. This factor is given by

$$\chi_{\phi_{j}} = \frac{K_{\phi_{j}} N_{\phi_{i}} n_{\phi_{j}}}{K_{\phi_{i}} N_{\phi_{j}}} , \qquad (28)$$

where N_{ϕ_i} is the number of basis states contain in the class $|\phi_i\rangle$ that has been acted on by H_f ; N_{ϕ_j} is the number of basis states in the new class $|\phi_j\rangle$; n_{ϕ_j} is the number of basis states in $|\phi_j\rangle$ generated when H_f acts on any member of $|\phi_i\rangle$; K_{ϕ_i} is the normalization factor of class $|\phi_i\rangle$, and K_{ϕ_j} is the normalization factor of $|\phi_j\rangle$. The results obtained for these parameters for six-site chain are tabulated in Table 1.

Table 1. Calculation of numerical weight χ_{ϕ_j} for six-site chain. $|R_0\rangle$, $|R_1\rangle$ and $|R_0\rangle$ are the representatives of $|\phi_0\rangle$, $|\phi_1\rangle$ and $|\phi_2\rangle$ respectively, $H_F|R_0\rangle$, $H_F|R_1\rangle$ and $H_F|R_2\rangle$ are the actions of the spin flipping term on the representatives.

Class
$$|\phi_0\rangle$$
 $|\phi_1\rangle$ $|\phi_2\rangle$ N_{ϕ_1} 6122 K_{ϕ_1} $\sqrt{6}$ $\sqrt{12}$ $\sqrt{2}$ $H_F|R_0\rangle$ $n_{\phi_0} = 0$ $n_{\phi_1} = 2$ $n_{\phi_2} = 0$ $H_F|R_1\rangle$ $n_{\phi_0} = 1$ $n_{\phi_1} = 2$ $n_{\phi_2} = 1$ $H_F|R_2\rangle$ $n_{\phi_0} = 0$ $n_{\phi_1} = 6$ $n_{\phi_2} = 0$

The action of H on the representative of a given class is shown below

$$H|1\rangle = H|000111\rangle = \frac{J}{2} [|001011\rangle + |100110\rangle + |000111\rangle]$$

From this operation, we have the following

 $|R_{o}\rangle = |000111\rangle$, $N_{\phi_{0}} = 6$, $N_{\phi_{1}} = 12$, $n_{\phi_{1}} = 2$, $K_{\phi_{0}} = \sqrt{6}$ and $K_{\phi_{1}} = \sqrt{12}$, where $|R_{o}\rangle$ is the representative of $|\phi_{o}\rangle$, $N_{\phi_{0}}$ is the number of basis states in $|\phi_{o}\rangle$, $N_{\phi_{1}}$ is the number of basis states in the new class $|\phi_{1}\rangle$ generated when H_{f} acts on any $|R_{0}\rangle$, $n_{\phi_{1}}$ is the number of basis states emanating from $|\phi_{1}\rangle$ in the single operation $H|R_{0}\rangle$, $K_{\phi_{0}}$ is the normalization constant for $|\phi_{o}\rangle$ and $K_{\phi_{1}}$ is the normalization constant for $|\phi_{1}\rangle$. Substituting these values into Eq. (28) gives

$$\chi_{\phi_1} = rac{K_{\phi_1} N_{\phi_0} n_{\phi_1}}{K_{\phi_0} N_{\phi_1}} = rac{\sqrt{12} \times 6 \times 2}{\sqrt{6} \times 12} = \sqrt{2}$$

Therefore, on account of Eq. (27), the action of H on $\left| \phi_{0} \right\rangle$ gives

$$H\big|\phi_0\big\rangle = \frac{J}{2}\big|\phi_0\big\rangle + \frac{J\sqrt{2}}{2}\big|\phi_1\big\rangle,$$

where the electronic weight of $|\phi_0\rangle$ is obtained from the diagonal spin interaction part of H. Similarly, the action of H on the representative of $|\phi_1\rangle$ gives

$$H|7\rangle = H|R_1\rangle = H|001011\rangle = \frac{J}{2} \left[|101010\rangle + |010011\rangle + |000111\rangle + |001101\rangle - |001011\rangle \right]$$

Here, we have three new basis states namely one for $|\phi_0\rangle$, two for $|\phi_1\rangle$ and one for $|\phi_2\rangle$. Using the information provided in the Table 2 above, the values of χ_{ϕ_0} , χ_{ϕ_1} and χ_{ϕ_2} are calculated below

$$\chi_{\phi_0} = \frac{K_{\phi_0} N_{\phi_1} \times n_{\phi_0}}{K_{\phi_1} N_{\phi_0}} = \frac{\sqrt{6} \times 12 \times 1}{\sqrt{12} \times 6} = \sqrt{2}$$

$$\chi_{\phi_{1}} = \frac{K_{\phi_{1}}N_{\phi_{1}} \times n_{\phi_{1}}}{K_{\phi_{1}}N_{\phi_{1}}} = \frac{\sqrt{12} \times 12 \times 2}{\sqrt{12} \times 12} = 2$$
$$\chi_{\phi_{2}} = \frac{K_{\phi_{2}}N_{\phi_{1}} \times n_{\phi_{2}}}{K_{\phi_{1}}N_{\phi_{2}}} = \frac{\sqrt{2} \times 12 \times 1}{\sqrt{12} \times 2} = \frac{6}{\sqrt{6}}$$

Therefore, the action of H on $\left|\phi_{0}\right\rangle$ gives

$$H|\phi_1\rangle = \frac{J\sqrt{2}}{2}|\phi_0\rangle + \frac{J}{2}|\phi_1\rangle + \frac{3J}{\sqrt{6}}|\phi_2\rangle$$

Finally, the action of H on the representative of $\left| \phi_{2} \right\rangle$ gives

 $H|19\rangle = H|101010\rangle = \frac{J}{2} \left[|011010\rangle + |110010\rangle + |100110\rangle + |101100\rangle - |101001\rangle + |001011\rangle - 3|101010\rangle \right]$ This gives six

new basis states belonging to $|\phi_1\rangle$. Using the information provided in Table 1 above, the value of χ_{ϕ_1} is calculated below

$$\chi_{\phi_1} = \frac{K_{\phi_1} N_{\phi_2} \times n_{\phi_1}}{K_{\phi_2} N_{\phi_1}} = \frac{\sqrt{12 \times 2 \times 6}}{\sqrt{2} \times 12} = \frac{6}{\sqrt{6}}$$

Therefore, the action of H on $|\phi_2\rangle$ gives

$$H|\phi_2\rangle = \frac{3J}{\sqrt{6}}|\phi_1\rangle - \frac{3J}{2}|\phi_2\rangle.$$

Hence, in the reduced basis $|\phi_0\rangle$, $|\phi_1\rangle$ and $|\phi_2\rangle$ a 3X3 Hamiltonian matrix is obtained as given by Eq. (29)

$$H = \begin{bmatrix} J/2 & J/\sqrt{2} & 0\\ J/\sqrt{2} & J/2 & 3J/\sqrt{6}\\ 0 & 3J/\sqrt{6} & -3J/2 \end{bmatrix}$$
(29)

This matrix can easily be diagonalized. The ground state energy is given by

$$E_g = \frac{1}{2} \left[-2J - J\sqrt{5} \right]$$

III. Eight- Site Heisenberg Chain

The Hilbert space of this system is of size $2^8=256$. Application of the quantum number S_{tot}^z to the above system will generate nine subspaces according to the quantum numbers: $S_{tot}^z = +4$, $S_{tot}^z = -4$, $S_{tot}^z = +3$, $S_{tot}^z = +2$, $S_{tot}^z = +1$, $S_{tot}^z = -3$, $S_{tot}^z = -2$, $S_{tot}^z = -1$ and $S_{tot}^z = 0$. The Hamiltonian is therefore block-diagonalized with respect to the quantum number S_{tot}^{z} . For the subspace of $S_{tot}^{z} = 0$, which contains the ground state wavefunction and energy, the number of states N_s is given by

$$N_s = \frac{N!}{\left[(N/2)! \right]^2} = \frac{8!}{(4!)^2} = 70$$
(30)

The basis states in this subspace of the Hilbert space are shown below.

$$\begin{aligned} |1\rangle &= |00001111\rangle, \ |2\rangle = ||10000111\rangle, \ |3\rangle = ||11000011\rangle, \ |4\rangle = ||11100001\rangle \\ |5\rangle &= ||11110000\rangle, \ |6\rangle = ||01111000\rangle, \ |7\rangle = ||00111100\rangle, \ |8\rangle = ||00011110\rangle \\ |9\rangle &= ||00010111\rangle, \ |10\rangle = ||10001011\rangle, \ |11\rangle = ||11000101\rangle, \ |12\rangle = ||11100010\rangle \end{aligned}$$

By making use of the translational and inversion symmetries in momentum space of K=0, the following reductions are obtained.

$$\begin{split} \left| \phi_{0} \right\rangle &= \frac{1}{\sqrt{8}} \left[\left| 1 \right\rangle + \left| 2 \right\rangle + \left| 3 \right\rangle + \left| 4 \right\rangle + \left| 5 \right\rangle + \left| 6 \right\rangle + \left| 7 \right\rangle + \left| 8 \right\rangle \right] \\ \left| \phi_{1} \right\rangle &= \frac{1}{4} \left[\left| 9 \right\rangle + \left| 10 \right\rangle + \left| 11 \right\rangle + \left| 12 \right\rangle + \left| 13 \right\rangle + \left| 14 \right\rangle + \left| 15 \right\rangle + \left| 16 \right\rangle \\ &+ \left| 17 \right\rangle + \left| 18 \right\rangle + \left| 19 \right\rangle + \left| 20 \right\rangle + \left| 21 \right\rangle + \left| 22 \right\rangle + \left| 23 \right\rangle + \left| 24 \right\rangle \right] \\ \left| \phi_{2} \right\rangle &= \frac{1}{4} \left[\left| 25 \right\rangle + \left| 26 \right\rangle + \left| 27 \right\rangle + \left| 28 \right\rangle + \left| 29 \right\rangle + \left| 30 \right\rangle + \left| 31 \right\rangle + \left| 32 \right\rangle \\ &+ \left| 33 \right\rangle + \left| 34 \right\rangle + \left| 35 \right\rangle + \left| 36 \right\rangle + \left| 37 \right\rangle + \left| 38 \right\rangle + \left| 39 \right\rangle + \left| 40 \right\rangle \right] \\ \left| \phi_{3} \right\rangle &= \frac{1}{\sqrt{8}} \left[\left| 41 \right\rangle + \left| 42 \right\rangle + \left| 43 \right\rangle + \left| 44 \right\rangle + \left| 45 \right\rangle + \left| 46 \right\rangle + \left| 47 \right\rangle + \left| 48 \right\rangle \right] \\ \left| \phi_{4} \right\rangle &= \frac{1}{4} \left[\left| 49 \right\rangle + \left| 50 \right\rangle + \left| 51 \right\rangle + \left| 52 \right\rangle + \left| 53 \right\rangle + \left| 54 \right\rangle + \left| 55 \right\rangle + \left| 56 \right\rangle \\ &+ \left| 57 \right\rangle + \left| 58 \right\rangle + \left| 59 \right\rangle + \left| 60 \right\rangle + \left| 61 \right\rangle + \left| 62 \right\rangle + \left| 63 \right\rangle + \left| 64 \right\rangle \right] \\ &= \frac{1}{9} \left[\left| 65 \right\rangle + \left| 66 \right\rangle + \left| 67 \right\rangle + \left| 68 \right\rangle \right] \\ &= \left| \phi_{6} \right\rangle &= \frac{1}{\sqrt{2}} \left[\left| 69 \right\rangle + \left| 70 \right\rangle \right] \end{split}$$

The Hamiltonian of this system is given by

$$\frac{J}{2} \Big[S_1^+ S_2^- + S_1^- S_2^+ + S_2^+ S_3^- + S_2^- S_3^+ + S_3^+ S_4^- + S_3^- S_4^+ + S_4^+ S_5^- + S_4^- S_5^+ + S_5^+ S_6^- \Big]
+ \frac{J}{2} \Big[S_5^- S_6^+ + S_6^+ S_7^- + S_6^- S_7^+ + S_7^+ S_8^- + S_7^- S_8^+ + S_8^+ S_1^- + S_8^- S_1^+ \Big]
+ J \Big[S_1^z S_2^z + S_2^z S_3^z + S_3^z S_4^z + S_4^z S_5^z + S_5^z S_6^z + S_6^z S_7^z + S_7^z S_8^z + S_8^z S_1^z \Big]$$
(31)

Table 2 provides the information for the determination of the numerical electronic weight of $|\phi_i\rangle$ (see Eq.27).

Table 2. Calculation of numerical weight χ_{ϕ_j} for eight- site chain. $|R_0\rangle$, $|R_1\rangle$,..., $|R_6\rangle$ are the representatives of $|\phi_0\rangle$, $|\phi_1\rangle$..., $|\phi_6\rangle$ respectively. $H_F|R_0\rangle$, $H_F|R_1\rangle$,..., $H_F|R_6\rangle$ are the actions of the spin flipping term on the representatives *Journal of the Nigerian Association of Mathematical Physics Volume* 22 (November, 2012), 9 – 20

Using the

information provided in the Table 2 for Eq. (28), the action of H on the various gives

$$H|\phi_{0}\rangle = J|\phi_{0}\rangle + \frac{J}{\sqrt{2}}|\phi_{1}\rangle$$

$$H|\phi_{1}\rangle = \frac{J}{\sqrt{2}}|\phi_{0}\rangle + J|\phi_{2}\rangle + \frac{J}{\sqrt{2}}|\phi_{3}\rangle$$

$$H|\phi_{2}\rangle = J|\phi_{1}\rangle + J|\phi_{4}\rangle$$

$$H|\phi_{3}\rangle = \frac{J}{\sqrt{2}}|\phi_{1}\rangle - J|\phi_{3}\rangle + J\sqrt{2}|\phi_{4}\rangle$$

$$H|\phi_{4}\rangle = J|\phi_{2}\rangle + J\sqrt{2}|\phi_{3}\rangle - J|\phi_{4}\rangle + J|\phi_{5}\rangle + J\sqrt{2}|\phi_{6}\rangle$$

$$H|\phi_{5}\rangle = J|\phi_{4}\rangle$$

$$H|\phi_{6}\rangle = J\sqrt{2}|\phi_{4}\rangle - 2J|\phi_{6}\rangle$$

The Hamiltonian matrix arising from these operations is given by

$$H = \begin{bmatrix} J & \frac{J}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\ \frac{J}{\sqrt{2}} & 0 & J & \frac{J}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & J & 0 & 0 & J & 0 & 0 \\ 0 & \frac{J}{\sqrt{2}} & 0 & -J & J\sqrt{2} & 0 & 0 \\ 0 & 0 & J & \frac{J}{\sqrt{2}} & -J & J & J\sqrt{2} \\ 0 & 0 & 0 & 0 & J & 0 & 0 \\ 0 & 0 & 0 & 0 & J\sqrt{2} & 0 & -2J \end{bmatrix}$$
(32)

This matrix can easily be diagonalized numerically. For example, the ground state energy at J=1 is -3.65109.

Symmetry Considerations in the Exact Diagonalization... *Ehika, Ataman and Idiodi J of NAMP* 5.0 Discussion Of Results

In this work, finite even chains up to eight sites were considered. For the four sites chain, the initial system size of 16 was blocked-diagonalized according to the subspaces of conserved S_{tot}^z of the system. For this system, the subspace of

 $S_{tot}^z = 0$ which contains the ground state energy of the system was reduced from size six to two by employing the translational symmetry of the system. Finally, six- and eight-site chains were reduced from initial system size of 64 and 256 to 20 and 70 respectively by using conservation of the quantum number S_{tot}^z . It was later reduced from 20 to 3 and from 70 to 7 by utilizing the translational and spin inversion symmetries of the system. On account of these symmetries, a simplified version of the Heisenberg model is obtained.

Conclusion

This paper has demonstrated how symmetries arising from the interaction topology or due to the structure and representation of the system and control Hamiltonian can be effectively utilized in reducing the size of the Hilbert space. Rather than applying these symmetries separately, it was shown in this work that the various symmetries of a system can be exploited at the same time to bring about a drastic reduction in the size of the Hilbert space. The four sites chain was reduced

from system size of 16 to 2, by concentrating only on the subspace of $S_{tot}^z = 0$ and utilizing the translational symmetry of the system. Finally, six and eight sites chain were reduced from initial system size of 64 and 256 to 3 and 7 respectively by exploiting the translational and spin inversion symmetry and the same time. On account of these symmetries, a simplified version of the Heisenberg model is obtained. This simplification makes it easier to apply the Heisenberg Hamiltonian to the

basis states of a finite system. The study in this work was restricted to the subspace of $S_{tot}^z = 0$, since the focus is on the

ground state properties of the system. This work though on small finite clusters has indeed elucidated the procedures that should be taken when performing large matrix numerical diagonalization. The reduction of the matrix into block-diagonal has the additional advantage that the particular eigenstates that emerge from the diagonalization are already partially characterized with respect to the quantum numbers that have been used to build up the Hamiltonian Sub-matrix.

The use of symmetries in exact diagonalization can be discussed using the

language of group theory. This formalism is often confusing and is not necessary. In this current work, a more practical approach is taken, with no reference to group theory terminology. Group theory is actually very useful when dealing with complex lattices, but the power of its formalism can perhaps be better appreciated after a thorough understanding of symmetry operations and block-diagonalization has been gained through less formal methods for simple lattices.

References

- Dagotto E., Joynt R. and Moreo A. (1990). Strongly correlated electronic systems with one hole: Dynamical properties. Phys.Rev.B41, pp9049-9073.
- [2] Dagotto E.(1994).Correlated electrons in high-temperature superconductors. Rev. Mod. Phys., 66, pp763-840.
- [3] Oleg A. S. and George F. R. (1996). Hole motion in the Ising antiferromagnet: An application of the recursion method. Phys. Rev. B53, pp2517-2522.
- [4] Ehika S., Igbinovia E.O. and Idiodi J.O.A. (2009). A Simplified formulation of the Lanczos technique for strongly correlated systems. AJP, Vol. 2, pp63-75.
- [5] L. M. Lederman and C. T. Hill. (2004). Symmetry and the Beautiful Universe. Prometheus Books, Amherst New York, pp1-363
- [6] Zee. A (2007). Fearful Symmetry: The search for beauty in modern physics. Princeton University Press, Princeton, New Jersey, pp3-8.
- [7] Lucas Jr. C.W. (2010). The Symmetry and Beauty of the Universe. Foundations of Science, Vol.13, pp 1-13.
- [8] Noether E. (1918). Invariant Variation Problems. Math- phys. Klasse 235 -257.
- [9] Byers N. (1999). E. Noether's discovery of the deep connection between symmetries and conservation laws. Isr. Math. Conf. Proc. 12, pp67–82
- [10] Coleman S.(1975). Secret symmetry: an introduction to spontaneous symmetry breakdown and gauge fields. Academic Press. New York, pp138-215.
- [11] Hanc J. Tuleja S. Hancova M. (2004). Symmetries and conservation laws: Consequences of Noether's theorem. Am. J. Phys., 72, pp 428–435.
- [12] Leon L. and Christopher T. H. (2005). Symmetry and the Beautiful Universe. Prometheus Books, Amherst, New York.
- [13] Wigner, E. P. (1937). On the Consequences of the Symmetry of the Nuclear Hamiltonian on the Spectroscopy of Nuclei. Phys. Rev. 51, pp106-119.
- [14] Manuosakis E. (1991). The spin- ¹/₂ Heisenberg antiferromagnet on a square lattice and its application to the cuprous oxides. Rev. Mod. Phys., 63, pp1-62.