Correlation Functions of the Antiferromagnetic Heisenberg Chains Using a New Version of Modified Lanczos Method

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Abstract

This work presents a detailed study of the diagonal spin-spin correlation function of the one dimensional antiferromagnetic Heisenberg model using a new version of modified Lanczos technique. The wavefunctions obtain at the end of the iterations provide a recipe for a formula that correctly computed the diagonal spin-spin correlation functions of the Heisenberg chains. The correlation functions for these Heisenberg chains are found to be translationally invariant and independent of the actual value of the antiferromagnetic constant J. The correlations are also found to be antiferromagnetic in the region $M \leq CL$, where CL is the correlation length and M is the separation between a reference spin and a spin under consideration.

1.0 Introduction

Most physical systems like semiconductors and most metals can be described as having non-interacting electrons. This simple approach is valid because the interaction (Coulomb) energy of electrons is much smaller than their kinetic energy. Another example is alkali atoms that undergo Bose condensation at low temperatures [1]. These atoms can be treated as non-interacting bosons because their scattering length (i.e. the length at which they interact with each other) is much smaller than the average distance between the particles. However, there are important systems for which the interactions between the particles are not weak. These systems are called strongly correlated systems. It is one of the most intensively studied areas of research in condensed-matter physics [2]. The term "strong correlation" describes the state of affair when the interaction energy U dominates in controlling the motion of the electron [3]. Due to this strong Coulomb repulsion U, electrons in these systems remain localized in their respective sites. Any attempt for an electron to hop to a neighbouring site thereby reducing its kinetic energy t will amount to double occupancy of some sites which cost U. These interactions play a major role in determining the properties of such systems. The presence of this large U, characterizes these systems as insulators. These insulators driven by strong coulomb repulsion are called Mott insulators [4]. They are indeed different from the band insulators that are characterized by a full and empty one electron band. More so, the band insulators will require the state to be metallic at half filling.

In These Mott insulators, the interactions between the electronic spins, charges, and orbitals produce a rich variety of electronic phases. The competition and/or cooperation among these correlated-electron phases can lead to the emergence of surprising electronic phenomena and functionalities and form the basis for a new type of electronics [5]. Electronic correlation is one of the most common and most useful statistics in condensed matter Physics. A correlation is a single number that describes the degree of relationship between two variables. In statistical mechanics, correlation function is a measure of the order in a system, as characterized by a mathematical correlation function, and describes how microscopic variables at different positions are correlated. In a spin system, it is the thermal average of the scalar product of the spins at two lattice points over all possible orderings [6]. The alignment that would naturally arise as a result of the interaction between spins is usually destroyed by thermal effects [7]. Electronic correlations can cause striking many-body effects like electronic localization, magnetism and charge ordering which cannot be described by the independent particle picture. The aim of this work is to study diagonal spin-spin correlation in the Heisenberg spin chains at different separations. The

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remainder of this paper is structured as follows. In Sec. 2, we present the antiferromagnetic Heisenberg Hamiltonian. Sec. 3 describes the version of modified Lanczos technique (MLT) used in this work. Application of MLT to some finite systems is examined in Sec. 4. Sec. 5 presents the calculations of diagonal spin-spin correlation function. Discussion of results is presented in Sec. 6. Sec. 7 concludes the presentation.

2.0 The Isotropic Antiferromagnetic Heisenberg Hamiltonian

At half-filling, hopping of electrons is highly forbidden due to the strong onsite electronic repulsion U. The model that captures the physics arising from spin-spin interaction of localized spins is the Heisenberg antiferromagnetic model. This model in one dimension and in the absence of external magnetic field is given by

$$H = J \sum_{i} \left[S_{i}^{z} S_{i+1}^{z} + \frac{1}{2} \left(S_{i}^{+} S_{i+1}^{-} + S_{i}^{-} S_{i+1}^{+} \right) \right]$$
(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. This model has been able to capture the magnetic properties of correlated quantum spin systems in different degrees of freedom, be it spin1/2 or spin-1 degree of freedom [8-10]. The linear chain Spin-1/2 Heisenberg antiferromagnet AFM is of fundamental importance in many-body physics, as it is one of the few systems where a nontrivial ground state is known exactly [11]. Some Quasi 1D antiferromagnetic chains have experimentally been realised [12-15]. The first problem when solving such a model is to describe the spectrum of its Hamiltonian. The second problem is to compute matrix elements of spin operators between two eigenvectors of H and then all correlation functions of spin operators. At zero temperature they reduce to the average value of products of spin operators in the lowest energy level state (the ground state).

3.0 The New Version of Modified Lanczos Technique

Because of exponential growth of the Hilbert space with system size and memory requirement of present day computers, direct exact diagonalization of strongly correlated electronic Hamiltonians is not feasible, even after exhausting all the symmetries of the system. The modified Lanczos technique (MLT) is a modification of the standard Lanczos technique (SLT) [16-18]. Contrary to SLT in which the size of the matrix still increases with system size, in MLT the size of the Hilbert space is compressed to two. The diagonalization process proceeds with 2x2 iterations. The version of MLT algorithm presented in this thesis is a modification of the previous ones used by [9, 19-21]. The approach employed in this thesis provides a more convenient way of obtaining the improved energy and wavefunction in each iteration [22].

As in the standard Lanczos technique [17] and its modifications [19], this method requires the selection of an initial trial vector $|\phi_0\rangle$ (normalized to one). If H acts on $|\phi_o\rangle$ the result can be written as

$$H|\phi_{0}\rangle = \frac{\langle\phi_{0}|H|\phi_{0}\rangle}{\langle\phi_{0}|\phi_{0}\rangle}|\phi_{0}\rangle + \left|\widetilde{\phi}_{0}\rangle, \qquad (2)$$

where $\left| \widetilde{\phi}_0 \right\rangle$ is a normalized new state vector orthogonal to $\left| \phi_0 \right\rangle$.

$$H = \begin{bmatrix} a_0 & b_0 \\ b_0 & c_0 \end{bmatrix}$$
(3)

This 2x2 matrix can easily be diagonalized. Its lowest eigenvalues a_1 is given by

$$a_{1} = \frac{a_{0} + c_{0} - \sqrt{(a_{0} + c_{0})^{2} - 4(a_{0}c_{0} - b_{0}^{2})}}{2}$$
(4)

Its corresponding eigenvector $|\phi_1\rangle$ is given by

$$\left|\phi_{1}\right\rangle = \alpha_{0}\left|\phi_{0}\right\rangle + \beta_{0}\left|\widetilde{\phi}_{0}\right\rangle,\tag{5}$$

where the electronic weights α_0 and β_0 of $|\phi_0\rangle$ and $|\tilde{\phi}_0\rangle$ respectively, are given by

$$\alpha_0 = \sqrt{\frac{b_0^2}{b_0^2 + (a_0 - a_1)^2}} \tag{6}$$

$$\beta_0 = -\sqrt{\frac{(a_0 - a_1)^2}{b^2 + (a_0 - a_1)^2}}$$
(7)

 a_1 and $|\phi_1\rangle$ are better approximations to E_0 (true ground state energy) and $|\Phi_0\rangle$ (true ground state wavefunction) than a_0 and $|\phi_0\rangle$ respectively. The method can be iterated by considering $|\phi_1\rangle$ as a new initial trial vector and repeating the steps from Eq. (2) to (5). In each iteration, the orthogonal pairs $(|\phi_0\rangle, |\tilde{\phi}_0\rangle)$, $(|\phi_1\rangle, |\tilde{\phi}_1\rangle)$, etc are normalized. The iteration terminates when $a_i \approx a_{i+1}$. For detailed description of this technique, see ref. [22].

4. APPLICATION OF MLT TO HEISENBERG CHAINS

In this section, the version of MLT described in section 3 will be applied to six- and eight-site Heisenberg chains.

1. APPLICATION OF MLT TO SIX- SITE HEISENBERG CHAIN

A six-site Heisenberg chain 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.1. In order to reduce the time of convergence when using MLT, it is





necessary first to reduce the size of the Hilbert space by utilizing the various symmetries of the system under study. Detailed description of the various symmetries of the Heisenberg chains will not be discussed in this current work. Such elaborate discussion of the symmetries of the Heisenberg model is currently under study. We will only utilize the result obtained from this study in implementing MLT on the six- and eight -site chains.

The Hilbert space of this system is of size $2^6=64$. 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

$$N_s = \frac{N!}{\left[(N/2)! \right]^2} = \frac{6!}{(3!)^2} = 20$$
(8)

The basis states in this subspace of the Hilbert space are

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

By making use of translational and spin-inversion or reflection symmetries in the momentum space of K=0, the following reductions are obtained:

$$\left|\phi_{0}\right\rangle = \frac{1}{\sqrt{6}}\left[\left|1\right\rangle + \left|2\right\rangle + \left|3\right\rangle + \left|4\right\rangle + \left|5\right\rangle + \left|6\right\rangle\right]\tag{9}$$

$$\left|\phi_{1}\right\rangle = \frac{1}{\sqrt{12}}\left[\left|7\right\rangle + \left|8\right\rangle + \left|9\right\rangle + \left|10\right\rangle + \left|11\right\rangle + \left|12\right\rangle + \left|13\right\rangle + \left|14\right\rangle + \left|15\right\rangle + \left|16\right\rangle + \left|17\right\rangle + \left|18\right\rangle\right]$$
(10)

$$\left|\phi_{2}\right\rangle = \frac{1}{\sqrt{2}}\left[\left|19\right\rangle + \left|20\right\rangle\right] \tag{11}$$

The Hamiltonian of this system is given by

$$H = \frac{J}{2} \Big[S_1^+ S_2^- + S_1^- S_2^+ + S_2^+ S_3^- + S_2^- S_3^+ + S_3^+ S_4^- + S_3^- S_4^+ + S_4^+ S_5^- + S_4^- S_5^+ + S_5^+ S_6^- \Big] + \frac{J}{2} \Big[S_5^- S_6^+ + S_6^+ S_1^- + S_6^- S_1^+ \Big] + J \Big[S_1^Z S_2^Z + S_2^Z S_3^Z + S_3^Z S_4^Z + S_4^Z S_5^Z + S_5^Z S_6^Z + S_6^Z S_1^Z \Big]$$
(12)

Having reduced the size of the system, the next step is the application of MLT to the reduced basis states as given in Eqs. (9), (10) and (11). Following the steps outlined in section 3, let $|\phi_1\rangle$ denoted by $|\varphi_0\rangle$ be the initial trial vector. When H in Eq. (12) acts on $|\varphi_0\rangle$, the results is

$$\begin{split} H|\varphi_{0}\rangle &= H|\phi_{1}\rangle = \frac{J}{\sqrt{2}}|\phi_{0}\rangle + \frac{J}{2}|\phi_{1}\rangle + \frac{J\sqrt{6}}{2}|\phi_{2}\rangle\\ a_{0} &= \langle\varphi_{0}|H|\varphi_{0}\rangle = \langle\phi_{1}|H|\phi_{1}\rangle = \frac{J}{2}\\ H^{2}|\varphi_{0}\rangle &= \left[\frac{J^{2}}{2\sqrt{2}} + \frac{J^{2}}{2\sqrt{2}}\right]|\phi_{0}\rangle + \left[\frac{J^{2}}{2} + \frac{J^{2}}{4} + \frac{6J^{2}}{4}\right]|\phi_{1}\rangle + \left[\frac{J^{2}\sqrt{6}}{4} - \frac{3J^{2}\sqrt{6}}{2\sqrt{2}}\right]|\phi_{2}\rangle\\ &= \frac{J^{2}}{\sqrt{2}}|\phi_{0}\rangle + \frac{9J^{2}}{4}|\phi_{1}\rangle - \frac{J^{2}\sqrt{6}}{2}|\phi_{2}\rangle\\ &\langle\varphi_{0}|H^{2}|\varphi_{0}\rangle = \frac{9J^{2}}{4}\\ b_{0} &= \left[\langle\varphi_{0}|H^{2}|\varphi_{0}\rangle - \left(\langle\varphi_{0}|H|\varphi_{0}\rangle\right)^{2}\right]^{1/2} = \left(\frac{9J^{2}}{4} - \frac{J^{2}}{4}\right)^{1/2} = J\sqrt{2} \end{split}$$

The vector $\left| \widetilde{arphi}_0
ight
angle$ orthogonal to $\left| arphi_0
ight
angle$ is given by

$$\left| \tilde{\varphi}_{0} \right\rangle = \frac{H \left| \varphi_{0} \right\rangle - \left\langle \varphi_{0} \left| H \right| \varphi_{0} \right\rangle \left| \varphi_{0} \right\rangle}{\left[\left\langle \varphi_{0} \left| H^{2} \right| \varphi_{0} \right\rangle - \left(\left\langle \varphi_{0} \left| H \right| \varphi_{0} \right\rangle \right)^{2} \right]^{1/2}} = \frac{H \left| \varphi_{0} \right\rangle - \left\langle \varphi_{0} \left| H \right| \varphi_{0} \right\rangle \left| \varphi_{0} \right\rangle}{b_{0}}$$

$$\begin{split} \left| \widetilde{\varphi}_{0} \right\rangle &= \frac{1}{2} \left| \phi_{0} \right\rangle + \frac{\sqrt{3}}{2} \left| \phi_{2} \right\rangle \\ H \left| \widetilde{\varphi}_{0} \right\rangle &= \frac{J}{4} \left| \phi_{0} \right\rangle + \left[\frac{J}{2\sqrt{2}} + \frac{3J\sqrt{2}}{4} \right] \left| \phi_{1} \right\rangle - \frac{3J\sqrt{3}}{4} \left| \phi_{2} \right\rangle \\ c_{0} &= \left\langle \widetilde{\varphi}_{0} \left| H \right| \widetilde{\varphi}_{0} \right\rangle = -J \end{split}$$

Therefore, the 2x2 Hamiltonian matrix arising from the orthogonal vectors $|\tilde{\varphi}_0\rangle$ and $|\varphi_0\rangle$ gives

$$H = \begin{bmatrix} a_0 & b_0 \\ b_0 & c_0 \end{bmatrix} = \begin{bmatrix} J/2 & J/\sqrt{2} \\ J/\sqrt{2} & -J \end{bmatrix}$$
(13)

The improved ground state energy and the corresponding wavefunction are respectively given by

$$a_{1} = \frac{1}{2} \left[a_{0} + c_{0} - \sqrt{(a_{0} + c_{0})^{2} - 4(a_{0}c_{0} - b_{0}^{2})} \right] = \frac{1}{4} \left[-J - J\sqrt{41} \right]$$
(14)
$$|a_{0}\rangle = a_{1}|a_{0}\rangle + \beta_{1}|\tilde{a}_{0}\rangle$$
(15)

$$\left|\varphi_{1}\right\rangle = \alpha_{0}\left|\varphi_{0}\right\rangle + \beta_{0}\left|\widetilde{\varphi}_{0}\right\rangle,\tag{15}$$

where α_0 and β_0 have been defined in Eqs. (6) and (7) respectively. Convergence was reached after the 5th iteration with the improved ground state wavefunction and energy given respectively as.

$$\left|\varphi_{5}\right\rangle = \sum_{i=0}^{2} \left(\alpha_{4}\sigma_{i} + \beta_{4}\lambda_{i}\right)\phi_{i}\right\rangle \tag{16}$$

$$a_{5} = \frac{1}{2} \left[a_{4} + c_{4} - \sqrt{\left(a_{4} + c_{4}\right)^{2} - 4\left(a_{4}c_{4} - b_{4}^{2}\right)} \right]$$
(17)

The numerical values of $a_1, a_2, ..., a_5$ are presented in Table 1. To check the validity and correctness of the version of MLT used in this work, the energy of the 5th iteration is compared with the exact result. The electronic weights α_4 and β_4 of the new vector $|\varphi_5\rangle$ assume their usual form as given in Eqs. (6) and (7) respectively. The parameters σ_i and λ_i are accumulated numerical weight of $|\phi_i\rangle$. The wave function in Eq. (16) can also be recast in the form

$$\left|\varphi_{5}\right\rangle = \sum_{i=0}^{2} X_{i} \left|\phi_{i}\right\rangle , \qquad (18)$$

where $X_i = (\alpha_4 \sigma_i + \beta_4 \lambda_i)$. The numerical values of X_i (i = 0, 1, 2) obtained at the end of the fifth iteration are:

 $X_0 = -0.120942$, $X_1 = -0.447260$ and $X_2 = 0.886119$. These values will be used to compute the diagonal spin-spin correlation function for six sites chain.

II. APPLICATION OF MLT TO SIX- EIGHT HEISENBERG CHAIN

An eight sites Heisenberg chain is shown in Fig. 2. 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. The size of this system is of $2^8 = 256$.



Fig.2: An eight-site Heisenberg chain. The topology of this system is that of a circle when subjected to periodic boundary conditions.

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

$$N_s = \frac{N!}{\left[\left(N/2 \right)! \right]^2} = \frac{8!}{\left(4! \right)^2} = 70$$
⁽¹⁹⁾

The basis states in this subspace of the Hilbert space are shown below. $|1\rangle = |00001111\rangle |2\rangle = |10000111\rangle |3\rangle = |11000011\rangle |4\rangle = |11100001\rangle$

$$\begin{split} |1\rangle &= |00001111\rangle, |2\rangle &= ||10000111\rangle, |3\rangle &= ||11000011\rangle, |4\rangle &= ||11100001\rangle \\ |5\rangle &= ||1110000\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 \\ |13\rangle &= |01110001\rangle, |14\rangle &= |10111000\rangle, |15\rangle &= |01011100\rangle, |16\rangle &= |00101110\rangle \\ |17\rangle &= |00011101\rangle, |18\rangle &= |10001110\rangle, |19\rangle &= |01000111\rangle, |20\rangle &= |10100011\rangle \\ |21\rangle &= |11010001\rangle, |22\rangle &= |11101000\rangle, |23\rangle &= |01110100\rangle, |24\rangle &= |00111010\rangle \\ |25\rangle &= |00011011\rangle, |26\rangle &= |10001101\rangle, |27\rangle &= |11000110\rangle, |28\rangle &= |01100011\rangle \\ |29\rangle &= |10110001\rangle, |30\rangle &= |11011000\rangle, |31\rangle &= |01101100\rangle, |32\rangle &= |0011010\rangle \\ |33\rangle &= |00100111\rangle, |34\rangle &= |10010011\rangle, |35\rangle &= |11001001\rangle, |36\rangle &= |11100100\rangle \\ |37\rangle &= |01110010\rangle, |38\rangle &= |00111001\rangle, |39\rangle &= |1001110\rangle, |40\rangle &= |01001110\rangle \\ |41\rangle &= |00101101\rangle, |42\rangle &= |1001011\rangle, |43\rangle &= |01001011\rangle, |44\rangle &= |0100101\rangle \\ |49\rangle &= |0010101\rangle, |46\rangle &= |01101001\rangle, |51\rangle &= |1100100\rangle, |52\rangle &= |0110010\rangle \\ |53\rangle &= |10110010\rangle, |54\rangle &= |0011001\rangle, |55\rangle &= |1001110\rangle, |56\rangle &= |0101100\rangle \\ |57\rangle &= |0011011\rangle, |58\rangle &= |1001101\rangle, |59\rangle &= |0101101\rangle, |60\rangle &= |1010010\rangle \\ |61\rangle &= |0010011\rangle, |62\rangle &= |1001001\rangle, |67\rangle &= |100100\rangle, |64\rangle &= |0100110\rangle \\ |65\rangle &= |0011001\rangle, |66\rangle &= |1001100\rangle, |67\rangle &= |1001010\rangle \\ |69\rangle &= |1010010\rangle, |70\rangle &= |0101010\rangle \\ |69\rangle &= |1010010\rangle, |70\rangle &= |0101010\rangle \\ |69\rangle &= |1010010\rangle, |70\rangle &= |0101010\rangle \\ |61\rangle &= |0010101\rangle, |66\rangle &= |1001001\rangle, |70\rangle &= |0100101\rangle \\ |61\rangle &= |0010011\rangle, |66\rangle &= |1001100\rangle, |70\rangle &= |0100101\rangle \\ |61\rangle &= |0010011\rangle, |66\rangle &= |1001100\rangle, |70\rangle &= |0100101\rangle \\ |61\rangle &= |0101001\rangle, |66\rangle &= |1001100\rangle, |70\rangle &= |0101010\rangle \\ |61\rangle &= |0101001\rangle, |66\rangle &= |1001100\rangle, |70\rangle &= |0101010\rangle \\ |69\rangle &= |1010010\rangle, |70\rangle &= |0101010\rangle \\ |69\rangle &= |1010010\rangle, |70\rangle &= |0100101\rangle \\ |61\rangle &= |0101001\rangle, |61\rangle &= |1001010\rangle, |61\rangle &= |1000100\rangle \\ |61\rangle &= |0011001\rangle, |61\rangle &= |1001000\rangle, |61\rangle &= |0100010\rangle \\ |61\rangle &= |0011001\rangle, |61\rangle &= |1001000\rangle, |61\rangle &= |0100010\rangle \\ |61\rangle &= |0011001\rangle, |61\rangle &= |1001000\rangle, |61\rangle &= |0100010\rangle \\ |61\rangle &= |00110001\rangle, |61\rangle &= |1000000\rangle, |61\rangle &= |1000000\rangle \\ |61\rangle &= |10$$

By making use of translational and spin-inversion or reflection symmetries in the momentum space of K=0, the following reductions are obtained:

$$\left|\phi_{0}\right\rangle = \frac{1}{\sqrt{8}}\left[\left|1\right\rangle + \left|2\right\rangle + \left|3\right\rangle + \left|4\right\rangle + \left|5\right\rangle + \left|6\right\rangle + \left|7\right\rangle + \left|8\right\rangle\right] \tag{20}$$

$$|\phi_{1}\rangle = \frac{1}{4} \begin{bmatrix} |9\rangle + |10\rangle + |11\rangle + |12\rangle + |13\rangle + |14\rangle + |15\rangle + |16\rangle \\ + |17\rangle + |18\rangle + |19\rangle + |20\rangle + |21\rangle + |22\rangle + |23\rangle + |24\rangle \end{bmatrix}$$
(21)

$$\left|\phi_{2}\right\rangle = \frac{1}{4} \begin{bmatrix} \left|25\right\rangle + \left|26\right\rangle + \left|27\right\rangle + \left|28\right\rangle + \left|29\right\rangle + \left|30\right\rangle + \left|31\right\rangle + \left|32\right\rangle \\ + \left|33\right\rangle + \left|34\right\rangle + \left|35\right\rangle + \left|36\right\rangle + \left|37\right\rangle + \left|38\right\rangle + \left|39\right\rangle + \left|40\right\rangle \end{bmatrix}$$
(22)

$$\left|\phi_{3}\right\rangle = \frac{1}{\sqrt{8}} \left[\left|41\right\rangle + \left|42\right\rangle + \left|43\right\rangle + \left|44\right\rangle + \left|45\right\rangle + \left|46\right\rangle + \left|47\right\rangle + \left|48\right\rangle\right]$$
(23)

$$\left|\phi_{4}\right\rangle = \frac{1}{4} \begin{bmatrix} |49\rangle + |50\rangle + |51\rangle + |52\rangle + |53\rangle + |54\rangle + |55\rangle + |56\rangle \\ + |57\rangle + |58\rangle + |59\rangle + |60\rangle + |61\rangle + |62\rangle + |63\rangle + |64\rangle \end{bmatrix}$$
(24)

$$\left|\phi_{5}\right\rangle = \frac{1}{2}\left[\left|65\right\rangle + \left|66\right\rangle + \left|67\right\rangle + \left|68\right\rangle\right] \tag{25}$$

$$\left|\phi_{6}\right\rangle = \frac{1}{\sqrt{2}} \left[\left|69\right\rangle + \left|70\right\rangle\right] \tag{26}$$

The classes $|\phi_0\rangle$, $|\phi_3\rangle$, $|\phi_5\rangle$ and $|\phi_6\rangle$ are unaffected by the spin-inversion symmetry.

The Hamiltonian of this system is given by

$$\frac{J}{2} \Big[S_{1}^{+} S_{2}^{-} + S_{1}^{-} S_{2}^{+} + S_{2}^{+} S_{3}^{-} + S_{2}^{-} S_{3}^{+} + S_{3}^{+} S_{4}^{-} + S_{3}^{-} S_{4}^{+} + S_{4}^{+} S_{5}^{-} + S_{4}^{-} S_{5}^{+} + S_{5}^{+} S_{6}^{-} \Big]
+ \frac{J}{2} \Big[S_{5}^{-} S_{6}^{+} + S_{6}^{+} S_{7}^{-} + S_{6}^{-} S_{7}^{+} + S_{7}^{+} S_{8}^{-} + S_{7}^{-} S_{8}^{+} + S_{8}^{+} S_{1}^{-} + S_{8}^{-} S_{1}^{+} \Big]
+ J \Big[S_{1}^{Z} S_{2}^{Z} + S_{2}^{Z} S_{3}^{Z} + S_{3}^{Z} S_{4}^{Z} + S_{4}^{Z} S_{5}^{Z} + S_{5}^{Z} S_{6}^{Z} + S_{6}^{Z} S_{7}^{Z} + S_{7}^{Z} S_{8}^{Z} + S_{8}^{Z} S_{1}^{Z} \Big]$$
(27)

The size of the system has now been reduced from 64 to 7. The next step is to apply MLT to the reduced Hilbert space. Following the steps outlined in section 3, let $|\phi_1\rangle$ denoted by $|\varphi_0\rangle$ be the initial trial vector. If H in Eq. (27) acts on $|\varphi_0\rangle$ in Eq. (20), the results is

$$H|\varphi_{0}\rangle = H|\phi_{3}\rangle = \frac{J}{\sqrt{2}}|\phi_{1}\rangle + J\sqrt{2}|\phi_{4}\rangle - J|\phi_{3}\rangle$$

$$a_{0} = \langle\varphi_{0}|H|\varphi_{0}\rangle = \langle\phi_{3}|H|\phi_{3}\rangle = -J$$

$$H^{2}|\varphi_{0}\rangle = \frac{J^{2}}{2}|\phi_{0}\rangle - \frac{J^{2}}{\sqrt{2}}|\phi_{1}\rangle + \left[\frac{J^{2}}{\sqrt{2}} + J^{2}\sqrt{2}\right]|\phi_{2}\rangle + \left[\frac{J^{2}}{2} + 3J^{2}\right]|\phi_{3}\rangle$$

$$-2J^{2}\sqrt{2}|\phi_{4}\rangle + J^{2}\sqrt{2}|\phi_{5}\rangle + 2J^{2}|\phi_{6}\rangle$$

$$\langle\varphi_{0}|H^{2}|\varphi_{0}\rangle = \frac{7J^{2}}{2}$$

$$b_{0} = \left[\langle\varphi_{0}|H^{2}|\varphi_{0}\rangle - \left(\langle\varphi_{0}|H|\varphi_{0}\rangle\right)^{2}\right]^{1/2} = \left(\frac{7J^{2}}{2} - J^{2}\right)^{1/2} = J\sqrt{\frac{5}{2}}$$

The vector $\left| \widetilde{arphi}_0
ight
angle$ orthogonal to $\left| arphi_0
ight
angle$ is given by

$$\begin{split} \left| \tilde{\varphi}_{0} \right\rangle &= \frac{H \left| \varphi_{0} \right\rangle - \left\langle \varphi_{0} \left| H \right| \varphi_{0} \right\rangle \left| \varphi_{0} \right\rangle}{\left[\left\langle \varphi_{0} \left| H^{2} \right| \varphi_{0} \right\rangle - \left(\left\langle \varphi_{0} \left| H \right| \varphi_{0} \right\rangle \right)^{2} \right]^{1/2}} = \frac{H \left| \varphi_{0} \right\rangle - \left\langle \varphi_{0} \left| H \right| \varphi_{0} \right\rangle \left| \varphi_{0} \right\rangle}{b_{0}} \\ &\left| \tilde{\varphi}_{0} \right\rangle = \frac{1}{\sqrt{5}} \left(\left| \varphi_{1} \right\rangle + 2 \left| \varphi_{4} \right\rangle \right) \\ H \left| \tilde{\varphi}_{0} \right\rangle &= \frac{J}{\sqrt{10}} \left| \varphi_{0} \right\rangle + \frac{3J}{\sqrt{5}} \left| \varphi_{2} \right\rangle + \frac{5J}{\sqrt{10}} \left| \varphi_{3} \right\rangle - \frac{2J}{\sqrt{5}} \left| \varphi_{4} \right\rangle + \frac{2J}{\sqrt{5}} \left| \varphi_{5} \right\rangle + \frac{4J}{\sqrt{10}} \left| \varphi_{6} \right\rangle \\ c_{0} &= \left\langle \tilde{\varphi}_{0} \left| H \right| \tilde{\varphi}_{0} \right\rangle = -\frac{4J}{5} \end{split}$$

Therefore, the 2x2 Hamiltonian matrix arising from the vectors $|\tilde{\varphi}_0\rangle$ and $|\varphi_0\rangle$ gives

$$H = \begin{bmatrix} a_0 & b_0 \\ b_0 & c_0 \end{bmatrix} = \begin{bmatrix} -J & J/\sqrt{5/2} \\ J/\sqrt{5/2} & -4J/5 \end{bmatrix}$$
(28)

The improved ground state energy and the corresponding wavefunction are respectively given by

$$a_{1} = \frac{1}{2} \left[a_{0} + c_{0} - \sqrt{(a_{0} + c_{0})^{2} - 4(a_{0}c_{0} - b_{0}^{2})} \right] = \frac{1}{10} \left(-9J - J\sqrt{251} \right)$$
(29)

$$|\varphi_1\rangle = \alpha_0 |\varphi_0\rangle + \beta_0 |\tilde{\varphi}_0\rangle \tag{30}$$

The ground state energy and wave function were found to converge reasonably well after the 10th iteration. The improve ground state wavefunction and energy obtained after the 10th iteration are

$$a_{10} = \frac{1}{2} \left[a_9 + c_9 - \sqrt{(a_9 + c_9)^2 - 4(a_9 c_9 - b_9^2)} \right]$$
(31)

$$\left|\varphi_{10}\right\rangle = \alpha_{9}\left|\varphi_{9}\right\rangle + \beta_{9}\left|\widetilde{\varphi}_{9}\right\rangle \tag{32}$$

The numerical values of $a_1, a_2, ..., a_{10}$ are presented in Table 2. The numerical weight α_9 and β_9 assume their form of Eqs. (6) and (7) respectively. The wavefunction in Eq. (32) can be recast in the form

$$\left|\varphi_{10}\right\rangle = \sum_{i=0}^{\circ} X_{i} \left|\phi_{i}\right\rangle, \tag{33}$$

where $X_i = \alpha_9 s_i + \beta_9 v_i$. The values of X_i obtained at the end of the tenth iteration are:

 $X_{0} = -0.021486, X_{1} = -0.139328, X_{2} = 0.218903, X_{3} = -0.388915, X_{4} = -0.657501,$

 $X_5 = 0.180346$ and $X_6 = 0.562246$. These values will be used to compute the diagonal spin-spin correlation function for eight-site chain.

Table 1. MLT results for six-site Heisenberg chain. ' a_i ' is the energy of the ith iteration and 'exact' is the exact ground state energy. These iterations were done with Mathematical 6.0 [23].

J	\mathbf{a}_1	a ₂	a ₃	\mathbf{a}_4	a ₅	exact
-3.00	5.55234	-0.782394	-4.48369	-4.99999	-4.50000	-4.50000
-2.00	3.70156	-0.521596	-2.98913	-3.00000	-3.00000	-3.00000
-1.50	2.77617	-0.391197	-2.24185	-2.25000	-2.25000	-2.25000
-1.00	1.85078	-0.260798	-1.49456	-1.50000	-1.50000	-1.50000
-0.80	1.48062	-0.208638	-1.19565	-1.20000	-1.20000	-1.20000
0.01	-0.01851	-0.021116	-0.02118	-0.02118	-0.02118	-0.02118
0.02	-0.03702	-0.042232	-0.04236	-0.04236	-0.04236	-0.04236
0.06	-0.11105	-0.126695	-0.12707	-0.12708	-0.12708	-0.12708
0.10	-0.18508	-0.211158	-0.21179	-0.21180	-0.21180	-0.21180

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J	\mathbf{a}_1	\mathbf{a}_2	a ₃	\mathbf{a}_4	a ₅	a ₆
-3.00	7.45289	-0.15090	-5.11178	-5.83848	-5.96068	-5.98436
-2.00	4.96860	-0.10060	-3.41186	-3.89232	-3.97378	-3.98957
-1.50	3.72645	-0.07545	-2.55889	-2.91924	-2.98034	-2.99218
-1.00	2.48430	-0.00503	-1.70593	-1.94616	-1.98689	-1.99479
-0.80	1.98744	-0.04024	-1.36474	-1.55693	-1.58951	-1.59583
0.01	-0.02484	-0.03309	-0.03557	-0.03627	-0.03645	-0.03649
0.02	-0.04969	-0.06617	-0.07114	-0.07253	-0.07290	-0.07299
0.06	-0.14906	-0.19852	-0.21343	-0.21759	-0.21869	-0.21897
0.10	-0.24843	-0.33086	-0.35571	-0.36265	-0.36448	-0.36495
1.00	-2.48430	-3.30859	-3.55711	-3.62653	-3.64478	-3.64948

Table 2. MLT results for eight-site Heisenberg chain. a_i is the energy of the ith iteration. These iterations were done with Mathematical 6.0 [23].

Continuation of Table .2 for the eight-site chain.

J	a ₇	a ₈	a9	a ₁₀
-3.00	-5.99166	-5.99517	-5.99718	-5.99835
-2.00	-3.99444	-3.99678	-3.99812	-3.99890
-1 50	-2.99583	-2.99758	-2.99859	-2.99917
-1.00	-1.99722	-1.99722	-1.99906	-1.99945
-0.80	-1.59778	-1.59871	-1.59925	-1.59956
0.01	-0.03651	-0.03651	-0.03651	-0.03651
0.02	-0.07301	-0.07301	-0.07302	-0.07302
0.06	-0.21904	-0.21906	-0.21906	-0.21907
0.10	-0.36507	-0.36510	-0.36511	-0.36511
1.00	-3.65068	-3.65099	-3.65107	-3.65109

5.0 Calculation of Diagonal Spin-Spin Correlation Function

Correlation function is a static property of strongly correlated fermionic systems. It is defined as the probability of finding an electron at site i when there is an electron at site j. This section presents the diagonal spin-spin correlation functions for four, six and eight Heisenberg chains. The diagonal spin-spin correlation function is given by

$$C_r = \left\langle S_i^z S_j^z \right\rangle \tag{34}$$

The correlation function for any Heisenberg cluster can be obtained by using Eqn. (35) as shown below

$$\left\langle S_i^z S_j^z \right\rangle = \sum_{i=0}^{N_c-1} \frac{X_i^2 Y_i}{4N_R} , \qquad (35)$$

where X_i is the electronic weight for corresponding class $|\phi_i\rangle$ or basis state, N_R is the number of basis states or representative in a particular class, Y_i is the correlation in a particular class or basis states, and N_c is the number of classes in the reduced Hilbert space.

I. Correlation Function for Six-Site Chain

The procedure for the calculation of Correlation function for six-site chain at separation m=1, 2 and 3 are shown in Tables 3, 4 and 5 respectively. The wavefunction obtained after the fifth Lanczos step has been used to set up these tables.

$\ket{\phi_i}$	X_{i}	X_i^2	N_R	Y_i	$X_i^2 Y_i / 4N_R$
$ \phi_0 angle$	-0.120942	0.0146227	6	2	0.00121891
$ \phi_1\rangle$	-0.447260	0.200410	16	-4	-0.0166701
$ \phi_2 angle$	0.886119	0.785331	2	-2	-0.1963333
Tal	ble 4. Calculation of	Correlation function	for six -sit	e chain a	at separation m=2
$ \phi_i\rangle$	X_{i}	X_i^2	N_R	Y_i	$X_i^2 Y_i / 4N_R$
$ \phi_0 angle$	-0.120942	0.0146227	6	-2	-0.00121891
$ \phi_1\rangle$	-0.447260	0.200410	16	-4	-0.0166701
$ \phi_2 angle$	0.886119	0.785331	2	2	0.1963333
Tal	ble 5. Calculation of	Correlation function	for six -sit	e chain a	at separation m=3
$\phi_i angle$	X_{i}	X_i^2	N_{R}	Y_i	$X_i^2 Y_i / 4N_R$
$\phi_0 \rangle$	-0.120942	0.0146227	6	-6	-0.00365674
ϕ_1	-0.447260	0.200410	16	4	0.01667010
ϕ_2	0.886119	0.785331	2	-2	-0.1963333

Table 3. Calculation of Correlation function for six -site chain at separation m=1

II. Correlation Function for Eight-Site Chain

The procedure for the calculation of Correlation function for eight-site chain at separation m=1, 2, 3 and 4, are shown below. The wavefunction obtained after the tenth Lanczos step has been used to set up these tables.

$ \phi\rangle$	<i>X</i> .	X. ²	N _p	Y.	$X_{1}^{2}Y_{1}/4N_{p}$
$ \varphi_i\rangle$	-0.021486	0.0004617	8	4	0.0000577076
$ \varphi_0\rangle$	-0.139328	0.0194123	16	0	0.0000000000
$ \varphi_1\rangle$	0.218903	0.0479185	16	0	0.000000000
$ \varphi_2\rangle$	0.388915	0.1512550	8	-4	-0.01890690
$ \Psi_3 $	-0.657501	0.4323080	16	-8	-0.054038400
$ \varphi_4 $	0.180346	0.0325247	4	0	0.000000000
$ \Psi_5\rangle$	0 562246	0 3161210	2	-2	-0.079030100
$ \varphi_6 \rangle$	0.002210	0.5101210	-	-	0.077050100

Table 6. Calculation of Correlation function for eight -site chain at separation m=1

$ \phi_i\rangle$	X_{i}	X_i^2	N_R	Y_i	$\frac{1}{X_i^2 Y_i / 4N_R}$
$ \phi_{0}\rangle$	-0.021486	0.0004617	8	0	0.00000000
$ \phi_1\rangle$	-0.139328	0.0194123	16	0	0.00000000
$ \phi_{2}\rangle$	0.218903	0.0479185	16	-8	-0.00598982
$ \phi_2\rangle$	0.388915	0.1512550	8	0	0.00000000
$ \phi_{\lambda}\rangle$	-0.657501	0.4323080	16	0	0.00000000
$ \phi_{\varepsilon}\rangle$	0.180346	0.0325247	4	-4	-0.00813117
$ \phi_6\rangle$	0.562246	0.3161210	2	2	0.07903010
1 ~ /					

Table 7 . Calculation of Correlation function for eight -site chain at separation m= 2

Table 8. Calculation of Correlation function for eight -site chain at separation m=3

$\ket{\pmb{\phi}_i}$	X_{i}	X_i^2	N_R	Y_i	$X_i^2 Y_i / 4N_R$
$ \phi_0 angle$	-0.021486	0.0004617	8	-4	-0.0000577076
$ \phi_1\rangle$	-0.139328	0.0194123	16	-8	-0.0024265400
$ \phi_2 angle$	0.218903	0.0479185	16	0	0.0000000000
$ \phi_{3}\rangle$	0.388915	0.1512550	8	4	0.0189069000
$ \phi_4\rangle$	-0.657501	0.4323080	16	0	0.0000000000
$ \phi_5\rangle$	0.180346	0.0325247	4	0	0.0000000000
$ \phi_6\rangle$	0.562246	0.3161210	2	-2	-0.0790301000

Table 9. Calculation of Correlation function for eight -site chain at separation m=4

$X_i^2 Y_i / 4N_R$	Y _i	N_R	X_i^2	X_{i}	$ \phi_i\rangle$
 -0.000115415	-8	8	0.0004617	-0.021486	$ \phi_0\rangle$
0.0000000000	0	16	0.0194123	-0.139328	$ \phi_1\rangle$
0.0000000000	0	16	0.0479185	0.218903	$ \phi_2\rangle$
-0.037813700	-8	8	0.1512550	0.388915	$ \phi_3\rangle$
0.0000000000	0	16	0.4323080	-0.657501	$ \phi_{4}\rangle$
0.0081311700	4	4	0.0325247	0.180346	$ \phi_5\rangle$
0.0790301000	2	2	0.3161210	0.562246	$ \phi_6 angle$
-0.037813700 0.0000000000 0.0081311700 0.0790301000	-8 0 4 2	8 16 4 2	0.1512550 0.4323080 0.0325247 0.3161210	0.388915 -0.657501 0.180346 0.562246	$egin{array}{c} \left oldsymbol{\phi}_3 ight angle \ \left oldsymbol{\phi}_4 ight angle \ \left oldsymbol{\phi}_5 ight angle \ \left oldsymbol{\phi}_6 ight angle \end{array}$

6.0 **Results And Discussion**

This section presents and discusses the results for the diagonal spin-spin correlation function for six and eight sites Heisenberg chain. These correlation functions for the various separations are summarized in Table 10. The six sites chain has both nearest neighbour (NN) and next nearest neighbour (NNN) spin-spin correlation functions arising from m=1 and m=2respectively, and an additional correlation function arising from m=3. The eight sites chain has four unique correlation functions due to separations m=1, 2, 3, and 4. Due to periodic boundary conditions, the correlation functions obtained for the longest distance for the various chains are equivalent to that of the shortest distance (NN). This behaviour is clearly obvious

in Table 10. For example, for the six and eight sites chains we have that $\langle S_1^Z S_2^z \rangle = \langle S_1^Z S_6^z \rangle$ and $\langle S_1^Z S_2^z \rangle = \langle S_1^Z S_8^z \rangle$

respectively. The correlation length which is defined as the distance in space beyond which the spins are uncorrelated with respect to the reference spin differs for the different chains. The correlation lengths for N=6 and 8 are 3 and 4 respectively.

The dependence of correlation function (CF) on the separation m for N= 6 and 8 is shown in Figs. 3 and 4 respectively. These Figures clearly show that the correlation function decays exponentially with distance. The correlation length (CL) from these curves is the value of m at which |CF| has its lowest value. The alternating values of +ve and -ve value for the CF is evidence that the spins are antiferromagnetically correlated. As observed from Table 10 and Figs. 3 and 4, correlation is found to vanish for m>CL. Thus, the CF obtained for m>CL are repetition of the ones obtained for m≤CL.

Table 10. Correlation functions for four, six and eight sites Heisenberg chains at separations m from the arbitrary chosen reference spin at site 1.

m	six sites	eight sites	
1	-0.52 N.7.84	-09159194180	
2	0.178440	0.06490920	
3	-0.183320	-0.0626075	
4	0.178440	0.0492321	
5	-0.211784	-0.0626075	
6		0.06490920	
7		-0.1519180	



Fig. 3. Correlation function for six- site chain





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7.0 Conclusion

This current work employed a new version of modified Lanczos technique (MLT) for the calculation of diagonal spinspin correlation function of six- and eight-site Heisenberg spin chains. First, the version of MLT employed in this paper was used to obtain the exact numerical ground state energy of six- and eight- site chains. The result obtained at the end of this iteration was used to develop a formula that correctly computed the correlation functions of the Heisenberg chains of six- and eight-site. The diagonal spin-spin correlation function (CF) for these Heisenberg chains were found to be antiferromagnetic in the region m \leq CL, where CL is the correlation length and m is the separation between a given spin and a reference spin. The correlation was found to vanish for m>CL. Thus, the CF obtained for m>CL are repetition of the ones obtained for m \leq CL. This shows that the CF is translationally invariant and independent of the actual value of J. The idea brought forward in this work is simple and can be generalized to other models and more complex systems.

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