Spin 1 Heisenberg Model (AKLT Model)

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1 History and Significance

The AKLT (Affleck-Kennedy-Lieb-Tasaki) Model is a mathematical model defined by Ian Affleck, Tom Kennedy, Elliott H. Lieb, and Hal Tasaki to explain the valence-bond ground state of antiferromagnetic materials [1]. This model is an extension of the one-dimensional Heisenberg spin chain model [2].

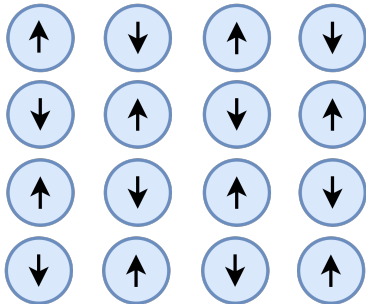

Figure 1: Alignment of Magnetic Moments in Antiferromagnets.

The motivation for defining this model is that in antiferromagnets, half of the magnetic moments are aligned in one direction and the rest are aligned in the opposite direction, due to which the net magnetic moment is zero. The ground state of this model is the same as they considered two out of every set of three neighboring sites, which are paired to form a valence bond or singlet. This leads to two spin halves for every site (s = 1); thus, the solution must be the wave function of the spin 1 system.

However, Hulthén further modified this model to find a solution for antiferromagnets. Still, this model is important in understanding several areas, such as Quantum states in extreme environments (e.g., Neutron Stars and Quark Matter), magnetar spin dynamics, etc.

2 Hamiltonian of AKLT Model

First, let us understand the concept of Valence bonds (or singlet).

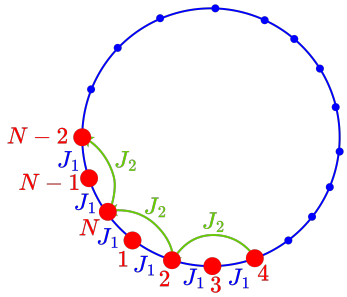

Figure 2: Majumdar Ghosh Model

In the Majumdar–Ghosh Model [3], which is represented as,

$$\mathcal{H} = J_1 \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \sum_i \vec{S}_i \cdot \vec{S}_{i+2} \tag{1}$$

where $\vec{S}$ is quantum spin operator with quantum number $S = \frac{1}{2}$. At the MG point (i.e. $J_2 = \frac{J_1}{2}$), the ground states of the MG Model are the tensor product of singlet states as,

$$|R_N\rangle = [1\ 2][3\ 4][5\ 6]\cdots[N-1\ N] \tag{2}$$

$$|C_N\rangle = [2\ 3][4\ 5][5\ 6]\cdots[N\ 1] \tag{3}$$

where,

$$[1\ 2] = \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle_{12} - |\downarrow\uparrow\rangle_{12}] \tag{4}$$

The two-qubit state in Eq. 4 is a singlet state,

$$\begin{aligned} S^2_{tot}[1\ 2] &= (\vec{S_1} + \vec{S_2})^2[1\ 2] = S(S+1)[1\ 2] \\ &= 0(0+1)[1\ 2] = 0[1\ 2] \\ S^2_{tot}[1\ 2] &= 0[1\ 2] \end{aligned} \tag{5}$$

The states in eq. 2 and eq. 3 are represented as,

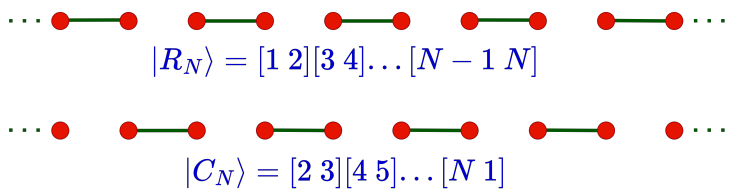

Figure 3: Ground State of MG Model at ($J_2 = \frac{J_1}{2}$)

These ground states have a translational symmetry broken from period 1 to period 2, which are ultrashort-range correlations. The bonds shown in green color in Fig. 3 are called valence bonds.

Now, let us extend the concept of valence bonds for higher spin. If a particle has spin S, then this spin can be constructed by $2S$ spin-$\frac{1}{2}$ particles. For example, if we have spin $S = 1$ particle, that can be constructed by $2 \times 1 = 2$ spin-$\frac{1}{2}$ particles, as $\frac{1}{2} + \frac{1}{2} = 1$.

Let us consider a linear 1-D lattice consisting of N sites. Between each pair of sites, there is a valence bond. So each site will have two spin-half particles, leading to a pair of spin-1 particles. So if we have N number of spin-1 sites, that can be constructed using 2N number of spin-half particles.

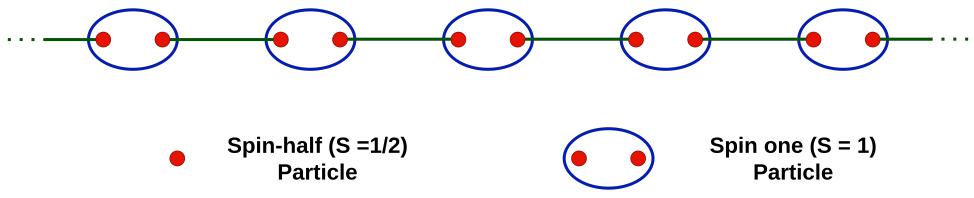

Figure 4: Ground State of AKLT Model

Unlike the dimerized state in Fig. 3, the state in Fig. 4 has unbroken translational symmetry.

Now we can construct the Hamiltonian for which this can be the ground state, also the presence of a valence bond between each neighboring pair implies that the total spin of such pairs cannot be 2.

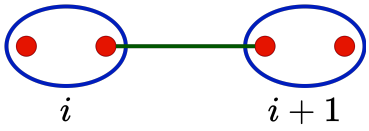

Figure 5: Neighboring Site Interaction

Let us try to understand the previous statement using the neighboring pair i and $i+1$ as shown in Fig. 5. Two of the spin-half particles are in the singlet state (particles connected by a green line). So the remaining two spin-half particles will combine to form the total spin S, as,

$$\begin{aligned} S &= |s_1 + s_2|, \cdots, |s_1 - s_2| \\ &= \left|\frac{1}{2} + \frac{1}{2}\right|, \cdots, \left|\frac{1}{2} - \frac{1}{2}\right| \end{aligned} \tag{6}$$

$$S = 1 \; and \; 0 \tag{7}$$

Hence, the pair of sites i and $i+1$ cannot have total spin S=2. Thus, we can choose our Hamiltonian to be the sum of projection operators onto Spin S=2 for each neighboring pair as,

$$\mathcal{H} = \sum_i P_2(\vec{S_i} + \vec{S}_{i+1}) \tag{8}$$

Now, one may think of a question: why didn't we choose projection operators onto spin S=$\frac{3}{2}$?

It is because the neighboring sites i and $i+1$ are S=1 particles, so $S_i = 1$ and $S_{i+1} = 1$. Hence, the outcomes for total spin are 2, 1, and 0. So the ground state, which is represented in Fig. 4 and Fig. 5, has to have a Hamiltonian made of projectors onto spin S=2. The eigenvalues of the projection operator P_2 are 0 and 1.

Now we try to find the expression of the projection operator P_2 in Eq. 8. As we know total spin operator for two neighboring spin sites ($S_i = 1$) can be written as,

$$\vec{S}_{tot} = \vec{S_i} + \vec{S}_{i+1} \tag{9}$$

$$X = \vec{S}_{tot}.\vec{S}_{tot} = S_{tot}^2 = \left(\vec{S_i} + \vec{S}_{i+1}\right)^2$$

$$X = S_{tot}^2 = \left(\vec{S_i} + \vec{S}_{i+1}\right)^2 \tag{10}$$

Now, we represent $S = 0$ state as $|0\rangle$, $S = 1$ state as $|1\rangle$ and $S = 2$ state as $|2\rangle$. If operator $X(S_{tot}^2)$ operates on spin state $|S\rangle$, then we observe,

$$X|S\rangle = S(S+1)|S\rangle \tag{11}$$

Using Eq. 11, we can calculate the following as,

$$X|0\rangle = 0(0+1)|0\rangle = 0|0\rangle \tag{12}$$

$$X|1\rangle = 1(1+1)|1\rangle = 2|1\rangle \tag{13}$$

$$X|2\rangle = 2(2+1)|2\rangle = 6|2\rangle \tag{14}$$

Hence, the matrix representation of X operator can be written as,

$$X = \begin{bmatrix} \langle 0|X|0\rangle & \langle 0|X|1\rangle & \langle 0|X|2\rangle \\ \langle 1|X|0\rangle & \langle 1|X|1\rangle & \langle 1|X|2\rangle \\ \langle 2|X|0\rangle & \langle 2|X|1\rangle & \langle 2|X|2\rangle \end{bmatrix}$$

$$X = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 6 \end{bmatrix} \tag{15}$$

Let us calculate the term $X(X-2I)$,

$$X(X-2I) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 6 \end{bmatrix} \begin{bmatrix} -2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 4 \end{bmatrix}$$

$$X(X-2I) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 24 \end{bmatrix} \tag{16}$$

From Eq. 16 we can write P_2 as,

$$P_2 = \frac{1}{24}X(X-2I) = \frac{1}{24}|2\rangle\langle 2| \tag{17}$$

Similarly, we can also calculate $(X-2I)(X-6I)$ as,

$$(X-2I)(X-6I) = \begin{bmatrix} -2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 4 \end{bmatrix} \begin{bmatrix} -6 & 0 & 0 \\ 0 & -4 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$(X-2I)(X-6I) = \begin{bmatrix} 12 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{18}$$

From Eq. 18 we can write P_0 as,

$$P_0 = \frac{1}{12}(X-2I)(X-6I) = \frac{1}{12}|0\rangle\langle 0| \tag{19}$$

Similarly, we can also calculate $X(X-6I)$ as,

$$X(X-6I) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 6 \end{bmatrix} \begin{bmatrix} -6 & 0 & 0 \\ 0 & -4 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$X(X-6I) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & -8 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{20}$$

From Eq. 20 we can write P_1 as,

$$P_1 = -\frac{1}{8}X(X-6I) = -\frac{1}{8}|1\rangle\langle 1| \tag{21}$$

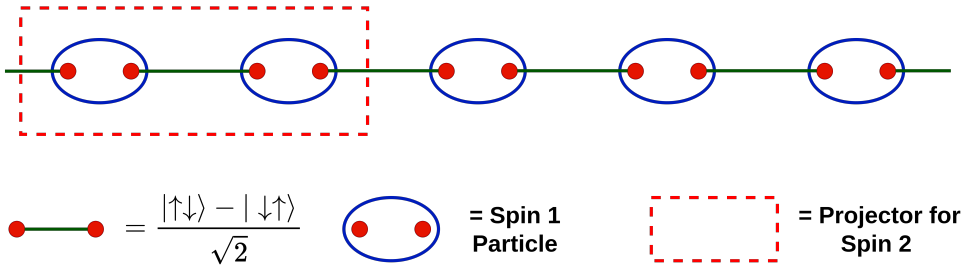

Figure 6: Ground State of AKLT Model

One can imagine the P_2 state as shown in Fig. 6. Now we calculate the algebraic expression of Eq. 17 as,

$$\begin{aligned} P_2 &= \frac{1}{24}[X^2 - 2X] \\ &= \frac{1}{24}[(\vec{S}_i + \vec{S}_j)^2(\vec{S}_i + \vec{S}_j)^2 - 2(\vec{S}_i + \vec{S}_j)^2] \\ &= \frac{1}{24}[(S_i^2 + S_j^2 + 2\vec{S}_i.\vec{S}_j)(S_i^2 + S_j^2 + 2\vec{S}_i.\vec{S}_j) - 2(S_i^2 + S_j^2 + 2\vec{S}_i.\vec{S}_j)] \end{aligned} \tag{22}$$

As we are working with spin $S = 1$, so $S_i^2 = 1(1+1) = 2$. So,

$$\begin{aligned} P_2 &= \frac{1}{24}[(2 + 2 + 2\vec{S}_i.\vec{S}_j)(2 + 2 + 2\vec{S}_i.\vec{S}_j) - 2(2 + 2 + 2\vec{S}_i.\vec{S}_j)] \\ &= \frac{1}{24}[(4 + 2\vec{S}_i.\vec{S}_j)(4 + 2\vec{S}_i.\vec{S}_j) - 2(4 + 2\vec{S}_i.\vec{S}_j)] \\ &= \frac{1}{24}[(16 + 16\vec{S}_i.\vec{S}_j + 4(\vec{S}_i.\vec{S}_j)^2) - (8 + 4\vec{S}_i.\vec{S}_j)] \\ &= \frac{1}{24}[8 + 12\vec{S}_i.\vec{S}_j + 4(\vec{S}_i.\vec{S}_j)^2] \\ &= \left[\frac{1}{3} + \frac{1}{2}(\vec{S}_i.\vec{S}_j) + \frac{1}{6}(\vec{S}_i.\vec{S}_j)^2\right] \end{aligned} \tag{23}$$

So, The Hamiltonian ($\mathcal{H}$) can be defined as,

$$\mathcal{H} = \sum_i \left[\frac{1}{3} + \frac{1}{2}\vec{S}_i.\vec{S}_{i+1} + \frac{1}{6}(\vec{S}_i.\vec{S}_{i+1})^2\right] \tag{24}$$

where $\vec{S}_i$ is a spin half operator acting on i^{th} spin, where $\vec{S}_i$ is defined as,

$$\vec{S}_i = S_i^x\hat{x} + S_i^y\hat{y} + S_i^z\hat{z} \tag{25}$$

where S_i^x, S_i^y and S_i^z are Spin components.

The constant term in the Hamiltonian will not affect the properties of the Hamiltonian; it will just shift the properties by some range so that we can take this term as a reference point. So, the Hamiltonian can be written as,

$$\mathcal{H} = \sum_i \left[\frac{1}{2}\vec{S}_i.\vec{S}_{i+1} + \frac{1}{6}(\vec{S}_i.\vec{S}_{i+1})^2\right] \tag{26}$$

Now, if we see carefully, there is a common factor of $\frac{1}{2}$ in both terms of the Hamiltonian, which will just scale the things and again not going to change the nature of the properties. So we can again take it common and neglect it. So the Hamiltonian will become,

$$\mathcal{H} = \sum_i \left[\vec{S}_i.\vec{S}_{i+1} + \frac{1}{3}(\vec{S}_i.\vec{S}_{i+1})^2\right] \tag{27}$$

Now, if each qubit has a spin angular momentum of half (i.e., $S = \frac{1}{2}$), this leads to a total spin angular momentum quantum number [4],

$$S = \begin{cases} 0 & \text{(singlet)} \\ 1 & \text{(triplet)} \end{cases}$$

We know,

$$\vec{S_1} \cdot \vec{S_2} = \frac{(S^2 - S_1^2 - S_2^2)}{2} \tag{28}$$

For the triplet case ($S = 1$),

$$\vec{S_1} \cdot \vec{S_2} = \left[\frac{1(1+1) - \frac{1}{2}(1+\frac{1}{2}) - \frac{1}{2}(1+\frac{1}{2})}{2}\right]\hbar^2 = \frac{1}{4}\hbar^2 \tag{29}$$

For the singlet case ($S = 0$),

$$\vec{S_1} \cdot \vec{S_2} = \left[\frac{0(0+1) - \frac{1}{2}(1+\frac{1}{2}) - \frac{1}{2}(1+\frac{1}{2})}{2}\right]\hbar^2 = -\frac{3}{4}\hbar^2 \tag{30}$$

Again, in terms of the Pauli spin matrix, we can write $\vec{S_1} = \frac{\hbar}{2}\vec{\sigma_1}$ and $\vec{S_2} = \frac{\hbar}{2}\vec{\sigma_2}$ [5]. This gives us,

$$\vec{\sigma_1} \cdot \vec{\sigma_2} = \frac{4}{\hbar^2}\vec{S_1} \cdot \vec{S_2} = \frac{4}{\hbar^2} \cdot \frac{1}{4}\hbar^2 = 1, \qquad \text{(for triplet)} \tag{31}$$

$$\vec{\sigma_1} \cdot \vec{\sigma_2} = \frac{4}{\hbar^2}\vec{S_1} \cdot \vec{S_2} = -\frac{4}{\hbar^2} \cdot \frac{3}{4}\hbar^2 = -3, \qquad \text{(for singlet)} \tag{32}$$

So let us rewrite our Hamiltonian in terms of Pauli Matrices,

$$\mathcal{H} = \frac{\hbar^2}{4}\sum_i \vec{\sigma}_i.\vec{\sigma}_{i+1} + \frac{1}{3}\left(\frac{\hbar^2}{4}\right)^2 \sum_i (\vec{\sigma}_i.\vec{\sigma}_{i+1})^2 \tag{33}$$

Now we can choose $\hbar$ as a unit, then our Hamiltonian becomes,

$$\mathcal{H} = \frac{1}{4}\sum_i \vec{\sigma}_i.\vec{\sigma}_{i+1} + \frac{1}{48}\sum_i (\vec{\sigma}_i.\vec{\sigma}_{i+1})^2 \tag{34}$$

If we simplify the Hamiltonian, it will look like this,

$$\mathcal{H} = \frac{1}{4}\sum_i (\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \sigma_i^z\sigma_{i+1}^z) + \frac{1}{48}\sum_i (\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \sigma_i^z\sigma_{i+1}^z)^2 \tag{35}$$

Since we know the spin for each particle, $\mathbf{s} = \frac{1}{2}$, we can calculate the number of basis states as

$$N = 2s + 1 \tag{36}$$

Substitute the value of $\mathbf{s}$ in Eq. 36, the total number of basis states will be 2. The basis states for this system are $|0\rangle$ and $|1\rangle$, which are the eigenvectors of σ_z with eigenvalues 1 and -1, respectively.

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{37}$$

In the Hamiltonian, for placing the lattice along different directions, we can use the fact that σ_i^α are spin

half operators acting on i^{th} spin, where σ^x, σ^y and σ^z are Pauli matrices,

$$\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma^y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{38}$$

and these Pauli matrices satisfy [6],

$$[\sigma_i^a, \sigma_j^b] = 2i\epsilon_{abc}\sigma_j^c\delta_{ij} \tag{39}$$

where, ϵ_{abc} is the Levi Civita symbol

$$\epsilon_{abc} = \begin{cases} +1 & \text{if (a,b,c)} \equiv \text{(1,2,3),(2,3,1),(3,1,2)} \\ -1 & \text{if (a,b,c)} \equiv \text{(3,2,1),(1,3,2),(2,1,3)} \\ 0 & \text{if a = b, b = c, c = a} \end{cases} \tag{40}$$

and, i and j represent the position of spin, and a,b, and c are the Pauli matrices (i.e. x, y, z).

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