Notes on the AKLT model and LSM theorem

W. Zhu[1]

[1] *Westlake Institute of Advanced Study,*

Westlake University, Hangzhou, P. C. China

Contents

In the case of 1D Heisenberg spin chains, the physics is especially interesting. We will focus on this problem in this chapter. For 1D Heisenberg model, there exists many famous exact solutions, and we will try to introduce one or two next. These exact solutions are quite important for the development of quantum magnetism and they outline the shape of quantum magnetism. So it is better to demonstrate some of these beautiful physics here.

A quite interesting story is, quantum spin chains develop some quite surprising differences between the cases of integer and half-integer spins. For half-integer spins $s = 1/2, 3/2, 5/2, ...$, we will see that quantum fluctuations destroy the long-range staggered magnetic order even at zero temperature. It turns out that the systems have gapless excitations, but they are not spin waves. On the other hand, for integer spin values $s = 1, 2, 3, ...$, the discreteness becomes relevant and the spin chain exhibits the so-called Haldane excitation gap. The origin of such a major qualitative difference is clearly revealed by a theorem by Lieb, Schultz, Mattis.

One may get more exact solutions based on the Bethe Ansatz and many others. In this course, we will neglect this part of discussion.

VALENCE BOND SOLID STATE

We discuss here a competing set of ground states to the Neel state, the valence bond states. Consider a state in which all atoms are in a singlet state with another atom, which we represent as a set of singlet bonds between sites (Fig. below). When the Heisenberg Hamiltonian acts on a pair of spins that are joined by a singlet, one finds $E = -J\frac{3}{4}$.

For a pair of spin half particles, the operator satisfy

$$S_iS_j = \frac{1}{2}[(S_i + S_j)^2 - S_i^2 - S_j^2] = \frac{1}{2}(S_{12}(S_{12} + 1) - \frac{1}{2}(\frac{1}{2} + 1) \times 2) \equiv \frac{1}{4} - P_{singlet} \quad (1)$$

where $P_{singlet}$ projects onto the singlet state. Here in spin-1/2 example, for singlet $S_{12} = 0$ while $S_{singlet} = 1$ for triplet.

The resonant valence bond state is a liquid, containing a superposition of all such states. The state is also called the quantum spin liquid. It turns out that in some situation this state could survive in the antiferromagnetic materials, but the experimental evidence remain elusive.

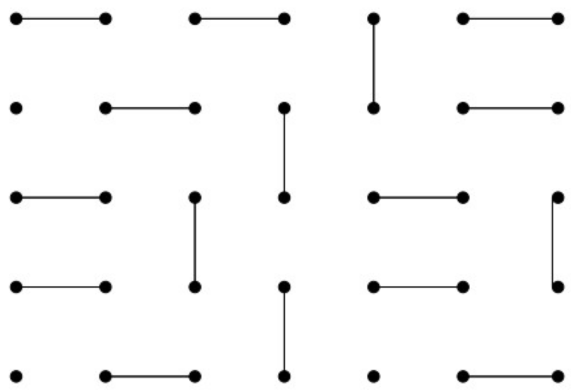


FIG. 1: The valence bond solid state.

Majumdar–Ghosh model

We introduce a second nearest-neighbor term in the spin chain model:

$$H^{MG} = J\sum_{i=1}^{N}(\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{2}\mathbf{S}_i \cdot \mathbf{S}_{i+2}) \tag{2}$$

Below we will show the ground state of this model is a dimer state or valence bond solid. The wave function is explicitly written as

$$|\psi_{\pm}\rangle = \prod_{n=1}^{N/2}(|\uparrow_{2n}\rangle|\downarrow_{2n\pm1}\rangle - |\downarrow_{2n}\rangle|\uparrow_{2n\pm1}\rangle)\frac{1}{\sqrt{2}} \tag{3}$$

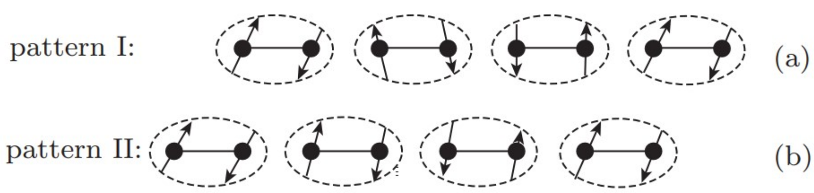
This is state is two-fold degenerated in 1D. The cartoon picture is as shown in Fig. **??**.

Let us rewrite the model as

$$\begin{aligned} H &= \frac{J}{2}\sum_{j}(\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \mathbf{S}_i \cdot \mathbf{S}_{i-1} + \mathbf{S}_{i-1} \cdot \mathbf{S}_{i+1}) \\ &= \frac{J}{4}\sum_{j}(\mathbf{S}_{i-1} + \mathbf{S}_{i+1} + \mathbf{S}_{i+1})^2 + const. \equiv= \frac{J}{4}\sum_{i}(\mathbf{J}_i)^2 \end{aligned} \tag{4}$$

where the total spin of a triad of spins at sites i is

$$\mathbf{J}_i = \mathbf{S}_{i-1} + \mathbf{S}_{i+1} + \mathbf{S}_{i+1} \tag{5}$$



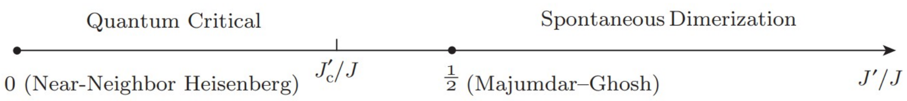


FIG. 2: Phase diagram of the $J - J'$ model, with nearest (J) and next-nearest (J') couplings of a spin-1/2 chain. The Majumdar–Ghosh (MG) model is a special point within the phase with spontaneous dimerization.

Its square has eigenvalues $J(J+1)$, where $J = 1/2, 3/2$.

The two exact ground states are made of nearest-neighbor pairs of spins forming singlets. The reason why they are exact ground states is the following. $\mathbf{J}_i$ is a sum of three-spin (in sequence) cluster terms, and the ground state of each term should have total spin-1/2 for the corresponding cluster. The two states of $|\psi_\pm\rangle$ have the property that, among each cluster of three neighboring spins, two of them form a singlet, guaranteeing that the total spin of the cluster is 1/2; they are thus the ground state of every term $\mathbf{J}_i$.

These singlet bonds formed by nearest neighbor spins are often called valence bonds (in analogy to the chemical bonds that are often referred to by the same name in chemistry), and such spontaneously dimerized states are also called valence bond solid (VBS).

In the Majumdar–Ghosh model the Lieb–Schultz–Mattis theorem (see below) is satisfied in a very unusual way: the ground state has double degeneracy, and higher exciations are gapped.

AKLT MODEL

In this section, we present detailed derivation of analytical results for AKLT model. We will demonstrate that, creating a boundary by cutting a valence bond in VBS state will lead to a fractional spin$-1/2$ forms near the boundary. We found that, despite the spatial oscillation due to the anti-ferromagnetic exchange, the spin magnetization exponentially decays to zero away from the boundary, which makes it available to define a edge spin localized in the vicinity of the boundary. Importantly, the net spin magnetization of edge spin is always quantized to fractional value.

We start from the well-known AKLT model[1], where the analytical solution will be important for the numerical results later on. The AKLT model placed on a open chain with

N sites can be described by

$$H_{AKLT} = \sum_{i=1}^{N-1} (\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 + \frac{2}{3}) = 2\sum_{i=1}^{N-1} P_{i,i+1}^{J=2} \tag{6}$$

where $\mathbf{S}$ is spin-1 operator. Each term $P_{i,i+1}^{J=2}$ projects the bond spin $\mathbf{J}_{i,i+1} = \mathbf{S}_i + \mathbf{S}_{i+1}$ onto the subspace of magnitude $J = 2$.

$$P_{i,i+1}^{J=2} \equiv \frac{1}{2}(\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \frac{1}{6}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 + \frac{1}{3} = \frac{1}{24} J_{i,i+1}^2 (J_{i,i+1}^2 - 2) \tag{7}$$

This operator annihilates total spin zero or one states, and gives unity on spin two states. If we introduce the basis of total spin states $|s_t, m_t\rangle$, where s_t is the total spin quantum number of $S_i + S_{i+1}$:

$$P^{J=2} = \sum_{m_t=-s_t,s_t} |2, m_t\rangle\langle 2, m_t| \tag{8}$$

Since Eq. 6 equivalent to spin projection operator, the exact zero energy ground state can be constructed accordingly. Here we utilize the Schwinger boson representation to express spin operators as $\hat{S}_j^+ = a_j^\dagger b_j$, $\hat{S}_j^z = \frac{1}{2}(a_j^\dagger a_j - b_j^\dagger b_j)$, where $a^\dagger$ and $b^\dagger$ satisfy the commutation relations $[a_j, a_j^\dagger] = [b_j, b_j^\dagger] = \delta_{ij}$ [2]. To reproduce the dimension of spin-1 Hilbert space at each site, we should impose the constraint that the total boson occupation number $a_j^\dagger a_j + b^\dagger b_j = 2$. With the help of Schwinger boson representation, the(un-normalized) ground state of Eq. 6 corresponds to a valence bond solid (VBS) of adjacent dimers (Fig. 3) [2]:

$$|\Phi_{VBS}\rangle = \prod_{\langle ij\rangle} (a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger)|0\rangle \tag{9}$$

We can show that

$$H_{AKLT}|\Phi_{VBS}\rangle = 0 \tag{10}$$

(Within the AKLT construction, it is the sum of the four spin 1/2s. Since two of them form a singlet, the possibility of $S = 2$ is eliminated, and S reduces to the sum of the remaining two spin-1/2s, thus $S = 0$ or 1.) Since, for each term in the AKLT model both $S = 0$ and $S = 1$ are ground states, the AKLT state is a ground state of the entire AKLT Hamiltonian.

There are two important properties of the VBS. First, the excitations are gapped, because breaking a singlet costs finite energy J. Second, the spin correlation is exponentially decay,

$$\langle \mathbf{S}_i \cdot \mathbf{S}_j\rangle \sim e^{-\frac{|i-j|}{\xi}}. \tag{11}$$

The proof needs the spin coherent state, as discussed below.

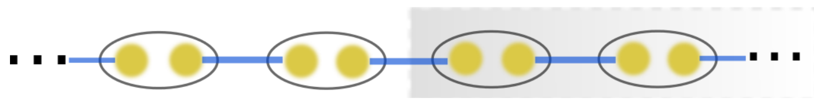


FIG. 3: Schematic plot of VBS as the exact ground state of spin-1 AKLT model. Each original spin-1 (black circle) is written as two spin$-1/2$ (yellow dot) in a triplet state. The ground state is then obtained by tensor product of singlet bonds (blue line) connecting nearest-neighbor adjacent spin$-1/2$, thus forming a crystalline pattern of valence bonds. Bipartitioning the chain into left and right part inevitably cuts one of valence bond, therefore two disentangled spin$-1/2$ spins form in the vicinity of the virtual boundary at the cut position.

Edge Spin of VBS state

Following the discussion in the main text, we consider the ground state of AKLT model in open boundary condition:

$$|\Phi_N(\alpha,\beta)\rangle = (a_1^\dagger)^{\frac{1}{2}+\alpha}(b_1^\dagger)^{\frac{1}{2}-\alpha}\prod_{i=1}^{N-1}(a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger)(a_N^\dagger)^{\frac{1}{2}+\beta}(b_N^\dagger)^{\frac{1}{2}-\beta}|0\rangle, \tag{12}$$

where α, β can be chosen as $\pm 1/2$, representing four-fold degenerate ground states with different boundary condition at site 1 and N. Using this wavefunction it is now straightforward to evaluate the magnetization on each site of the open chain. Next we perform the calculation on $|\Phi(\alpha = 1/2, \beta = 1/2)\rangle$ and the results for the other three ground states are similar.

First we noticed that $|\Phi\rangle$ is unnormalized so let us determine the normalization factor

$\langle\Phi|\Phi\rangle$:

$$\langle\Phi(\frac{1}{2},\frac{1}{2})|\Phi(\frac{1}{2},\frac{1}{2})\rangle = \langle 0|a_N\prod_{i=1}^{N-1}(a_ib_{i+1}-b_ia_{i+1})a_1a_1^\dagger\prod_{i=1}^{N-1}(a_i^\dagger b_{i+1}^\dagger-b_i^\dagger a_{i+1}^\dagger)a_N^\dagger|0\rangle$$
$$=\prod_{i=1}^{N}[\int\frac{2S+1}{4\pi}d\Omega_i]|u_1|^2|u_N|^2\prod_{i=1}^{N-1}[\frac{1-\Omega_i\cdot\Omega_{i+1}}{2}]$$
$$=\prod_{i=1}^{N}[\int\frac{2S+1}{4\pi}d\Omega_i]|u_1|^2|u_N|^2[4\pi\sum_{l_1=0}^{\infty}\frac{C_{l_1}}{2l_1+1}\sum_{m_1=-l_1}^{l_1}Y_{l_1,m_1}(\Omega_1)Y^*_{l_1,m_1}(\Omega_2)][4\pi\sum_{l_2=0}^{\infty}\frac{C_{l_2}}{2l_2+1}\sum_{m_2=-l_2}^{l_2}Y_{l_2,m_2}($$
$$...[4\pi\sum_{l_{N-1}=0}^{\infty}\frac{C_{l_{N-1}}}{2l_{N-1}+1}\sum_{m_{N-1}=-l_{N-1}}^{l_{N-1}}Y_{l_{N-1},m_{N-1}}(\Omega_{N-1})Y^*_{l_{N-1},m_{N-1}}(\Omega_N)]$$
$$=\frac{(2S+1)^N}{4\pi}\sum_{l_1,l_2,...,l_{N-1}}\frac{C_{l_1}}{2l_1+1}\frac{C_{l_2}}{2l_2+1}...\frac{C_{l_{N-1}}}{2l_{N-1}+1}\delta_{l_1,l_2}\delta_{l_2,l_3}...\delta_{l_{N-2},l_{N-1}}$$
$$=(2S+1)^N[C_0^{N-1}\frac{1}{4}+(\frac{C_1}{3})^{N-1}\frac{1}{4}\frac{1}{3}]=(2S+1)^N[\frac{1}{2^{N+1}}+(-)^{N-1}\frac{1}{2^{N+1}}\frac{1}{3^N}]$$

where we used

$$\int d\Omega\cos^2\frac{\theta}{2}Y_{l,m}(\Omega)=\int d\Omega\frac{1+\cos\theta}{2}Y_{l,m}(\Omega)=\frac{\sqrt{4\pi}}{2}\delta_{l=0}\delta_{m=0}+\frac{1}{2}\sqrt{\frac{4\pi}{3}}\delta_{l=1}\delta_{m=0} \qquad (13)$$

Next, with the help of the relation $\hat{S}=\int\frac{(S+1)(2S+1)}{4\pi}\hat{\Omega}|\Omega\rangle\langle\Omega|$, we calculate the magnetization at the site 1 (the last site N is equivalent):

$$\langle\Phi(\frac{1}{2},\frac{1}{2})|S_1^z|\Phi(\frac{1}{2},\frac{1}{2})\rangle=\langle\Phi(\frac{1}{2},\frac{1}{2})|\int\frac{(S+1)(2S+1)}{4\pi}\Omega_1^z|\Omega_1\rangle\langle\Omega_1||\Phi(\frac{1}{2},\frac{1}{2})\rangle$$
$$=(S+1)\prod_{i=1}^{N}[\int\frac{(2S+1)}{4\pi}\Omega_i^z]|u_1|^2|u_N|^2\Omega_1\prod_{i=1}^{N-1}[\frac{1-\Omega_i\cdot\Omega_{i+1}}{2}]$$
$$=(S+1)\prod_{i=1}^{N}[\frac{2S+1}{4\pi}d\Omega_i]|u_1|^2|u_N|^2\Omega_1[4\pi\sum_{l_1=0}^{\infty}\frac{C_{l_1}}{2l_1+1}\sum_{m_1=-l_1}^{l_1}Y_{l_1,m_1}(\Omega_1)Y^*_{l_1,m_1}(\Omega_2)][4\pi\sum_{l_2=0}^{\infty}\frac{C_{l_2}}{2l_2+1}\sum_{m_2=-l_2}^{l_2}$$
$$...[4\pi\sum_{l_{N-1}=0}^{\infty}\frac{C_{l_{N-1}}}{2l_{N-1}+1}\sum_{m_{N-1}=-l_{N-1}}^{l_{N-1}}Y_{l_{N-1},m_{N-1}}(\Omega_{N-1})Y^*_{l_{N-1},m_{N-1}}(\Omega_N)]$$
$$=(S+1)\frac{(2S+1)^N}{4\pi}\sum_{l_1,l_2,...,l_{N-1}}\frac{C_{l_1}}{2l_1+1}\frac{C_{l_2}}{2l_2+1}...\frac{C_{l_{N-1}}}{2l_{N-1}+1}\delta_{l_1,l_2}\delta_{l_2,l_3}...\delta_{l_{N-2},l_{N-1}}$$
$$=(S+1)(2S+1)^N[\frac{1}{2^{N+1}}\frac{1}{3}+(-)^{N-1}\frac{1}{2^{N+1}}\frac{1}{3^N}]=(2S+1)^N[\frac{1}{2^{N+1}}\frac{2}{3}+2(-)^{N-1}\frac{1}{2^{N+1}}\frac{1}{3^N}]$$

where we used the relations Eq. 13 and

$$
\begin{aligned}
&\int d\Omega \cos^2\frac{\theta}{2}\cos\theta Y_{l,m}(\Omega) = \int d\Omega \frac{1+\sqrt{\frac{4\pi}{3}}Y_{10}(\Omega)}{2}\sqrt{\frac{4\pi}{3}}Y_{10}(\Omega)Y_{l,m}(\Omega) \\
&= \frac{1}{2}[\sqrt{\frac{4\pi}{3}}\delta_{l=1}\delta_{m=0} + \sqrt{\frac{4\pi}{3}}\sqrt{\frac{4\pi}{3}}\sqrt{\frac{3*3*(2l+1)}{4\pi}}\begin{pmatrix} 1 & 1 & l \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & l \\ 0 & 0 & m \end{pmatrix}] \\
&= \frac{1}{2}[\sqrt{\frac{4\pi}{3}}\delta_{l=1}\delta_{m=0} + \frac{\sqrt{4\pi}}{3}\delta_{l=0}\delta_{m=0} + (l \geq 2)]
\end{aligned} \tag{14}
$$

Finally, we have

$$
\begin{aligned}
\langle S_1^z \rangle = \frac{\langle \Phi(\frac{1}{2},\frac{1}{2})|S_1^z|\Phi(\frac{1}{2},\frac{1}{2})\rangle}{\langle \Phi(\frac{1}{2},\frac{1}{2})|\Phi(\frac{1}{2},\frac{1}{2})\rangle} &= \frac{(2S+1)^N[\frac{1}{2^{N+1}}\frac{2}{3} + 2(-)^{N-1}\frac{1}{2^{N+1}}\frac{1}{3^N}]}{(2S+1)^N[\frac{1}{2^{N+1}} + (-)^{N-1}\frac{1}{2^{N+1}}\frac{1}{3^N}]} \\
&= \frac{\frac{2}{3} + 2(-)^{N-1}\frac{1}{3^N}}{1 + (-)^{N-1}\frac{1}{3^N}}
\end{aligned} \tag{15}
$$

Furthermore, we can proof the general expression for any site i:

$$
\langle S_i^z \rangle = (-)^{i-1}\frac{\frac{2}{3}(\frac{1}{3})^{i-1} + 2(-)^{N-1}\frac{1}{3^N}3^{i-1}}{1 + (-)^{N-1}\frac{1}{3^N}} \tag{16}
$$

Hence, in the thermodynamic limit we have two important observations. First, the spin magnetization has the real space distribution as

$$
\langle S_i^z \rangle \rightarrow \frac{2}{3}(-\frac{1}{3})^{i-1} = (-)^{i-1}\frac{2}{3}e^{-(i-1)\ln 3} \tag{17}
$$

This explicitly shows that the spin magnetization is decreasing exponentially away from the boundary of the chain with a length scale equal to $\xi = \ln 3$, which is consistent with the correlation length in the bulk (using periodic boundary condition). This leads to the picture that emergent spin is localized near the open boundary therefore we can define the emergent spin near the boundary as the edge spin. Second, the total net spin magnetization of edge spin is

$$
\Delta S^z|_{edge} = \lim_{N\rightarrow\infty}\sum_{i\in edge}\langle S_i^z\rangle \rightarrow \sum_i \frac{2}{3}(-\frac{1}{3})^{i-1} = \frac{1}{2} \tag{18}
$$

Spin Coherent State

In order to calculate the quantities using AKLT wavefunction, it is convenient to introduce the concept of spin coherent state [2]. Spin coherent states are a family of spin states created by applying the rotation operator R to the maximally polarized state $|S,S\rangle$:

$$|\hat{\Omega}\rangle = R(\theta,\phi)|S,S\rangle = e^{iS^z\phi}e^{iS^y\theta}|S,S\rangle \tag{19}$$

where the unit vector $\hat{\Omega} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ parametrizes the spin coherent state. $\theta \in [0,\pi]$ is the latitude and $\phi \in [-\pi,\pi]$ is longitude.

We introduce two schwinger bosons to represent the spin operators as follows:

$$S^+ = a^+b, S^- = b^+a, S^z = \frac{1}{2}(a^+a - b^+b) \tag{20}$$

The spin magnitude S defines the physical subspace

$$n_a + n_b = 2S. \tag{21}$$

The spin states are given by

$$|S,m\rangle = \frac{(a^+)^{S+m}}{\sqrt{(S+m)!}}\frac{(b^+)^{S-m}}{\sqrt{(S-m)!}}|0\rangle \tag{22}$$

where S, m respectively labels the $\mathbf{S}^2$ and S^z eigenvalues, $|0\rangle$ is the Schwinger bosons vaccuum. For example, the spin-1/2 states are given in the second quantized notation as

$$|\uparrow\rangle = a^+|0\rangle, |\downarrow\rangle = b^+|0\rangle \tag{23}$$

For spin-1 states are :

$$|\uparrow\rangle \sim a^+a^+|0\rangle, |\downarrow\rangle \sim b^+b^+|0\rangle, |0\rangle \sim a^+b^+|0\rangle \tag{24}$$

Schwinger bosons are useful for calculating matrix elements of spin operators. Under the rotation operation,

$$\begin{pmatrix} (a')^+ \\ (b')^+ \end{pmatrix} = R \begin{pmatrix} a^+ \\ b^+ \end{pmatrix} R^{-1} = e^{iS^y\theta}e^{iS^z\phi}\begin{pmatrix} a^+ \\ b^+ \end{pmatrix} = \begin{pmatrix} u & v \\ -v^* & u^* \end{pmatrix}\begin{pmatrix} a^+ \\ b^+ \end{pmatrix} \tag{25}$$

where

$$u = \cos\frac{\theta}{2}e^{i\frac{\phi}{2}}, v = \sin\frac{\theta}{2}e^{-i\frac{\phi}{2}}. \tag{26}$$

Next we introduce the spin coherent state wave function:

$$|\hat{\Omega}\rangle \equiv \frac{(ua^\dagger + vb^\dagger)^{2S}}{\sqrt{(2S)!}}|0\rangle = \sqrt{(2S)!}\sum_m \frac{u^{S+m}v^{S-m}}{\sqrt{(S+m)!(S-m)!}}|S,m\rangle, \tag{27}$$

and for a point $\Omega = (\theta, \phi)$ on the unit sphere. Here we have already fixed the $U(1)$ gauge degree of freedom since it has no physical content. The spin coherent state defined this way satisfies several useful conditions (leaving for homework), such as

$$\hat{\Omega}\cdot\hat{S}|\hat{\Omega}\rangle = S|\hat{\Omega}\rangle, \tag{28}$$

$$\langle 0|a^{S+l}b^{S-l}|\hat{\Omega}\rangle = \sqrt{(2S)!}u^{S+l}v^{S-l}, \tag{29}$$

and the completion relation

$$\int \tfrac{(2S+1)d\hat{\Omega}}{4\pi}|\Omega\rangle\langle\Omega| \tag{30}$$

$$= \tfrac{(2S+1)}{2}\int_{-1}^{1} d(\cos\theta)\sum_m (\tfrac{1+\cos\theta}{2})^{S+m}(\tfrac{1-\cos\theta}{2})^{S-m}\tfrac{(2S)!}{(S+m)!(S-m)!}|S,m\rangle\langle S,m| \tag{31}$$

$$= \sum_m |S,m\rangle\langle S,m| = 1. \tag{32}$$

Taking the advantage of spin coherent representation, we can calculate the quantities using the ground state of AKLT model. For example, the normalization factor of the ground state of AKLT model is obtained by:

$$\begin{aligned} N_0 &= \langle VBS|VBS\rangle = \langle VBS|\prod_i[\int \frac{(2S+1)d\hat{\Omega}_i}{4\pi}]|\Omega_i\rangle\langle\Omega_i||VBS\rangle \\ &= \prod_i\int \frac{(2S+1)d\hat{\Omega}_i}{4\pi}|u_iv_{i+1} - v_iu_{i+1}|^2 \\ &= \prod_i\int \frac{(2S+1)d\hat{\Omega}_i}{4\pi}[\frac{1-\hat{\Omega}_i\cdot\hat{\Omega}_{i+1}}{2}]. \end{aligned} \tag{33}$$

To explicitly complete the integral, we need the relation

$$\begin{aligned} &\frac{1-\hat{\Omega}_i\cdot\hat{\Omega}_j}{2} = \frac{1}{2} - \frac{1}{4}(\Omega_i^\dagger\Omega_j^- + \Omega_i^-\Omega_j^\dagger) + \frac{1}{2}\Omega_i^z\Omega_j^z \\ &= 4\pi[\frac{1}{2}Y_{00}(\hat{\Omega}_i)Y_{00}^*(\hat{\Omega}_j) - \frac{1}{6}Y_{1,-1}(\hat{\Omega}_i)Y_{1,-1}^*(\hat{\Omega}_j) - \frac{1}{6}Y_{1,0}(\hat{\Omega}_i)Y_{1,0}^*(\hat{\Omega}_j) - \frac{1}{6}Y_{1,1}(\hat{\Omega}_i)Y_{1,1}^*(\hat{\Omega}_j)] \\ &= 4\pi\sum_{l=0}^{\infty}\frac{C_l}{2l+1}\sum_{m=-l}^{l}Y_{l,m}(\hat{\Omega}_i)Y_{l,m}^*(\hat{\Omega}_j) \end{aligned}$$

and

$$C_0 = \frac{1}{2}, C_1 = -\frac{1}{2}, C_{k>1} = 0. \tag{34}$$

Here we also introduced the spherical harmonics function $Y_{l,m}(\mathbf{\Omega})$:

$$Y_{0,0}(\mathbf{\Omega}) = \frac{1}{\sqrt{4\pi}}, Y_{1,-1}(\mathbf{\Omega}) = \sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi}, Y_{1,0}(\mathbf{\Omega}) = \sqrt{\frac{3}{4\pi}}\cos\theta, Y_{1,1}(\mathbf{\Omega}) = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\phi} \tag{35}$$

In the integral calculation, the orthogonal relation will be very helpful:

$$\int d\hat{n} Y_{l,m}(\hat{\Omega}) Y^*_{l',m'}(\hat{\Omega}) = \delta_{l,l'}\delta_{m,m'} \tag{36}$$

LIEB-SCHULTZ-MATTIS THEOREM

The original Lieb–Schultz–Mattis theorem states that, for half-integer antiferromagnetic chain, the separation between the ground and first excited state energies, $|E_1 - E_0|$, vanishes in the thermodynamic limit.

The generalized LSM theorem: For a lattice model with half-odd-spin in each unit cell, the ground state is either gapless or gapped with degeneracy. So the gapped paramagnet without degeneracy is impossible.

This theorem is very helpful in the study of spin liquid. That is, for spin-1/2 lattice like triangular and kagome, the ground state could be:

- Gapless: 1) magnetic order with spin rotation symmetry spontaneously broken; or 2) gapless spin liquid.
- Gapped: 1) Valence-bond solid with lattice symmetry spontaneously broken; or 2) Gapped spin liquid.

Fermion system

The physical picture is the following.

Let us consider a 1D spinless Hubbard model with periodic boundary condition ($c_L \equiv c_0$):

$$H = t \sum_j (c_j^+ c_{j+1} + h.c.) + V \sum_j n_j n_{j+1} \tag{37}$$

Translation operator T commutes with the Hamiltonian,

$$T c_j T^{-1} = c_{j+1}, [T, H] = 0 \tag{38}$$

Question: How to write down the operator form of T?

Suppose the ground state is $H|\Psi_0\rangle = E_0|\Psi_0\rangle$, where $|\Psi_0\rangle$ is very complicated but we don't need to know it exactly.

This model has a continuous $U(1)$ symmetry, which means the total number of particles is conserved:

$$e^{i\theta N} = e^{i\theta \sum_j n_j} \tag{39}$$

Next we introduce an operator U which is defined as

$$U = \exp(\sum_j \frac{2\pi i j}{L} n_j) \tag{40}$$

By applying it to electron operator

$$U^+ c_j U = c_j e^{2\pi i j/L} \tag{41}$$

This is operator consistent with the periodic boundary condition

$$U^+ c_0 U = c_0, U^+ c_L U = c_L \tag{42}$$

Next we calculate the following quantity

$$U^+ H U = t \sum_j (e^{-2\pi i/L} c_j^+ c_{j+1} + e^{2\pi i/L} c_j c_{j+1}^+) + V \sum_j n_j n_{j+1} \tag{43}$$

$$\Rightarrow U^+ H U - H = t\frac{2\pi}{L} \sum_j (c_j^\dagger c_{j+1} - c_{j+1}^\dagger c_j) + t(\frac{2\pi}{L})^2 \sum_j (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) + ... \tag{44}$$

After the average, we have

$$\langle \Psi_0 | U^+ H U - H | \Psi_0 \rangle = O(\frac{1}{L}) \tag{45}$$

The reason is as following. $i(c_j^\dagger c_{j+1} - c_{j+1}^\dagger c_j)$ is the current operator. In a time-reversal symmetric system, the stable ground state should not take any current, so it must vanish.

Does it mean anything?

$$\langle \Psi_0 | U^+ H U - H | \Psi_0 \rangle \equiv E_U - E_0 = O(\frac{1}{L}) \tag{46}$$

which means the state $U|\Psi_0\rangle$ has almost the same energy with the ground state $|\Psi_0\rangle$, i.e. the system is gapless.

Here there is a loop-hole, we need to exclude a trivial case: $T|\Psi_0\rangle = e^{ig}|\Psi_0\rangle$.

Say, the ground state takes momentum $T|\Psi_0\rangle = e^{iP_0}|\Psi_0\rangle$. So,

$$U^+ T U = e^{i2\pi \sum_j n_j / L} T = e^{2\pi \nu i} T \tag{47}$$

where the filling factor $\nu = \frac{\sum_j n_j}{L} = \frac{N}{L}$. We can deduce that

$$T(U|\Psi_0\rangle) = e^{iP_0 + 2\pi i \nu} U|\Psi_0\rangle \tag{48}$$

If ν is not integer, $|\Psi_0\rangle$ and $U|\Psi_0\rangle$ are different states, because they take different quantum numbers.

Next we have the LSM theorem as following: A quantum many-body system in 1D with global U(1) symmetry and lattice translation symmetry, at a fractional (non-integer) filling factor ν, the system should be gapless excitations above the ground state, or degenerate ground states below gap. A trivial insulator/paramagnet with a single ground state is forbiden.

Spin-1/2 system

Next we go to prove the LSM theorem in spin-1/2 system. We try to elucidate this theorem in one-dimensional spin-1/2 anti-ferromagnetic chain:

$$H = \sum_{\langle ij \rangle} S_i^z S_j^z + \frac{1}{2}(S_i^+ S_j^- + h.c.) \tag{49}$$

Suppose the ground state is $H|\Psi_0\rangle = E_0|\Psi_0\rangle$, where $|\Psi_0\rangle$ is very complicated but we don't need to know it exactly. Since it is antiferromagnetic model, the ground state should have $\sum_n S_n^z = 0$.

We define two operators first. The first operator is translation operator T. Translation operator T commutes with the Hamiltonian,

$$TS_jT^{-1} = S_{j+1}, [T, H] = 0. \tag{50}$$

We assume the eigenvalue of translational operation is

$$T\Psi_0 = e^{ig}\Psi_0 \tag{51}$$

The second operator is U_k for $k = 2\pi/L$:

$$U_k \equiv \exp(ik \sum_n nS_n^z). \tag{52}$$

Here operator U is very important. It has a non-trivial commutation relation with T:

$$TU_kT^{-1} = \exp(ik \sum_n nS_{n+1}^z) = U_k \exp(ikNS_1^z) \exp(-ik \sum_n S_n^z) = -U_k \exp(-ik \sum_n S_n^z) \tag{53}$$

where we used the condition $e^{i2\pi S_1^z} = e^{i\pi\sigma_z} = I\cos\pi + i\sin\pi\sigma_z = -I$. Please note that, this condition can be generalized to

$$e^{i2\pi S^z} = \begin{cases} -1, S = \frac{1}{2}, \frac{3}{2}, ... \\ 1, S = 1, 2, ... \end{cases} \tag{54}$$

So the half-integer spin is different from the integer spin. In the half-integer spin we have the orthogral condition for the following state $|\Psi_k\rangle$, but not for integer spin.

Next we consider the state

$$\Psi_k = U_k\Psi_0 = \exp(ik\sum_n nS_n^z)\Psi_0 \tag{55}$$

where $k = 2\pi/N$.

We first prove that Ψ_k is orthogonal to the ground state:

$$\langle\Psi_0|\Psi_k\rangle = \langle\Psi_0|U_k|\Psi_0\rangle = \langle\Psi_0|TU_kT^{-1}|\Psi_0\rangle = -\langle\Psi_0|U_k|\Psi_0\rangle = -\langle\Psi_0|\Psi_k\rangle \tag{56}$$

where we used the condition for $\sum_n S_n^z = 0$ for the ground state. So it must be vanish, which is the orthogonal condition for Ψ_0 and Ψ_k.

$$\langle\Psi_0|\Psi_k\rangle = -\langle\Psi_0|\Psi_k\rangle = 0 \tag{57}$$

Next we calculate the energy difference between Ψ_k and Ψ_0. We need the following relations

$$U_k^{-1}S_n^xU_k = S_n^x\cos(kn) + S_n^y\sin(kn) \tag{58}$$

$$U_k^{-1}S_n^yU_k = -S_n^x\sin(kn) + S_n^y\cos(kn) \tag{59}$$

$$U_k^{-1}S_n^zU_k = S_n^z \tag{60}$$

which lead to

$$\begin{aligned} &U_k^{-1}S_n^xS_{n+1}^xU_k = (S_n^x\cos(kn) + S_n^y\sin(kn))(S_{n+1}^x\cos(k(n+1)) + S_{n+1}^y\sin(k(n+1))) \\ &= S_n^xS_{n+1}^x\cos(kn)\cos(k(n+1)) + S_n^yS_{n+1}^y\sin(kn)\sin(k(n+1)) \\ &+ S_n^yS_{n+1}^x\sin(kn)\cos(k(n+1)) + S_n^xS_{n+1}^y\cos(kn)\sin(k(n+1)) \end{aligned} \tag{61}$$

$$\begin{aligned} &U_k^{-1}S_n^yS_{n+1}^yU_k = (-S_n^x\sin(kn) + S_n^y\cos(kn))(-S_{n+1}^x\sin(k(n+1)) + S_{n+1}^y\cos(k(n+1))) \\ &= S_n^xS_{n+1}^x\sin(kn)\sin(k(n+1)) + S_n^yS_{n+1}^y\cos(kn)\cos(k(n+1)) \\ &- S_n^yS_{n+1}^x\cos(kn)\sin(k(n+1)) - S_n^xS_{n+1}^y\sin(kn)\cos(k(n+1)). \end{aligned} \tag{62}$$

We find

$$
\begin{aligned}
&\langle\Psi_k|H|\Psi_k\rangle = \langle\Psi_0|U_k^{-1}HU_k|\Psi_0\rangle \\
&= \langle\Psi_0|H + (\cos(k)-1)\sum_n(S_n^xS_{n+1}^x + S_n^yS_{n+1}^y) + \sin(k)\sum_n(S_n^xS_{n+1}^y - S_n^yS_{n+1}^x)|\Psi_0\rangle \\
&= E_0 + (-\frac{1}{2}(\frac{2\pi}{N})^2 - O(N^{-4}))\langle\Psi_0|\sum_n(S_n^xS_{n+1}^x + S_n^yS_{n+1}^y)|\Psi_0\rangle + \sin(k)\langle\Psi_0|\sum_n(S_n^xS_{n+1}^y - S_n^yS_{n+1}^x)|\Psi_0\rangle \\
&\leq E_0 + \frac{2\pi^2}{N}\times const.
\end{aligned}
\tag{63}
$$

The second term must have zero expectation in the ground state. The reason is as following. The definition of x, y could be switched, $S^x \to S^y, S^y \to S^x$. Under this rotation, the second term is odd, changing a sign, which means that it should vanish due to the symmetry reason. In the first term, the sum $\sum_n$ gives an order N, which cancels a factor of N in the final result.

To sum up, the energy gap vanishes if the chain is infinite long ($N \to \infty$).

For spin-1/2 chain, there are many interesting stories. For example, here we introduce the famous *Marshall theorem*, which states that the ground state of spin-1/2 anti-ferromagnetic chain has the same sign for all basis.

We consider the one-dimensional spin-1/2 anti-ferromagnetic chain:

$$H = \sum_{\langle ij\rangle} S_i^zS_j^z + \frac{1}{2}(S_i^+S_j^- + h.c.) \tag{64}$$

On all even sites, we make a canonical transformation ($S_j^x \to -S_j^x$, $S_j^y \to -S_j^y$, $S_j^z \to S_j^z$),

$$H' = \sum_{\langle ij\rangle} S_i^zS_j^z - \frac{1}{2}(S_i^+S_j^- + h.c.) \tag{65}$$

H' and H should take the same properties.

Since $[S^z, H] = 0$, let us consider only states with $S^z = 0$ next. A complete set of states in this subspace have configurations (Φ_μ) with $N/2$ spin-ups and $N/2$ spin downs. The general wave function can be expressed as

$$\Psi = \sum_\mu c_\mu\Phi_\mu, \tag{66}$$

and the coefficients c_μ satisfy the equations

$$(E-\epsilon_\mu)c_\mu = \frac{1}{2}\sum_{\nu(\mu)} c_\nu, (\epsilon_\mu \Phi_\mu = \sum_{ij} S_i^z S_j^z \Phi_\mu) \tag{67}$$

Without loss of generality, we take c_μ as real numbers.

Next we need to proof the following lemma-1: For any ground state with $S^z = 0$, all $c_\mu \neq 0$. The proof is as following. Suppose the contrary, i.e. for some ground state Ψ_0 having the ground state energy E_0,

$$c_{\mu_1,\mu_2,\ldots,\mu_p} = 0. \tag{68}$$

We get the Schrodinger equations

$$0 = \frac{1}{2}\sum_{\nu(\mu)} c_\nu \tag{69}$$

At least one of these equations have none trivial solution with $c_\nu \neq 0$; therefore it implies that there are nonzero coefficients c_μ with both signs. Next we consider a trial function Ψ_0':

$$\Psi_0' = \sum_\mu |c_\mu| \Phi_\mu \tag{70}$$

On the one hand, Ψ_0' is not an eigenstate because

$$|c_{\mu_{1,2,\ldots,p}}| = 0 \texttt{but} 0 \neq \frac{1}{2}\sum_{\nu(\mu)} c_\nu \tag{71}$$

Due to the variational principle, we have for its energy

$$E_0' > E_0 \tag{72}$$

On the other hand, explicit evaluation gives

$$E_0' = \sum_\mu \epsilon_\mu c_\mu^2 - \frac{1}{2}\sum_{\mu\nu} |c_\mu||c_\nu| \tag{73}$$

$$E_0 = \sum_\mu \epsilon_\mu c_\mu^2 - \frac{1}{2}\sum_{\mu\nu} c_\mu c_\nu \tag{74}$$

from which it follows that

$$E_0' \leq E_0. \tag{75}$$

Here the condition $E_0' \leq E_0$ contradicts with $E_0' > E_0$. Thus the original suppose is incorrect. So lemma-1 is correct.

Next we will have the lemma-2: For every ground state with $S^z = 0$, all c_μ have the same sign.

This comes from Eq. 73 directly. The equality sgn is only achieved by the ground state itself. This occurs if and only if, all terms $c_\mu c_{\mu'}$ are positive.

It is now obvious that there can be only one ground state with $S^z = 0$; otherwise, the several states would all have all positive coefficients and so could not be orthogonal to one another.

HALDANE CONJECTURE

Based on the above examples, Haldane conjectured that spin-$1/2, 3/2, ...$ chains are gapless, but the spin-$1, 2, 3...$ are gapped. The discussion will be presented elsewhere.

Homework: Please prove the following relations using the spin coherent state:

$$\hat{\Omega} \cdot \hat{S}|\hat{\Omega}\rangle = S|\hat{\Omega}\rangle, \tag{76}$$

$$\langle 0|a^{S+l}b^{S-l}|\hat{\Omega}\rangle = \sqrt{(2S)!}u^{S+l}v^{S-l}, \tag{77}$$

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