AKLT

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References

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1 Motivation

Spin chains have been studied extensively in condensed matter physics. The simplest and most well-known example is that of the spin-1/2 Heisenberg model, given by

$$H = J \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1}, \tag{1}$$

with $J > 0$, the solution of which was essentially given by Hans Bethe (1931). The antiferromagnet exhibits a gapless spectrum in the the thermodynamic limit and power-law correlations. Specifically, the quantum fluctuations are significant enough to wipe out Néel order.

Are power-law correlations and a gapless spectrum generic of spin chains?

1.1 Lieb-Schultz-Mattis theorem

This important theorem shows that for any half-odd-integer S spin chain with a reasonably local Hamiltonian satisfying translational and rotational invariance, that either

- the spectrum has zero gap i.e. is massless

- the ground state is degenerate i.e. spontaneously breaks parity (site-reflection).

Consider a finite chain of even length L and periodic boundary conditions. We denote one of potentially many ground states byt $|\psi_0\rangle$, respecting parity and rotational invariance. The key point of the proof is to construct a state $|\psi_1\rangle$ which is orthogonal to $|\psi_0\rangle$ and has a low expectation energy i.e.

$$\langle\psi_1|\psi_0\rangle = 0, \qquad \langle\psi_1|(H - E_0)|\psi_1\rangle = \mathcal{O}(L^{-1}), \tag{2}$$

with $H|\psi_0\rangle = E_0|\psi_0\rangle$. $|\psi_1\rangle$ may or may not be an eigenstate, but if we can satisfy (2) then such an eigenstate does exist. Labelling the sites from $-L/2, \cdots L/2 - 1$, we define the unitary operator

$$U = \exp\left[\frac{i\pi}{l}\sum_{j=-l}^{l}(j+l)S_j^z\right], \qquad |\psi_1\rangle = U|\psi_0\rangle. \tag{3}$$

This operator creates a 2π twist of spins about the z-axis over a length $2l+1$. We take l to be $\mathcal{O}(L)$. We must now show that the two criteria of (2) are satisfied. Due to the assumed rotational symmetry, a uniform twist over the entire chain is cost-free and therefore we expect a slow twist to be cheap, so for $|i| \leq |l|$

$$\begin{aligned} U^\dagger S_i^\pm U &= e^{-i\pi/l(l+i)[S_i^z,\ ]}S_i^\pm = e^{\pm\frac{i\pi}{l}(i+l)}, \\ U^\dagger S_i^+ S_{i+1}^- U &= e^{-i\pi/l}S_i^+ S_{i+1}^-. \end{aligned} \tag{4}$$

Considering the Heisenberg chain for illustrative purposes

$$\begin{aligned} \delta E &= \langle\psi_1|(H - E_0)|\psi_1\rangle, \\ &= \frac{J}{2}\langle\psi_0|\sum_i\left[(e^{-i\pi/l}-1)S_i^+S_{i+1}^- + (e^{i\pi/l}-1)S_i^-S_{i+1}^+\right]|\psi_0\rangle. \end{aligned} \tag{5}$$

If the system is parity-invariant, we can write

$$\begin{aligned} \delta E &= J\,(\cos\pi/l - 1)\sum_i\langle\psi_0|S_i^+S_{i+1}^-|\psi_0\rangle, \\ &\sim e_0 l(\cos\pi/l - 1) = \mathcal{O}(l^{-1}). \end{aligned} \tag{6}$$

This easily generalises to a large number of local Hamiltonians i.e. δE will be the expectation value of a local operator times a quantity of $\mathcal{O}(l^{-1})$.

So far, we haven't relied on any properties of the particular representation of SU(2), but we still need that $\langle\psi_1|\psi_0\rangle = 0$, otherwise we may still have that, as $l \to \infty$, $|\psi_1\rangle \to |\psi_0\rangle$, which will tell us very little. The orthogonality is simply implied by the parity of the two states being opposite. Specifically, we take the twist operation of (3) and combine this with $S_i^z \to -S_{-i}^z$ i.e.

$$U = \exp\left[\frac{i\pi}{l}\sum_{j=-l}^{l}(j+l)S_j^z\right], \qquad |\psi_1\rangle = U\exp\left[-2\pi i\sum_{j=-l}^{l}S_j^z\right]|\psi_0\rangle \tag{7}$$

The energy of this new $|\psi_1\rangle$ is unchanged but, as the sum contains an *odd* number of spins, the exponential simply reduces to $2\pi i(n-s)$ $n \in \mathbb{Z}$. Therefore, for s integer/half-odd integer, $|\psi_1\rangle$ is parity even/odd respectively, relative to the ground state. Hence, for half-odd integer, both of the criteria are satisfied.

This means that as $L \to \infty$, there may be a gapless, particle-like excitation with negative parity, *or* parity may be spontaneously broken with two ground states and a gap above each. An example of this is dimer configurations e.g. $|\psi\rangle = |\alpha_1, \alpha_2, \alpha_3, \alpha_4, \cdots\rangle \varepsilon^{\alpha_1,\alpha_2}\varepsilon^{\alpha_3,\alpha_4}\cdots$.

1.2 Haldane conjecture

This proof can be made more rigorous, but still only holds for half-odd integer spin chains. What about generic integer spin chains? For large spins, one can map such spin chains onto an O(3) non-linear sigma model. From this, Haldane conjectured that the Heisenberg antiferromagnet is *gapped* for integer spin, but not for half-odd integer spin.

2 Majumdar-Ghosh model

A natural extension to the spin-1/2 Heisenberg model is the J_1-J_2 model, which accounts for a next-nearest-neighbour exchange interaction. This has the general form of

$$H = J_1 \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+2} \tag{8}$$

This Hamiltonian has, a priori, richer physics than the Heisenberg model, as one might expect that the J_2 term could introduce frustration into the system. The specific case where $J_1 = J = 2J_2$ is known as the *Majumdar-Ghosh model* viz.

$$H_{\mathrm{MJ}} = J \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{J}{2} \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+2} \tag{9}$$

2.1 Exact ground state of MJ

The reason that the MJ model has a special name is that it is possible to find exactly the (twofold degenerate) ground state of this model. This is most easily achieved by considering the operator

$$\mathbf{S}_i^{\mathrm{tr}} := \mathbf{S}_{i-1} + \mathbf{S}_i + \mathbf{S}_{i+1} \tag{10}$$

This has the property that

$$\mathbf{S}_i^{\mathrm{tr}} \cdot \mathbf{S}_i^{\mathrm{tr}} = 2\mathbf{S}_i \cdot (\mathbf{S}_{i-1} + \mathbf{S}_{i+1}) + 2\mathbf{S}_{i-1} \cdot \mathbf{S}_{i+1} \tag{11}$$

If this is summed over all of the spins, we recover the Majumdar-Ghosh Hamiltonian up to a constant, i.e.

$$H_{\mathrm{MG}} = \frac{J}{4} \sum_i \left(\mathbf{S}_i^{\mathrm{tr}}\right)^2 + \text{const.}. \tag{12}$$

In order to find the ground state of the Hamiltonian, we would want to find the ground state of this operator. In fact, we can put a lower bound on the energy of the ground state straight away:

$$\langle H_{\mathrm{MG}} \rangle \geq \frac{J}{4} \sum_i \frac{3}{4} = \frac{3JN}{16} \tag{13}$$

Therefore, if we can find a state which saturates this bound, then we must have found a ground state. The real question to answer, therefore, is *can we find a spin*-1/2 *state for every triplet of sites*? Let's try to construct one!

$$|\uparrow\rangle_{123} := (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\,|\uparrow\rangle \tag{14}$$

Naively, we would take some sort of spin-singlet coupled to another spin, to give a total $S^z = 1/2$, specifically the state defined in (14). This might put us in the $S = 3/2$ space, but also might put us in the $S = 1/2$ space or indeed a combination of both! But, it is plausible that this, in fact, *is* the appropriate state: why? Well, we could calculate

$$(S^{\mathrm{tr}})^2\,(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\,|\uparrow\rangle \tag{15}$$

But instead consider the action of $S^{\mathrm{tr}\pm}$ on these states. As the first two spins are in the singlet state, this just acts as a *single* $S = 1/2$ raising/lowering operator, and therefore this must sweep out the $S = 1/2$ subspace. This is in the $S^{\mathrm{tr}} = 1/2$ subspace for the spin being *up or down* and therefore we can immediately write down two states which saturate the bound on the ground-state energy

$$|\mathrm{MG1}\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\,(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\ldots \tag{16}$$

And, due to translation invariance of the Hamiltonian, this shifted by one site. We use the notation

$$|\mathrm{MG1}\rangle = [12][34][56]\ldots \tag{17}$$
$$|\mathrm{MG2}\rangle = [23][45][67]\ldots \tag{18}$$

It is also clear that these are the *only* two states which saturate this bound and are therefore all of the ground states of the model. For a finite system without PBCs, the two states are non-degenerate, and the splitting is exponentially small in the system size. These states can be pictorially represented by "dimerisation" or "valence-bonding" of the spin-1/2s in the chain.

3 AKLT Model

As the The Majumdar-Ghosh model may be viewed as a sum of projectors of three neighbouring spins onto an $S = 3/2$ space. What exactly does this mean? We could view this as the statement that *if we are seeking* a ground state of the dimerised form i.e. we want

the ground state to be comprised of triples of $S = 1/2$, then the easiest way to do this is to project into the orthogonal subspace and these states will *necessarily* have zero energy. How would we construct this? Well, for composing three spin-1/2s, we must either be in an $S = 1/2$ or $S = 3/2$ state, so we can just project away the $S = 1/2$ state, i.e. $(S^{\text{tr}})^2 - 1/2$ would do this!

AKLT's idea was to take this idea to try to say something about spin-chains of *higher spin*. Note that there is an important philosophical departure from typical condensed matter physics: normally the idea is to write down a model of a system observed in experiment and determine various properties about said system, such as ground state, excitations, correlation functions etc. In this case, the perspective is turned on its head: we cook up a specific state and then engineer a "parent Hamiltonian" for which this is the ground state.

To do this, we must generalise the notion of a valence bond. The key observation is that a spin S state can be represented by symmetrisation over $2S$ spin-1/2s. A valence bond (i.e. spin singlet) occurs when all of these $2s$ spin-1/2s terminate on another site.

Imagine we have a spin-1 chain, this is described by symmetrising pairs of spin-1/2s for each site, we then make valence bonds to neighbouring sites. For this to be the ground state we must project out the spin-2 component for adjacent sites, as spin singlets preclude the largest spin between pairs occurring. All we need to do is to set the Hamiltonian to be the projector onto local spin-2 pairs to have the constructed state be the ground state i.e. consider

$$(\mathbf{S}_i + \mathbf{S}_{i+1})^2((\mathbf{S}_i + \mathbf{S}_{i+1})^2 - 2), \tag{19}$$

which gives the total Hamiltonion as

$$H_{\mathbf{AKLT}} = \sum_i \left(\frac{1}{2}\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{6}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 + \frac{1}{3}\right). \tag{20}$$

Note that this doesn't guarantee anything about uniqueness or correlation length, which is the crucial question. If we take periodic boundary conditions, then the ground state *is* unique. The state is, however, simple enough that some properties can be calculated.

We write the local wavefunction on each site by ψ_α and define

$$\psi_{\alpha\beta} = \frac{1}{\sqrt{2}}\left(\psi_\alpha \otimes \psi_\beta + \psi_\beta \otimes \psi_\alpha\right) \tag{21}$$

We also take the "metric" to be the antisymmetric tensor, writing $\psi^\alpha = \varepsilon^{\alpha\beta}\psi_\beta$ with $\varepsilon^{\uparrow,\downarrow} = 1$. The constructed state is then written as

$$\chi_{\alpha_1}^{\alpha_{N+1}} = \psi_{\alpha_1,\alpha_2}\psi^{\alpha_2,\alpha_3}\cdots\psi^{\alpha_N,\alpha_{N+1}}. \tag{22}$$

As the inner product $\psi^{\dagger\alpha_1}\psi_{\alpha_2} = \delta_{\alpha_2}^{\alpha_1}$ we can calculate the norm of this state. First, we end up with terms on each site of the form

$$\delta_{\alpha_i}^{\beta_i}\delta_{\alpha_{i+1}}^{\beta_{i+1}} + \delta_{\alpha_{i+1}}^{\beta_i}\delta_{\alpha_i}^{\beta_{i+1}}. \tag{23}$$

Verify, for the un-antisymmetrised terms:

$$\frac{1}{2}\left(\psi^{\dagger\beta_i}\psi^{\dagger\beta_{i+1}}+\psi^{\dagger\beta_{i+1}}\psi^{\dagger\beta_i}\right)\left(\psi_{\alpha_i}\psi^{\alpha_{i+1}}+\psi_{\alpha_{i+1}}\psi^{\alpha_i}\right)=\delta^{\beta_i}_{\alpha_i}\delta^{\beta_{i+1}}_{\alpha_{i+1}}+\delta^{\beta_i}_{\alpha_{i+1}}\delta^{\beta_i}_{\alpha_{i+1}} \tag{24}$$

and for the antisymmetrised we find

$$\varepsilon^{\beta_i,\beta_i'}\varepsilon^{\beta_{i+1},\beta_{i+1}'}\varepsilon^{\alpha_i,\alpha_i'}\varepsilon^{\alpha_{i+1},\alpha_{i+1}'}\left(\delta^{\beta_i'}_{\alpha_i'}\delta^{\beta_{i+1}'}_{\alpha_{i+1}'}+\delta^{\beta_i'}_{\alpha_{i+1}'}\delta^{\beta_{i+1}'}_{\alpha_i'}\right) \tag{25}$$

using $\varepsilon^{ij}\varepsilon^{ik}=\delta_{ik}$ we have the same as in the previous case. So, we now need to expand out the product and do the sum: if we consider

$$\sum_{\alpha_2,\beta_2}\left(A\delta_{\alpha_1,\beta_1}\delta_{\alpha_2,\beta_2}+\delta_{\alpha_2,\beta_1}\delta_{\alpha_1,\beta_2}\right)\left(\delta_{\alpha_2,\beta_2}\delta_{\alpha_3,\beta_3}+\delta_{\alpha_2,\beta_3}\delta_{\alpha_3,\beta_2}\right) \tag{26}$$

This is given by

$$(3A+1)\delta_{\alpha_1,\beta_1}\delta_{\alpha_3,\beta_3}+\delta_{\alpha_1,\alpha_3}\delta_{\beta_1,\beta_3} \tag{27}$$

We can solve this recurrence relation to give

$$\chi^{\dagger\beta_1}_{\ \ \beta_{N+1}}\chi^{\alpha_{N+1}}_{\alpha_1}=\frac{3^N-1}{2}\delta^{\beta_1}_{\alpha_1}\delta^{\alpha_{N+1}}_{\beta_{N+1}}+\delta^{\beta_1}_{\beta_{N+1}}\delta^{\alpha_{N+1}}_{\alpha_1} \tag{28}$$

In the periodic chain, this is simply

$$\chi^{\dagger\beta_1}_{\ \ \beta_1}\chi^{\alpha_1}_{\alpha_1}=3^N+3. \tag{29}$$

We can also calculate the correlation function $\langle S^\alpha_0 S^\beta_r\rangle$ via the same approach as AKLT originally did, but we will look at it differently.

4 A glimpse of matrix product states

We can write the state of (22) in a different form. We first label the pairs of sites $\{a_1,b_1\},\{a_2,b_2\},\cdots$. The state can then always be written as

$$|\psi\rangle=\sum_{\mathbf{a}}\sum_{\mathbf{b}}c_{\mathbf{ab}}|\mathbf{ab}\rangle. \tag{30}$$

where $|\mathbf{a}\rangle=|\mathbf{a_1},\cdots,\mathbf{a_N}\rangle$, $|\mathbf{b}\rangle=|\mathbf{b_1},\cdots,\mathbf{b_N}\rangle$. We are then forced to have singlets between b_i and a_{i+1}, which for each pair site we can write as

$$\begin{aligned}|\Sigma^{(i)}\rangle&=\sum_{b_i,a_{i+1}}\Sigma_{b_i,a_{i+1}}|b_i\rangle|a_{i+1}\rangle,\\ \Sigma&=\begin{pmatrix}0 & \frac{1}{\sqrt{2}}\\ -\frac{1}{\sqrt{2}} & 0\end{pmatrix}.\end{aligned} \tag{31}$$

The state with all of these singlet bonds now reads

$$|\psi_\Sigma\rangle = \sum_{\mathbf{a}} \sum_{\mathbf{b}} \Sigma_{b_1,a_2}\Sigma_{b_2,a_3}\cdots\Sigma_{b_N,a_1}|\mathbf{a}\rangle|\mathbf{b}\rangle, \tag{32}$$

note that this is a product state across the "internal sites" of the composite spins. We now need to symmetrise to reduce the spin-1/2s to spin-1s, as before. We can do this by projecting with

$$M^\sigma_{ab}|\sigma\rangle\langle ab|, \tag{33}$$

which projects the configiuration $|ab\rangle$ into the spin-1 state $|\sigma\rangle$ on each site. We take

$$M^+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad M^0 = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{pmatrix}, \qquad M^- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{34}$$

Doing this projection, we find the total projection operator is

$$\sum_{\boldsymbol{\sigma}} \sum_{\mathbf{ab}} M^{\sigma_1}_{a_1,b_1}\cdots M^{\sigma_L}_{a_L,b_L}|\boldsymbol{\sigma}\rangle\langle\mathbf{ab}|, \tag{35}$$

and therefore the AKLT state is given by

$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} \mathrm{Tr}\left[M^{\sigma_1}\Sigma\cdots M^{\sigma_L}\Sigma\right]|\boldsymbol{\sigma}\rangle. \tag{36}$$

Defining $\widetilde{A}^\sigma = M^\sigma\Sigma$, we can write this as

$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} \mathrm{Tr}\left[\widetilde{A}^{\sigma_1}\cdots\widetilde{A}^{\sigma_L}\right]|\boldsymbol{\sigma}\rangle. \tag{37}$$

This is known as a matrix product state. For the AKLT model, the ground state is precisely of this form, with A given by 2×2 matrices. Encoding the full quantum state in essentially three matrices is very efficient and can reduce the calculation of various physical quantities to fast linear algebra calculations. Upon normalising we have

$$\begin{gathered} |\psi\rangle = \sum_{\boldsymbol{\sigma}} \mathrm{Tr}\left[A^{\sigma_1}\cdots A^{\sigma_L}\right]|\boldsymbol{\sigma}\rangle, \\ A^+ = \begin{pmatrix} 0 & \sqrt{\frac{2}{3}} \\ 0 & 0 \end{pmatrix}, \qquad A^0 = \begin{pmatrix} -\frac{1}{\sqrt{3}} & 0 \\ 0 & \frac{1}{\sqrt{3}} \end{pmatrix}, \qquad A^- = \begin{pmatrix} 0 & 0 \\ -\sqrt{\frac{2}{3}} & 0 \end{pmatrix}. \end{gathered} \tag{38}$$

Just to clarify, this is done by evlauating

$$\begin{aligned} \langle\psi|\psi\rangle &= \sum_{\sigma_i,\sigma_i'} \langle\boldsymbol{\sigma}'|\boldsymbol{\sigma}\rangle \mathrm{Tr}\left[A^{\sigma_1'}\cdots A^{\sigma_N'}\right]\mathrm{Tr}\left[A^{\sigma_1}\cdots A^{\sigma_N}\right], \\ &= \mathrm{Tr}\left(\sum_{\sigma_1} A^{\sigma_1 *}\otimes A^{\sigma_1}\right)\cdots\left(\sum_{\sigma_1} A^{\sigma_N *}\otimes A^{\sigma_N}\right), \\ &= \mathrm{Tr}\, E^N. \end{aligned} \tag{39}$$

with

$$E = \sum_{\sigma} A^{\sigma *} \otimes A^{\sigma} = \begin{pmatrix} \frac{1}{3} & 0 & 0 & \frac{2}{3} \\ 0 & -\frac{1}{3} & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & 0 \\ \frac{2}{3} & 0 & 0 & \frac{1}{3} \end{pmatrix}, \tag{40}$$

(N.B. This is (92), which is incorrect in Schollwöck), which has eigenvalues $1, -1/3, -1/3, -1/3$, which means that for $L \to \infty$ this is exponentially well normalised. To calculate the correlator, we will just consider the correlator $\langle S_r^+ S_0^- \rangle$. With the MPS formulation, this is simply

$$\langle \psi | S_r^+ S_0^- | \psi \rangle = \sum_{\{\sigma_i, \sigma_i'\}} \langle \boldsymbol{\sigma}' | S_r^+ S_0^- | \boldsymbol{\sigma} \rangle \mathrm{Tr} \left[A^{\sigma_0'} \cdots A^{\sigma_{N-1}'} \right] \mathrm{Tr} \left[A^{\sigma_0} \cdots A^{\sigma_{N-1}} \right]. \tag{41}$$

The matrix element is trivial and enforces $\sigma_r' = \sigma_r + 1$, $\sigma_0' = \sigma_0 - 1$. We therefore, similarly to before, just need to calcuate

$$\langle \psi | S_r^+ S_0^- | \psi \rangle = \mathrm{Tr} \left[\left(A^+ \otimes A^0 + A^0 \otimes A^- \right) E^{r-1} \left(A^- \otimes A^0 + A^0 \otimes A^+ \right) E^{N-r-1} \right]. \tag{42}$$

This is simple linear algebra and can be done exactly for the 4×4 matrices we are dealing with, yielding

$$\begin{aligned} \langle \psi | S_r^+ S_0^- | \psi \rangle &= \frac{4}{3}(-1)^r 3^{-r} + \frac{4}{3}(-1)^{L-r} 3^{-L+r}, \\ \lim_{N \to \infty} \langle \psi | S_r^+ S_0^- | \psi \rangle &= \frac{4}{3}(-1)^r 3^{-r}. \end{aligned} \tag{43}$$

This shows that the correlation function of this local variable is exponentially localised. AKLT also go on to show that the energy gap is finite and various other features of the model.