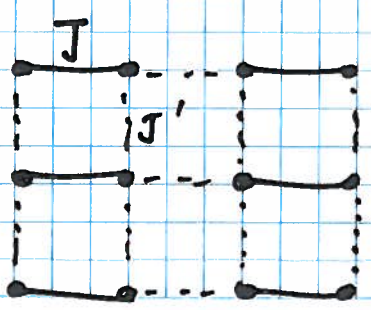
IV - Gapped systems

From the previous sections it is clear that if the spectrum of an antiferromagnet is soft enough, quantum fluctuations will destroy the classical order. This raises the natural question of the nature of the ground state and of the excitations above the ground state. In this section, we are going to discuss a number of situations in which quantum fluctuations have been shown to stabilize a ground state which is essentially a product wave function of local singlets, with the consequence that there is a gap to triplet excitations.

① Coupled dimers:

Let us consider the (Spin 1/2) AF Heisenberg model on the square lattice, and let us reduce the magnitude of some couplings so as to transform the system into a model of weakly coupled dimers:



As long as J and J' are both positive, which is the case we will concentrate on, it is clear that the

classical ground state is still the Néel configuration since it fully satisfies all bonds. One might be tempted to believe that the system will thus remain a Néel antiferromagnet down to $J'=0$.

To demonstrate that this is not so, the most efficient way to proceed is to start from the $J'=0$ case, and to treat J' as a perturbation.

When $J'=0$, the system is a collection of independent dimers coupled by J. The spectrum of 2 spins-$1/2$ coupled by J consists of one singlet and one triplet. Indeed,

$$\mathcal{H} = J\,\vec{S}_1\cdot\vec{S}_2 = \frac{J}{2}\left[(\vec{S}_1+\vec{S}_2)^2 - \vec{S}_1^2 - \vec{S}_2^2\right]$$

$$= \frac{J}{2}(\vec{S}_1+\vec{S}_2)^2 - \frac{3}{4}J$$

If $S_{tot}=0$, $E_s = -\frac{3}{4}J$, while if $S_{tot}=1$, $E_t = \frac{1}{4}J$.

Let us denote by $|S\rangle$ the singlet and by $|T_{-1}\rangle$, $|T_0\rangle$ and $|T_1\rangle$ the three triplets with $S^z_{tot} = -1, 0$ and 1 respectively:

$$|S\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right),\quad |T_{-1}\rangle = |\downarrow\downarrow\rangle,\quad |T_0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right),\quad |T_1\rangle = |\uparrow\uparrow\rangle.$$

The unperturbed ground state can then be written as

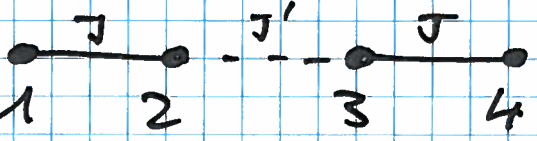
$$|GS\rangle = |s \cdots s\rangle = |s\rangle \otimes |s\rangle \otimes \cdots \otimes |s\rangle$$

where the product runs over all dimers of the lattice. Its energy is given by $E_0 = -\frac{3}{4} J \frac{N}{2}$.

The first excited state is obtained by promoting one singlet into a triplet. The energy is equal to $E_0 + J$, and the degeneracy is equal to $3 \times \frac{N}{2}$, where $\frac{N}{2}$ is the number of dimers, and 3 keeps track of the 3 possible values of S^z_{tot} (-1, 0 or 1).

Let us now treat J' as a perturbation. Since the ground state is now degenerate we can calculate the 1st order correction as $\langle GS | \mathcal{H}(J') | GS \rangle$.

$\mathcal{H}(J')$ is a sum of terms that couple two dimers in the simplest possible way:



$$J' \vec{S}_2 \cdot \vec{S}_3 = J' \left(S_2^z S_3^z + \frac{1}{2} \left(S_2^+ S_3^- + S_2^- S_3^+ \right) \right)$$

$$|S\rangle_{12} = \frac{1}{\sqrt{2}} \left(|\uparrow_1 \downarrow_2\rangle - |\downarrow_1 \uparrow_2\rangle \right)$$

$$S_2^z |S\rangle_{12} = \frac{1}{2\sqrt{2}} \left(-|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right) = -\frac{1}{2} |T_0\rangle$$

$$S_2^+ |S\rangle_{12} = \frac{1}{\sqrt{2}} |\uparrow\uparrow\rangle = \frac{1}{\sqrt{2}} |T_1\rangle$$

$$S_2^- |S\rangle_{12} = \frac{1}{\sqrt{2}} (-|\downarrow\downarrow\rangle) = -\frac{1}{\sqrt{2}} |T_{-1}\rangle$$

So, by applying any term of $\vec{S}_2 \cdot \vec{S}_3$, we transform the singlet on bond (12) into a triplet. The scalar product of the resulting states with $|GS\rangle$ with them vanish.

So, the first order correction to the ground state energy vanishes: $E_0^{(1)} = 0$.

Let us now turn to the 1st excited state. Since it is degenerate, we have to turn to degenerate perturbation theory. Since S^z_{tot} commutes with the Hamiltonian, we can do this separately for the sectors $S^z_{tot} = -1, 0$ and 1. Let us do it for $S^z_{tot} = 1$. A bases of the degenerate subspace is given by

$$|m\rangle = |S \cdots T_1 \cdots S\rangle$$

triplet on bond m

We need to calculate $\langle m | \mathcal{H}^{(1)} | m \rangle$, and to diagonalize this matrix. Let us choose a specific J' bond. It can only couple the state with triplets emanating from the ends of this bond. So, let us calculate

$$\langle T_1 |_{12} \otimes \langle S |_{34} \; J' \vec{S}_2 \cdot \vec{S}_3 \; |S\rangle_{12} \otimes |T_1\rangle_{34}$$

We have already calculated the effect of $S_2^+ S_2^-$ and S_2^z on $|S\rangle_{12}$. Let us calculate the effect of the component of $\vec{S}_3$ on $|T_1\rangle$:

$$S_3^z |T_1\rangle = \frac{1}{2} |T_1\rangle$$

$$S_3^+ |T_1\rangle = 0$$

$$S_3^- |T_1\rangle = |\downarrow\uparrow\rangle = \frac{1}{\sqrt{2}} \left(-|S\rangle_{34} + |T_0\rangle_{34} \right)$$

$$\rightarrow \vec{S}_2 \cdot \vec{S}_3 \left(|S\rangle_{12} \otimes |T_1\rangle_{34} \right)$$

$$= -\frac{1}{2} |T_0\rangle_{12} \otimes \frac{1}{2} |T_1\rangle_{34} + \frac{1}{2} \frac{1}{\sqrt{2}} |T_1\rangle_{12} \otimes \frac{1}{\sqrt{2}} \left(-|S\rangle_{34} + |T_0\rangle_{34} \right)$$

$$\Rightarrow \langle T_1|_{12} \otimes \langle S|_{34} \, J' \vec{S}_2 \cdot \vec{S}_3 \, |S\rangle_{12} \otimes |T_1\rangle_{34}$$

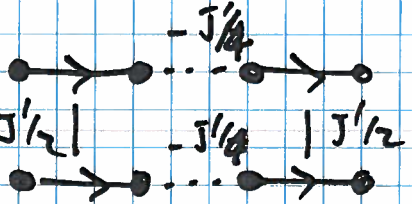
$$= -\frac{J'}{4}$$

So the effect of J' is to let $|T_1\rangle$ jump with amplitude $-J'/4$.

The only subtelty is the sign of the hopping. It is easy to check that if we had taken $\vec{S}_2 \cdot \vec{S}_4$, the sign would be opposite, as well as for $\vec{S}_1 \cdot \vec{S}_3$, while it would be the same for $\vec{S}_1 \cdot \vec{S}_4$. So, if dimers are coupled by two bonds in the geometry $J'(\vec{S}_2 \cdot \vec{S}_3 + \vec{S}_1 \cdot \vec{S}_4)$, the total amplitude will be $-J'/2$, while

if it is $J'(\vec{S}_1 \cdot \vec{S}_3 + \vec{S}_2 \cdot \vec{S}_4)$, it will be $J'/2$.

Let us come back to the square lattice. To keep track of the convention for the singlet which spin is $\uparrow$ in the wave-function with + sign, we draw an arrow from that spin to the other one.



The matrix elements $\langle m | \mathcal{H}(J) | n \rangle$ thus correspond to those of a particle hopping on a square lattice with amplitude $-J/4$ horizontally and $J'/2$ vertically.

The spectrum is given by:

$$\varepsilon_{\vec{k}} = -\frac{J'}{2}\cos k_x + J' \cos k_y .$$

The bottom of the band is at $k_x = 0$, $k_y = \pi$, with energy $-\frac{3}{2}J'$.

So, to first order in perturbation, the lowest energy in the 1st excited state branch is equal to $J - \frac{3}{2}J'$.

This theory predicts that there is a

transition at $J' = \frac{2}{3} J$. Below that value, there is a gap to triplet excitations. Above that value the gap closes, and we must be back to a Néel antiferromagnet with low-lying spin wave excitations.

This picture is confirmed by Quantum Monte Carlo simulations, and the transition takes place at $J'/J = 0.5237...$

The same theory applied to a ladder predicts that the gap persists up to $J'/J = 1$. In fact, field theory arguments suggest that the gap persists as long as $J/J' > 0$.

② J_1-J_2 chain :

The previous example is somewhat trivial since the dimerization has been put by hand. Let us now turn to situations where the dimerization appears spontaneously.

The first example where such an effect has been discovered is the Majumdar-Ghosh point $J_2 = J_1/2$ of the spin $\frac{1}{2}$ J_1-J_2 chain defined by the Hamiltonian:

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

Proposition : When $J_2 = J_1/2$, the states

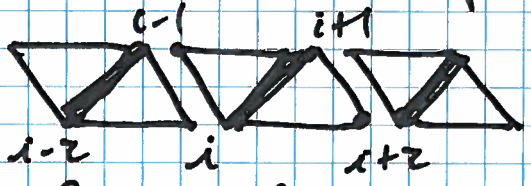
$|\Psi_e\rangle = \prod_{i \text{ even}} |S\rangle_{i,i+1}$ and $|\Psi_o\rangle = \prod_{i \text{ odd}} |S\rangle_{i,i+1}$ are ground states of $\mathcal{H}$.

Demonstration : As usual, we shall proceed in two steps.

① Prove that they are eigenstates.

② Prove that they minimize the energy.

① It is sufficient to prove it for one state since $\mathcal{H}$ is translationally invariant. Since $J_1 = 2J_2$ we can represent the model in the following way



where each bond is a coupling of strength J_2 and write the Hamiltonian

$$\mathcal{H} = \sum_{i \text{ even}} \left(2J_2 \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \vec{S}_{i-1} \cdot (\vec{S}_i + \vec{S}_{i+1}) + J_2 \vec{S}_{i+2} \cdot (\vec{S}_i + \vec{S}_{i+1}) \right).$$

Now, if we consider $\prod_{i \text{ even}} |S\rangle_{i,i+1}$, $\vec{S}_i$ and $\vec{S}_{i+1}$ are in a singlet state. Then,

$$\left(S_i^\alpha + S_{i+1}^\alpha\right)|S\rangle_{i,i+1} = 0 \quad \text{for} \quad \alpha = x, y, z$$

$$\Rightarrow \vec{S}_{i-1}\cdot\left(\vec{S}_i + \vec{S}_{i+1}\right) = 0 \quad \text{and} \quad \vec{S}_{i+2}\cdot\left(\vec{S}_i + \vec{S}_{i+1}\right) = 0$$

Finally, $\mathcal{H} \prod_{i\,\text{even}} |S\rangle_{i,i+1} = \sum_{i\,\text{even}} 2J_2 \times \left(-\frac{3}{4}\right) \prod_{i\,\text{even}} |S\rangle_{i,i+1}$

$$= -\frac{3}{4} J_2 N \prod_{i\,\text{even}} |S\rangle_{i,i+1}.$$

So $\prod_{i\,\text{even}} |S\rangle_{i,i+1}$ is an eigenstate for $J_2 = J_{1/2}$ with eigenvalue $-\frac{3}{4} J_2 N$. The same is of course true for the odd wave function by symmetry.

② To prove that this minimizes the energy, let us partition the Hamiltonian in a different way:

$$\mathcal{H} = \sum_i J_2 \left(\vec{S}_i \cdot \vec{S}_{i+1} + \vec{S}_i \cdot \vec{S}_{i+2} + \vec{S}_{i+1} \cdot \vec{S}_{i+2}\right) = \sum_i \mathcal{H}_\Delta(i)$$

Now, $\vec{S}_i \cdot \vec{S}_{i+1} + \vec{S}_i \cdot \vec{S}_{i+2} + \vec{S}_{i+1} \cdot \vec{S}_{i+2} = \frac{1}{2}\left[\left(\vec{S}_i + \vec{S}_{i+1} + \vec{S}_{i+2}\right)^2 - 3 \times \frac{3}{4}\right]$

The lowest eigenvalue is reached when S_{tot} is minimal, and for 3 spins $1/2$ the minimal value is $1/2$

$$\Rightarrow \min\left\langle \mathcal{H}_\Delta(i) \right\rangle = -\frac{3}{4} J_2.$$

so, $\langle H \rangle \geq \sum_i \min \langle h_\Delta(i) \rangle = -\frac{3}{4} J_2 N$.

Since we found two states with energy $-\frac{3}{4} J_2 N$, they must be the ground states.

It seems plausible that triplet excitations will be gapped, and this indeed confirmed by numerical simulations. In fact, the J_1-J_2 AFM $S = 1/2$ chain is gapless up to $J_2/J_1 \simeq 0.2411$ and is gapped above that value.

(3) Spin 1 chain:

In the lectures on path integrals it has been shown that there is a fundamental difference between half-integer and integer spin chains. Half-integer spin chains have a non trivial Berry phase, while integer spin chains don't. As a consequence, their long wavelength properties can be expected to be different. In the lectures on bosonization it was shown that half-integer spin chains have algebraic correlations. By contrast, integer spin chains are gapped. Rather than going back to the non-linear sigma model, let us show that the ground state is more or less a product of singlets.

More precisely, we are going to construct a wave function which creates spin-$\frac{1}{2}$ singlets on all bonds of a chain. This wave function is a spin-1 wavefunction, and it is the ground state of a Hamiltonian which is not too different from the $S=1$ Heisenberg model.

To construct this wave-function, it is useful to introduce yet another representation of spin operators with bosons known as Schwinger bosons.

Consider 2 types of bosons at a given site: $a^\dagger, a$ and $b^\dagger, b$.

Prop 1: The composite operators

$$\begin{cases} S^+ = a^+ b \\ S^- = b^+ a \\ S^z = \frac{1}{2}(a^+ a - b^+ b) \end{cases}$$

satisfy the SU(2) commutation relations

$$\begin{cases} [S^+, S^-] = [S^x + iS^y, S^x - iS^y] = 2S^z \\ [S^+, S^z] = [S^x + iS^y, S^z] = -iS^y - S^x = -S^+ \\ [S^-, S^z] = [S^x - iS^y, S^z] = -iS^y + S^x = S^- \end{cases}$$

Proof: $[a^+ b, b^+ a] = a^+ [b, b^+ a] + [a^+, b^+ a] b$

$$= a^+ a - b^+ b = 2S^z$$

$$\left[a^+ b, \frac{1}{2}(a^+ a - b^+ b)\right] = \frac{1}{2}[a^+ b, a^+ a] - \frac{1}{2}[a^+ b, b^+ b]$$

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

$$\left[b^+ a, \frac{1}{2}(a^+ a - b^+ b)\right] = \frac{1}{2}[b^+ a, a^+ a] - \frac{1}{2}[b^+ a, b^+ b]$$

$$= \frac{1}{2} b^+ a + \frac{1}{2} a b^+ = b^+ a$$

Prop. 2: $\vec{S}^2 = S(S+1)$ if the constraint $a^+ a + b^+ b = 2S$ is imposed.

Proof: $\vec{S}^2 = S^{x2} + S^{y2} + S^{z2}$

$$= \frac{1}{4}(S^+ + S^-)^2 - \frac{1}{4}(S^+ - S^-)^2 + S^{z2}$$

$$= \frac{1}{4}(a^+ b + b^+ a)^2 - \frac{1}{4}(a^+ b - b^+ a)^2 + \frac{1}{4}(a^+ a - b^+ b)^2$$

$$= \frac{1}{2}(a^+ b b^+ a + b^+ a a^+ b) + \frac{1}{4}(a^+ a + b^+ b)^2 - (a^+ a b^+ b)$$

$$= \frac{1}{2}(a^+ a + a^+ a b^+ b + a^+ a b^+ b + b^+ b) + \frac{1}{4}(a^+ a + b^+ b)^2 - a^+ a b^+ b$$

$$= \frac{1}{2}\left(a^\dagger a + b^\dagger b\right) + \frac{1}{4}\left(a^\dagger a + b^\dagger b\right)^2 = S + S^2 = S(S+1) \quad \blacksquare$$

Prop. 3: Consider 2 spins $\frac{1}{2}$ i and j. The wave-fund $|\phi\rangle = \frac{1}{\sqrt{2}}\left(a_i^\dagger b_j^\dagger - a_j^\dagger b_i^\dagger\right)|0\rangle$ is the singlet.

Proof: ① It is normalized?

$$\frac{1}{2}\langle 0|(a_i b_j - a_j b_i)(a_i^\dagger b_j^\dagger - a_j^\dagger b_i^\dagger)|0\rangle$$

$$= \frac{1}{2}\langle 0|a_i b_j a_i^\dagger b_j^\dagger|0\rangle + \frac{1}{2}\langle 0|a_j b_i a_j^\dagger b_i^\dagger|0\rangle$$

$$= \frac{1}{2}\langle 0|(1+a_i^\dagger a_i)(1+b_j^\dagger b_j)|0\rangle + \frac{1}{2}\langle 0|(1+a_j^\dagger a_j)(1+b_i^\dagger b_i)|0\rangle$$

$$= \frac{1}{2} + \frac{1}{2} = 1 .$$

② $S_{tot}^-|\phi\rangle = (S_i^- + S_j^-)|\phi\rangle = 0$?

$$(S_i^- + S_j^-)|\phi\rangle = \left(b_i^\dagger a_i + b_j^\dagger a_j\right)\frac{1}{\sqrt{2}}\left(a_i^\dagger b_j^\dagger - a_j^\dagger b_i^\dagger\right)|0\rangle$$

$$= \frac{1}{\sqrt{2}}\left(b_i^\dagger a_i a_i^\dagger b_j^\dagger - b_j^\dagger a_j a_j^\dagger b_i^\dagger\right)|0\rangle$$

$$= \frac{1}{\sqrt{2}}\left(b_i^\dagger b_j^\dagger - b_j^\dagger b_i^\dagger\right)|0\rangle = 0 .$$

③ $S_{tot}^z|\phi\rangle = 0$? Yes, because there is always 1 a and 1 b. $\blacksquare$

Now, consider the wavefunction

$$|BS\rangle = 2^{-N/2}\prod_i \left(a_i^\dagger b_{i+1}^\dagger - a_{i+1}^\dagger b_i^\dagger\right)|0\rangle , \quad N = \#\text{ of sites}$$

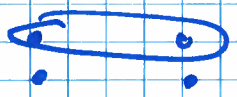
Prop. 4: This corresponds to 1 spin 1 per site.

Proof: Consider the operator $a_i^\dagger a_i + b_i^\dagger b_i$. In each

term of the wave function, there is either a factor $a_i^\dagger a_j^\dagger$, a factor $a_i^\dagger b_j^\dagger$ or a factor $b_i^\dagger b_j^\dagger$. So the wave function is an eigenstate of $a_i^\dagger a_i + b_i^\dagger b_i$ with the eigenvalue 2.

Parent Hamiltonian:

Now let us look for a Hamiltonian of which this wave-function could be the ground state. If we consider a pair of spin 1, the total spin could be either 0, 1 or 2. Now, if a wave function contains a singlet of spin $\frac{1}{2}$ on a bond, it sounds plausible that it cannot be a state of spin 2 for the total spin on that bond. This is intuitive if we consider a spin 1 as made of two spins $\frac{1}{2}$ - if two spins build a singlet, the other 2 can build a singlet or a triplet, and the total spin is at most 1.



Let's prove it. The operator $S_i^z + S_j^z$ is given by $\frac{1}{2}(a_i^\dagger a_i + a_j^\dagger a_j - b_i^\dagger b_i - b_j^\dagger b_j)$

Since the wave function contains a factor $(a_i^\dagger b_j^\dagger - a_j^\dagger b_i^\dagger)$, the total number of $a^\dagger$ operators is at most 3, and that of $b^\dagger$ operators at least 1. So, the largest possible eigenvalue of $S_i^z + S_j^z$ is $\frac{1}{2}(3-1) = 1$.

Now, the total wavefunction is a singlet since it is a product of singlets. So $S^+_{tot}|VBS\rangle = 0$. If $|VBS\rangle$ contains a component with $S_{tot(i,j)} = 2$ and $S^z_{tot(i,j)} = 1$, it has to be multiplied by a function of spins $k \neq i,j$ that must also have $S_{tot} = 2$ since $|VBS\rangle$ is a global singlet, with $S^z_{tot} = -1$.

So applying S^+_{tot} will create a state with $S_{tot(i,j)} = 2$ and $S^z_{tot(i,j)} = 2$, which cannot be cancelled by any term of $|VBS\rangle$ since these terms are not present. This contradicts the fact that $|VBS\rangle$ is a singlet. So there can be no component with $S_{tot(i,j)} = 2$ and $S^z_{tot(i,j)} = 1$.

If there was a component with $S_{tot(i,j)} = 2$ and $S^z_{tot(i,j)} = 0$, the same argument leads to a component $S_{tot(i,j)} = 2$, $S^z_{tot(i,j)} = 1$ in $S^+_{tot}|VBS\rangle$ which cannot be cancelled.

So, $|VBS\rangle$ contains no component with $S = 2$ for a pair of neighbouring sites. Hence,

$$\sum_{\langle i,j \rangle} P^{(i,j)}_{S=2} |VBS\rangle = 0$$

where $P_{S=2}^{(i,j)}$ is the projector on $S_{tot}=2$ for the pair (i,j). Since the smallest possible eigenvalue of a projector is 0, this implies that $|\psi_{GS}\rangle$ is a groundstate of $\sum_{\langle i,j\rangle} P_{S=2}^{(i,j)}$.

How does this projector look like?
We look for an operator such that satisfies

$$P_{S=2}\,|\psi(S=0)\rangle = 0 \qquad (1)$$

$$P_{S=2}\,|\psi(S=1)\rangle = 0 \qquad (2)$$

$$P_{S=2}\,|\psi(S=2)\rangle = |\psi(S=2)\rangle \qquad (3)$$

where $|\psi(S=i)\rangle$ is any state of total spin i.

Now, $\vec{S}_i\cdot\vec{S}_j = \frac{1}{2}\vec{S}_{tot}^{\,2} - 2$

$$\Rightarrow \vec{S}_i\cdot\vec{S}_j\,|\psi(S=0)\rangle = -2\,|\psi(S=0)\rangle$$

$$\vec{S}_i\cdot\vec{S}_j\,|\psi(S=1)\rangle = -\,|\psi(S=1)\rangle$$

$$\vec{S}_i\cdot\vec{S}_j\,|\psi(S=2)\rangle = |\psi(S=2)\rangle$$

So the operator $\frac{1}{\alpha}(\vec{S}_i\cdot\vec{S}_j+2)(\vec{S}_i\cdot\vec{S}_j+1)$ satisfies conditions (1) and (2), and the third condition is fulfilled if $\alpha=6$

$$\rightarrow P_{S=2} = \frac{1}{6}(\vec{S}_i\cdot\vec{S}_j+2)(\vec{S}_i\cdot\vec{S}_j+1)$$

$$\boxed{P_{S=2} = \frac{1}{2}\left(\vec{S}_i\cdot\vec{S}_j + \frac{1}{3}(\vec{S}_i\cdot\vec{S}_j)^2 + \frac{2}{3}\right)}$$

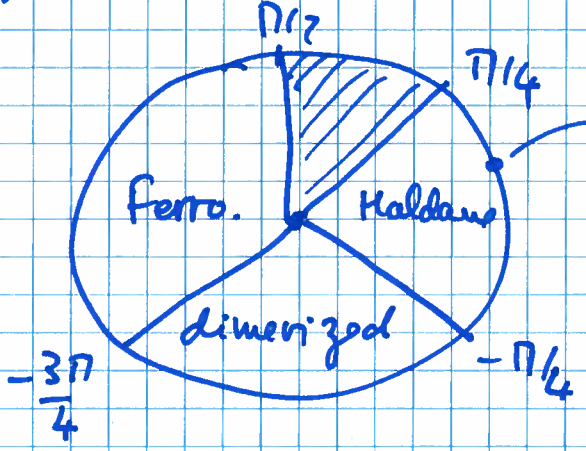
Finally, $|VBS\rangle$ is the ground state of

$$\mathcal{H}_{AKLT} = \sum_i \left(\vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3} (\vec{S}_i \cdot \vec{S}_{i+1})^2 \right)$$

The term $(\vec{S}_i \cdot \vec{S}_j)^2$ is called a biquadratic interaction. Intensive numerical and analytical investigations of the generalization

$$\mathcal{H} = \sum_i \left(\cos\theta \, \vec{S}_i \cdot \vec{S}_{i+1} + \sin\theta \, (\vec{S}_i \cdot \vec{S}_{i+1})^2 \right)$$

have revealed that the model of which $|VBS\rangle$ is the ground state and the spin-1 Heisenberg chain with nearest-neighbour interactions are in the same phase.



AKLT = Affleck. Kennedy. Lieb-Tasaki