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7 Quantum spin systems, quantum computing

7.1 Quantum mechanics

We start with a crash course in the basics of quantum mechanics that is relevant to quantum spin systems and quantum computation.

In classical mechanics the state of the system is given by some point in the phase space. There is an energy function (Hamiltonian) defined on the phase space. This is just an ordinary real-valued function. If we have a single particle this is a function of its position x and momentum p. The equations of motion (Hamiltonian formulation) are then

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q} \tag{1}$$

In quantum mechanics the state of the system is given by a unit vector ψ in some compex Hilbert space. The energy of the system is now a linear operator H acting on this Hilbert space and the equations of motion are the Schrodinger equation

$$i\hbar \frac{\partial}{\partial t}\psi(t) = H\psi(t) \tag{2}$$

Consider a single particle moving in a potential $V(x)$. Classically the energy is $\frac{p^2}{2m} + V(x)$, where p is the momentum of the particle and x is its position. A point in phase space is (x, p). In QM the Hilbert space is $L^2(\mathbb{R}^3)$ over the complex numbers. p is replaced by the operator $i\hbar\nabla$, $V(x)$ becomes the operator of multiplication by $V(x)$ and the Schrodinger eq. is

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\Delta + V(x)\right]\psi(x,t) \tag{3}$$

Note that this is an unbounded self-adjoint operator on $L^2(\mathbb{R}^3)$. We will not be considering such systems. From now on we will choose our units so that $\hbar = 1$.

The simplest system is a single spin 1/2 particle. Its state space is a two dimensional complex Hilbert space. (All Hilbert spaces in this chapter will be complex.) The spin operator is a vector of operators.

$$\mathbb{S} = \frac{1}{2}(\sigma^x, \sigma^y, \sigma^z) \tag{4}$$

With the standard choice of basis, the Pauli spin matrices are given by

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

If you take a classical charged particle and spin it about some axis, classical E and M says it will have a magnetic moment μ proportional to its spin angular momentum S. So $\mu = \gamma S$ where μ and S are vectors and γ is a scalar. So if you put it in a magnetic field B, the energy will be $H = -\mu \cdot B$ where μ is a the magnetic moment (a vector).

If we put our quantum mechanical spin 1/2 particle in a magnetic field B then the Hamiltonian is $H = -\gamma B \cdot \mathbb{S}$ where the constant γ depends on the type of particle. Electrons and protons are both have spin 1/2 but the electon has a much larger γ.

Suppose the field is in the positive z direction with magnitude B, so $H = -\frac{\gamma B}{2}\sigma^z$. We can easily solve the Schrondinger equation since H is diagonal. Let (a, b) be the state at time 0. So a, b are complex with $|a|^2 + |b|^2 = 1$ Let $\psi(t) = (a(t), b(t))$. Note that since H does not depend on time, the solution of the SE can be written in terms of a matrix exponential

$$\psi(t) = \exp(itH)\psi(0) \tag{5}$$

Since σ^z is diagonal it is trivial to compute the matrix exponential

$$\exp(itH) = \exp(it\gamma B\sigma^z/2) = \begin{pmatrix} \exp(it\gamma B/2) & 0 \\ 0 & \exp(-it\gamma B/2) \end{pmatrix} \tag{6}$$

So we have

$$\psi(t) = (a\exp(i\gamma Bt/2), b\exp(-i\gamma Bt/2)) \tag{7}$$

Now suppose we put the field in the x direction. The solution of the SE is

$$\exp(itH) = \exp(it\gamma B\sigma^x/2) \tag{8}$$

Since σ^x is not diagonal the matrix exponential is not trivial, but it is still pretty simple since $(\sigma^x)^2 = 1$ Expand the exponential in a power series and we find

$$\exp(it\gamma B\sigma^x/2) = \cos(t\gamma B/2)I + i\sin(t\gamma B/2)\sigma^x \tag{9}$$

Apply this to the intial vector and we find

$$\begin{aligned} \psi(t) &= \cos(t\gamma B/2)(a,b) + i\sin(t\gamma B/2)(b,a) && (10)\\ &= (a\cos(t\gamma B/2) + ib\sin(t\gamma B/2), b\cos(t\gamma B/2) + ia\sin(t\gamma B/2)) && (11)\end{aligned}$$

7.1.1 Measurement

Quantum Mechanics is intrinsically random. If we have a single particle with wave function $\psi(x,t)$, then the particle is not located at a single point. Instead $|\psi(x,t)|^2$ is the probability density that the particle is located at x. **Explain density**

If O is a self-adjoint operator with discrete spectrum and we measure O, then the possible outcomes are the eigenvalues of O. If λ is an eigenvalue and P_λ the orthogonal projection onto its eigenspace, then the probability of getting λ when we measure O is $< \psi|P_\lambda|\psi >$ where ψ is the state of the system. Note that since $\sum_\lambda P_\lambda = I$ and $||\psi|| = 1$, the sum of the probabilities is 1 as it must be.

If we put our single spin 1/2 particle in a magnetic field then the Hamiltonian is $H = -\frac{h}{2}\sigma^z$. This will cause the spin to precess. See the notes provided by Prof. Faris for details of this.

7.1.2 Combining two quantum systems

In quantum mechanics if we combine two systems, one of which has state space $\mathbb{H}_1$ and the other has state space $\mathbb{H}_2$, then the state space for the combined system is the tensor product $\mathbb{H}_1 \otimes \mathbb{H}_2$.

Review tensor product of two Hilbert spaces

If the two systems are just two spin 1/2's, then the state space for the two spins is $\mathbb{C}^2 \otimes \mathbb{C}^2$ which is 4 dimensional.

Define spin operators for 1 and 2.

Recall that in the classical setting, the ferromagnetic interaction between two spins (with values in S^{N-1}) was $-\sigma_1 \cdot \sigma_2$. In the quantum case the

ferromagnetic interaction betwen the two spins is the operator

$$H = -S_1 \cdot S_2 \tag{12}$$

We now find the eigenstates of H. Up to a factor of $1/4$ this is the same as finding the eigenstates of $\sigma_1 \cdot \sigma_2$. We start by considering ground states - the states with the smallest eigenvalue. First consider the Hamiltonian $\sigma_1 \cdot \sigma_2$ for two spins. We split it into two pieces $\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y$ and $\sigma_1^z \sigma_2^z$ which we will refer to as the jump piece and the diagonal piece. The Hilbert space is 4d with a basis $|++>, |-->, |+->, |-+>$. The diagonal piece acts as

$$|++> \ \rightarrow \ |++>, \quad |--> \rightarrow |-->, \tag{13}$$
$$|+-> \ \rightarrow \ -|+->, \quad |-+> \rightarrow -|-+> \tag{14}$$

while the jump piece acts as

$$|++> \ \rightarrow \ 0, \quad |--> \rightarrow 0, \tag{15}$$
$$|+-> \ \rightarrow \ 2|-+>, \quad |-+> \rightarrow 2|+-> \tag{16}$$

So we we consider the operator $E_{12} = \frac{1}{2}(\sigma_1 \cdot \sigma_2 + 1)$ then we have

$$E_{12} \quad |++> \rightarrow |++>, \quad E_{12}|--> \rightarrow |-->, \tag{17}$$
$$E_{12} \quad |+-> \rightarrow |-+>, \quad E_{12}|-+> \rightarrow |+-> \tag{18}$$

Note that E_{12} just interchanges the spins at 1 and 2. (We called it E_{12} for exchange.) The operator E_{12} has two eigenvalues. Eigenvalue +1 has multiplicity 3 and eigenvalue -1 has multiplicity 1. The eigenvectors for eigenvalue 1 are

$$|++>, |-->, \frac{1}{\sqrt{2}}(|+-> + |-+>) \tag{19}$$

and the eigenvector for eigenvalue -1 is

$$\frac{1}{\sqrt{2}}(|+-> - |-+>) \tag{20}$$

There is a triplet (3d subspace) of ground states (spin 1) and a singlet (1d subspace) of an excited state. If we consider the antiferromagnet then we have a 1d ground state and a 3d excited state.

7.2 Quantum spin systems

We consider spin 1/2 quantum spin systems. We will consider general spin later.

Suppose we have a finite subset Λ of a lattice. At each site in the lattice we have a two dimensional state space for the spin 1/2 at that site. So the state space for the system on Λ is the tensor product over $i \in \Lambda$ of $\mathbb{H}_i$. So the state space for Λ has dimension $2^{|\Lambda|}$. The ferromagnetic Hamitonian with open boundary conditions is

$$H = -\sum_{<ij>} \sigma_i \cdot \sigma_j \tag{21}$$

For the antiferromagnetic Hamiltonian the definition is the above without the minus sign. Unlike the classical case, even if the lattice is bipartitite these two Hamiltonians are not equivalent. More precisely there is no unitary operator on the Hilbert space which transforms the ferromagnetic H into the antiferromagnetic H. This is an important point. The physics of the ferromagnet and the antiferromagnet are different.

In the classical case the Heisenberg Hamiltonian has a rotational symmetry - if we rotate the spins at all the sites by the same rotation, then the value of the Hamiltonian is unchanged. There is a similar symmetry for our quantum model with Hamiltonian (21). To be precise, it is an $SU(2)$ symmetry rather than an $SO(3)$ symmetry. We illustrate it with a special case of the "rotation". Let $U_i(\theta) = \exp(i\theta\sigma_i^z)$. This is a unitary operator whose inverse is $U_i(-\theta) = \exp(-i\theta\sigma_i^z)$. Clearly, $U_i(-\theta)\sigma_i^z U_i(\theta) = \sigma_i^z$. A little computation shows that the same conjugation transforms the 2d vector (σ_i^x, σ_i^y) into $R(\sigma_i^x, \sigma_i^y)$ where R is a rotation in the xy plane. It follows that if we define $U = \prod U_i$, then $U^{-1}HU = H$.

As we will see, even the ground state can be very non-trivial. Previously we found the eigenstates, in particular the ground states, for a quantum spin system with just two sites. Now consider more than two sites. So for the ferromagnetic case we consider

$$H = -\sum_{<ij>} E_{ij} \tag{22}$$

The state with + at all sites is an eigenstates with eigenvalue E equal to minus the number of bonds. Same for the state with - at all sites. But that is only two ground states. We expect more given the symmetry (infinitely

many in the infinite volume limit). For a subset X of Λ, let Ψ_X the the state with $+$ on X and $-$ on $\Lambda \setminus X$. Fix a integer k and consider the state

$$\Psi^k = \sum_{X:|X|=k} \Psi_X \tag{23}$$

It is easy to see that for every bond $< ij >$ we have $E_{ij}\Psi^k = \Psi^k$ Hence Ψ^k is an eigenstate of H with the same eigenvalue as the all $+$ state. This construction gives $|\Lambda| + 1$ ground states. These ground states are said to be unfrustrated. For every bond $< ij >$ the energy $< \Psi^k | E_{ij} | \Psi^k >$ is equal to the smallest eigenvalue of E_{ij}.

The ground states of the antiferromagnet are more complicated. We first consider a ring of four sites. So

$$H = E_{12} + E_{23} + E_{34} + E_{14} \tag{24}$$

One can explicitly diagonalize this Hamiltonian (the matrix is 16 by 16 but there is a lot of symmetry). You find there is a unique lowest eigenstate, and its energy it strictly greater than four times the lowest eigenvalue of a single E_{ij}. We say the system is frustated.

We can see this frustration without explicitly digaonalizing H. First consider just $E_{12} + E_{34}$. Its unique ground states is the spin singlet on sites 1,2 tensor with the spin singlet on spins 3,4. But this state is not an eigenstate of the rest of the Hamiltonian $E_{23} + E_{14}$. So the expectation of $E_{23} + E_{14}$ is this state will be greater that the lowest eigenvalue of $E_{23}+E_{14}$. Is impossible to find a state that simultaneously minimizes the energy of each individual term in the Hamiltonain.

So far we have been considering the quantum analog of the $N = 3$ model from the last chapter (in which the spins took) values on the usual sphere in $\mathbb{R}^3$. The quantum analog of the **rotator model** ($N = 2$ - spin values on the circle) is

$$H = -\sum_{<ij>} (S_i^x S_j^x + S_i^y S_j^y) \tag{25}$$

This is often called the quantum XY model. The above is the ferromagnetic model - note the minus sign. For this model the ferromagnet and the antiferromagnet are equivalent in the sense that there is a unitary operator U such that $UH_F U^{-1} = H_{AF}$. For spins 1/2 we can take U to be

$$U = \prod_{i:even} \sigma_i^z \tag{26}$$

where the product is over the "even" sublattice. Note that since $(\sigma^z)^2 = 1$, $U^{-1} = U$. And U is self-adjoint, so it is unitary. A little calculation shows

$$\sigma_i^z \sigma_i^\alpha \sigma_i^z = -\sigma_i^\alpha \tag{27}$$

for $\alpha = x, y$. So $UH_F U^{-1} = H_{AF}$.

The analog of the classical model with $N = 1$, the Ising model, is

$$H = -\sum_{<ij>} S_i^z S_j^z \tag{28}$$

This is an operator on a Hilbert space, but it is a diagonal operator. So in fact this quantum model is just the usual (classical) Ising model.

General spin

For spins 1/2, at each site there is a two-dimensional Hilbert space and a triplet of operators S^x, S^y, S^z acting on it. One can easily check that they satisfy the commutations relations

$$[S^\alpha, S^\beta] = i\epsilon_{\alpha\beta\gamma} S^\gamma \tag{29}$$

where $\epsilon_{\alpha\beta\gamma}$ is zero if α, β, γ are not all different and is ± 1 if they are different. The sign is $+1$ if α, β, γ are in cyclic order and -1 if anticyclic order. These are the commutation relations of the Lie algebra $su(2)$. (There is a factor of i difference ...) Spin 1/2 is a two dimensional representation of $su(2)$. Particles can have spin $S = 1/2, 1, 3/2, 2, ...$ For spin S the spin operators still satisfy the above commutation relations but now they act on a space of dimension $2S + 1$. (So S^x, S^y, S^z are $2S + 1$ by $2S + 1$ matrices. For a quantum spin system we then have a Hilbert space of dimension $2S + 1$ at each site and we tensor them together.

Until now we have focused on the ground states which are relavant for zero temperature. We now consider nonzero temperature (finite β). In the classical setting we had a probability measure defined on spin configurations.
Review this

For quantum spin systems $\exp(-\beta H)$ is an operator. The partition function is

$$Z = Tr(\exp(-\beta H)) \tag{30}$$

For our models the state space at each site is finite dimensional, so if we consider a finite volume then H is an operator on a finite dimensional space

and we can think of it (and of $\exp(-\beta H)$) as a giant matrix. The trace is then the usual matrix trace. For an operator O (an "observable") on the Hilbert space we define its expected value at inverse temperature β to be

$$< O > \frac{1}{Z} Tr(O \exp(-\beta H)) \tag{31}$$

Examples of some O's:

- H itself. Then $< H >$ is the average energy
- For a unit vector n, consider $n \cdot \sigma_0$. Its expectation is the average magnetization at site 0.
- $\sigma_0 \cdot \sigma_j$. If we look at $< \sigma_0 \cdot \sigma_j > - < \sigma_0 > \cdot < \sigma_j >$ this is like the covariance between the spin at the origin and the spin at 0. We can look for LRO by seeing whether $< \sigma_0 \cdot \sigma_j >$ converges to zero (no LRO) or not (LRO). We are thinking of the ferromagnet here.

Infinite volume limit

First consider a finite volume. An observable just means an operator on the state space of the finite volume system. Let $\mathbb{A}_\Lambda$ be the space of observables on the space for Λ. A **state** ω is a linear operator from $\mathbb{A}_\Lambda$ to $\mathbb{C}$ on the space of observables such that
(1) $\omega(A^*A) \geq 0$ for all $A \in \mathbb{A}_\Lambda$ (positive)
(2) $\omega(I) = 1$ (nonnegative)

Unit vectors in the state space give states but there are states that do not come from unit vectors. **MORE**

The observables are bounded linear operators on a finite dimensional Hilbert space, so they are a C^* algebra. It is possible to take a limit of this algebra to construct the space of quasi-local observables. Then an infinite volume state ω on the space of quasi-local observables is a linear functional that is positive and normalized.

Intuitively ground states are states with the lowest eigenvalue. An infinite volume ground state is a state ω such that

$$\omega(A^*[H, A]) \geq 0 \tag{32}$$

for all local observables A. Explain why $[H, A]$ makes sense.

Intuition behind this def

It is possible to define the spectral gap in the infinite volume limit, but you need the GNS construction for this.

Interesting questions:

- Is there LRO - breaking of the continuous (or in some cases discrete) symmetry at low temperatures? This would mean that there are multiple equilibrium states.
- Do correlations decay like a power law or exponentially for low temperatures?
- Is there a spectral gap?
- For the antiferromagnet is there LRO in the ground state, and hence multiple ground states in the infinite volume limit?
- Do correlations in the ground state(s) decay like a power law or exponentially?

quantum fluctuations can act like thermal fluctations

Uniqueness of the ground state: A word of caution. It is tempting to study the ground state for a finite system and use this to conclude whether or not there is a unique or multiple ground states in the infinite volume limit. Don't do this. **Explain why**

Spectral gap: This refers to the gap (or lack of a gap) between the ground state energy and the first excited state. There is a definition in the infinite volume limit but we did not give it. Again, it is tempting to try to study this by studying the difference between the lowest eigenvalue and the next to lowest for a finite system and seeing what happens as the volume goes to infinity. Don't do this. **Explain why**

In the antiferromagnet if there is LRO the spin will tend to have nearest neighbors anti-aligned. This is calle Néel order. For the antiferromagnet we should look at

$$\lim_{|j|\to\infty} (-1)^j < \sigma_0 \cdot \sigma_j > \tag{33}$$

where $(-1)^j$ is defined to be 1 on the even sublattice and -1 on the odd sublattice.

Exercises:

7.2.1 (3 points) Let n be a 3d unit vector. Let $U_i = \exp(i\theta n \cdot \sigma_i)$. Let $U = \prod_i U_i$. Note that the U_i and U are unitary operators. Show that $U(-\theta)HU(\theta) = H$ where H is the Heisenberg Hamiltonian (ferromagnetic or antiferromagnetic). This is the SU(2) symmetry of the quantum Heisenberg model.

7.2.2 (4 points) Consider the quantum spin antiferromagnet on a ring of four sites with $S = 1/2$. So the Hamiltonian is

$$H = E_{12} + E_{23} + E_{34} + E_{14} \tag{34}$$

where E_{ij} is the exchange operator that interchanges the spins at sites i and j. The Hilbert space has dimension $2^4 = 16$. The lowest eigenvalue of E_{ij} is -1. So $H \geq -4$. Find lowest eigenvalue of H. You should find that it is stricly greater than -4. Remark: The brute force approach is to just diagonalize the 16 by 16 matrix using a computer. This model has a lot of symmetry. (You can rotate the square of sites and reflect it. Also the operator $\sigma_1^z + \sigma_2^z + \sigma_3^z + \sigma_4^z$.) All this symmetry can reduce the search for the ground state to eigenproblems with small dimension.

7.2.3 (4 points) Let Ψ^k be the ground state for the ferromagnet defined in (23). Let i, j be sites (not necessarily nearest neighbors). Compute the expectation of $\sigma_i \cdot \sigma_j$ in the state Ψ^k, i.e., compute $< \Psi^k | \sigma_i \cdot \sigma_j | \Psi^k >$. Hint: you can rewrite $\sigma_i \cdot \sigma_j$ in terms of E_{ij}.

7.3 Existence of long range order - symmetry breaking

Just as in the classical case, a continuous symmetry in two dimensions precluded LRO.

Theorem 1. *(Hohenberg - Mermin - Wagner) Consider the quantum rotator model in two dimensions on a square lattice with nearest neighbor coupling. Then for all temperatures the rotation symmetry is not broken - no LRO.*

In three and higher dimensions we expect broken symmetry (LRO) at low temperatures in both the ferromagnet and antiferromagnet. But this has only been proved for the antiferromagnet.

Theorem 2. *(Dyson,Lieb,Simon) Consider the quantum Heisenberg model in three and more dimensions on a square lattice with nearest neighbor couplings. For all spins ($S = 1/2, 1, 3/2, \cdots$) the antiferromagnet has Néel LRO at low temperatures. There are multiple equilibrium states which break the continuous symmetry*

Theorem 3. *Consider the quantum Rotator model in three and more dimensions on a square lattice with nearest neighbor couplings. For all spins ($S = 1/2, 1, 3/2, \cdots$) the ferromagnet has LRO and the antiferromanet has Néel LRO at low temperatures. There are multiple equilibrium states which break the continuous symmetry*

Open problem: Prove LRO in the ferromagnet at low temperatures for $d \geq 3$.

The ground state of the antiferromagnet is quite nontrivial and in two dimensions it is an interesting, non-trivial question whether or not there is LRO (and hence multiple ground states that break the symmetry).

Theorem 4. *In three dimensions in all the cases where it is proved that there is LRO at low temperatures there is LRO in the ground state. Furthermore, in two dimensions there is LRO in the Heisenberg model ground states if $S \geq 1$ and in the rotator model for all S.*

Open problem: Prove LRO in the Heisenberg antiferromagnet ground states for two dimensions and $S = 1/2$.

Anisotropic model - Peierls argument

7.4 Quantum spin chains

For quantum systems there can be interesting physics in the ground state of one dimensional systems.

For spin 1/2 in one dimension the model is Bethe ansatz solvable. This solution shows that there is power law decay of the correlations in the ground state.

Digression on translation symmetry breaking in classical systems

Frustrated spin 1/2 chain

$$H = \sum_i \sigma_i \cdot \sigma_{i+1} + g \sum_i \sigma_i \cdot \sigma + i + 2 \tag{35}$$

with $g > 0$. **Explain why this is frustrated**

For $g = 0$ this is the usual nearest-neighbor Heisenberg spin 1/2 chain. The Bethe ansatz solution shows it has power law decay of the two point function.

For $g > 0.2411...$ the translational symmetry is broken - there are two ground states related by a translation by one lattice site. **Picture:**

If $g = 0.5$ the ground states are simple and explicit One ground state is formed by put the pairs $\{1, 2\}$, $\{3, 4\}$ into the single state and then taking a tensor product of these states. This model is known as the Majumdar-Gosh model.

two dimensions - VBS and RVB

Spin 1 and the Haldane phase

The Heisenberg model has an $su(2)$ symmetry. It is also translation invariant. Are there any other Hamiltonians with these properties. (Of course one can mutiply the Hamiltonian by a constant and add a constant to it.) We could try to construct others by adding in powers of $S_i \cdot S_j$. However, $(\sigma_i \cdot \sigma_j)^2$ is a linear combination of $\sigma_i \cdot \sigma_j$ and the identity, so for spin 1/2 we do not get any new Hamiltonians this way. In fact, the Heisenberg Hamiltonians is the only translation invariant, nearest-neighbor, $su(2)$ invariant Hamiltonian.

For $S = 1$, $(S_i \cdot S_j)^2$ is not a linear combinations of I and $S_i \cdot S_j$. So we can consider a more general Hamiltonian

$$H = J_1 \sum_i S_i \cdot S_{i+1} + J_2 \sum_i (S_i \cdot S_{i+1})^2 \tag{36}$$

Of course the physics really only depends on the ratio J_2/J_1. This is the most general translation invariant, $su(2)$ invariant Hamiltonian for $S = 1$. (For $S = 1$ $(S_i \cdot S_j)^3$ is a linear combination of I, $S_i \cdot S_j$ and $(S_i \cdot S_j)^2$.)

Initially people thought that the $S = 1$ Heisenberg model ($J_2 = 0$) behaves like the $S = 1/2$ model. Duncan Haldane argued that it (and all integer spin chains, i.e., $S = 1, 2, 3, ...$ should behave quite differently - exponential decay of correlations and a spectral gap.

For $J_2/J_1 = 1/3$ this model is solvable (not Bethe ansatz). One can compute the correlations and see they decay exponentially with correlation length $1/\ln(3)$. This model has also been proved to have a spectral gap. These results have been extended to a small neighborhood of $J_2/J_1 = 1/3$.

To explain why this particular model is solvable we need a bit of discussion of the tensor product of two spin 1's. Some representation theory shows that this tensor product is the direct sum of three subspaces - one each for spin $= 0, 1, 2$. We have

$$H = \sum_i \left[\frac{1}{3} + \frac{1}{2} S_i \cdot S_{i+1} + \frac{1}{6} (S_i \cdot S_{i+1})^2 \right] = \sum_i P^{(2)}_{i,i+1} \tag{37}$$

where $P^{(2)}_{i,i+1}$ is the orthogonal projection onto the states on sites i and $i+1$ with spin 2. If it is possible to find a state whose restriction to any two adjacent sites has no component in the spin 2 subspace, then that state is a ground state. If this is possible then there is no frustration in the model. More results for this model are explored in one of the homework problems.

Figure 1 shows the conjectured phase diagram.

Exercises:

7.4.1 (3 points) Consider the Majumdar-Gosh model.

(a) Show that the two states we said were ground states are indeed ground states.

(b) (3 points) Compute the correlation functions $< \sigma_i \cdot \sigma_j >$ and $< \sigma_i >$ in one of these ground states. Here σ_i is the usual vector of sigma matrices. So $< \sigma_i >$ is a vector (whose components are complex numbers).

7.4.2 Consider the spin-1 chain with Hamiltonian

$$H = \sum_i \left[\frac{1}{3} + \frac{1}{2} S_i \cdot S_{i+1} + \frac{1}{6} (S_i \cdot S_{i+1})^2 \right] = \sum_i P^{(2)}_{i,i+1} \tag{38}$$

where $P^{(2)}_{i,i+1}$ is the orthogonal projection onto the states on sites i and $i+1$ with spin 2. An orthonormal basis for the states on two sites with spin 2 is

$$e_1 = (++), \quad e_2 = [(+0) + (0+)]/\sqrt{2} \tag{39}$$

$$e_3 = [2(00) + (+-) + (-+)]/\sqrt{6} \tag{40}$$

$$e_4 = [(-0) + (0-)]/\sqrt{2}, \quad e_5 = (--) \tag{41}$$

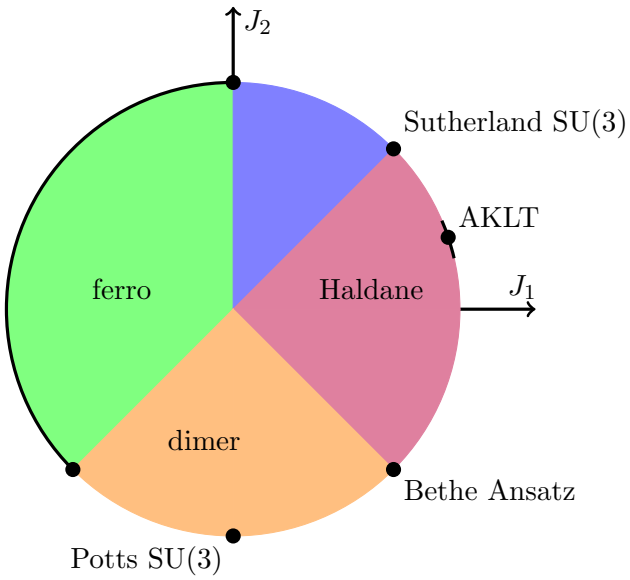

Figure 1: Conjecture phase diagram of general $S = 1$ spin chain. Courtesy of Bruno Nachtergaele, Robert Sims.

With periodic boundary conditions there is a unique ground state. The basis in which the S_i^z are diagonal can be denoted by $|A>$ where A ranges over all strings of $+, 0, -$. For an A in which the the number of $+$'s equals the number of $-$'s and the non-zero entries alternate between $+$ and $-$ we define

$$\psi(A) = (-1)^m \, 2^k \tag{42}$$

where k is the number of pairs of $+,-$ and m is the number of odd sites with $+$ or $-$. For example, $\psi(0 - + - 00 + -0+) = 2^3$ since $k = 3$ and $m = 2$. For all other A define $\psi(A) = 0$. Then we let

$$\Omega = \sum_A \psi(A)|A> \tag{43}$$

(a) (3 points) Show that $P^{(2)}_{i,i+1}\Omega = 0$ for all i, and hence it is a ground state.
(b) (5 points) Compute $< \Omega | S_i \cdot S_j | \Omega >$. For a simpler computation you can compute $< \Omega | S_i^z S_j^z | \Omega >$. Conclude that the correlation length is $1/ln(3)$.