Chapter 3

Basic quantum statistical mechanics of spin systems

3.1 Spins and $SU(2)$ symmetry

Even though the first chapter discussed classical ferromagnets, ferromagnetism is an inherently quantum-mechanical phenomenon.

The Hamiltonian of a single quantum spin is built from the spin operators S^x, S^y and S^z, These operators satisfy the commutation relations of the $su(2)$ Lie algebra

$$[S^a, S^b] = i\epsilon_{abc}S^c \tag{3.1}$$

where ϵ_{abc} is the completely antisymmetric tensor with $\epsilon_{xyz} = 1$. This algebra is familiar as the algebra of generations of rotations (i.e. the components of the angular momentum). Here, the rotation is *not* in the position of the spins, but rather in its "direction" (in quotes because it is of course not possible to measure all three components of a quantum spin).

The HIlbert space of a quantum spin is defined by choosing a *representation* of the spin operators. A representation of a Lie algebra is a set of three matrices satisfying the commutation relations, for $su(2)$ given by (3.1). An *irreducible* representation is a set of matrices such that no unitary transformation $US^aU^\dagger$ block-diagonalizes all three matrices. From the theory of Lie algebras, it is known that for $su(2)$ there is exactly one set (up to unitary transformations) of irreducible $n \times n$ matrices for each integer n. For reasons soon to be apparent, it is customary to write $n = 2s + 1$ for all integers and half-integers s. The index s is typically called, somewhat confusingly, the "spin" of the particle. A single spin-s quantum particle at a fixed point in space therefore has a Hilbert space $\mathbb{C}^{2s+1}$, so the matrices S^a all are $(2s+1) \times (2s+1)$. An orthonormal basis is given by the eigenstates of any one of the matrices. It does not matter which one; any such basis chosen can be "rotated" (in spin space!) to any other.

For $s = 0$, the matrices all consist of the number zero; not surprisingly, this is called the *trivial* representation. For $s = 1/2$, it gets interesting; $S^a = \sigma^a\hbar/2$, where the σ^a are the Pauli matrices

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

The eigenstates of S^z for spin-1/2 particles are typically called spin "up" and "down". For $s = 1$, the matrices can be written to have entries $(S^a)_{bc} = i\epsilon_{abc}$.

The eigenvalues of $S^a/\hbar$ in the spin-S representation are given by $(s, s-1, \cdots -s)$. This follows from the following elegant argument. Define the *raising* and *lowering* operators S^+ and S^- by

$$S^{\pm} = \frac{1}{2}(S^x \pm iS^y) .$$

In terms of these operators the $su(2)$ Lie algebra is

$$[S^+, S^-] = \hbar S^z/2, \qquad [S^z, S^{\pm}] = \hbar S^{\pm} .$$

The latter relation means that for any eigenstate of S^z obeying $S_z|m\rangle = m\hbar\rangle$, the state $S^+|m\rangle$ is either 0 or is an eigenstate with eigenvalue $(m+1)\hbar$:

$$S^z S^+ |m\rangle = (m+1)\hbar S^+|m\rangle$$

. Since the matrices are $(2s+1)$-dimensional, $S^z/\hbar$ has $(2s+1)$ eigenvalues, and so in an irreducible representation they must take on the value $s, s-1, \cdots - s$.

In a given representation, one can consider products and sums of the spin operators, given simply by multiplying and adding the corresponding matrices. An important one is the combination

$$\vec{S} \cdot \vec{S} \equiv S^x S^x + S^y S^y + S^z S^z$$

This operator, known in the theory of Lie algebras as the quadratic Casimir, commutes with each of the generators S^a. As a result, it must be proportional to the identity in a given irreducible representation. This is a consequence of fundamental result in the theory of representations, called *Schur's Lemma*:

> Let V be the vector space associated with a finite-dimensional irreducible representation of an algebra A over $\mathbb{C}$. Then let $\phi : V \to V$ be a homorphism, i.e. $\phi(av) = a\phi(v)$ for any $a \in A$ and $v \in V$. Then $\phi = \lambda I$, where I is the identity matrix.

A vector space V "over $\mathbb{C}$" means that multiplying a vector by a complex number gives another vector in V. It turns out that in the spin-s representation of $su(2)$, the constant is quite simply

$$\vec{S} \cdot \vec{S} = s(s+1)\hbar^2 I \tag{3.2}$$

This formula can be verified easily for spin 1/2 and spin 1 by using the explicit matrices.

One can of course consider quantum-mechanical "spins" based on algebras larger than $su(2)$. One reason for doing so is it gives a way of introducing a small parameter into the theory in order to do perturbative computations. Namely, if the "spin" is in a representation of the Lie algebra $su(n)$ or $sp(n)$, it is possible to take n large and do computations as a power series in $1/n$.

The fact that a quantum-mechanical spin has a fixed "magnitude" in the sense of (3.2) is the reason why it is typical to consider only classical spins of fixed magnitude. In fact, a classical fixed-magnitude spin can be recovered simply by taking the limit $s \to \infty$ and $\hbar \to 0$ with $s\hbar$ fixed. Taking $\hbar \to 0$ in (3.1) shows that the different components of the spin commute, as classical spins do. From (3.2) it then follows that these classical spins indeed have fixed magnitude $s\hbar$ in this limit.

3.2 Hamiltonians for many spins

A single quantum-mechanical spin (or a collection of non-interacting spins) is not particularly difficult to understand, and thorough discussions can be found in many books on statistical mechanics. The situation gets much more interesting (and difficult) in interacting many-body systems.

The simplest way to model a magnetic many-body systems to consider spins fixed at the sites on a lattice. Each set $\vec{S_i}$ for fixed i satisfies the $su(2)$ commutation rules

$$[S^a_j, S^b_k] = i\delta_{jk}\epsilon_{abc}S^c_j \tag{3.3}$$

with spin operators on different sites commuting Henceforth, Planck's constant in these spin systems is set to $\hbar = 1$. A convenient shorthand for these three matrices at site i is $\vec{S} = (S^x_i, S^y_i, S^z_i)$, so that e.g.

$$\vec{S_1} \cdot \vec{S_2} \equiv S^x_1 S^x_2 + S^y_1 S^y_2 + S^z_1 S^z_2$$

The Hilbert space of a many-spin system is the *tensor product* of the Hilbert space for each individual spin. A tensor product of two Hilbert spaces V and W is another Hilbert space, denoted $V \otimes W$. Each element of $V \otimes W$ is comprised of an element $v \in V$ and an element $w \in W$ such that $(\lambda v) \otimes w = v \otimes (\lambda w) = \lambda(v \otimes w)$ for any complex number λ. [1] The inner product is defined by the product:

$$\langle v_1 \otimes w_1 | v_2 \otimes w_2 \rangle = \langle v_1 | v_2 \rangle \langle w_1 | w_2 \rangle \ .$$

The full Hilbert space for N spin-s particles is therefore the tensor product of N Hilbert spaces $\mathbb{C}^2$, written in shorthand as $(\mathbb{C}^{2s+1})^{\otimes N}$. In this tensor product language,

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[1] There is another way to put two vector spaces together called the *direct product* . As with the tensor product, each element of the direct $V \times W$ is comprised of an element from V and an element from W. The difference is that here $(\lambda v) \times w \neq \lambda(v \times w)$. Instead, $\lambda(v \times w) = \lambda v \times \lambda w$. As a result, each v and w corresponds to a unique vector $v \times w$, as opposed to the tensor product case, where for example $v \otimes 0 = 0$ for any v. A well-known example of a direct product is combining the vectors along the x-axis with vectors along the y axis $\mathbb{R}$ to get vectors in the plane: $\mathbb{R}^2 = \mathbb{R} \times \mathbb{R}$.

the spin operators S_i^a at site i acts on the full Hilbert space, but non-trivially only on the ith spin. In shorthand,

$$S_i^a \equiv I \otimes I \otimes \cdots \otimes I \otimes S^a \otimes I \otimes ...$$

Operators need not decompose purely into a product of operators on the individual spins, but can be a sum of them.

An important set of operators is the *total spin*:

$$\mathcal{S}^a = \sum_{i=1}^{N} S_i^a \ . \tag{3.4}$$

If the Hamiltonian commutes with these, then the full system is $su(2)$ symmetric. By direct computation, it is straightforward to check that each of the three components of the "total" spin

$$\vec{\mathcal{S}} = \sum_i \vec{S}_i$$

commutes with any "dot product":

$$[\vec{\mathcal{S}}, \vec{S}_i \cdot \vec{S}_j] = 0 \ .$$

This commutes with any dot product, just like for ordinary vectors. It is important to remember though that $\vec{S}_i$ is a vector whose components are each matrices/operators.

The simplest example of an $su(2)$-symmetric spin Hamiltonian is therefore the nearest-neighbor *Heisenberg model*, where

$$H = -J \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j \tag{3.5}$$

Since the spin-1/2 operators can be written in term of Pauli matrices, the spin-1/2 Heisenberg Hamiltonian on a chain in terms of raising/lowering operators is then:

$$H = -J \sum_{i=1}^{N} \left(\frac{1}{2} (\sigma_i^+ \sigma_{i+1}^- + \sigma_i^- \sigma_{i+1}^i) + \frac{1}{4} \sigma_i^z \sigma_{i+1}^z \right) \tag{3.6}$$

As in the classical case, $J > 0$ is the *ferromagnetic* case, where the diagonal terms in the Hamlitonian favorable spins aligning, while $J < 0$ is the *antiferromagnetic* case, where the diagonal terms favor antialignment. However, as opposed to the classical case, quantum ferromagnets and antiferromagnets behave very differently even on lattices without geometric frustration, as will be described in depth in the next section.

The Heisenberg Hamiltonian commutes with the $\mathcal{S}^a$ by construction. It is then quite interesting to look the "magnitute" of the total spin, $\vec{\mathcal{S}} \cdot \vec{\mathcal{S}}$. Schur's Lemma does not immediately apply, because the $\mathcal{S}^a$ are reducible. The representation theory of $su(2)$

explains how to decompose the tensor products of representations into their irreducible components. In physics, this is often known as "angular momentum multiplication". The simplest example is what happens with with the Hilbert space of two spin-1/2 particles, the tensor product of two spin-1/2 representations of $su(2)$. The four states in the Hilbert space can be decomposed into the triplet representation and the singlet representation:

$$\text{triplet}: \quad |\uparrow\uparrow\rangle,\ \tfrac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle),\ |\downarrow\downarrow\rangle \tag{3.7}$$

$$\text{singlet}: \qquad \tfrac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \tag{3.8}$$

It is easy to check that the three states in (3.7) have eigenvalues of $\mathcal{S}^\ddagger$ given by 1, 0, and -1 respectively, and that $\mathcal{S}^\pm$ map these states onto each other (or annihilate them) The singlet is annihilated by all the $\mathcal{S}^a$. Schematically, we this decomposition is denoted by the *fusion rule*

$$(1/2) \otimes (1/2) = (0) + (1)\ .$$

In general, the tensor product of $su(2)$ representations with spin s_1 and s_2 contains all the representations with spins $|s_1 - s_2|, |s_1 - s_2| + 1, \ldots, s_1 + s_2$, each appearing once. This is typically denoted by the fusion rule

$$(s_1) \otimes (s_2) = \sum_{s=|s_1-s_2|}^{s_1+s_2} (s). \tag{3.9}$$

It is important to note that the fusion rule only says which representations appear in the tensor product; it does not give the precise decomposition as in (3.7) and (3.8). The explicit coefficients relating the basis elements are called Clebsch-Gordon coefficients, and are quite tedious to work out in general. Luckily, they are not needed in many cases; it suffices to know the fusion rules. The fusion rules are associative, so that the tensor product of multiple spins can be found by fusing two at a time, e.g.

$$(1/2) \otimes (1/2) \otimes (1/2) = \big((0) + (1)\big) \otimes (1/2) = (3/2) + (1/2) + (1/2)\ .$$

A check is that the dimensions of the representations adds up properly: $2\times2\times2 = 4+2+2$. This example also illustrates that with multiple spins, the same kind of representation can appear multiple times. Here, this means there are two linearly-independent ways of making a total-spin-1/2 representation out of three spin-1/2 particles.

The Heisenberg Hamiltonian is the only $su(2)$-invariant nearest-neighbor spin Hamiltonian for spin-1/2 particles. Some well-known generalizations break the $su(2)$ symmetry. The unimaginatively named XXZ Hamiltoninan allows for varying the coupling in front of the diagonal term:

$$H_{\text{XXZ}} = -\sum_{i=1}^{N} \left(J_\perp (\sigma_i^+ \sigma_{i+1}^- + \sigma_i^- \sigma_{i+1}^+) + \frac{J_z}{2} \sigma_i^z \sigma_{i+1}^z \right)\ . \tag{3.10}$$

It is easy to check that this Hamiltonian still commutes with $\mathcal{S}^z$, and so preserves a $U(1)\times\mathbb{Z}_2$ symmetry. In the language of rotations of classical spins, the $U(1)$ corresponds to rotations around the z axis, while the $\mathbb{Z}_2$ corresponds to flipping all the spins, i.e. sending each $\sigma^x_i \to \sigma^x_i$, $\sigma^y_i \to -\sigma^y_i$, $\sigma^z_i \to -\sigma^z_i$.[2] A still more general Hamiltonian, the even more unimaginatively named XYZ case, preserves only the spin-flip symmetry:

$$H_{XXZ} = -\sum_{i=1}^{N} \left(J_x\sigma^x_i\sigma^x_{i+1} + J_y\sigma^y_i\sigma^y_{i+1} + J_z\sigma^z_i\sigma^z_{i+1} \right) \ . \tag{3.11}$$

None of these Hamiltonians correspond to a quantum version of the Ising model. Later in this chapter, one will be derived.

3.3 Ferromagnets and antiferromagnets

Unless there's geometric frustration, in classical systems there seems to be not much difference between ferromagnets and antiferromagnets. For example, with nearest neighbor interactions, geometric frustration occurs for lattices that are not bipartite. In a bipartite lattice, the sites can be divided into two sublattices such that nearest neighbors always belong to different sublattices. A nearest-neighbor antiferromagnetic interaction in a classical model on a bipartite lattice can typically be changed into a ferromagnetic one by redefining the spin to by a flip (e.g. ↑↔↓ in the Ising model) on all sites on one of the sublattices, but not the other. The physics of such classical antiferromagnets is therefore essentially equivalent to that of the ferromagnets.

Antiferromagnetic quantum systems on non-bipartite lattices also exhibit interesting behavior. But the interesting thing is that on bipartite lattices, there are a number of important difference between quantum ferromagnets and antiferromagnets. In this section, this will be illuminated by studying the spin-1/2 Heisenberg Hamiltonian on two and four sites; the essential physics is already apparent.

Analyzing the Heisenberg interaction $-J\vec{S}_1\cdot\vec{S}_2$ across a single bond is very illuminating. For spin-1/2, this is simply a 4×4 matrix:

$$\begin{aligned}\vec{S}_1\cdot\vec{S}_2 &= \sum_{i=1}^{4}\left(\frac{1}{2}(\sigma^+_i\sigma^-_{i+1} + \sigma^-_i\sigma^+_{i+1}) + \frac{1}{4}\sigma^z_i\sigma^z_{i+1}\right) \\ &= \frac{1}{4}\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & -1 & 2 & 0\\ 0 & 2 & -1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}\end{aligned}$$

where this matrix acts on the basis $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$. Diagonalizing this matrix is obviously not difficult, but it is illuminating to first group the states into representations

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[2] One needs to flip two of the three S^z in order to preserve the commutation relations.

of the $su(2)$ symmetry. Since the $su(2)$ fusion rule is $(1/2)\otimes(1/2) = (0)+(1)$, these states can be grouped into the $s = 1$ triplet representation and the $s = 0$ singlet representation, as defined in (3.7) and (3.8). It is simple to check that $\vec{\mathcal{S}}\cdot\vec{\mathcal{S}} = s(s+1)$ in the two cases, and that while the singlet is annihilated by all three generators $\vec{\mathcal{S}}$, acting with $\mathcal{S}^+$ and $\mathcal{S}^-$ takes members of the triplet to each other.

Each member of the triplet has eigenvalue $-J/4$ under $\vec{S}_1 \cdot \vec{S}_2$, while the singlet has eigenvalue $+J/4$. One important difference between the ferromagnet $J > 0$ and the antiferromagnet $J < 0$ is now readily apparent. There are multiple ground states of the ferromagnet: each member of the triplet has the minimum energy $-J$, while the antiferromagnetic ground state, the singlet, is unique. Moreover, the antiferromagnetic ground state is invariant under the $su(2)$ symmetry, whereas the ferromagnetic ground states are not.

Additional insight comes from solving the Heisenberg model on a four-site chain. The Hilbert space is now 16 dimensional, but by exploiting symmetry the Hamiltonian can be block-diagonalized into much smaller blocks. The magnetization $\mathcal{S}^z$ commutes with H, so they can be diagonalized simultaneously. For periodic boundary conditions, *translation invariance* proves another powerful constraint. The translation operator $\mathcal{T}$ simply shifts the spins by one site mod N: $\mathcal{T}^{-1}\vec{S}_i\mathcal{T} = \vec{S}_{i+1}$. The Hamiltonian commutes with $\mathcal{T}$ when the boundary conditions are periodic, and $\mathcal{T}$ commutes with $\mathcal{S}^z$ as well. Thus H can be broken into blocks acting with on states with a fixed eigenvalue of $\mathcal{T}$ and $\mathcal{S}^z$.

Since $\mathcal{T}^N = 1$ for an N-site chain, the eigenvalues of $\mathcal{T}$ are $e^{i2\pi n/N}$ for integer n. It is customary to define the corresponding *momentum* as $k \equiv 2\pi n/N$. The (unnormalized) eigenstates of $\mathcal{T}$ are then of the form

$$\sum_{n=0}^{N-1} e^{-i2\pi n/N}\mathcal{T}^n|s\rangle = |s\rangle \ + \ e^{-i2\pi/N}\mathcal{T}|s\rangle \ + \ \ldots \ + \ e^{i2\pi/N}\mathcal{T}^{-1}|s\rangle$$

For four sites, using translation invariance already diagonalizes the entire Hamlitonian save for $m = 0$ and $k = 0$ or π. The corresponding eigenstates are

$$\begin{aligned} |A\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\uparrow\downarrow\rangle + e^{-i\pi k}|\downarrow\uparrow\downarrow\uparrow\rangle)\ , \\ |B\rangle &= \frac{1}{2}((|\uparrow\uparrow\downarrow\downarrow\rangle + e^{-i\pi k}|\downarrow\uparrow\uparrow\downarrow\rangle + \ldots)\ . \end{aligned}$$

The Hamiltonian on these $k = 0$ or π states is

$$-J\begin{pmatrix} -1 & \sqrt{2}\cos(\pi k/2) \\ \sqrt{2}\cos(\pi k/2) & 0 \end{pmatrix}$$

The eigenvalues in these sectors are therefore $-J$ and $2J$ for $k = 0$ and J and 0 for $k = \pi$. Again organizing the eigenstates into $su(2)$ multiplets gives for the energy levels divided by $-J$:

$$\begin{array}{rc} \text{quintuplet :} & 1 \\ \text{triplets :} & \cos(\pi k)\ (\text{ for } k \neq 0) \\ \text{singlets :} & -2, 0 \text{ for } k = 0, \pi \ \text{ respectively.} \end{array}$$

The $su(2)$ invariance allows the construction of the entire multiplet once one of the states is known.

As with two sites, the ferromagnetic ground state is a multiplet, whereas the antiferromagnetic is a singlet. For a general N-site ferromagnet, the completely ferromagnetic states (all spins up or all spins down) are exact ground states of H. This suggests using an order parameter for ferromagnetism. A ferromagnetic order parameter is simply the quantum analog of the magnetization, the expectation value of the z component of the total spin:

$$\langle \text{g.s.}|\mathcal{S}^z|\text{g.s.}\rangle = \sum_{i=1}^{N} \langle \text{g.s.}|S_i^z|\text{g.s.}\rangle \ .$$

This is not a particularly great order parameter: as with the classical case, this will vanish if there is a symmetry under spin flip. A better one is $\langle \text{g.s.}|(\mathcal{S}^z|)^2|\text{g.s.}\rangle$. The completely ferromagnetically ordered states (all spins up or all spins down) are both eigenstates of $\mathcal{S}^\ddagger$ with the maximum magnitude of eigenvalue, N^2, and are ground states of the Hamiltonian.

The antiferromagnetic situation is very different. The staggered magnetization, or *Néel order parameter*, is commonly used to understand antiferromagnetic order. It can only be defined on bipartite lattices. Label the sites so that the odd sites are on one sublattice, and the even sites the other, and consider the operator

$$\mathcal{N} \equiv \sum_{i=1}^{N} (-1)^i S_i^z$$

A "Néel state" has eigenvalue N^2 under $\mathcal{N}^2$, i.e. the spins are spin up on one sublattice and spin down on the other, like state $|A\rangle$ for four sites. Note, however, that $\mathcal{N}$, opposed to $\mathcal{S}^z$. does not commute with the Hamiltonian, and the Néel state is *not an eigenstate* of the Heisenberg Hamiltonian. This is a huge difference between ferromagnets and antiferromagnets even on bipartite lattices, not just on geometrically frustrated ones.

For example, for four sites and $J < 0$ the ground state is a spin singlet and translation invariant. The properties are quite typical of antiferromagnetic ground states. The diagonal terms are J and 0 for the translation-invariant Néel state $|A\rangle$ and the other state $|B\rangle$ respectively, so indeed this favors the Néel state. However, the off-diagonal terms in the Hamiltonian, mean that the eigenstate is proportional to $\sqrt{2}|A\rangle + |B\rangle$. Thus while the translation-invariant Néel state $|A\rangle$ has the largest magnitude in the ground state, the other state $|B\rangle$ is also present.

Since the exact ferromagnetic ground states are known, the energy of the lowest-energy excited states can also be computed. Consider the states with $\mathcal{S}^z = N/2 - 1$ on N-site spin-1/2 chain, i.e. with $N - 1$ up spins and one down spin. WIth periodic boundary conditions, there is only one given state with each momentum $k = 2\pi a/N$. These states are commonly called *spin waves*. The ground state energy of the ferromagnet for N sites is $-NJ/4$, because each nearest-neighbor term contributes $-J/4$, and the off-diagonal terms annihilate this state. The diagonal term for any of the $\mathcal{S}^z = N/2 - 1$ states is $-NJ/4 + J$ because there are two broken bonds, each adding an energy $J/2$. The contribution of the off-diagonal terms is the same $-J\cos(\pi k)$ as in the four-site case. The energy $E(k)$ of a spin wave of momentum k is therefore the difference between this energy and that of the ground state:

$$E(k) = J(1 - \cos(\pi k)) \ . \tag{3.12}$$

$E(k) \geq 0$, with the zero-energy state the one with zero momentum; this is part of the ground-state multiplet. The lowest-energy excited states have momentum near zero. For them, the energy is quadratic:

$$E(k) \approx Jk^2/2 \ ,$$

a characteristic feature of ferromagnets. This ferromagnet is *gapless*; there exist excitations of arbitrarily small energy in the limit $N \to \infty$, vanishing here as $1/N^2$.

This function $E(k)$ is an example of a *dispersion relation*. The spin waves can be thought of as *quasiparticles*, excitations that behave like particles in that they have a definite relation between their momentum and energy, and when Fourier-transformed back to position space they are localized. There is no guarantee that in a many-body system, the low-lying excitations will be quasiparticle-like, but in a remarkable number of systems, they are. The fact that $E(k) \geq 0$ is a quantum version of the Peierls argument: if it were less than zero, then the ground state wouldn't be a ground state!

3.4 Rewriting a Hamiltonian in terms of projectors

It is often useful to rewrite a Hamiltonian as a sum of projection operators, especially if a form can be found where the coefficients are all positive. This can be done for both the Heisenberg ferromagnet and antiferromagnets, and illuminates greatly the distinction between the two.

A projector in general is an operator that squares to itself: $P^2 = P$. Its eigenvalues therefore can be only zero or one. Any Hamiltonian that can be written in such a form necessarily has non-negative eigenvalues. The proof of this statement is simple. Consider an eigenstate $|E\rangle$ of $H = \sum_i \alpha_i P_i$ where all the α_i are non-negative and each P_i is hermitian. Then

$$E = \langle E|H|E\rangle = \sum_i \alpha_i \langle E|P_i|E\rangle \ .$$

Consider now just one of the terms in this sum and expand $|E\rangle$ in a complete set of eigenstates of this P_i, i.e. $|E\rangle = \sum_j \beta_{ij}|i;j\rangle$. The eigenvalues λ_{ij} of a given P_i must be zero or one, and so non-negative. Therefore

$$\langle E|P_i|E\rangle = \sum_j \lambda_{ij}|\beta_{ij}|^2 \geq 0 \ .$$

Therefore each term in the sum for E is non-negative, yielding

$$E \geq 0.$$

Moreover, it follows that the only way to get $E = 0$ is if each projector P_i *individually* annihilates $|0\rangle$: $P_i|0\rangle = 0$ for all i. Such a state is a ground state, and Hamiltonians which have such a ground state are called in the quantum information world *frustration free.*

A projector $P^{(s)}$ onto spin s gives 1 when acting on a collection of spins whose total spin is s, and 0 otherwise. A projector onto m spins can be built up by taking products of the operators $(\sum_{i=1}^m \vec{S}_i)\cdot(\sum_{i=1}^m \vec{S}_i) - j(j+1)$. For example, there are two projectors $P^{(0)}$ and $P^{(1)}$ acting on two spin-1/2 particles, since $(1/2)\otimes(1/2) = (0) + (1)$. They are given by

$$\begin{aligned} P^{(1)}(\vec{S}_1+\vec{S}_2) &= \frac{1}{2}\Big((\vec{S}_1+\vec{S}_2)\cdot(\vec{S}_1+\vec{S}_2)\Big) \\ P^{(0)}(\vec{S}_1+\vec{S}_2) &= -\frac{1}{2}\Big((\vec{S}_1+\vec{S}_2)\cdot(\vec{S}_1+\vec{S}_2) - 2\Big) \end{aligned}$$

Note that the sum of all projectors is 1, since all states belong to some $su(2)$ multiplet. Since $\vec{S}_i\cdot\vec{S}_i = 3/4$ for a spin-1/2 particle,

$$P^{(1)}(\vec{S}_i+\vec{S}_{i+1}) = 3/4 + \vec{S}_1\cdot\vec{S}_2 \ , \qquad P^{(0)}(\vec{S}_i+\vec{S}_{i+1}) = 1/4 - \vec{S}_1\cdot\vec{S}_2 \ ,$$

The spin-1/2 Heisenberg Hamiltonian therefore can be rewritten as a sum of projectors with positive coefficients in both ferromagnetic and antiferromagnetic cases. After an overall shift by a constant,

$$H = J\sum_{i=1}^N P^{(0)}(\vec{S}_i+\vec{S}_{i+1}) \ .$$

In the ferromagnetic case, this is a sum of projectors with positive coefficients. Each of these projectors annihilates any ferromagnetic ground state. This is obvious for the completely aligned states, since $P^{(0)}$ annihilates any pair of spins that are the same. It is not as obviously true for other parts of the ferromagnetic ground-state multiplet, but follows from the facts that $\mathcal{S}^{\pm}$ commute with the Hamiltonian and act on the completely aligned states to give the rest of the multiplet. Thus the ferromagnetic Heisenberg Hamiltonian is frustration free.

The antiferromagnetic spin-1/2 Heisenberg Hamiltonian can also be rewritten as a sum of projectors with positive coefficients.

$$H = -J \sum_{i=1}^{N} P^{(1)}(\vec{S}_i + \vec{S}_{i+1}) \ .$$

Here, however, there is no state annihilated by all the projectors. This is simple to see by checking explicitly just for three spins in a row. The antiferromagnetic Heisenberg Hamiltonian is therefore not frustration free, another way of seeing the difference between it and the ferromagnetic one.

A final comment on the term "frustration-free" is essential to avoid potential confusion. In some Hamiltonians that are frustration-free, such as the Majumdar-Ghosh one described in the next section, one can reasonably describe the interaction as being *frustrated*, in the sense that different terms in the Hamiltonian favor different types of order. To avoid confusion, a better way of describing such interactions is as *competing.* The point is that there are many different types of ordering possible in a system, and rewriting the Hamiltonian in different ways can highlight whether a resulting term favors or disfavors some type of order. Having competing interactions does not preclude a system being frustration-free, since it is entirely possible that the end result will be a system with a different type of order. A beautiful illustration of this is in the valence-bond solids discussed next.

3.5 Exact ground states for a few antiferromagnets: valence-bond solids

Finding the exact ground state in closed form of an antiferromagnet for N large is typically impossible. Only in a few special cases can the ground state be computed exactly. These, however, are not Néel states, and in fact have a vanishing value of the $\mathcal{N}^2$. Studying them, however is quite illuminating. Not only does it provide an exact ground state in an interacting quantum system, but gives a way of displaying the rich types of behavior possible for antiferromagnets. In this section I will discuss two examples of a different kind of ordering.

Different antiferromagnetic ground states can occur when there are *competing interactions.* These occur when different types of order are favored by different terms in the Hamiltonian. This is nicely illustrated in the *Majumdar-Ghosh* (MG) Hamiltonian. This acts on spin-1/2 particles on an N site chain, but contains a next-nearest-neighbor interaction in addition to the Heisenberg term:

$$H_{MG} = \sum_i \left(\vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{2} \vec{S}_i \cdot \vec{S}_{i+2} \right) \ . \tag{3.13}$$

The diagonal part of the second term favors making spins two sites apart *oppositely* aligned. This thus is an impediment to Néel order, where spins two sites apart are aligned. Thus the two interactions are *competing*, in that they seem to favor different types of order. This results in the MG ground state having another kind of antiferromagnetic order: it is a *valence-bond solid*.

Like the Heisenberg Hamiltonians, the antiferromagnetic MG Hamiltonian is a sum of projectors with positive coefficients. Even though the interactions in the MG Hamiltonian are antiferromagnetic, it has a zero-energy ground state, as opposed to the Heisenberg antiferromagnet. In fact, for periodic boundary conditions and an even number of sites, it has two.

The two terms in the MG Hamiltonian has a relative coefficient 1/2, carefully chosen so that it can be written as the sum of projectors acting on three consecutive spins:

$$H = \sum_i P^{(3/2)}(\{i, i+1, i+2\}) \ .$$

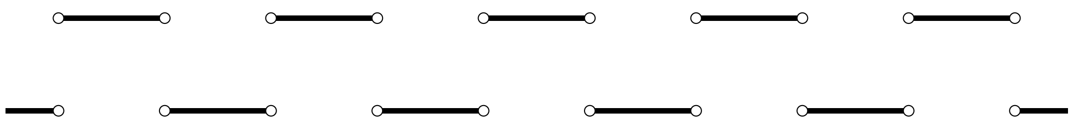
This is not difficult to check (HW). For simplicity I now label the spins in the projector just by their site indices. The zero-energy ground states are found by noting a fact about the fusion rule

$$(1/2) \otimes (1/2) \otimes (1/2) = \big((0) + (1)\big) \otimes (1/2) = (3/2) + (1/2) + (1/2)$$

for three spins: the spin-3/2 state for three spins can be found only by fusion a third spin with the spin-1 state of the two spins. Since this fusion can be done in any order, this means that any two of the three consecutive spins in the MG chain must have spin 1 for the three to have total spin 3/2. Thus if any two of the three spins are in a singlet, $P^{(3/2)}(\{i, i+1, i+2\})$ must annihilate the state. Therefore the state

$$\cdots \otimes (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \otimes (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \otimes \ldots$$

is annihilated by *every* $P^{(3/2)}(\{i, i+1, i+2\})$. The singlet state between two sites is often denoted pictorially by a "dimer", a line drawn between the two. For an even number of sites and periodic boundary conditions, there are two dimer coverings of the chain, e.g. for 10 sites



Each of these states has exactly zero energy. For N even and free boundary conditions instead of periodic, there are five ground states: the end spins are not part of any dimer in one of the coverings and so can be any of the four possible values. In current parlance, these are zero-energy "edge modes": the spin at the end can be flipped without changing the energy.

A singlet state is called a *valence* bond, so such ground states are called *valence-bond solids'*. These ground states are clearly of antiferromagnetic type, since the overall state is a spin singlet. However, they are *not* Néel ordered:

$$\langle\text{dimer}|\, \mathcal{N}^2 \,|\text{dimer}\rangle = N$$

for either dimer state, and so the normalized operator $\mathcal{N}^2/N^2$ vanishes in the large N limit. These ground states are clearly ordered, however; for example the dimer order parameter

$$\langle\text{dimer}|\, \sum_i P^{(0)}(\{i, i+1\}) \,|\text{dimer}\rangle \propto N.$$

Moreover, the spin-spin correlator

$$\langle\text{dimer}|\, S_i^a S_j^a \,|\text{dimer}\rangle = 0 \qquad \text{for } |i-j| > 1;$$

spins beyond nearest-neighbors are completely uncorrelated, so the decay is not even exponential. As is typical of chains with exponentially decaying correlators, the MG chain is gapped.

Finding such Hamiltonians for spin-1/2 requires having next-nearest neighbor interactions. The only $su(2)$-invariant Hamiltonian with nearest-neighbor interactions for spin-1/2 systems is the Heisenberg one, because $\vec{S}_1 \cdot \vec{S}_2$ and its powers are the only $su(2)$ invariants involving two spins. However, in the spin-1/2 case, the higher powers can be reduced to the original. This is because $P^{(1)}(\{i, i+1\})P^{(0)}(\{i, i+1\}) = 0$, and rewriting the projectors in terms of $\vec{S}_1 \cdot \vec{S}_2$ gives $(\vec{S}_1 \cdot \vec{S}_2)^2 = 3/16 - \vec{S}_1 \cdot \vec{S}_2$.

This is not true for higher spins. Consider two spin-1 particles, where the fusion rule is

$$(1) \otimes (1) = (0) + (1) + (2) \ .$$

The projectors here involve the square of $\vec{S}_1 \cdot \vec{S}_2$, e.g.

$$P^{(2)}(\{i, i+1\}) = \frac{1}{3} + \frac{1}{2}\vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{6}(\vec{S}_i \cdot \vec{S}_{i+1})^2 \ .$$

so the trick used for spin-1/2 will not get rid of squares, but only cubes. Thus there is a one-parameter family of $su(2)$-invariant nearest-neighbor spin-1 Hamiltonians

$$H_1 = \sum_i \cos(\theta)\vec{S}_i \cdot \vec{S}_{i+1} + \sin(\theta)(\vec{S}_i \cdot \vec{S}_{i+1})^2 \ . \tag{3.14}$$

This Hamiltonian has a variety of phases and critical points as a function of θ to which will return later. One very interesting point of this spin-1 chain is similar to the Majumdar-Ghosh chain in many ways. This is $\cos(\theta) = 3\sin(\theta)$, and is called the AKLT chain.[3] At this point, each term in the Hamiltonian is simply proportional to the projector $P^{(2)}$:

$$H_{AKLT} = \sum_i P^{(2)} \ . \tag{3.15}$$

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[3] I. Affleck, T. Kennedy, E. Lieb and H. Tasaki, Comm. Math. Phys. **115**, 477 (1982)

Like the MG chain, the exact ground-state can be found, and is a valence-bond solid.

The VBS nature of the AKLT ground state is not immediately obvious, but can be found by a clever trick. First consider a state space of $2N$ *spin-1/2* particles, two for each site on the original lattice. This space is 2^{2N}-dimensional. Let the states $\psi_1 =\uparrow\rangle$ and $\psi_2 = |\downarrow\rangle$ at a given site. Then an orthogonal (but not normalized) basis for the spin-1 triplet is found by combining the two spin-1/2 particles at each site into ψ_{11}, $\psi_{12} = \psi_{21}$, and ψ_{22} where

$$\psi_{\alpha\beta} = \frac{1}{\sqrt{2}}(\psi_\alpha \otimes \psi_\beta + \psi_\alpha \otimes \psi_\beta) \ .$$

These states form an $su(2)$ triplet (+,0,-), with S^z values (1,0,-1) respectively:

$$\psi_{11} = \sqrt{2}(+), \qquad \psi_{12} = \psi_{21} = (0), \qquad \psi_{22} = \sqrt{2}(-) \ ;$$

note the first and last are not normalized. The Hilbert space for the original spin-1 chain is therefore has a basis

$$\psi_{\alpha_1\beta_1} \otimes \psi_{\alpha_2\beta_2} \otimes \cdots \otimes \psi_{\alpha_N\beta_N} \ .$$

This space is indeed 3^N dimensional.

Each bond on the original spin-1 chain has four spin-1/2 particles associated with it. The key obvervation is that *any pair* of these four particles must be in a triplet state for the operator $P^{(2)}$ to be non-vanishing. This follows from the fusion rules

$$(1/2) \otimes (1/2) \otimes (1/2) \otimes (1/2) = ((0) + (1)) \otimes ((0) + (1)) \ ;$$

the only way to get (2) overall is from $(1) \otimes (1)$. The AKLT Hamiltonian therefore annihilates any state where *any* two of the four are in a spin-singlet state. For example the state on two sites $\psi_{11}\psi_{21} - \psi_{12}\psi_{11}$ is annihilated by $P^{(2)}$. Unlike the Heisenberg case, there is a state that is annihilated by each of the projectors:

$$\epsilon^{\beta_1\alpha_2}\epsilon^{\beta_2\alpha_3} \ldots \epsilon^{\beta_N\alpha_1}\psi_{\alpha_1\beta_1} \otimes \psi_{\alpha_2\beta_2} \otimes \cdots \otimes \psi_{\alpha_N\beta_N}$$

(not yet normalized). This is a dimer state with the dimers connecting the spin-1/2 particles:

Here it is important to remember that $\psi_{12} = \psi_{21}$ at each site, so the dimer really is symmetric with respect to the two spin-1/2 particles at each site.

For free boundary conditions, the AKLT chain has zero-energy "edge modes" like the MG chain. What is somewhat curious is that they can be thought of as having spin-1/2, even though the chain is made up only of spin-1 particles! The point is that if one thinks of the edge modes as being particles, there are two of them, one at each end of the chain. Yet the net spin of the chain must be zero or one, so the only way to think of a two-particle state with these values is to treat the individual particles as having spin-1/2! This is readily apparent in the dimer picture of the ground state, where there is a spin-1/2 at each end not part of any dimer.

The AKLT chain has exponentially decaying spin-spin correlators, with correlation length ln(3). It is gapped, as is typical of chains with exponentially decaying correlators. This intuitively plausible, but difficult to prove. Gaps are difficult to prove in general because that lower bounds on the energy are much more difficult to find. Upper bounds are much easier to find using variational methods, but are useless for proving a gap. Nevertheless, AKLT proved in their original paper that this chain is gapped. This is a result of great interest, because it gives a strong indication that the nearby Heisenberg model ($\theta = 0$) is also gapped. This was a great surprise when Haldane first argued this, because folk wisdom had it that the spin-1 Heisenberg chain would behave like the gapless spin-1/2 chain. I will describe both these situations later in this book.