Chapter 7

Gapped frustrated quantum magnets

When quantum fluctuations are strong enough to destroy long-range magnetic order, one natural possibility is that spin-spin correlations decay exponentially. In that case, the excitations can be expected to ressemble those of a finite system of dimension ξ^D, where ξ is the correlation length and D the dimensionality. Now, in finite systems, the spectrum is quantized, and the spectrum has a gap of order $v2\pi/L$, where v is the typical velocity and L the linear size of the system. So a disordered antiferromagnet can be expected to have a gap of order $\Delta \propto Ja/\xi$, where J is a typical coupling constant and a the lattice parameter. This can be demonstrated explicitly in the case of dimerized models, where strong antiferromagnetic bonds lead to a ground state that is essentially a product of singlets on these bonds. What is specific to frustrated magnets is that the formation of local singlets can be spontaneous, the dimerization then implying the breaking of the translation symmetry.

7.1 Dimerized square lattice

A simple example to demonstrate that quantum fluctuations can lead to a spin gap is the dimerized antiferromagnetic Heisenberg model on the square lattice, where the coupling constant is equal to J on a set of dimers in columnar geometry such that each site belongs to one and only one dimer, and is reduced to $J' < J$ on the other bonds (see Fig. 7.1). As long as J and J' are both positive, it is clear that the classical ground state is still the Néel configuration since it fully satisfies all bonds. However, in the limit $J' \to 0$,

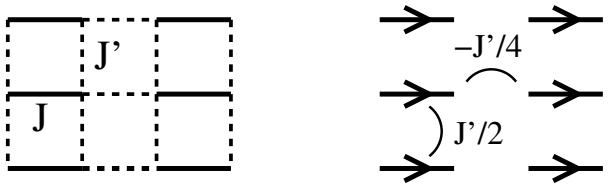

Figure 7.1: Dimerized square lattice. Left: Definition of the intra-dimer coupling constants J and of the inter-dimer coupling constants J'. Right: Arrows defining the convention of the singlets, and hopping amplitudes for one triplet.

the spectrum becomes very soft, and the correction to the magnetization diverges in that limit.

To study the excitation spectrum in that limit, let us start from the case $J' =$ and treat J' as a perturbation. When $J' = 0$, the system is a collection of independent dimers coupled by J. The spectrum of a dimer has two eigenstates, a singlet and a triplet. Indeed,

$$J\vec{S}_1 \cdot \vec{S}_2 = \frac{J}{2}[(\vec{S}_1 + \vec{S}_2)^2 - \vec{S}_1^2 - \vec{S}_2^2] = \frac{J}{2}\vec{S}_{\rm tot}^2 - \frac{3}{4}J$$

where $\vec{S}_{\rm tot} = \vec{S}_1 + \vec{S}_2$ is the total spin. Now, from the theory of the addition of angular momenta, we known that

$$\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$$

implying that $\vec{S}_{\rm tot}^2$ takes two values of the form $S_{\rm tot}(S_{\rm tot}+1)$ with $S_{\rm tot} = 0$ or 1. The eigenvalues of the singlet ($S_{\rm tot} = 0$) and of the triplet ($S_{\rm tot} = 1$) are thus given by

$$E_{\rm s} = -\frac{3}{4}J, \quad E_{\rm t} = \frac{1}{4}J.$$

Let us denote by $|S\rangle$ the singlet wave-function, and by $|T_{-1}\rangle$, $|T_0\rangle$ and $|T_1\rangle$ those of the three triplets with $S^z_{\rm tot} = -1$, 0 and 1 respectively. They are given by

$$|S\rangle = \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$$

and

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

When necessary, we will add indices referring to the sites of the lattice: $|S\rangle_{ij} = (|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle)/\sqrt{2}$, etc.

The unperturbed ground state can be written as

$$|GS\rangle = |S\rangle \otimes |S\rangle \otimes ... \otimes |S\rangle,$$

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. Its energy equal to $E_0 + J$, and its degeneracy is equal to $3 \times \frac{N}{2}$, where $\frac{N}{2}$ is the number of dimers, and the factor 3 keeps track of the three possible values of S^z_{tot}, -1, 0 or 1.

Let us now treat J' as as perturbation. Since the ground state is non degenerate, we can calculate the first order correction as $\langle GS|\mathcal{H}(J')|GS\rangle$, where $\mathcal{H}(J')$ is the Hamiltonian describing the inter-dimer coupling. $\mathcal{H}(J')$ is a sum of terms that couple two dimers. Let's consider two singlets $|S\rangle_{12}$ and $|S\rangle_{34}$ such that sites 2 and 3 are nearest neighbours. The operator $J'\vec{S}_2 \cdot \vec{S}_3$ can be written as

$$J'\vec{S}_2 \cdot \vec{S}_3 = J'[S^z_2 S^z_3 + \frac{1}{2}(S^+_2 S^-_3 + S^-_2 S^+_3)].$$

Now,

$$S^z_2|S\rangle_{12} = \frac{1}{2\sqrt{2}}(-|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle) = -\frac{1}{2}|T_0\rangle_{12},$$

$$S^+_2|S\rangle_{12} = \frac{1}{\sqrt{2}}|\uparrow_1\uparrow_2\rangle = \frac{1}{\sqrt{2}}|T_1\rangle_{12}, \quad S^-_2|S\rangle_{12} = \frac{1}{\sqrt{2}}(-|\downarrow_1\downarrow_2\rangle) = -\frac{1}{\sqrt{2}}|T_{-1}\rangle_{12}.$$

So, by applying any term of $J'\vec{S}_2 \cdot \vec{S}_3$ to $|S\rangle_{12}$, we transform it into a triplet. The scalar product of the resulting state with $|GS\rangle$, which is a product of singlets, will thus vanish. The first order correction to the ground state energy therefore vanishes: $E^{(1)}_0 = 0$.

Let us now turn to the first 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 calculation separately in the sectors $S^z_{\text{tot}} = -1$, 0 or 1. Let us do it for $S^z_{\text{tot}} = 1$. A basis of the degenerate subspace is given by

$$|n\rangle = |S\rangle \otimes ...|T_1\rangle \otimes ... \otimes |S\rangle$$

where n is the position of the only dimer that is not a singlet but a $|T_1\rangle$. To solve the problem to first order, we need to calculate $\langle n|\mathcal{H}(J')|m\rangle$ and to

diagonalize this matrix. Let us choose a specific J' bond. It can only couple the states with triplets connected to 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 components of $\vec{S}_3$ on $|T_1\rangle_{34}$:

$$S_3^z|T_1\rangle_{34} = \frac{1}{2}|T_1\rangle_{34}, \quad S_3^+|T_1\rangle_{34} = 0,$$

$$S_3^-|T_1\rangle_{34} = |\downarrow_3\uparrow_2\rangle = \frac{1}{\sqrt{2}}(-|S\rangle_{34} + |T_0\rangle_{34}).$$

This implies that

$$\vec{S}_2 \cdot \vec{S}_3\ |S\rangle_{12} \otimes |T_1\rangle_{34} = -\frac{1}{2}|T_0\rangle_{12} \otimes |T_1\rangle_{34} + \frac{1}{2}\frac{1}{\sqrt{2}}|T_1\rangle_{12} \otimes \frac{1}{\sqrt{2}}(-|S\rangle_{34} + |T_0\rangle_{34})$$

leading to

$$\langle T_1|_{12} \otimes \langle S|_{34}\ J'\vec{S}_2 \cdot \vec{S}_3\ |S\rangle_{12} \otimes |T_1\rangle_{34} = -\frac{J'}{4}.$$

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

The only subtlety is the sign of the hopping. It is easy to check that if we had considered $\vec{S}_2 \cdot \vec{S}_4$, 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 with total operator $J'(\vec{S}_2 \cdot \vec{S}_3 + \vec{S}_1 \cdot \vec{S}_4)$, the total hopping amplitude will be $-J'/2$, while they are coupled by $J'(\vec{S}_1 \cdot \vec{S}_3 + \vec{S}_2 \cdot \vec{S}_4)$, it will be $J'/2$.

Let us come back to the square lattice. To keep track of the sign convention for the singlets, we draw an arrow going from site i to site j to represent $|S_{ij}\rangle$ (see Fig. 7.1). For the columnar state, the horizontal hoppings have amplitude $-J'/4$, while the vertical hoppings have amplitude $J'/2$. The effective Hamiltonian to first order with matrix elements $\langle n|\mathcal{H}(J')|m\rangle$ thus corresponds to a tight binding problem defined on the lattice of the centers of the bonds, with lattice parameters $2a$ resp. a horizontally and vertically, with dispersion

$$\epsilon_{\vec{k}} = -\frac{J'}{2}\cos(2k_x a) + J'\cos(k_y a).$$

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

Finally, to first order in perturbation, the lowest energy in the branch of the first excited state is equal to $J - \frac{3}{2}J'$. Therefore, this theory predicts that there is a gap as long as $J' < \frac{2}{3}J$. At that point, the gap closes, and

the system must then develop long-range Néel order with gapless spin-wave excitations.

This conclusion is qualitatively confirmed by Quantum Monte Carlo simulations, which have shown that the transition takes place at $J'/J \simeq 0.5237$.

7.2 Frustration and dimer singlets

Let us now see under which conditions frustration leads to ground states built with dimer singlets. We will mostly discuss spin-1/2 systems.

7.2.1 Spin-1/2 triangle

$$H = \frac{J}{2}\left[\vec{S}_{\rm tot}^2 - \sum_i \vec{S}_i^2\right] \tag{7.1}$$

The ground state minimize $\vec{S}_{\rm Tot}^2$. For 3 spin 1/2, the basics of angular momentum addition leads to:

$$\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1 \tag{7.2}$$

$$\frac{1}{2} \otimes \left(\frac{1}{2} \otimes \frac{1}{2}\right) = \frac{1}{2} \otimes 0 \oplus \frac{1}{2} \otimes 1 = \frac{1}{2} \oplus \frac{1}{2} \oplus \frac{3}{2} \tag{7.3}$$

There are two doublets (spin 1/2 states), hence 4 states that minimize the energy. The ground state energy is

$$E_0 = \frac{J}{2}\left[\frac{3}{4} - 3 \times \frac{3}{4}\right] = -\frac{3}{4}J \tag{7.4}$$

Let's determine the ground state wave-function. It is actually easy to construct ground state wave-functions. Indeed, consider the state

$$|\psi\rangle = |\sigma\rangle_1 \otimes \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} \tag{7.5}$$

$$= |\sigma\rangle_1 \otimes |S\rangle_{23} \tag{7.6}$$

Since spins 2 and 3 form a singlet,

$$\vec{S}_1 \cdot \left(\vec{S}_2 + \vec{S}_3\right)|\psi\rangle = \vec{S}_1 \cdot \vec{S}_{23}\,|\psi\rangle = 0 \tag{7.7}$$

This is most simply shown as follow:

$$\vec{S}_1 \cdot \left(\vec{S}_2 + \vec{S}_3\right) = S_1^z\,(S_2^z + S_3^z) + \frac{1}{2}[S_1^+\,(S_2^- + S_3^-) + S_1^-\,(S_2^+ + S_3^+)] \tag{7.8}$$

where all terms gives 0 when applied to $|S\rangle_{23}$.

Finally,

$$H|\psi\rangle = J\vec{S}_2\cdot\vec{S}_3|\psi\rangle = -\frac{3}{4}J|\psi\rangle \tag{7.9}$$

Now, one can construct 6 such states:

$$|\sigma_i\rangle\otimes|S\rangle_{jk}, \quad j\neq k, \quad j,k\neq i, \quad \sigma_i=\uparrow \text{ or } \downarrow$$

But there are only 4 ground states! Where is the problem? These states are not orthogonal. Indeed,

$$\begin{aligned}&|\uparrow_1\rangle\otimes|S\rangle_{23}+|\uparrow_2\rangle\otimes|S\rangle_{31}+|\uparrow_3\rangle\otimes|S\rangle_{12}\\ =&\frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\downarrow\rangle-|\uparrow\downarrow\uparrow\rangle+|\downarrow\uparrow\uparrow\rangle-|\uparrow\uparrow\downarrow\rangle+|\uparrow\downarrow\uparrow\rangle-|\downarrow\uparrow\uparrow\rangle\right)=0\end{aligned}$$

To construct the 4 ground states, one can choose states that correspond to the two-dimensional representation of the C_3 group (rotation by $2\pi/3$ around the z axis):

$$\begin{aligned}|\mathrm{L},\uparrow\rangle &= \frac{1}{\sqrt{3}}\left(|\uparrow\uparrow\downarrow\rangle+\omega|\uparrow\downarrow\uparrow\rangle+\omega^2|\downarrow\uparrow\uparrow\rangle\right)\\ |\mathrm{R},\uparrow\rangle &= \frac{1}{\sqrt{3}}\left(|\uparrow\uparrow\downarrow\rangle+\omega^2|\uparrow\downarrow\uparrow\rangle+\omega|\downarrow\uparrow\uparrow\rangle\right)\\ |\mathrm{L},\downarrow\rangle &= \frac{1}{\sqrt{3}}\left(|\downarrow\downarrow\uparrow\rangle+\omega|\downarrow\uparrow\downarrow\rangle+\omega^2|\uparrow\downarrow\downarrow\rangle\right)\\ |\mathrm{R},\downarrow\rangle &= \frac{1}{\sqrt{3}}\left(|\downarrow\downarrow\uparrow\rangle+\omega^2|\downarrow\uparrow\downarrow\rangle+\omega|\downarrow\uparrow\uparrow\rangle\right)\end{aligned}$$

with $\omega = e^{2i\pi/3}$, and L, R stand for left and right.

So, for the spin 1/2 triangle, there is a clear tendency to form singlets in the ground state.

Triangles with $S > 1/2$

The rules of the addition of angular momenta lead to:

$$S\otimes S = 0\oplus 1\oplus\cdots\oplus 2S, \quad S\otimes(S\otimes S) = ?$$

If S is half-integer, $S-\frac{1}{2}$ and $S+\frac{1}{2}$ appear in the sequence $0,1,\ldots,2S$ and they both yield a doublet (a spin-1/2) when coupled to S in $S\otimes(S\otimes S)$. So the ground state is a 2-fold degenerate doublet.

If S is integer, S appears in the sequence $0, 1, \ldots, 2S$, and it gives rise to a unique singlet in $S \otimes (S \otimes S)$. So the ground state in a non-degenerate singlet.

However, the ground state is no longer a simple product state if $S \geq 1$. A state $|\sigma_1\rangle \otimes |S\rangle_{23}$ is still an eigenstate, but its energy is that of a singlet built out of two spins, $-JS(S+1)$. The ground state energy of the triangle is, however, given by the minimum of $\vec{S}^2_{\text{tot}}$:

$$\frac{J}{2}\left[\vec{S}^2_{\text{tot}} - 3S(S+1)\right] = \begin{cases} \frac{J}{2}\left[\frac{3}{4} - 3S(S+1)\right] & \text{for half-integer spin} \\ -J\frac{3}{2}S(S+1) & \text{for integer spin} \end{cases}$$

For integer spin, it is clear that the ground state energy is smaller that of the product state $|\sigma_1\rangle \otimes |S\rangle_{23}$. For half-integer spin,

$$E_{\text{Product}} - E_{\text{GS}} = \frac{J}{2}\left[S(S+1) - \frac{3}{4}\right] \begin{cases} = 0 \text{ for } S = \frac{1}{2} \\ > 0 \text{ for } S > \frac{1}{2} \end{cases}$$

The tendency to form dimer singlets on equilateral triangles is thus limited to spins 1/2.

7.2.2 $J_1 - J_2$ chain

Consider the spin-1/2 $J_1 - J_2$ chain, also known as the zigzag chain (see Fig.7.2), defined by the Hamiltonian

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

Proposition

At the Majumdar-Ghosh point $J_1 = 2J_2$, the two states with a singlet on every other J_1 bond

$$|\psi_{\text{even}}\rangle = \prod_{i \text{ even}} |S\rangle_{i\ i+1} \quad \text{and} \quad |\psi_{\text{odd}}\rangle = \prod_{i \text{ odd}} |S\rangle_{i\ i+1}$$

are degenerate ground states.

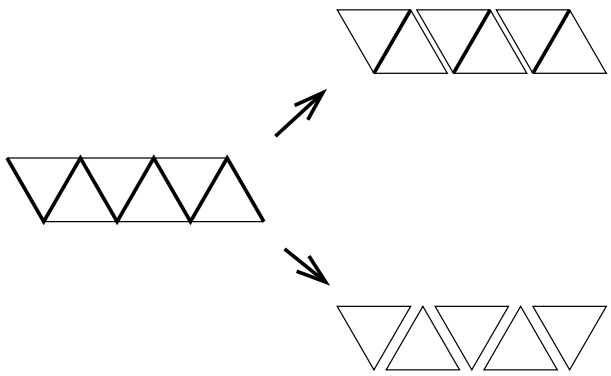

Figure 7.2: J_1-J_2 chain. Left: Representation as a zigzag chain. Thick lines: J_1 bonds; thin lines: J_2 bonds. Right panels: Alternative representations at the Majumdar-Ghosh point $J_1 = 2J_2$. Pairs of parallel J_2 bonds connecting the same points correspond to a J_1 bond. Top right: Representation as a sum of Hamiltonians centered on every other J_1 bond. Bottom right: representation as a sum of triangles with J_2 bonds.

Proof

We will proceed in two steps: i) Prove that they are eigenstates; ii) Prove that they minimize the energy.

Since the Hamiltonian is translationally invariant, and since one state can be obtained form the other one by a translation by one lattice site, it will have the same properties, and it is sufficient to prove these properties for one state, say $|\psi_{\rm even}\rangle$.

To prove i), and taking into account the fact that $J_1 = 2J_2$, it is convenient to split the Hamiltonian as (see Fig.7.2, top right panel):

$$H = \sum_{i\ \rm even} h_i, \quad h_i = 2J_2\vec{S}_i\cdot\vec{S}_{i+1} + J_2\vec{S}_{i-1}\cdot(\vec{S}_i+\vec{S}_{i+1}) + J_2\vec{S}_{i+2}\cdot(\vec{S}_i+\vec{S}_{i+1}).$$

Then, since in $|\psi_{\rm even}\rangle$ the spins $\vec{S}_i$ and $\vec{S}_{i+1}$ are in a singlet state for i even, the last two terms of all h_i give zero, as in the triangle, and the first terms are diagonal with energy $-(3/4)2J_2$. So $|\psi_{\rm even}\rangle$ is an eigenstate of H with energy $-(3/4)J_2N$.

To prove ii), it is more convenient to write the Hamiltonian as a sum over triangles (see Fig.7.2, bottom right panel):

$$H = \sum_i h_\Delta(i), \quad h_\Delta(i) = J_2(\vec{S}_i\cdot\vec{S}_{i+1} + \vec{S}_i\cdot\vec{S}_{i+2} + \vec{S}_{i+1}\cdot\vec{S}_{i+1}). \tag{7.10}$$

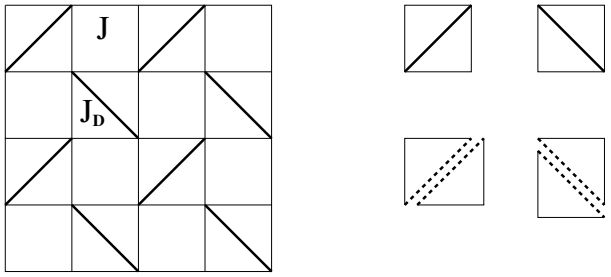

Figure 7.3: Shastry-Sutherland model. The Hamiltonian can be seen as a collection of square plaquettes with diagonal bonds (top right) or as a collection of isosceles triangles with two bonds of strength J and one bond of strength $J_D/2$.

The ground state energy of $h_\Delta(i)$ is $-(3/4)J_2$. The variational principle implies that

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

Since $|\psi_{\text{even}}\rangle$ is an eigenstate of H with energy $-(3/4)J_2N$, it is a ground state. And, as noticed above, $|\psi_{\text{odd}}\rangle$ must also be a ground state.

So, at the Majumdar-Ghosh point, the $J_1 - J_2$ chain has two degenerate ground states that are exact products of singlets. In these states, the correlation length is equal to zero (spin-spin correlations do not extend beyond first neighbors), and one can expect the spectrum to be gapped. This is true, but the proof is more subtle than one could naively imagine because the elementary excitations are domain walls between the two possible ground states, not just a triplet moving in a sea of singlets. These excitations carry a spin-1/2 and are often referred to as spinons. They must be created in pairs, but they are deconfined, and the spectrum is a two-spinon continuum. Still it can be shown that the dispersion of these spinons is gapped, and accordingly the spectrum of the Majumdar-Ghosh chain is gapped. More generally, the spin-1/2 $J_1 - J_2$ chain has been shown to be dimerized with a gapped spectrum for $J_2/J_1 > 0.2411...$

For larger spins, the products of singlets are still eigenstates when $J_1 = 2J_2$, but there are not ground states, a consequence of the fact that for $S \geq 1$, the ground state of an equilateral triangle is not a product state involving a dimer singlet.

7.2.3 Shastry-Sutherland model

In 1981, Shastry and Sutherland have generalized this construction to two-dimensions. The model is defined for arbitrary spin S, but for simplicity we will concentrate on $S = 1/2$. It can be seen as a square lattice with some diagonal bonds (see Fig.7.3).

Proposition

If we denote by $\mathcal{D}$ the set of diagonal bonds, the wave-function

$$|\psi_{\rm dimer}\rangle = \prod_{(ij)\in\mathcal{D}} |S\rangle_{ij}$$

is an eigenstate.

Proof

If one denotes by J the couplings that build the square lattice, and by J_D the diagonals couplings, the Hamiltonian can be rewritten as a sum of plaquette Hamiltonians defined on each plaquette with a diagonal bond J_D and square bonds J (see Fig.7.3, top right). Then, if the spins coupled by the diagonal bond form a singlet, the other interactions give zero because they couple a spin to a singlet, and the diagonal term contributes $-S(S+1)J_D$ to the energy. So, for spin-1/2, $|\psi_{\rm dimer}\rangle$ is an eigenstate of energy $-(3/4)J_D N/2$.

This energy does not depend on J. So clearly it cannot be the lowest energy for any J. Indeed, if $J_D = 0$, the ground state is the Néel state with a negative ground state energy proportional to J while this state has zero energy. However, if $J = 0$, the product of singlets $|\psi_{\rm dimer}\rangle$ is clearly the ground state. In our quest for ground states built out of dimer singlets, the relevant question is the value of the ratio J/J_D up to which $|\psi_{\rm dimer}\rangle$ is the ground state. Shastry and Sutherland found a lower bound to this critical ratio using a simple variational argument. To this end, they have noticed that the Hamiltonian can also be written as a sum of N isosceles triangles with two bonds of strength J and one bond of strength $J_D/2$ (see Fig.7.3, bottom right). Since the triangle is no longer equilateral, a product state involving a dimer singlet can minimize the energy. Indeed, denoting by 1 the site coupled to the other two by J and the other two sites by 2 and 3,

the Hamiltonian of such a triangle can be written

$$\begin{aligned} h_\Delta =& \frac{J}{2}\left(\vec{S}_{\rm tot}^2 - \vec{S}_1^2 - \vec{S}_{23}^2\right) + \frac{J_D}{4}\left(\vec{S}_{23}^2 - \vec{S}_2^2 - \vec{S}_3^2\right) \\ =& \frac{J}{2}\vec{S}_{\rm tot}^2 + \left(\frac{J_D}{4} - \frac{J}{2}\right)\vec{S}_{23}^2 - \frac{J}{2}\vec{S}_1^2 - \frac{J_D}{4}\left(\vec{S}_2^2 + \vec{S}_3^2\right) \end{aligned}$$

where $\vec{S}_{23} = \vec{S}_2 + \vec{S}_3$. The ground state energy will be reached when the spins $\vec{S}_2$ and $\vec{S}_3$ form a singlet as long as the coefficient of $\vec{S}_{23}^2$ is positive, i.e. as long as $J_D > 2J$, or equivalently as long as $J < J_D/2$. If that is the case, the ground state energy of each triangle is equal to $-(3/4)J_D/2$, and since there are N triangles, the variational principle implies that the ground state energy of H is bounded from below by $-(3/4)J_DN/2$. This bound is saturated by $|\psi_{\rm dimer}\rangle$, which shows that this wave function is a ground state at least as long as $J < J_D/2$. Numerical investigations of this model have shown that $|\psi_{\rm dimer}\rangle$, which is always an eigenstate of H, actually remains the ground state as long as $J/J_D < 0.675$.

The variational argument has been extended by Shastry and Sutherland to arbitrary spin S, leading to the conclusion that the product of singlets on the diagonal bonds is the ground state as long as $J_D > 2(S+1)J$, or equivalently $J < J_D/[2(S+1)]$.

In that case, the ground state is unique. Elementary excitations are thus constructed as in the dimerized Heisenberg model by promoting a local singlet into a triplet, and the spectrum remains gapped as long as the ground state is a product of singlets, as has been shown by numerical investigations of the model.

7.3 Resonance between valence-bond singlets

In situations where several dimer coverings are in competition, the energy is sometimes minimized by a resonance between products of dimer singlets. In this section, we demonstrate this mechanism in the case of four spins. The possibility to stabilize resonating valence-bond (RVB) phases is discussed in the next chapter.

7.3.1 Tetrahetron

Let us start by deriving the ground state of a tetrahedron, or equivalently of a square plaquette with diagonal bonds of equal strength (see Fig. 7.4).

Since this is a complete graph, the Hamiltonian can be written:

$$H = \frac{J}{2}\vec{S}_{\rm tot}^2 - \frac{J}{2}\sum_{i=1}^{4}\vec{S}_i^2$$

Let us first discuss the general case of spins S. Since $S\otimes S = 0\oplus 1\oplus\cdots\oplus 2S$, $(S\otimes S)\otimes(S\otimes S)$ contains $2S+1$ singlets. The ground state is thus a $(2S+1)$-fold degenerate singlet.

It is easy to construct ground states. For instance, the product of two dimer singlets constructed out of different pairs is a singlet, hence a ground state. This leads in general to three ground states since there are three ways of partitioning four sites into two pairs.

For $S = \frac{1}{2}$, since there are $2\frac{1}{2}+1 = 2$ singlet states, these three states cannot be independent. And indeed,

$$|S\rangle_{23}\otimes|S\rangle_{14} + |S\rangle_{12}\otimes|S\rangle_{43} - |S\rangle_{13}\otimes|S\rangle_{24} \tag{7.11}$$

$$= \frac{1}{2}\left[|\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle - |\uparrow\downarrow\uparrow\downarrow\rangle - |\downarrow\uparrow\downarrow\uparrow\rangle\right. \tag{7.12}$$

$$+ |\uparrow\downarrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle \tag{7.13}$$

$$\left. - |\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle\ \right] = 0 \tag{7.14}$$

So the ground state manifold of a spin-1/2 tetrahedron is spanned by two products of dimer singlets.

7.3.2 Square plaquette

This situation with degenerate products of singlet wave functions in the ground state should be contrasted to less frustrated situations. For this, let us consider the spin-1/2 $J_1 - J_2$ plaquette (see Fig. 7.4):

$$\begin{aligned}
H =& J_1\left(\vec{S}_{13}\cdot\vec{S}_{24}\right) + \frac{J_2}{2}\left[\vec{S}_{24}^2 - \vec{S}_2^2 - \vec{S}_4^2\right] + \frac{J_2}{2}\left[\vec{S}_{13}^2 - \vec{S}_1^2 - \vec{S}_3^2\right]\\
=& \frac{J_1}{2}\left[\vec{S}_{\rm tot}^2 - \vec{S}_{13}^2 - \vec{S}_{24}^2\right] + \frac{J_2}{2}\left[\vec{S}_{24}^2 - \vec{S}_2^2 - \vec{S}_4^2\right] + \frac{J_2}{2}\left[\vec{S}_{13}^2 - \vec{S}_1^2 - \vec{S}_3^2\right]\\
=& \frac{J_1}{2}\vec{S}_{\rm tot}^2 + \frac{J_2 - J_1}{2}\left[\vec{S}_{13}^2 + \vec{S}_{24}^2\right] - \frac{J_2}{2}\sum_i \vec{S}_i^2
\end{aligned}$$

The ground state always has $S_{\rm tot} = 0$, but depending on the sign of $J_2 - J_1$, S_{13} and S_{24} will be minimal or maximal:

- $J_2 < J_1$: $S_{13} = S_{24} = 1$

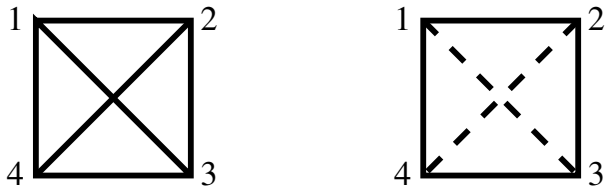

Figure 7.4: Left: Square plaquette with diagonal couplings equal to the side ones. It is equivalent to a tetrahedron and is thus a complete graph (all sites are coupled to each other). Right: Square plaquette with side bonds J_1 (solid lines) and diagonal bonds J_2 (dashed lines). The numbering of the sites corresponds to that used in the main text.

- $J_2 > J_1$: $S_{13} = S_{24} = 0$
- $J_2 = J_1$: $S_{13} = S_{24} = 0$ or 1

For the simple square plaquette ($J_2 = 0$), the Hamiltonian reduces to

$$H = \frac{J_1}{2}[\vec{S}^2_{\text{tot}} - \vec{S}^2_{13} - \vec{S}^2_{24}]$$

The ground state is obtained for $S_{13} = S_{24} = 1$, and its energy is equal to $-2J$.

Now, to construct a singlet of two spins 1, one can start from the state $|S = 2, S^z = 2\rangle = |11\rangle$ and apply S^-_{tot} to get $|S = 2, S^z = 1\rangle \propto |10\rangle + |01\rangle$ and $|S = 2, S^z = 0\rangle \propto |1-1\rangle + |-11\rangle + 2|00\rangle$. In the sector $S^z_{\text{tot}} = 1$, the state orthogonal to $|S = 2, S^z = 1\rangle$ is $|S = 1, S^z = 1\rangle \propto |10\rangle - |01\rangle$, from which we obtain $|S = 1, S^z = 0\rangle \propto |1-1\rangle - |-11\rangle$ by application of S^-_{tot}. Finally, the singlet is the state orthogonal to $|S = 2, S^z = 0\rangle$ and $|S = 1, S^z = 0\rangle$ in the sector $S^z_{\text{tot}} = 0$. It is given by $|S = 0, S^z = 0\rangle \propto |1-1\rangle + |-11\rangle - |00\rangle$.

So the ground state of the square plaquette is, up to a normalization constant,

$$|\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle - \frac{1}{2}(|\uparrow\downarrow\uparrow\downarrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle.$$

It is easy to check, by expanding the corresponding singlets, that this wave function is equal, up to an overall factor, to

$$|S\rangle_{12} \otimes |S\rangle_{34} + |S\rangle_{14} \otimes |S\rangle_{23}.$$

So the ground state can be thought of as a resonance between dimer singlet coverings. Note that the ground state energy, $-2J$, is smaller than that of

each component, which is the sum of the energies of two singlets and is equal of $-(3/2)J$. There is an energy gain due to the resonance.

It has been suggested in 1973 by Anderson and Fazekas that this construction can be generalized to more complicated lattices, and that some systems might have a ground state that corresponds to a resonance between dimer singlet coverings, a state they named a resonating valence bond (RVB) state. This possibility is explored in the next chapter in the context of simpler models known as Quantum Dimer Models.