Solvable Lattice Models: Lecture 1

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Lattice models were introduced in statistical mechanics in order to study realistic systems. Statistical mechanics will *not* be a focus of this course. Indeed, it turns out that solvable lattice models have important connections with representation theory, for example of quantum groups regarding the underlying mechanism, and other areas such as representation theory of p-adic groups, algebraic combinatorics, algebraic geometry, and conformal field theory. We will review the statistical mechanical origins of the theory, referring to Baxter [1] for much more information, before turning away to other subjects.

1 Thermodynamics

The purpose of this section is to give a quick impressionistic treatment of statistical mechanics. Since we will soon migrate away from this subject, we will not try for any depth.

Statistical mechanics is a development from thermodynamics. Thermodynamics was an empirical discovery which started with the theory of gases, motivated by considerations related to engines and refrigeration.

We recommend the Feynman Lectures in Physics, I.44 for an introduction to Thermodynamics. Thermodynamics can be *axiomatized* in the form of several laws, most importantly the *second law of thermodynamics* which contains a subtle and important concept, entropy. The laws of Thermodynamics are sometimes stated thus:

(1) Energy is conserved in a closed system.

(2) Entropy is increasing.

(3) If the temperature is decreased to zero, entropy approaches a fixed value, called the *residual entropy*.

The concept of entropy is of great importance, and universal in its surprising applicability to different areas, such as information theory and black holes. It has important philosophical implications, since it gives a direction to the arrow of time. This is paradoxical since the laws of physics are invariant under time reversal (CPT symmetry).

We take for granted the concept of energy, and its conservation. In thermodynamics and statistical mechanics, it is important to take into account both closed systems, that do not interact with their environment, and systems that do interact. Thus we imagine that energy can be put into a system, or extracted from it. *Work* can be described as energy that is extracted from a system, for example by operating a piston or generating electricity.

Heat is a form of energy that we now understand to be due to the kinetic energy of molecules in a substance. Carnot, whose investigations of the steam engine led to the concepts of thermodynamics, thought of heat as a fluid like water, that can flow from higher levels to lower, and in the process can be made to do work. The first law of thermodynamics can be expressed in the formula

$$dU = dQ + dW,$$

where U is a variable expressing the total amount of energy in the system, Q is the amount of heat, and W is a variable expressing work, energy that is put into a system, or extracted from it.

As Carnot realized, certain processes are reversible. We may imagine a perfectly efficient engine, with frictionless parts, where energy is put in in the form of fire or electricity, and mechanical work is extracted. But other processes, such as friction, are irreversible. In friction, work is transformed into heat, and this is energy that can never be extracted from the system. A processes involving friction is irreversible.

Again, if a system consists of two bodies of different temperatures, energy can be extracted as work by a mechanism such as a dipping bird. But if heat flows from one body to the other, until they reach the same temperature, the energy still exists, but can no longer be extracted as work. Thus the cooling of a hot object is an irreversible process.

The second law of thermodynamics regulates such irreversible processes. The second law postulates that there is a quantity S, called *entropy* that can only increase. Irreversible processes are precisely those that increase the entropy. Conversely, a process is reversible if it does not increase entropy. A system is at *maximal entropy* the entropy can no longer increase. An example would be a system in thermal equalibrium, where all parts are at the same temperature.

Also related to the second law is the notion of *free energy*. This is the amount of energy that can be extracted from a system as useful work. Thus the entropy of the system is maximal if the free energy is zero.

2   Statistical Mechanics and the Partition Function

The physical basis for thermodynamics is *statistical mechanics*. Thus heat is understood as being the kinetic energy of atoms and molecules, and the laws of thermodynamics can be derived from statistical considerations.

We will consider a system with many possible states, which is not strictly subject to the first law, in that not all states have the same energy. The source of this uncertainty is usually interaction with the environment. For example, one considers a system that is in contact with a heat bath at a constant temperature. The system itself is assigned a temperture that may be constant, or could vary within the medium. The system may also depend on other parameters, such as pressure or the strength of an applied electromagnetic field.

An important question that is investigated in Statistical Mechanics is the behavior of a system at a phase transition point. We may consider the melting or boiling of a substance as an example. In an idealized form, we may imagine the process as follow. In a "frozen" state, there are correlations between the local structure of the system at locations that are separated in distance, but in the "melted" form, there are no such correlations. The phase

transition point or critical temperature is the value where the structure changes from frozen to melted.

A statistical mechanical system $\mathfrak{S}$ is an ensemble of *states*. Each state $\mathfrak{s}$ has an energy $e(\mathfrak{s})$, and there is a probability measure on $\mathfrak{S}$, with high energy states being less probable. The system may depend on some external parameters, notably the *temperature* of the system. The probability of the state $\mathfrak{s}$ with energy $E(\mathfrak{s})$ is proportional to $\beta(\mathfrak{s}) = e^{-E(\mathfrak{s})/kT}$, where k is *Boltzmann's constant*. Since the sum of the probabilities must be 1, the actual probability is

$$\frac{1}{Z}\beta(\mathfrak{s}), \qquad Z = Z(\mathfrak{S}, T) := \sum_{\mathfrak{s}} \beta(\mathfrak{s}).$$

The quantity $\beta(\mathfrak{s})$ is called the *Boltzmann weight* of the state, and the quantity Z is called the *partition function*. Note that as the temperature increases, energetic states become more probable.

The partition function is a powerhouse in statistical mechanics. For example the mean energy is

$$\langle E \rangle := \frac{1}{Z} \sum_{\mathfrak{s}} \beta(\mathfrak{s})\, E(\mathfrak{s}) = kT^2 \frac{\partial}{\partial T} \log(Z).$$

The free energy, which we recall is the amount of energy that can be extracted from the system as work, equals

$$F = -kT \, \log(Z),$$

and the entropy is

$$S = k \, \log(Z) + \frac{1}{kT}\langle E \rangle.$$

If the partition function depends on other parameters such as a magnetic field strength, differentiating with respect to those will yield other values of significance.

The partition function also occurs in other areas of physics, such as quantum field theory. For us, the partition function will be a main object of study, even though we will soon leave its origins in statistical mechanics behind.

3   Ice

Linus Pauling computed the entropy and free energy of ice by means of a three-dimensional lattice model.

In an ice crystal we will consider two oxygen atoms adjacent if they share a hydrogen bond. They then form a graph Γ that is nearly 4-regular in that each oxygen atom, except those at the boundary of the crystal, have 4 neighbors. (Here we are ignoring a detail about boundary edges, and we will give a proper discussion of Γ below in Section 5.

Ice has many possible crystalline structures. Under normal conditions, Ice I_h is the usual one. This crystal occurs in sheets or layers. The graph is bivalent. Each layer is a tesselated by hexagons, with oxygen atoms at their vertices. Furthermore, each atom has a bond with one in either the layer above or below, depending on its valence.

Here is the hexagonal Ice I_h lattice, showing the segments joining a sample Oxygen atom (green) to its four neighbors.
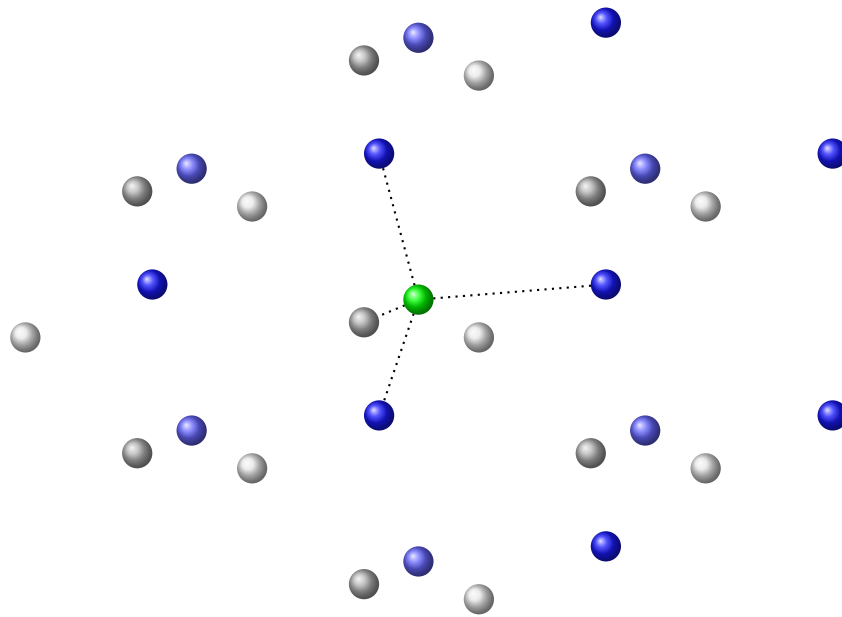
Here is the graph Γ showing two adjacent layers.
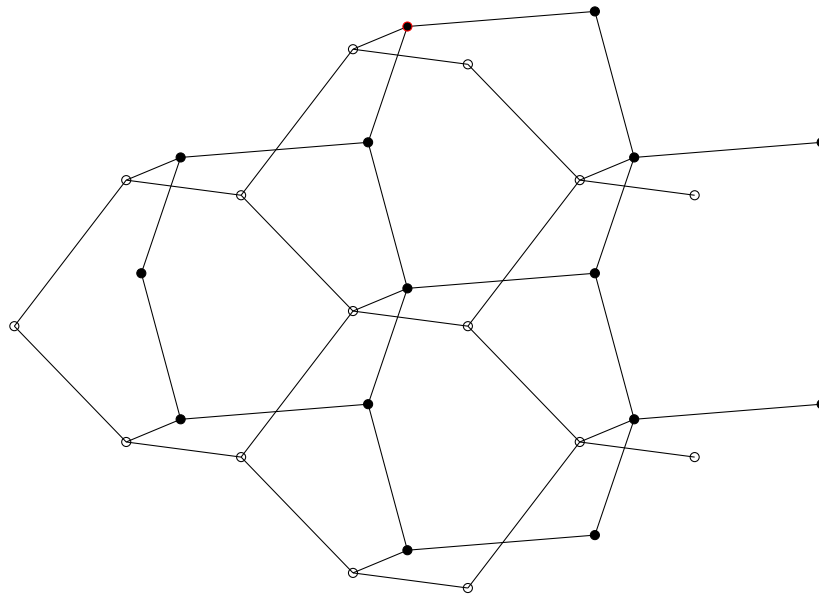
While the location of the oxygen atoms is fixed, and forced into a crystalline pattern, the location of the hydrogen nuclei (protons) is another matter. Due to its position in the periodic table, oxygen is allowed two covalent bonds. The oxygen atom will therefore borrow electrons from two hydrogen atoms. This causes the protons to lie on the segments between two adjacent oxygen atoms, but each proton will be closer to one or the other of the two oxygen atoms. There are many possible configurations, which are subject to quantum superposition.
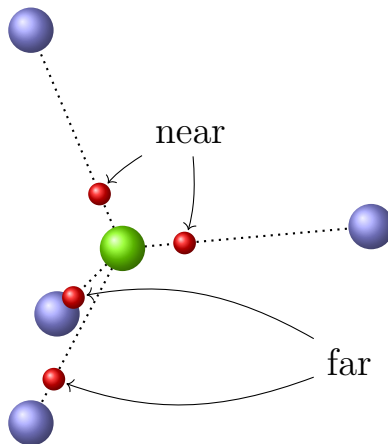
We may represent this graphically by making the graph Γ into a *directed* graph. We decorate the edges with arrows, each pointing towards the hydrogen atom on the edge.
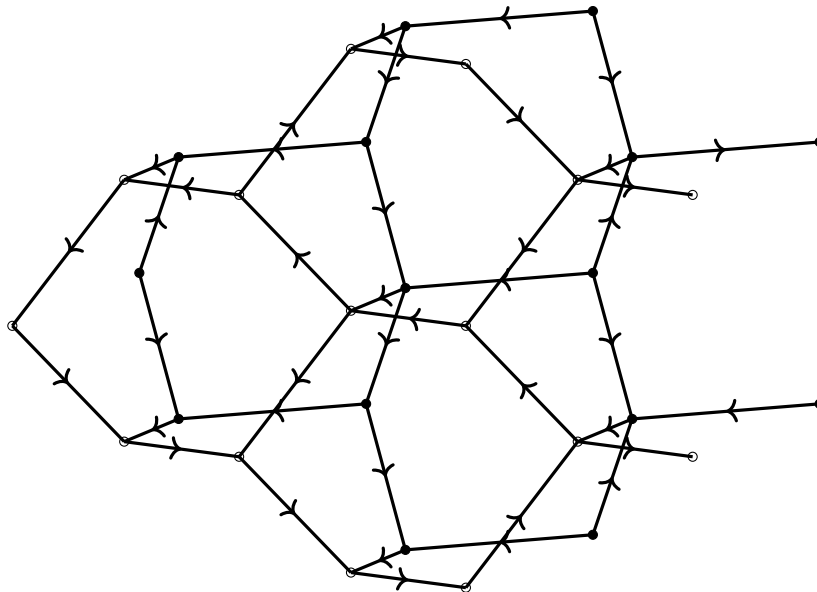
Then we obtain the following model: we have a 4-regular graph, based on the three-dimensional hexagonal lattice. A state of the system is a refinement of the graph to a directed graph, with every vertex having two incoming and two outgoing arrows.

4 Ice

Linus Pauling computed the entropy and free energy of ice by means of a three-dimensional lattice model.

For example we may consider ice (frozen H_2O) where the larger oxygen atoms have fixed locations at the vertices of a grid. In its usual form (called Ice I_h) these oxygen atoms are arranged in a three-dimensional hexagonal lattice. We can envision the oxygen atoms as lying on the vertices of a three-dimensional hexagonal crystal lattice. Each oxygen atom will have four neighbors, lying at the vertices of a tetrahedron. We may consider the 4-regular

graph Γ whose vertices are the oxygen atoms and whose edges are the segments joining them to the four nearby atoms.

5   A class of lattice models

5.1   Graphs

We have formalized the ice crystal into a system based on a *graph*, which is almost but not the same as a graph in the usual combinatorial definition. Let us define a graph to be a set of *vertices* and a set of *edges* with an incident relation, that some edges are *through* or *adjacent to* certain vertices. We will assume that every edges is through either exactly two vertices, or a single vertex. The edges that are through a single vertex will be called *boundary edges*. The edges that connect two vertices are *interior edges*.

As an example, let us consider this graph:

$$\tag{1}$$
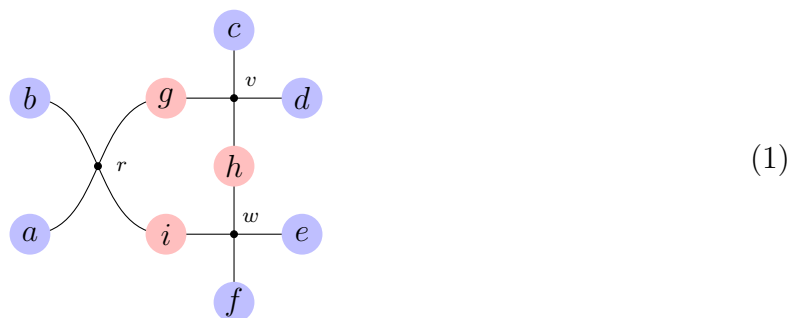
Here we have a graph with three vertices, labeled v, w and r. There are nine edges, labeled a, b, c, d, e, f and g, h, i. The edges a, b, c, d, e, f are boundary edges.

The graph is *planar* if it can be embedded in the plane. **We will consider mainly planar 4-regular graphs.** The Ice I_h graph is 4-regular, but not planar. On the other hand, the graph (1) is planar.

5.2   Spins

In the class of models we will consider, every edge e will be assigned a set Σ_e of possible states, called *spins*. In the Ice models, the spins are the two possible orientations of the arrow that points towards the hydrogen atom. We will require that the spins of the boundary edges are fixed, and are part of the data describing the system. On the other hand, the spins of the interior edges are variable.

5.3   States

A *state* of the model is an assignment of an element of its spinset to every edge of the model. We will assume that the boundary spins have fixed assignments. Indeed, this will be part of the data describing the model.

Almost always there will be local constraints at each vertex on the possible configurations of spins adjacent to a particular vertex. We will call a state in which these constraints are satisfied at every vertex *admissible*.

For example in the Ice I_h model that we have described, the spins are directions or orientations of the edges, which we can represent by arrows, and the constraint is that there there are two "in" arrows and two "out" arrows. This means that there are $\binom{4}{2} = 6$ possible configurations of local spins at the vertex.

5.4   Boltzmann weights

Every admissible configuration $\mathfrak{s}$ is therefore a state of the system $\mathfrak{S}$, which is the ensemble of all states. It is to be assigned a *Boltzmann weight* $\beta(\mathfrak{s})$. We will assume that this is a product of *local Boltzmann weights* $\beta_v(\mathfrak{s})$ at each vertex v:

$$\beta(\mathfrak{s}) = \prod_v \beta_v(\mathfrak{s}),$$

where $\beta_v(\mathfrak{s})$ depends only on the configuration of spins at the edges adjacent to the vertex. We can extend this definition to states that are not admissible by defining $\beta_v(\mathfrak{s}) = 0$ if the local configuration is not admissible. Then $\beta(\mathfrak{s}) = 0$ for inadmissible states $\mathfrak{s}$.

The partition function is

$$Z(\mathfrak{S}) = \sum_{\mathfrak{s}} \beta(\mathfrak{s}).$$

We may sum over all states, or over admissible states.

6   The Six Vertex Model

Certain lattice models are called *solvable* since algebraic methods based on the Yang-Baxter equation, which will be a major focus of this course, allow the partition function to be computed exactly. Historically the first example was Onsager's 1944 study of the 2-dimensional Ising model. However we will start with an even simpler model, the *six-vertex model*, which is also related to ice.

Solvable lattice models are almost exclusively 2-dimensional. This means that the underlying graph is planar. The Ice I_h model that we considered is not solvable as far as we know, and its graph is not planar.

While Pauling had considered the realistic problem of 3-dimensional Ice and heuristically computed the number of states, one can also consider 2-dimensional Ice, in which the oxygen atoms are restricted to a plane, and form a crystal with the oxygen atoms at the vertices of a square lattice. This was investigated by Nagle [7], after which Lieb [6, 4, 5] and Sutherland [8] found exact solutions for the entropy problem. For 2-dimensional Ice, Lieb found that the residual entropy was $kN \log(W)$ with $W = (4/3)^{3/2}$.

The mathematical model of 2-dimensional ice is the famous 6-vertex model, which is the archetype of a large class of important solvable lattice models. It is realistic enough to have a phase transition, which was of great interest to the early investigators. We will therefore discuss it at length.

The six-vertex model is nearly identical to the I_h models we have discussed, except that the underlying crystal is 2-dimensional, based on a square lattice. We will give two versions of the Boltzmann weights. Recall that the spinset of an edge is a set of possible states. For the six-vertex model, the spinset has cardinality two. In one version of the six vertex model, the spinset of an edge is an orientation. The Boltzmann weights depend on six parameters, a_1, a_2, b_1, b_2, c_1 and c_2, which may depend on the vertex v, so we may write $a_1(v)$, etc. We label the possible states as follows:

a_1	a_2	b_1	b_2	c_1	c_2
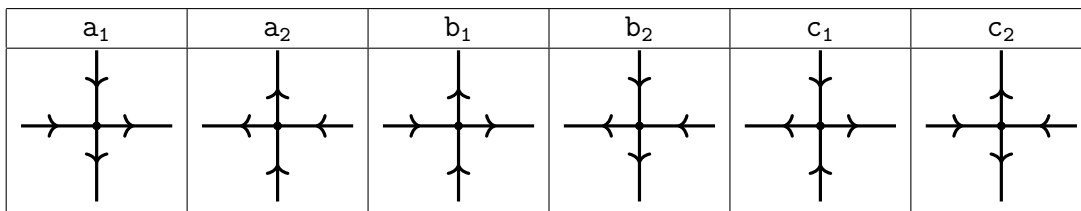
On the other hand, it will also be convenient to dispense with the orientation and take the spinset to be the 2-element set $\{+, -\}$. Then the labeling of the states is as follows:

a_1	a_2	b_1	b_2	c_1	c_2
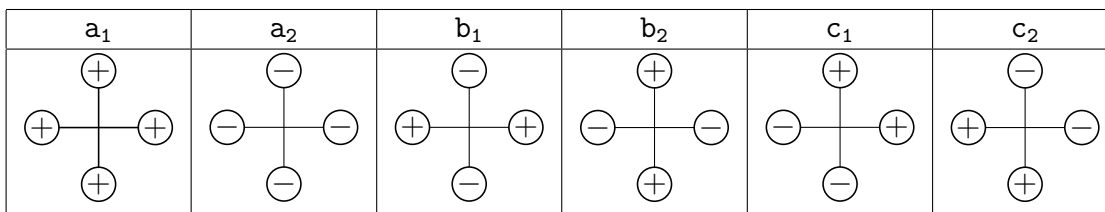
Although the lattice model will be based on a rectangular grid, we will also encounter vertices that are in a rotated orientation, and we will use the following labels for these.

| a_1	a_2	b_1	b_2	c_1	c_2
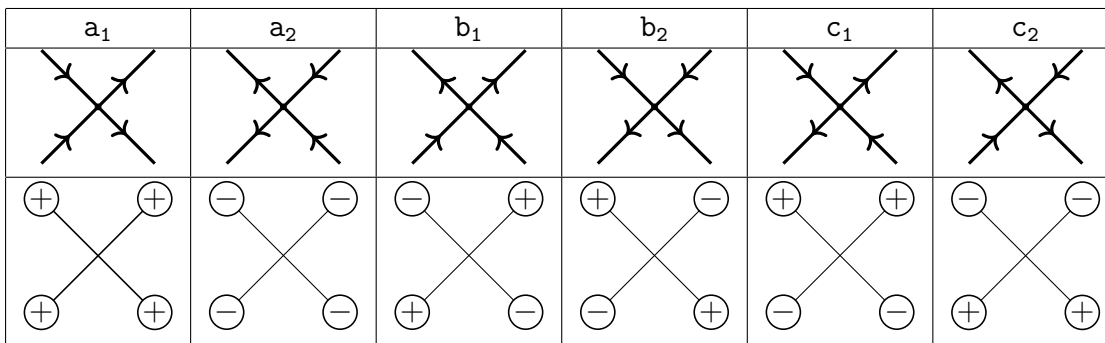
7   Solvability

Baxter introduced an important method of studying certain vertex models, and he used it to solve not just the six-vertex model, but the more difficult eight-vertex model, and with it the XYZ Heisenberg spin chain, a related quantum mechanical problem. This method is based on the *Yang-Baxter equation*, so named by Faddeev. The study of the Yang-Baxter

equation leads to interesting mathematics, namely braided categories and quantum groups. Indeed, historically, the six-vertex model was a key example.

We will consider vertices in a model (as described in Section 5) as being associated with a set of Boltzmann weights. We will say that a class of models is *solvable* if when v and w are vertices that can occur adjacent to each other in the class, there is another type of vertex that we will denote r such that the two following systems are equivalent:
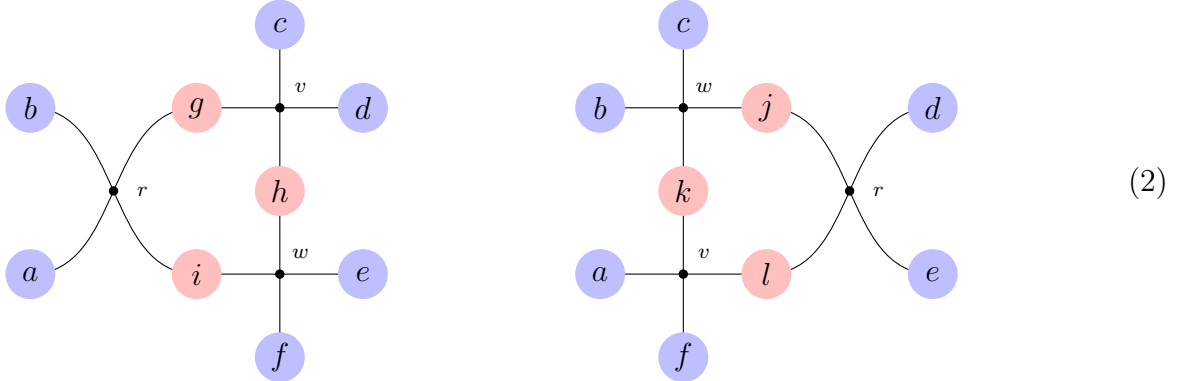
This means that for every possible assignment of spins to the six boundary edges a, b, c, d, e, f, the partition functions of the two systems are equivalent. Thus we sum over all possible assignments of spins to the interior edges, g, h, i on the left-hand side, or j, k, l on the right-hand side. If this is so, we say the *Yang-Baxter equation* is satisfied for these vertices v, w, r.

We will consider two families of solutions to the Yang-Baxter equation within the six-vertex model.

7.1 Field-Free Six-Vertex Model

The vertex v with Boltzmann weights $a_i(v)$, $b_i(v)$ and $c_i(v)$ will be called *field-free* if $a_1(v) = a_2(v)$, $b_1(v) = b_2(v)$ and $c_1(v) = c_2(v)$. We will suppress the subscript in the field free case and write just $a(v) = a_1(v) = a_2(v)$. We will make the following assumptions:

Assumption 7.1. *In addition to the field-free assumption that $a_1 = a_2$, $b_1 = b_2$, $c_1 = c_2$ we will assume that $a \neq 0$ and that $b \neq \pm c$.*

Let

$$\Delta(v) = \frac{a^2(v) + b^2(v) - c^2(v)}{2a(v)b(v)}.$$

Note that this requires $a(v)$ and $b(v)$ to be nonzero, and we will assume this for v, w and r in the next theorem. We will relax that assumption in Lecture 4. (In Lecture 4 we will continue to assume $a(v) \neq 0$ but we will allow $b = 0$.)

**Assumption 7.2.** *We will assume that $\Delta \neq 0, 1, -1$.*

Assumption 7.1 is essential, and needed to obtain a reasonable theory. Assumption 7.2 should be removed. The assumption that $\Delta \neq 0$ is because we will treat that case in detail as part of the free-fermionic case in later lectures. The assumption that $\Delta \neq 1, -1$ is out of caution since though these cases are important. (They are phase transition points.) Some of our algebra might be wrong if $\Delta = \pm 1$.

Theorem 7.1 (Baxter). *Let $\Delta \in \mathbb{C}$, and let v and w be two field-free six-vertex model vertices with $\Delta(v) = \Delta(w) = \Delta$. In addition to the requirement in Assumption 7.1 that $a(v)$ and $a(w)$ are nonzero, let us assume that $b(v)$ and $b(w)$ are nonzero. Then there is another field-free six-vertex model vertex r such that the Yang-Baxter equation (2) is satisfied. We have $a(r)^2 + b(r)^2 - c(r)^2 = 2a(r)\,b(r)\,\Delta$, so if $b(r) \neq 0$ then $\Delta(r) = \Delta$.*

Proof. We claim that there are three equations that must be satisfied for the Yang-Baxter equation to be satisfied. First take $(a, b, c, d, e, f) = (+, +, -, +, -, +)$. The left-hand side of the Yang-Baxter equation has one admissible state:
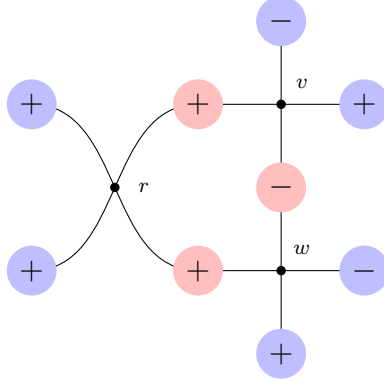
This has Boltzmann weight $b(v)c(w)a(r)$. On the other hand, there are two admissible states on the right-hand side:
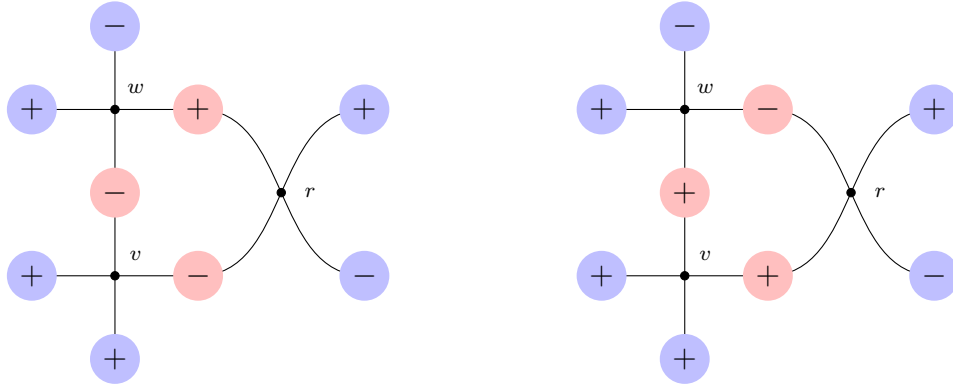
These have weights $c(v)b(w)c(r)$ and $a(v)c(w)b(r)$. So we obtain the equation

$$b(v)c(w)a(r) = c(v)b(w)c(r) + a(v)c(w)b(r). \tag{3}$$

Taking $(a, b, c, d, e, f) = (+, +, -, -, +, +)$ gives

$$c(v)a(w)a(r) = c(v)b(w)b(r) + a(v)c(w)c(r), \tag{4}$$

and taking $(a, b, c, d, e, f) = (+, -, +, -, +, +)$ gives

$$b(v)a(w)c(r) = c(v)c(w)b(r) + a(v)b(w)c(r). \tag{5}$$

Taking other combinations of a, b, c, d, e, f give a total of 12 equations altogether, but they turn out to be these same three equations, repeated. So we need to show that we can construct the vertex r to satisfy (3–5).

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Since $\Delta(v) = \Delta(w)$ we have

$$(a(v)^2 + b(v)^2 - c(v)^2)a(w)b(w) = (a(w)^2 + b(w)^2 - c(w)^2)a(v)b(v).$$

This identity implies that

$$\frac{b(v)a(w)b(w) - a(v)b(w)^2 + a(v)c(w)^2}{a(w)} = \frac{a(v)b(v)a(w) - a(v)^2b(w) + c(v)^2b(w)}{b(v)},$$

and we define this to be $a(r)$. Then we define

$$b(r) = b(v)a(w) - a(v)b(w), \qquad c(r) = c(v)c(w).$$

Now it may be checked that the identities (3), (4), (5) are satisfied. For example, to prove (3), the right-hand side equals

$$c(w)(a(v)b(v)a(w) - a(v)^2b(w) + c(v)^2b(w))$$

and using the second expression for $a(r)$ this equals $a(r)c(w)b(v)$. We leave the other two cases to the reader. Checking that $\Delta(r) = \Delta$ is an easy calculation. $\qquad\square$

We will explain later how this Yang-Baxter equation can be applied to study the partition functions for the field-free two-dimensional ice models, and what some of the applications are.

7.2   The Free-Fermionic Six Vertex Model

The second case where there is solvability is the *free-fermionic case*. Here the relevant Yang-Baxter equation was found (partly) by Korepin around 1981. See [3], page 126, with referencces to earlier literature. Later Brubaker, Bump and Friedberg rediscovered this in a slightly more general form and gave applications. See [2]. Within the six-vertex model, this is a very interesting example with important generalizations.

We will call the six-vertex model vertex v *free-fermionic* if

$$a_1(v)a_2(v) + b_1(v)b_2(v) = c_1(v)c_2(v).$$

We are of course dropping the field free-condition.

Theorem 7.2 (Korepin-Izergin; Brubaker-Bump-Friedberg). *Let v and w be free-fermionic vertices. Then there is a free-fermionic vertex r such that the Yang-Baxter equation is satisfied.*

References

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