Knot Theory and Statistical Mechanics

Richard Altendorfer *
Dept. of Physics and Astronomy
Bloomberg Center
3400 N. Charles Street
Baltimore, MD 21218

Abstract
In this paper, a connection between statistical mechanics and knot theory will be established. The investigation is restricted to spin models, which can be defined on a link diagram (replacing the lattice of the model). By imposing certain conditions on the Boltzmann weights the partition function of the system may yield a link invariant, i.e. the partition function depends only on the link as a three-dimensional entity and not on the chosen diagram.

*e-mail: richard@bohr.pha.jhu.edu
1 Spin models

A spin model is a statistical mechanical model defined on a graph with vertices \( \{v\} \) and edges \( \{e\} \) [1]. The vertices acquire values of a finite set \( \theta \) of "spins" with \( |\theta| = n \). A state is a function \( \sigma : \{v\} \rightarrow \theta (|\{v\}| = V) \). A nearest neighbour interaction model is defined by an energy function

\[
E : \theta \times \theta \rightarrow \mathbb{R}
\]

so that the energy of an edge joining vertices \( v_a \) and \( v_b \) is

\[
E(a, b) := E(\sigma(v_a), \sigma(v_b))
\]

With the definition

\[
w(a, b) := e^{-\beta E(a, b)}
\]

the partition function \( Z \) reads

\[
Z = \sum_{\sigma} e^{-\beta \sum_{e} E(a, b)} = \sum_{\sigma} \prod_{e} w(a, b)
\]

As an example, the two-dimensional Ising model on a square lattice is defined by \( \theta = \{-1, 1\} \). Hence \( \sigma(v_i) = \pm 1 \forall i \), where \( i \) enumerates the lattice sites. The energy function is

\[
E(a, b) := J \sigma(v_a) \sigma(v_b)
\]

with \( J \) being the interaction energy.

![Figure 1: Ising model: sample state on a rectangular lattice](image-url)

Clearly, the assignment \( \theta = \{-1, 1\} \) is arbitrary and can be modified by a redefinition of the interaction energies. Therefore, throughout this paper the more fundamental quantity \( w(a, b) := e^{-\beta E(a, b)} \) will be used.
2 How can a spin model be related to a link diagram?

At first glance, link diagrams and spin models seem to be quite unrelated. In general, spin models are defined on a periodic lattice (an exception is the Bethe lattice) and must be endowed with an interaction term, whereas link diagrams have an irregular shape and are specified by under/overcrossings.

Figure 2: A link diagram

The question is: “How can a link diagram be identified with a graph without losing information about the link?”

The obvious procedure is to project the link diagram onto a two-dimensional plane and to identify the crossings with vertices and the strings between the crossings with edges. This must be rejected, however, as the crucial information about the link, its knottedness, - encoded in the under/overcrossings - is lost. The following recipe does preserve the characteristics of a link [2, 3, 4]:

1. Shade the regions of a link diagram like a chequer-board. (This can always be done in a consistent way, i. e. no occurrence of adjacent regions of the same colour, because only four-valent crossings are present in a link diagram.)

2. Extract a graph from the link diagram by taking the shaded regions as vertices and the crossings as edges.

3. Assign different Boltzmann weights \( w_\pm(a, b) \) to an under-/overcrossing.
The normalized partition function for such a spin model is defined as [2, 4]

\[ Z_L^S := \left( \frac{1}{\sqrt{n}} \right)^{V-1} \sum_{\sigma} \prod_{c} w_\pm(a, b). \]  \hspace{1cm} (2.1)

Although the intermediate goal of identifying a link diagram with a spin model has been accomplished, the relevance of this procedure is not self-evident, especially when taking into account that many new arbitrary parameters \( w_\pm(a, b) \) had to be introduced. This will become clear when recalling what knot theory is all about: ambient isotopy.
3 When will a spin model be invariant under ambient isotopy?

In knot theory, ambient isotopy [5, 2] defines an equivalence class of links which are related by continuous deformations of knots, i.e., deformations without cutting the strings of the link. These deformations can be effected by the three Reidemeister moves. The above recipe of identifying a link diagram with a spin model suggests investigating the effect of the Reidemeister moves on the partition function $Z_L^S$ (2.1). A true equivalence of the link diagram and the spin model could be established, if the partition function $Z_L^S$ were invariant under the Reidemeister moves. In general, this invariance can not be expected as the Boltzmann weights $w_\pm(a, b)$ can be arbitrarily chosen. Imposing invariance of $Z_L^S$ under the Reidemeister moves will therefore lead to constraints on $w_\pm(a, b)$ [2]. The derivation of these constraint equations is as follows:

Reidemeister I:

\[
\Rightarrow \sum_{x \in \theta} w_+(a, x) = \sqrt{n} \quad (3.1)
\]
\[ \Rightarrow w_-(a,a) = 1 \]  \hspace{1cm} (3.2)

The two shading possibilities generate in fact only one condition, since invariance under the third Reidemeister move (3.7) relates the equations (3.1) and (3.2):

\[ A := w_-(b,b) = \frac{1}{\sqrt{n}} \sum_{x \in \theta} w_+(a,x) \frac{1}{\theta} = 1. \]  \hspace{1cm} (3.3)

Under the first Reidemeister move, the partition function transforms into

\[ Z_L^S = A^{\pm 1} Z_{L'}^S. \]  \hspace{1cm} (3.4)

The condition (3.3) turns out to be too restrictive, but can be absorbed into a proper normalization of \( Z_L^S \) [4].
Reidemeister II:

\[ \Rightarrow w_+(a, b)w_-(a, b) = 1 \quad (3.5) \]

\[ \Rightarrow \sum_{x \in \theta} w_-(a, x)w_+(x, b) = n\delta(a, b) \quad (3.6) \]
Reidemeister III:

\[ \Rightarrow \sum_{x \in \Theta} w_+ (a, x) w_+ (b, x) w_-(c, x) = \sqrt{n} w_+ (a, b) w_+ (b, c) w_-(c, a) \]  \hspace{1cm} (3.7)

ii) The opposite shading is analogous to case i) and leads to the same constraint equation.

In statistical mechanics, this relation is known as the star-triangle relation [1]. It relates two spin models that have the same nearest neighbour interaction, but are defined on different lattices - the honeycomb lattice and its dual lattice, the triangular lattice.

Figure 4: a) Dual lattices: honeycomb and triangular lattice b) Star-triangle relation

For such a pair of spin models it can be shown [1] that for certain interaction energies \( E(a, b) \) (e.g. the Ising model and the \( n \)-state Potts model), contributions of subgraphs of the dual lattices can be related by

\[ \sum_{x \in \Theta} e^{-\beta(E(a, x) + E(b, x) + E(c, x))} = \text{Re}^{-\beta(E(a, b) + E(b, c) + E(c, a))} \]  \hspace{1cm} (3.8)
with some normalization constant $R$. The importance of this relation became clear when Baxter solved the two-dimensional Ising model defined on a honeycomb and a triangular lattice merely on the basis of this relation. By "solution" the free energy per lattice site in the thermodynamic limit is understood. The star-triangle relation is a simple version of the ubiquitous Yang-Baxter equation, which appears in different fields like two-dimensional field theories and quantum groups.

Invariance under the second and the third Reidemeister move leads to the following constraint equations for the Boltzmann weights $w_{\pm}(a, b)$ [2]:

\[
\begin{align*}
  w_{\pm}(a, b) & = w_{\pm}(b, a) \\
  w_+(a, b)w_-(a, b) & = 1
\end{align*}
\]

\[
\sum_{x \in \Theta} w_-(a, x)w_+(x, b) = n\delta(a, b)
\]

\[
\sum_{x \in \Theta} w_+(a, x)w_+(b, x)w_-(c, x) = \sqrt{n}w_+(a, b)w_-(b, c)w_-(c, a)
\]

(3.9)

Hence one looks for solutions of (3.9).

Among the simplest spin models is the $n$-state Potts model. Its Boltzmann weight is given by

\[
w_{\pm}(a, b) = \begin{cases} X & \text{if } a = b \\
Y & \text{if } a \neq b \end{cases}
\]

(3.10)

where $X$ and $Y$ are arbitrary energy levels. For $n = 2, 3$ the solution of (3.9) and (3.10) is unique [4]:

\[
w_+(a, b) = \begin{cases} 1 & \text{if } a = b \\
-\frac{1}{t} & \text{if } a \neq b \end{cases}
\]

(3.11)

\[
w_-(a, b) = \begin{cases} 1 & \text{if } a = b \\
-\frac{1}{t} & \text{if } a \neq b \end{cases}
\]

(3.12)

with

\[
2 + t + \frac{1}{t} = n.
\]

(3.13)

For $n > 3$ the complete set of solutions is not known.

The interpretation of the obtained solution leads to an immediate problem: the Boltzmann weights $w_{\pm}(a, b)$ are not positive definite and can even be complex. Hence a $Z_L^S$ obtained by inserting $w_{\pm}(a, b)$ into $Z_L^S$ is not an ordinary partition function from the statistical mechanics' point of view. On the other hand, $Z_L^S$ is by construction invariant under ambient isotopy and is therefore a knot invariant. By establishing the above described connection between link diagrams and spin models, a knot invariant can be found or recovered for every conceivable spin model (assuming that (3.9) can be solved).
In the case of the $n$-state Potts model it can be shown that [4]:

$$Z_L^S = \left(\frac{1}{\sqrt{n}}\right)^{V-1} \sum_\sigma \prod_\epsilon w_\epsilon(a, b)$$

$$= Z_L^S(t)$$

$$\sim V_L(t) \quad \text{(the Jones polynomial)}$$

(3.14)

Note that by (3.13) $t$ is fixed ($n = 2 \iff t = i$; $n = 3 \iff t = e^{i\pi/2}$), whereas in the original definition of the Jones polynomial [2], $t$ was an undetermined variable.

4 Conclusion

The association of a link diagram with a spin model can lead to the (re-)discovery of link invariants (e.g. the Jones Polynomial). This is achieved by imposing invariance under ambient isotopy - represented by invariance under the Reidemeister moves - on the partition function of the spin model. Following the above described procedure entails a set of algebraic equations, which can be solved uniquely for $n$-state Potts models with $n = 2, 3$.

References


