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Complexity classification of the six-vertex model

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ABSTRACT

We prove a complexity dichotomy theorem for the six-vertex model. For every setting of the parameters of the model, we prove that computing the partition function is either solvable in polynomial time or #P-hard. The dichotomy criterion is explicit.

1. Introduction

A primary purpose of complexity theory is to provide classifications to computational problems according to their inherent computational difficulty. While computational problems can come from many sources, a class of problems from statistical mechanics has a remarkable affinity to what is naturally studied in complexity theory. These are the *sum-of-product* computations, a.k.a. *partition functions* in physics.

Well-known examples of partition functions from physics that have been investigated intensively in complexity theory include the Ising model and Potts model [10,8,7,12]. Most of these are spin systems. Spin systems as well as the more general counting constraint satisfaction problems (#CSP) are special cases of Holant problems [5] (see Section 2 for definitions). Roughly speaking, Holant problems are tensor networks where edges of a graph are variables while vertices are local constraint functions; by contrast, in spin systems vertices are variables and edges are (binary) constraint functions. Spin systems can be simulated easily as Holant problems, but Freedman, Lovász and Schrijver proved that simulation in the reverse direction is generally not possible [6]. In this paper we study a family of partition functions that fit the Holant problems naturally, but not as a spin system. This is the *six-vertex model*.

The six-vertex model in statistical mechanics concerns crystal lattices with hydrogen bonds. Remarkably it can be expressed perfectly as a family of Holant problems with 6 parameters for the associated signatures, although in physics people are more focused on regular structures such as lattice graphs, and asymptotic limit. In this paper we study the partition functions of six-vertex models purely from a complexity theoretic view, and prove a complete classification of these Holant problems, where the 6 parameters can be arbitrary complex numbers.

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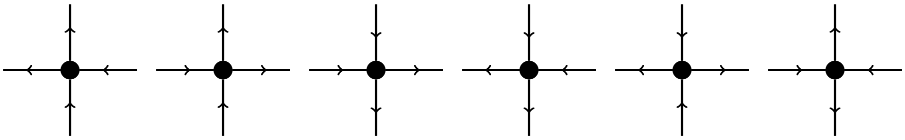

Fig. 1. Valid configurations of the six-vertex model.

The first model in the family of six-vertex models was introduced by Linus Pauling in 1935 to account for the residual entropy of water ice [17]. Suppose we have a large number of oxygen atoms. Each oxygen atom is connected by a bond to four other neighboring oxygen atoms, and each bond is occupied by one hydrogen atom between two oxygen atoms. Physical constraint requires that the hydrogen is closer to either one or the other of the two neighboring oxygens, but never in the middle of the bond. Pauling argued [17] that, furthermore, the allowed configuration of hydrogen atoms is such that at each oxygen site, exactly two hydrogens are closer to it, and the other two are farther away. The placement of oxygen and hydrogen atoms can be naturally represented by vertices and edges of a 4-regular graph. The constraint on the placement of hydrogens can be represented by an orientation of the edges of the graph, such that at every vertex, exactly two edges are oriented toward the vertex, and exactly two edges are oriented away from it. In other words, this is an *Eulerian orientation*. Since there are $\binom{4}{2} = 6$ local valid configurations, this is called the six-vertex model. In addition to water ice, potassium dihydrogen phosphate KH_2PO_4 (KDP) also satisfies this model.

The valid local configurations of the six-vertex model are illustrated in Fig. 1. There are parameters $\epsilon_1, \epsilon_2, \ldots, \epsilon_6$ associated with each type of the local configuration. The total energy E is given by $E = n_1\epsilon_1 + n_2\epsilon_2 + \ldots + n_6\epsilon_6$, where n_i is the number of local configurations of type i. Then the partition function is $Z = \sum e^{-E/k_B T}$, where the sum is over all valid configurations, k_B is Boltzmann's constant, and T is the system's temperature. Mathematically, this is a *sum-of-product* computation where the sum is over all Eulerian orientations of the graph, and the product is over all vertices where each vertex contributes a factor $c_i = c^{\epsilon_i}$ if it is in configuration i $(1 \le i \le 6)$ for some constant c.

Some choices of the parameters are well-studied. On the square lattice graph, when modeling ice one takes $\epsilon_1 = \epsilon_2 = \ldots = \epsilon_6 = 0$. In 1967, Elliott Lieb [14] famously showed that, as the number N of vertices approaches ∞, the value of the "partition function per vertex" $W = Z^{1/N}$ approaches $\left(\frac{4}{3}\right)^{3/2} \approx 1.5396007\ldots$ (Lieb's square ice constant). This matched experimental data 1.540 ± 0.001 so well that it is considered a triumph. The case $\epsilon_1 = \epsilon_2 = \ldots = \epsilon_6 = 0$ is precisely the problem of counting the number of Eulerian orientations on 4-regular graphs. Mihail and Winkler [16] showed that counting the number of Eulerian orientations (on a general even degree graph, called an Euler graph) is #P-hard, and gave a fully polynomial randomized approximation scheme (fpras) for it. Huang and Lu [9] proved that the problem remains #P-hard for 4-regular graphs, which is exactly the special case for the six-vertex model with $\epsilon_1 = \epsilon_2 = \ldots = \epsilon_6 = 0$. They proved this by a reduction from the #P-hardness of $T_G(3,3)$, the evaluation at $(3,3)$ of the Tutte polynomial T_G, due to Las Vergnas [11]. On (4-regular) *planar* graphs, $T_G(3,3)$ is actually exactly equivalent to a specific six-vertex model; in the notation of Section 2, it is specified by the signature matrix $\begin{bmatrix} 0&0&0&1 \\ 0&1&2&0 \\ 0&2&1&0 \\ 1&0&0&0 \end{bmatrix}$. Welsh has pointed out that $T_G(0,-2)$ is equivalent to counting the number of Eulerian orientations on 4-regular graphs [21]. Luby, Randall and Sinclair [15] gave sampling algorithms for Eulerian orientations on simply connected regions of the grid graph with boundary conditions.

There are other well-known choices in the six-vertex model family. The KDP model of a ferroelectric is to set $\epsilon_1 = \epsilon_2 = 0$, and $\epsilon_3 = \epsilon_4 = \epsilon_5 = \epsilon_6 > 0$. The Rys F model of an antiferroelectric is to set $\epsilon_1 = \epsilon_2 = \epsilon_3 = \epsilon_4 > 0$, and $\epsilon_5 = \epsilon_6 = 0$. When there is no ambient electric field, the model chooses the zero field assumption: $\epsilon_1 = \epsilon_2$, $\epsilon_3 = \epsilon_4$, and $\epsilon_5 = \epsilon_6$. Historically these are widely considered among the most significant applications ever made of statistical mechanics to real substances. In classical statistical mechanics the parameters are all real numbers while in quantum theory the parameters are complex numbers in general.

In this paper, we give a complete classification of the complexity of calculating the partition function Z on any 4-regular graph defined by an arbitrary choice parameter values $c_1, c_2, \ldots, c_6 \in \mathbb{C}$. (To state our theorem in strict Turing machine model, we take $c_1, c_2, \ldots, c_6$ to be *algebraic* numbers.) Depending on the setting of these values, we show that the partition function Z is either computable in polynomial time, or it is #P-hard, with nothing in between. The dependence of this dichotomy on the values $c_1, c_2, \ldots, c_6$ is explicit.

A number of complexity dichotomy theorems for counting problems have been proved previously. These are mostly on spin systems, or on #CSPs (counting Constraint Satisfaction Problems), or on Holant problems with *symmetric* local constraint functions. #CSP is the special case of Holant problems where EQUALITIES of all arities are auxiliary functions assumed to be present. Spin systems are a further specialization of #CSP, where there is a single binary constraint function (see Section 2). The six-vertex model cannot be expressed as a #CSP problem. It is a Holant problem where the constraint functions are *not symmetric*. Thus previous dichotomy theorems do not apply. This is the first complexity dichotomy theorem proved for a class of Holant problems on *non-symmetric* constraint functions and without auxiliary functions assumed to be present.

However, one important technical ingredient of our proof is to discover a direct connection between some subset of the six-vertex models with spin systems. Another technical highlight is a new interpolation technique that carves out subsums