# Approximate sampling and COUNTING FOR SPIN MODELS IN GRAPHS 

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#### Abstract

We approach the problems of approximate sampling and counting in spin models on graphs, surveying the most significant results in the area and introducing the necessary background from statistical physics. We pay particular attention to the general algorithm design frameworks developed by Weitz and Barvinok, as well as to the newer results on counting and sampling independent sets of given size. In addition, we discuss the adaptation of the arguments behind these results to count and sample colorings with fixed color sizes, explaining in detail the current research line we are undertaking.


Keywords: spin model, statistical physics, hard-core model, approximate counting, approximate sampling, combinatorics, graph theory

MSC2020: 05C85

## Resumen

En este trabajo abordamos los problemas de muestreo y conteo aproximado en modelos de espines en grafos, recopilando los resultados más significativos del campo e introduciendo el conocimiento previo necesario del área de la física estadística. En particular, prestamos especial atención a los métodos generales de diseño de algorismos desarrollados por Weitz y Barvinok, así como a los avances recientes en cuanto al conteo y muestreo de conjuntos independientes de un tamaño dado. Así mismo, discutimos cómo se podrían adaptar estos argumentos al problema de contar y muestrear coloraciones con el tamaño de cada color fijo, explicando en detalle la línea de investigación que estamos llevando a cabo actualmente.

Palabras claves: modelo de espines, física estadística, hard-core model, conteo aproximado, muestreo aproximado, combinatoria, teoría de grafos

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## Resum

En aquest treball abordem els problemes de mostreig i comptatge aproximat en models d'espins en grafs, recopilant els resultats més significatius de l'àrea i introduïnt els coneixements previs necessaris del camp de la física estadística. En particular, prestem especial atenció als mètodes generals de disseny d'algorismes desenvolupats per Weitz i Barvinok, així com els avenços recents en matèria de comptatge i mostreig de conjunts independents de mida donada. Així mateix, discutim com es podrien adaptar aquests arguments als problemes de comptatge i mostreig de coloracions amb les mides de cada color fixades, explicant amb detall la línia de recerca actual que estem duent a terme.

Paraules clau: model de spins, física estadística, hard-core model, comptatge aproximat, mostreig aproximat, combinatòria, teoria de grafs

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## Chapter 1

## Introduction

The aim of this thesis is to provide an introduction to the problem of approximately sampling and counting in spin models on graphs, surveying the general results from the last three decades and focusing at the end on the newer results for structures of fixed size.

Chapter 2 constitutes a self-contained introduction to the concepts from statistical physics that are used throughout the thesis. Though we often make an effort to provide the necessary physical intuition behind the definitions, the view is heavily shifted towards a combinatorial interpretation, so we omit much of the content that would typically appear in an introductory statistical physics course. For a rigorous mathematical take on the subject that still covers the whole breadth of the topic, we recommend the textbook by Friedli and Velenik [FV17].

Chapter 3 introduces the main problems of approximate sampling and counting, describing both the original results by Jerrum and Sinclair that raised interest on the topic and introducing two of the main methods used to construct efficient approximate counting algorithms nowadays: the correlation decay argument by Weitz, based on the self-avoiding tree construction, and the polynomial interpolation argument by Barvinok. Though most of the proofs of this chapter have appeared in various papers, we have made an effort to compile the most significant ones and reexplain them without assuming much previous knowledge about the topic.

Chapter 5 builds on Chapter 3 by exploring a variation of the same problems, in which we try to design algorithms that only count (or sample) the objects that have a certain given size. For the counting and sampling of independent sets, we describe the significant advances that have been achieved in the last few years. For the counting and sampling of colorings with given sizes, which is still mostly unexplored, we provide a detailed description of a future line of research to approach the problem.

Chapter 4 deviates a bit from the general line of the rest of the thesis, focusing on the problem of proving the existence of colorings with certain given color sizes. This does not bear much relation with the general topic, but it is a prerequisite for the design of sampling algorithms for colorings in

Chapter 5.

## Chapter 2

## Fundamentals of Statistical Physics

### 2.1 Introduction

In this chapter we introduce the main tools from statistical physics that we will use to study combinatorial problems. Many of the definitions and examples are taken from Per22, Per20, and [FV17. First, however, we give a short introduction on what is the kind of problems that statistical physics deals with and why the probabilistic and statistical approach is useful for studying deterministic physical systems.

### 2.1.1 Why statistical physics?

In classical physics, in order to accurately model the behaviour of a system with $n$ particles, one needs to use Newton's laws to construct a system of equations with $6 n$ variables, 3 for the position of each particle and 3 for the velocity. Thus, to model a macroscopic object of, say, a mole of particles, we would need to solve a system of the order of $10^{24}$ equations, which is totally unfeasible. The same is true for the Lagrangian or Hamiltonian reformulations of classical mechanics, which do not change the total number of variables one needs to compute.

One way to approach this issue is that of thermodynamics, which completely ignores the underlying constituents of matter and focuses only on macroscopic properties, deriving their governing equations by empirical methods. That method allowed early 19th century physicists to derive the equation of state of an ideal gas $P V=n R T$ without having any knowledge about the existence of atoms, relying only on experimental data.

This approach provides a certain robustness to thermodynamics that many other branches of physics lack. Indeed, if a new fundamental particle were to be discovered tomorrow, all the standard model of subatomic physics would need to be rewritten from scratch, while thermodynamics would remain largely unaffected, as it does not base its validity on any assumptions about the microscopic constituents of matter. This is what Albert Einstein meant when he stated that "[Thermodynamics]
is the only physical theory of universal content which I am convinced will never be overthrown".
However, having to derive the equations of state from experiments is an incredibly arduous process, and it is very limited in terms of what can one achieve with it. The field of statistical physics, as we understand it today, was created in the end of the 19th century in order to deal with these issues, providing an alternative and more rigorous way of proving the results given by classical thermodynamics.

The basic idea of statistical physics is that, instead of keeping track of all the microscopic variables (e.g. position and velocity of each particle), we can describe the system by specifying the probability distribution that these microscopic variables follow. Intuitively, we imagine having a large number of independent copies of our system, each of them with the same macroscopic state (i.e. in the case of an ideal gas, same pressure, volume and temperature), but each with a different microscopic state. Then we ask about the probability that one of these copies chosen at random (not necessarily uniformly, see the discussion on entropy maximization) will have a certain microscopic value.

Once we have a probabilistic microscopic description of the system, we can approximate any macroscopic quantity by computing its expected value in the probabilistic model. By the law of large numbers, (and with some extra assumptions that are followed by all reasonable macroscopic quantities of interest) this probabilistic approximation will be very close to the real value.

### 2.1.2 Microscopic description and ensembles

Suppose we have a physical system, and let $\Sigma$ be the set of the microscopic states of the system (which we assume for simplicity to be finite). The energy of the system can be calculated from its microscopic description (by computing the interaction between each pair of particles ${ }^{1}$ ), giving a map $\mathcal{H}: \Sigma \longrightarrow \mathbb{R}$ that associates each state to its energy. This map is called the Hamiltonian of the system.

As explained before, the statistical physics approach consists on defining a probability measure $\mu: \Sigma \longrightarrow[0,1]$, and considering that any macroscopic observable $A: \Sigma \longrightarrow \mathbb{R}$ can be approximated by $\mathbb{E}_{\mu}[A]$. The specific measure $\mu$ that we choose will depend on the restrictions we impose on the system. Typically, the 3 following cases are considered:

- Microcanonical ensemble: the system cannot exchange either particles or energy with its surroundings.
- Canonical ensemble: the system cannot exchange particles but it can exchange energy with its surroundings (i.e. it is in contact with a thermal bath at constant temperature).
- Grand canonical ensemble: the system can exchange either particles or energy with its

[^0]surroundings (i.e. it is contact with a thermal bath at constant temperature and with a particle reservoir with constant chemical potentials for each of the different types of particles).

We take as an axiom that the probability measure $\mu$ chosen should be the one with maximum Shannon entropy over those that agree with the restrictions of the system:

Maximum Entropy Principle ([Jay57], [FV17]): For a given probability measure $\mu: \Sigma \longrightarrow \mathbb{R}$, let $S(\mu):=-\sum_{\sigma \in \Sigma} \mu(\sigma) \log \mu(\sigma)$ be its Shannon entropy. Then, the $\mu$ that best describes our knowledge of the system is the one that maximizes $S(\mu)$ over all $\mu$ compatible with the restrictions on the system.

Remark. In all of the 3 ensembles we consider that the system is in equilibrium. This is often defined informally by saying that a physical system is in equilibrium if its macroscopic variables do not change with time. However, this characterization is not entirely accurate. Even in a system in equilibrium, microscopic changes occur constantly, which imply fluctuations on the value of the macroscopic variables. What it means to be in equilibrium is that the timescale of this fluctuation is much smaller than that of our measuring procedures. Thus, when we measure a certain macroscopic variable, we will obtain the average of the fluctuations, which will be a constant value.

In statistical physics, we consider that a measurement over a long enough timescale is equivalent to taking an average with respect to the probability measure $\mu$. Then, for example, if the system has a measured internal energy of $U$, that means that our measure has to satisfy that $\mathbb{E}_{\mu}[\mathcal{H}]=U$. Hence, allowing energy to fluctuate (by putting the system in contact with a thermal bath), induces a restriction on $\mu$ that does not exist in the microcanonical ensemble, in which we are restricted to states with $\mathcal{H}(\sigma)=U$. As will be seen next, this extra restriction implies that the probability measure $\mu$ will not be uniform.

### 2.1.3 Microcanonical ensemble

In the microcanonical ensemble, the system is isolated from its surroundings both in terms of energy and particle exchange, so it can only exist in microstates $\sigma$ with energy $\mathcal{H}(\sigma)=U$ and number of particles $\mathcal{N}(\sigma)=N$. Therefore, the measure on microstates will be the one that maximizes the Shannon entropy over those with support in $\Sigma^{\prime}=\{\sigma \in \Sigma: \mathcal{N}(\sigma)=N, \mathcal{H}(\sigma)=U\}$. By a classical result, the maximizer is the uniform measure:

Proposition 2.1. Let $X$ be a finite ground set, and let $\mu: X \longrightarrow[0,1]$ be a probability measure on $X$. Let $\mu^{\text {unif }}$ be the uniform probability measure on $X$ (i.e. $\mu^{\text {unif }}(x):=1 /|X|$ for all $x \in X$ ). Then,

$$
S(\mu) \leq S\left(\mu^{u n i f}\right)
$$

with equality if, and only if, $\mu=\mu^{u n i f}$.

Proof. First note that the function $f(x)=x \log x$, defined for all $x \geq 0$ (with $f(0):=0$ ), is strictly
convex, since $f^{\prime \prime}(x)=1 / x>0$ for all $x>0$. Then, by Jensen's inequality,

$$
\begin{aligned}
S(\mu) & =-\sum_{x \in X} \mu(x) \log \mu(x)=-\sum_{x \in X} f(\mu(X)) \leq \\
& \leq-|X| f\left(\frac{1}{|X|} \sum_{x \in X} \mu(x)\right)=-|X| f(1 /|X|)=S\left(\mu^{\mathrm{unif}}\right)
\end{aligned}
$$

As $f$ is strictly convex, the equality will only hold if all the averaged points are the same, that is, if $\mu(x)=1 /|X|$ for all $x \in X$.

Remark. As an aside, this property of the entropy is what allows it to be used as a tool in enumerative combinatorics. For any probability measure, its entropy will be at most $S\left(\mu^{\text {unif }}\right)=\log (|X|)$, so one can derive a lower bound on $|X|$ by computing the entropy of any probability measure on $X$. This is the idea behind the recent advances in the Union-Closed Conjecture (see Gil22]). For an accessible introduction to entropy techniques in combinatorics, see Gal14.

### 2.1.4 Canonical ensemble

In the canonical ensemble, we consider a system in contact with a thermal bath at constant temperature, so the energy is allowed to fluctuate (while keeping the average value $\mathbb{E}_{\mu}[\mathcal{H}]=U$ ). Thus, the measure that maximizes the entropy will be the solution to the following optimization problem:

$$
\begin{align*}
\operatorname{minimize} & \sum_{\sigma \in \Sigma} \mu(\sigma) \log \mu(\sigma) \\
\text { subject to } & \sum_{\sigma \in \Sigma} \mu(\sigma)=1  \tag{2.1}\\
& \sum_{\sigma \in \Sigma} \mu(\sigma) \mathcal{H}(\sigma)=U
\end{align*}
$$

Proposition 2.2. (Theorem 12.1.1 from CT05]) For any feasible $U$ (i.e. $\inf _{\sigma} \mathcal{H}(\sigma) \leq U \leq$ $\left.\sup _{\sigma} \mathcal{H}(\sigma)\right)$, the solution to 2.1 is given by

$$
\mu(\sigma)=\frac{1}{Z(\beta)} e^{-\beta \mathcal{H}(\sigma)}
$$

where $\beta \in \mathbb{R}$ is the only value that makes $\mathbb{E}_{\mu}[\mathcal{H}]=U$, and $Z(\beta):=\sum_{\sigma \in \Sigma} e^{-\beta \mathcal{H}(\sigma)}$ is the normalizing factor.

Proof. We solve 2.1 with the method of Lagrange multipliers. The Lagrange function is

$$
L(\mu)=\sum_{\sigma \in \Sigma} \mu(\sigma) \log \mu(\sigma)+\alpha\left(\sum_{\sigma \in \Sigma} \mu(\sigma)-1\right)+\beta\left(\sum_{\sigma \in \Sigma} \mu(\sigma) \mathcal{H}(\sigma)-U\right)
$$

At the optimum, $\nabla L=0$, so the derivative with respect to each $\mu(\sigma)$ has to be zero. This gives us the form of the distribution:

$$
\frac{\partial L}{\partial \mu(\sigma)}=\log \mu(\sigma)+1+\alpha+\beta \mathcal{H}(\sigma)=0 \Longrightarrow \mu(\sigma)=e^{-\beta \mathcal{H}(\sigma)} e^{-1-\alpha}
$$

By imposing that these all sum to 1 , we get the desired normalization factor, and by imposing that $\mathbb{E}_{\mu}[\mathcal{H}]=U$, we get the condition on $\beta$.

Proposition 2.2 implies that, when working with systems where the energy is allowed to fluctuate (but the number of particles is not), the probability of being on a certain microscopic state $\sigma \in \Sigma$ is proportional to $e^{-\beta \mathcal{H}(\sigma)}$, where $\beta \in \mathbb{R}$ is some constant value depending on the mean energy of the system. This is the motivation behind the definition of a Gibbs measure in the next section, which is supposed to model this behaviour for the case of an abstract spin model on a graph (not necessarily representative of any physical system).

### 2.2 Spin models on graphs

In the previous section we have assumed that the state space $\Sigma$ is finite. There are also statistical physics models that deal with a continuous state space, but usually one tries to discretize the problem so $\Sigma$ is finite, or at least countably infinite. This raises the question of how to translate a real-world problem, in which space and time are continuous, into a discrete representation.

The usual approach is to divide the space into a 3-dimensional lattice, with cells of negligible size. Then we can describe the positions of the particles by the cell that they are in (not caring about their specific position inside the cell). This immediately suggests defining a graph $G$ in which the vertices are the discretized cells, and there is an edge between two cells if they are close enough that a particle in one will interact noticeably with a particle in the other. These kind of models are expressed abstractly as spin models on graphs:

Definition 2.1 (Spin configuration). Given a graph $G$ and a finite set of spins $\Omega$, we define a configuration $\sigma \in \Omega^{V(G)}$ as an assignment of a spin from $\Omega$ to each vertex of the graph $G$. For simplicity of notation, we usually denote $\sigma(v)$ as $\sigma_{v}$.

Definition 2.2 (Spin model). Given a graph $G$ and a finite set of spins $\Omega$, we define a spin model on $G$ as a Hamiltonian $\mathcal{H}: \Omega^{V(G)} \longrightarrow \mathbb{R} \cup\{+\infty\}$ that assigns an energy to every spin configuration. We require that the Hamiltonian respects the structure of the graph, that is, that it takes the form

$$
\mathcal{H}(\sigma)=\sum_{v \in V(G)} f\left(\sigma_{v}\right)+\sum_{u v \in E(G)} g\left(\sigma_{u}, \sigma_{v}\right)
$$

for some functions $f: \Omega \longrightarrow \mathbb{R}$ and $g: \Omega \times \Omega \longrightarrow \mathbb{R} \cup\{+\infty\}$.

Remark. From a physical point of view, each spin represents the internal state of the particle on the cell. Then the function $g$ from the Hamiltonian measures the energy due to the interaction between particles in different cells (restricted only to the edges of $G$, as we consider negligible all other interactions), while function $f$ measures the energy added to the system by the internal state of the particle. Usually this latter effect is thought of as having an external field that interacts differently with each kind of spin (e.g. a magnetic field that interacts differently with each particle depending on the orientation of its magnetic dipolar moment).

Remark. This formalism can also be used to model systems with a variable number of particles. In this case, we choose as spin set $\Omega=\{0,1\}$, representing whether the cell is occupied or not by a particle. As the number of particles of the system can vary, in this case we should work with the grand canonical ensemble. Doing a very similar calculation to the one on the previous section, we find that the grand canonical ensemble induces the measure:

$$
\mu(\sigma) \propto e^{-\beta(\mathcal{H}(\sigma)+\nu N)}
$$

where $N$ is the number of particles and $\nu$ is a constant that can be identified with the chemical potential of the particle reservoir in contact with the system. For our purposes it will not matter whether we are working with the canonical or grand canonical ensemble, as we can define an auxiliary Hamiltonian $\tilde{\mathcal{H}}(\sigma):=\mathcal{H}(\sigma)+\mu N$, incorporating the $\mu N$ term into the $f$ function.

Definition 2.3 (Gibbs measure, partition function). Given a spin model on a graph $G$, defined by a Hamiltonian $\mathcal{H}$, and given a constant $\beta \in \mathbb{R}$, we define the Gibbs measure associated to the model with parameter $\beta$ as the probability measure on the space of $\operatorname{spin}$ configurations $\Omega^{V}$ given by

$$
\mu_{G, \beta}(\sigma):=\frac{1}{Z(\beta)} e^{-\beta \mathcal{H}(\sigma)}
$$

where $Z(\beta):=\sum_{\sigma \in \Omega^{V}} e^{-\beta \mathcal{H}(\sigma)}$, the so-called partition function, is the required normalization constant.

Definition 2.4 (Hard constraint). We say that a spin model on graphs has a hard constraint if there is some pair of spins $\omega, \tilde{\omega} \in \Omega$ such that $g(\omega, \tilde{\omega})=+\infty$.

Remark. For $\beta \in \mathbb{R}^{+}$, states with less energy are favored by $\mu_{G, \beta}$, so an infinite value of $g$ means that the interaction between spins $\omega$ and $\tilde{\omega}$ is so energetically unfavorable that it will occur with probability zero. This can be used to forbid certain structures in the spin configurations. For example, for $\Omega=\{1, \ldots, q\}$, we can model proper $q$-colorings of the graph by imposing a hardconstraint $g(i, i)=+\infty$ for all $i \in \Omega$. Then, configurations with a monochromatic edge will be given probability zero by $\mu_{G, \beta}$.

We will now introduce three examples of spin models in graphs. The Ising model is one of the most classical examples of a statistical physics model (as it is one of the simplest models with a phase
transition), while the hard-core model and the Potts model will be used extensively in the following chapters to study independent sets and colorings, respectively.

Example 2.1 (Ising model). The Ising model was proposed by Lenz in 1920 as a simplified model of ferromagnetism. In one dimension, one can imagine $n$ particles in a row, each with its magnetic dipole moment pointing either up or down (represented by spins +1 and -1 ). We assume that each particle only interacts with its two nearest neighbors, and that the interaction is ferromagnetic (that is, particles "tend" to have the same spin as their neighbors). Formally, this is modeled by taking $\beta>0$ and the Hamiltonian

$$
\mathcal{H}(\sigma)=\sum_{i=1}^{n-1}-\sigma_{i} \sigma_{i+1}
$$

so that the energy $\mathcal{H}(\sigma)$ is higher the more pairs of neighboring particles there are with different spin, and thus the probability of these configurations $\mu_{G, \beta}(\sigma) \propto e^{-\beta \mathcal{H}(\sigma)}$ is lower.

According to the formalism introduced earlier, this one-dimensional version corresponds to taking the graph $G=P_{n}$ (a path with $n$ vertices). Similarly, one can define a $d$-dimensional version of the Ising model by taking $G$ to be a $d$-dimensional lattice. In section 2.5 we will see how, for $d \geq 2$, the $d$-dimensional model has a very significant qualitative difference to the 1 -dimensional version, as it exhibits a phase transition.

Remark. From a combinatorics perspective, the Ising model can be thought of as a distribution on the cuts of the graph $G$ (by taking the vertices with spin +1 to be one side of the cut and the vertices with spin -1 to be the other). Then, each cut has weight proportional to $e^{-2 \beta|\partial E|}$, where $\partial E:=\left\{i j \in E: \sigma_{i} \neq \sigma_{j}\right\}$ is the set of edges that "cross" the cut.

By the same argument used in Proposition 2.2, one can show that the Gibbs distribution from the Ising model is the one that maximizes the entropy over all the distributions on the set of cuts of $G$ with a given expected number of crossing edges (actually, Theorem 12.1.1 from [CT05] is stated in more generality than Proposition 2.2 and can be applied to prove this directly).

Example 2.2 (Hard-core model). The hard-core model attempts to model the situation of having an ideal (i.e. non-interacting) gas with a variable number of particles in a lattice. The width and height of the cells of the lattice is chosen smaller than the radius of the particles, so that two particles in adjacent cells would overlap. Hence, the model imposes the restriction that no two neighboring cells can be occupied at the same time.

Under the previous formal framework, for a general graph $G$ (not necessarily a lattice), we define the hard-core model with spins $\Omega=\{0,1\}$ ( 1 corresponding to the vertex being occupied by a particle, and 0 to the vertex being unoccupied) and the Hamiltonian given by $f\left(\sigma_{v}\right)=-\sigma_{v}$, and $g(1,1)=+\infty, g(0,0)=g(0,1)=g(1,0)=0$.

Then, the probability of a certain spin assignment is

$$
\mu_{G, \beta}(\sigma) \propto e^{-\beta \mathcal{H}(\sigma)}=e^{\beta|V|_{1}} \mathbb{1}_{V \in \mathcal{I}(G)}
$$

where $V$ is the set of vertices with $\sigma_{v}=1$, and $\mathcal{I}(G)$ is the set of independent sets of the graph. The term $\mathbb{1}_{V \in \mathcal{I}(G)}$ comes from the hard constraint imposed by $g$, under the assumption that $\beta>0$.

Note that (restricting first $\mu$ only to the configurations that correspond to independent sets), the probability of a certain configuration only depends on the number of occupied vertices. The quantitative nature of the dependence is determined by the parameter $\lambda:=e^{\beta} \in \mathbb{R}^{+}$, usually called fugacity or activity. For $\lambda<1$, states with lower number of vertices will be more probable; while for $\lambda>1$, states with higher number of vertices are favored. For $\lambda=1, \mu$ corresponds to the uniform distribution on $\mathcal{I}(G)$.

Expressing everything in terms of the fugacity (and identifying spin configurations by the set of occupied vertices $I \in \mathcal{I}(G)$ ), the Gibbs measure of the hard-core model becomes

$$
\mu_{G, \lambda}(I)=\frac{1}{Z(\lambda)} \lambda^{|I|}
$$

with partition function

$$
Z(\lambda)=\sum_{I \in \mathcal{I}(G)} \lambda^{|I|}
$$

This partition function is known in combinatorics as the independence polynomial of the graph, and can be seen as the generating function of the sequence $\left\{i_{k}\right\}_{k}$, where $i_{k}$ is the number of independent sets of $G$ with $k$ vertices. Thus, one can obtain a lot of information about the independent sets of the graph by knowing $Z(\lambda)$. For instance, the independence number $\alpha(G)$ (i.e. the size of the biggest independence set of $G$ ) corresponds to the degree of $Z(\lambda)$, while the total number of independent sets of the graph is $Z(1)$.

The partition function of the hard-core model is also closely related to the probability generating function of $|I|$, where $I \sim \mu_{G, \lambda}$. Indeed, taking $P(t):=\operatorname{pgf}(|I|)$, we have that

$$
P(t)=\sum_{k \geq 0} \underbrace{i_{k}(G) \frac{\lambda^{k}}{Z(\lambda)}}_{\operatorname{Pr}[|I|=k]} t^{k}=\frac{Z(\lambda t)}{Z(\lambda)}
$$

Example 2.3 (Potts model). The Potts model is a generalization of the Ising model to more than 2 spins. It is defined by the set of spins $\Omega=\{1, \ldots, q\}$, for some $q>2$, and the Hamiltonian

$$
\mathcal{H}(\sigma)=-\sum_{u v \in E} \mathbb{1}_{\sigma_{u}=\sigma_{v}}=-M_{G}(\sigma)
$$

where $M_{G}(\sigma)$ is the number of monochromatic edges under the spin assignment $\sigma$. In graph theory the concept of assigning an integer to each vertex is known as coloring, so in this model we will refer to spins as colors and we will say that edges that have the same spin on both endpoints are monochromatic. This Hamiltonian induces the Gibbs measure

$$
\mu_{G, \beta}(\sigma)=\frac{1}{Z(\beta)} e^{\beta M_{G}(\sigma)}
$$

where $Z(\beta)=\sum_{\sigma} e^{\beta M_{G}(\sigma)}$.
Often in graph theory one is interested in proper colorings, i.e. colorings with no monochromatic edges. We can force $\mu$ to be only supported on proper colorings by imposing a hard constraint on $g$. In this case, we will also introduce a fugacity $\lambda_{i}$ for each color $i \in[q]$, so the Gibbs measure ends up being

$$
\mu_{G, \boldsymbol{\lambda}}(\sigma)=\frac{1}{Z(\boldsymbol{\lambda})}\left(\prod_{v \in V} \lambda_{\sigma_{v}}\right) \prod_{u v \in E} \mathbb{1}_{\sigma_{u} \neq \sigma_{v}}
$$

where $\boldsymbol{\lambda}=\left(\lambda_{1}, \ldots, \lambda_{q}\right)$ is the vector of fugacities of the colors.
Note that, if we take $\lambda_{1}=\cdots=\lambda_{q}=: \lambda \in \mathbb{R}$, each proper coloring is weighted by the same factor $\lambda^{n}$, so the distribution is uniform over all proper colorings. Taking a different fugacity for each color allows us to break the symmetry, prioritizing the colorings that have more occurrences of the colors with greater $\lambda_{i}$.

### 2.3 Cumulants and joint cumulants

We will see that from the partition function we can recover very easily the cumulants of the random variable $\mathcal{H}(\sigma)$. Let us first introduce the necessary definitions:

Definition 2.5 (cumulant generating function, $n$-th order cumulant). Let $X$ be a random variable with finite moments. We define the cumulant generating function $K_{X}(t):=\log \mathbb{E}\left[e^{t X}\right]$ as the logarithm of the moment generating function. If $K_{X}(t)$ is analytic at $t=0$, we then define the $n$ - $t h$ order cumulant of $X$ as the $n$-th coefficient in the Taylor series of $K_{X}$ around $0: \kappa_{n}(X):=K_{X}^{(n)}(0)$.

Note that the cumulant generating function receives its name because it is the exponential generating function of the cumulants $\left\{\kappa_{n}(X)\right\}_{n \geq 1}$ :

$$
K_{X}(t)=\sum_{n \geq 1} \kappa_{n}(X) \frac{t^{n}}{n!}
$$

(there is no independent term because $K_{X}(0)=0$ from its definition).
The cumulants can be seen as analogues to the moments, as $\kappa_{1}(X)=\mathbb{E}[X], \kappa_{2}(X)=\operatorname{Var}[X]$,
and $\kappa_{3}(X)$ is the third central moment. From then on the cumulants do not exactly coincide with moments, though we can still express ones in function of the others. We are going to use the following two properties of the cumulants:

Proposition 2.3. The $n$-th order cumulant is an homogeneous function of degree $n$, i.e. $\kappa_{n}(\lambda X)=$ $\lambda^{n} \kappa_{n}(X)$, for any $\lambda \in \mathbb{R}$.

Proof. Let $g(t)=\lambda t$. By definition,

$$
K_{\lambda X}(t)=\log \mathbb{E}\left[e^{t \lambda X}\right]=K_{X}(\lambda t)=K_{X}(g(t))
$$

Thus, each derivative of $K_{\lambda X}(t)$ brings out a constant $\lambda$ factor, corresponding to $g^{\prime}(t)$. Hence,

$$
K_{\lambda X}^{(n)}(t)=\lambda^{n} K_{X}(\lambda t)
$$

so $\kappa_{n}(\lambda X)=\lambda^{n} \kappa_{n}(X)$.
Proposition 2.4. Let $X$ be a random variable with $\mathbb{E}[X], \mathbb{E}\left[X^{2}\right]<\infty$. Then, $X$ follows a normal distribution if, and only if, $\kappa_{n}(X)=0$ for all $n \geq 3$.

Proof.
$(\Longrightarrow)$ The forward direction is by direct computation. For $X \sim N\left(\mu, \sigma^{2}\right)$, the moment generating function is

$$
\mathbb{E}\left[e^{t X}\right]=\int_{-\infty}^{+\infty} e^{t x} \frac{1}{\sqrt{2 \pi} \sigma} e^{-(x-\mu)^{2} / 2 \sigma^{2}} d x
$$

We rewrite the exponent to get rid of the linear term in $x$ :

$$
t x-\frac{(x-\mu)^{2}}{2 \sigma^{2}}=t(x-\mu)-\frac{(x-\mu)^{2}}{2 \sigma^{2}}+t \mu=-\left(\frac{x-\mu}{\sqrt{2} \sigma}+\frac{t \sigma}{\sqrt{2}}\right)^{2}+\frac{t^{2} \sigma^{2}}{2}+t \mu
$$

Therefore, we can transform this integral into a Gaussian integral by doing the change of variable $y \leftarrow x-\mu+t \sigma^{2}$, giving

$$
\mathbb{E}\left[e^{t X}\right]=\frac{1}{\sqrt{2 \pi} \sigma} \int_{-\infty}^{+\infty} e^{\mu t+\frac{1}{2} \sigma^{2} t^{2}} e^{-y^{2} / 2 \sigma^{2}} d y=\frac{1}{\sqrt{2 \pi} \sigma} e^{\mu t+\frac{1}{2} \sigma^{2} t^{2}} \sqrt{2 \pi} \sigma=e^{\mu t+\frac{1}{2} \sigma^{2} t^{2}}
$$

Then the cumulant generating function is $K_{X}(t)=\mu t+\frac{1}{2} \sigma^{2} t^{2}$, so the cumulants of order $n \geq 3$ vanish.
$(\Longleftarrow)$ In general the distribution of a random variable might not be uniquely determined by its moments or cumulants. However, uniqueness is guaranteed as long as the moment generating function does not blow up around $t=0$ :

Theorem 2.5 (Theorem 30.1 from [Bil95]). Let $X$ be a random variable whose moment generating function $\mathbb{E}\left[e^{t X}\right]$ has a positive radius of convergence around the point $t=0$. Then, the distribution of $X$ is uniquely determined.

In our case, we have a random variable $X$ with $\kappa_{n}(X)=0$ for $n \geq 3$ and $\kappa_{1}(X), \kappa_{2}(X)<\infty$ (due to the fact that $\kappa_{1}(X)=\mathbb{E}[X]$ and $\left.\kappa_{2}(X)=\mathbb{E}\left[X^{2}\right]-\mathbb{E}[X]^{2}\right)$. Then, the moment generating function is $\mathbb{E}\left[e^{t X}\right]=e^{\kappa_{1}(X) t+\frac{1}{2} \kappa_{2}(X) t^{2}}$, which is analytic at $t=0$. Therefore, by the previous theorem the distribution of $X$ is uniquely determined (and so $X$ follows a normal distribution with mean $\kappa_{1}(X)$ and variance $\kappa_{2}(X)$ ).

Remark. The backwards implication from Proposition 2.4 admits an strengthening due to Marcinkiewicz:
Theorem 2.6 (Theorem 2-bis from Mar39]). Let $X$ be a random variable. If there exists an $r \in \mathbb{Z}^{+}$ such that $\log \mathbb{E}\left[e^{t X}\right]=a_{1} t+\cdots+a_{r} t^{r}$ for some $a_{1}, \ldots, a_{r} \in \mathbb{R}$, then $r \leq 2$.

This relaxes the condition from Proposition 2.4. we no longer need to prove that $\kappa_{n}(X)=0$ for all $n \geq 3$, we have enough with proving it for all but a finite number of values of $n$.

Due to the particular form of Gibbs measures, we are able to obtain a lot of information about the distribution from just the partition function. In particular, we can recover the expected value, variance and higher-order cumulants of $\mathcal{H}$ by taking successive derivatives of $\log Z(\beta)$ with respect to $\beta$ :

Proposition 2.7. For $k \geq 1$, we can recover the $k$-th order cumulant of $\mathcal{H}$ as

$$
\kappa_{k}(\mathcal{H})=(-1)^{k} \frac{d^{k}}{d \beta^{k}} \log Z(\beta)
$$

Proof. Notice that we can express the moment generating function of $\mathcal{H}$ as

$$
\mathbb{E}\left[e^{t \mathcal{H}}\right]=\sum_{\sigma} \frac{e^{-\beta \mathcal{H}(\sigma)}}{Z(\beta)} e^{t \mathcal{H}(\sigma)}=\frac{Z(\beta-t)}{Z(\beta)}
$$

Thus, the cumulant generating function is $K_{\mathcal{H}}(t)=\log Z(\beta-t)-\log Z(\beta)$ and the $k$-th order cumulant takes the value

$$
\kappa_{k}(\mathcal{H})=\left.\frac{d^{k}}{d t^{k}}(\log Z(\beta-t)-\log Z(\beta))\right|_{t=0}=(-1)^{k}(\log Z)^{(k)}(\beta)
$$

provided that $k \geq 1$.
This last proposition is very useful because in many models $\mathcal{H}$ is related to the size of a certain structure in the graph (e.g. size of an independent set for the hard-core model or number of
monochromatic edges for the Potts model), so knowing probabilistic information about $\mathcal{H}$ allows us to prove structural graph theory results.

Even if we are only interested in the univariate partition function $Z(\beta)$, it is often useful to define a multivariate version:

Definition 2.6 (Multivariate partition function). Given a partition function $Z(\lambda)$, we define the corresponding multivariate partition function as

$$
Z(\lambda, t):=\sum_{\sigma} e^{-\beta \mathcal{H}(\sigma)} \prod_{v \in V} e^{t_{v} \sigma_{v}}
$$

Note that we can recover the original partition function by taking $\mathbf{t}=\mathbf{0}$.
We say that the vector $\mathbf{t}$ corresponds to the external field, that favors positive or negative spins (depending on its sign). If $\mathbf{t}=(t, \ldots, t)$ for some $t \in \mathbb{R}$, we say that the external field is uniform, i.e. that it acts on the same way in each vertex.

Remark. In section 2.5 we will see that the partial derivatives of the multivariate partition function with respect to the external fields give the correlation between the marginals of different vertices.

### 2.4 Temperature and energy/entropy trade-off

As we are dealing with spin models in an abstract way, we have not yet assigned any meaning to the parameter $\beta$. From the physics perspective, $\beta$ represents a constant inversely proportional to the temperature of the system ( $\beta=1 / k T$, where $k$ is the Boltzmann constant). We will not define formally what the temperature means, as this lies outside the scope of our work, but the analogy of $\beta$ with the inverse of the temperature can be used to give some intuition about the effect of $\beta$ to the properties of the Gibbs distribution.

Recall that the Gibbs measure of a configuration $\sigma$ is proportional to $e^{-\beta \mathcal{H}(\sigma)}$, where the Hamiltonian $\mathcal{H}(\sigma)$ measures the energy of $\sigma$. Then, as $\beta$ grows, configurations with lower energy are favored, until at the limit $\beta \rightarrow \infty$ we have that $\mu_{G, \beta}$ is only supported on the configurations that minimize the energy. We call these configurations the ground states (in contraposition to excited states, which are states in which the energy of the system is bigger than the minimum possible energy).

In contrast, when $\beta$ gets smaller, the energy of a configuration becomes less relevant, until at $\beta=0$ we have that all states are equally probable, regardless of their energy ${ }^{2}$ Then, the probability of a certain macroscopic event only depends on the number of microscopic configurations that are compatible with the macroscopic event (which is related to the entropy).

For a constant $0<\beta<+\infty$, we have a trade-off between the energetic and the entropic effects.

[^1]As an example, consider the hard-core model from example 2.2. There we associate configurations with independent sets $I \in \mathcal{I}(G)$ and the energy of a configuration is given by $\mathcal{H}(I):=-|I|$, so $\mu_{G, \lambda}(I) \propto \lambda^{|I|}$, where $\lambda:=e^{\beta}$. Consider the macroscopic event " $|I|=k$ ". For $\beta \rightarrow \infty$, we have that the probability of this event only depends on whether $k$ is the maximum size of an independent set (i.e. the minimum energy):

$$
\left.\operatorname{Pr}[|I|=k]\right|_{\lambda=+\infty}= \begin{cases}1, & \text { if } k=\alpha(G) \\ 0, & \text { if } k \neq \alpha(G)\end{cases}
$$

On the other hand, if $\beta=0$, the probability of the event " $|I|=k$ " depends on the number of independent sets with $|I|=k$ (i.e. the entropy):

$$
\left.\operatorname{Pr}[|I|=k]\right|_{\lambda=1}=\frac{i_{k}(G)}{|\mathcal{I}(G)|}
$$

For $\beta$ positive but finite, we have the aforementioned trade-off:

$$
\operatorname{Pr}[|I|=k] \propto i_{k}(G) \cdot \lambda^{k}
$$

where $i_{k}(G)$ is the contribution of the entropy and $\lambda^{k}$ is the contribution of the energy.
From a combinatorics perspective, the case with $\beta \rightarrow \infty$ corresponds to the extremal object (the object that minimizes the energy), while the case with $\beta=0$ corresponds to an object drawn uniformly at random. For $0<\beta<+\infty$ we interpolate between randomness and optimization.

### 2.5 Phase transitions

One of the fundamental themes of statistical physics is how the qualitative behaviour of the extreme cases $\beta=0$ and $\beta=+\infty$ persists as long as $\beta$ is small enough or large enough. In some models, there are specific values of $\beta$ for which the qualitative behaviour of the model changes drastically (i.e. the model changes from behaving like the $\beta=0$ case to behaving like the $\beta=+\infty$ case). This is what is known as phase transition.

### 2.5.1 Marginals and correlation

In order to formally define phase transitions, we have to introduce the notion of correlation between vertices. We will define everything for the hard-core model but it can be easily extended to other 2-spin systems $3^{3}$

Definition 2.7 (marginal probability). Given a vertex $v \in G$, we define the marginal probability

[^2]of $v$ as $\mu_{v}:=\operatorname{Pr}\left[\sigma_{v}=1\right]$ (that is, probability that vertex $v$ is occupied). Similarly, for a subset of vertices $S \subseteq V$, we define the joint marginal $\mu_{S}:=\operatorname{Pr}\left[\bigcap_{v \in S}\left(\sigma_{v}=1\right)\right]$ (also called $k$-point correlation function, where $k:=|S|)$.

Definition 2.8 (truncated 2-point correlation function). For a pair of vertices $u, v \in V$, we define their truncated 2-point correlation function as $\kappa(u, v):=\mu_{u, v}-\mu_{u} \mu_{v}$ (i.e. the usual covariance between $\sigma_{u}$ and $\sigma_{v}$, understood as indicator random variables).

Here truncated refers to the fact that we are substracting $\mu_{u} \mu_{v}$ to it, so $\kappa(u, v)=0$ if $\sigma_{u}$ and $\sigma_{v}$ are uncorrelated.

To generalize the notion of correlation to more than 2 spins, we observe that we can characterize it in terms of derivatives of the multivariate partition function with respect to the external field:

Proposition 2.8. For a given vertex $v \in V$,

$$
\mu_{v}=\left.\frac{\partial}{\partial t_{v}} \log Z(\lambda, \mathbf{t})\right|_{\mathbf{t}=0}
$$

and for a given pair of vertices $u, v \in V$,

$$
\kappa(u, v)=\left.\frac{\partial^{2}}{\partial t_{u} \partial t_{v}} \log Z(\lambda, \mathbf{t})\right|_{\mathbf{t}=0}
$$

Proof. The proof follows from direct computation. The first derivative is:

$$
\frac{\partial}{\partial t_{v}} \log Z(\lambda, \mathbf{t})=\frac{1}{Z(\lambda, \mathbf{t})} \frac{\partial}{\partial t_{v}} \sum_{I \in \mathcal{I}(G)} \lambda^{|I|} \prod_{v \in V} e^{t_{v}}=\frac{1}{Z(\lambda, \mathbf{t})} \sum_{\substack{I \in \mathcal{I}(G) \\ I \ni v}} \lambda^{|I|} \prod_{v \in V} e^{t_{v}}
$$

so taking $\mathbf{t}=\mathbf{0}$ we get

$$
\left.\frac{\partial}{\partial t_{v}} \log Z(\lambda, \mathbf{t})\right|_{\mathbf{t}=\mathbf{0}}=\frac{1}{Z(\lambda)} \sum_{\substack{I \in \mathcal{I}(G) \\ I \ni v}} \lambda^{|I|}=\operatorname{Pr}[v \in I]
$$

Deriving a second time (and using the previous result) we obtain

$$
\begin{aligned}
\left.\frac{\partial}{\partial t_{u}}\left(\frac{1}{Z(\lambda, \mathbf{t})} \frac{\partial}{\partial t_{v}} Z(\lambda, \mathbf{t})\right)\right|_{\mathbf{t}=\mathbf{0}} & =\left.\frac{\frac{\partial^{2}}{\partial t_{u} \partial t_{v}} Z(\lambda, \mathbf{t}) \cdot Z(\lambda, \mathbf{t})-\frac{\partial}{\partial t_{u}} Z(\lambda, \mathbf{t}) \frac{\partial}{\partial t_{v}} Z(\lambda, \mathbf{t})}{Z(\lambda, \mathbf{t})^{2}}\right|_{\mathbf{t}=\mathbf{0}}= \\
& =\left(\frac{1}{Z(\lambda)} \sum_{\substack{I \in \mathcal{I}(G) \\
u, v \in I}} \lambda^{|I|}\right)-\left(\left.\left.\frac{1}{Z(\lambda)} \frac{\partial}{\partial t_{u}} Z(\lambda, \mathbf{t})\right|_{\mathbf{t}=\mathbf{0}} \cdot \frac{1}{Z(\lambda)} \frac{\partial}{\partial t_{v}} Z(\lambda, \mathbf{t})\right|_{\mathbf{t}=\mathbf{0}}\right)= \\
& =\operatorname{Pr}[u, v \in I]-\operatorname{Pr}[u \in I] \cdot \operatorname{Pr}[v \in I]=\kappa(u, v)
\end{aligned}
$$

Inspired by this last proposition, we can generalize the notion of correlation to more than 2 vertices:
Definition 2.9 (truncated $k$-point correlation function). Given $k$ vertices $v_{1}, \ldots, v_{k}$, we define their truncated $k$-point correlation function $\kappa\left(v_{1}, \ldots, v_{k}\right)$ as

$$
\kappa\left(v_{1}, \ldots, v_{k}\right):=\left.\frac{\partial}{\partial t_{v_{1}} \cdots \partial t_{v_{k}}} \log Z(\lambda, \mathbf{t})\right|_{\mathbf{t}=\mathbf{0}}
$$

Remark. The definition of truncated $k$-point correlation function is analogous to how one defines the joint cumulants of a random vector by taking derivatives on the joint cumulant generating function $K_{X_{1}, \ldots, X_{k}}(\mathbf{t}):=\log \mathbb{E}\left[e^{t_{1} X_{1}+\cdots+t_{k} X_{k}}\right]$.

### 2.5.2 Correlation decay

Informally speaking, we say that a model exhibits correlation decay if, for any vertex $v$, knowing the spin of a vertex far from $v$ does not give us much information about the spin of $v$. We can define it more rigorously using the 2-point correlation function:

Definition 2.10 (exponential decay of 2-point correlations). Let $\mathcal{G}$ be an infinite family of graphs. Let $\left\{\mu_{G}\right\}_{G \in \mathcal{G}}$ be a collection of Gibbs measures, one for each graph in $\mathcal{G}$. We say that these exhibit exponential decay of correlations if there exist constants $A, B>0$ such that

$$
|\kappa(u, v)| \leq A e^{-B \cdot \operatorname{dist}(u, v)}
$$

for all $G \in \mathcal{G}$ and for all $u, v \in V(G)$.
Remark. Though we have stated it in more generality, we are usually dealing with a family of graphs $\mathcal{G}=\left\{G_{n}\right\}_{n \in \mathbb{N}}$, where each $G_{n}$ has $n$ vertices. Thus, if we choose a pair of vertices $u_{n}, v_{n} \in G_{n}$ such that $\operatorname{dist}\left(u_{n}, v_{n}\right) \rightarrow \infty$ as $n \rightarrow \infty$, we have that the 2 -point correlation $\kappa\left(u_{n}, v_{n}\right)$ decays exponentially fast (with respect to $\operatorname{dist}\left(u_{n}, v_{n}\right)$ ) as $n \rightarrow \infty$.

Notice that for $\beta=0$ the spin of each vertex is independent, so $\kappa(u, v)=0$ for any $u, v \in V$. Hence, correlation decay is trivial for $\beta=0$. In most models, this behaviour still persists if we take $\beta$ small enough, as the dependence between vertices is still "small". This is a common theme in probabilistic combinatorics: a group of correlated variables still exhibit some of the properties of independent variables as long as their dependence is quantifiably "small" (for example, if they only depend on a small subset of other variables, in Local Lemma style).

For some models the correlation decay persists for all $\beta \in \mathbb{R}^{+}$:
Example 2.4. The hard-core model on the family of paths $\mathcal{G}=\left\{P_{n}\right\}_{n \geq 1}$ exhibits correlation decay for all possible values of $\lambda$.

Example 2.5. The one-dimensional Ising model (i.e. the Ising model on the family of paths $\left.\mathcal{G}=\left\{P_{n}\right\}_{n \geq 1}\right)$ exhibits correlation decay for all possible values of $\beta$.

For other models, however, there exists a threshold on $\beta$ beyond which correlation decay no longer holds. This is what is known as a phase transition:

Definition 2.11 (phase transition). We say that a spin model on a certain family of graphs $\mathcal{G}$ exhibits a phase transition if there exists a critical value $\beta_{c}$ such that the model exhibits correlation decay for $\beta<\beta_{c}$ but it does not for $\beta>\beta_{c}$.

In the next two sections we will see two alternative characterizations of phase transitions: the first given by the analyticity of the limit of the free energy, and the second given by the uniqueness of the Gibbs measure on the infinite lattice.

### 2.5.3 Analyticity of free energy

Definition 2.12 (infinite volume pressure / free energy). Let $\mathcal{G}=\left\{G_{n}\right\}_{n \geq 1}$ be a family of graphs, where each $G_{n}$ has $n$ vertices. We define the free energy (per unit volume) or volume pressure as the function of $\beta$ given by the point-wise limit

$$
f(\beta):=\lim _{n \rightarrow \infty} \frac{1}{n} \log Z_{G_{n}}(\beta)
$$

Remark. The free energy is only well-defined when the above limit exists.
The free energy gives us a different way to formalize the notion of phase transition:
Definition 2.13 (phase transition, order of the phase transition). We say that a model exhibits a phase transition if there exists a critical value $\beta_{c}$ such that the free energy $f(\beta)$ is not analytic at $\beta_{c}$.
We define the order of the phase transition as the lowest derivative that is not continuous. For example, we say that the phase transition is of the first order if $f^{\prime}$ is discontinuous at $\beta_{c}$, and we say that the phase transition is of the second order if $f^{\prime}$ is continuous but $f^{\prime \prime}$ is not. In the case that $f \in \mathcal{C}^{\infty}$ but it is not analytic, we say that the phase transition is of infinite order.

Remark. This definition of phase transition is not always equivalent to the one based on correlation decay (though there exist some conditions such that one implies the other).

Example 2.6 (Hard-core model on paths). Consider the hard-core model on the family of paths $\mathcal{G}=\left\{P_{n}\right\}_{n \geq 1}$. We have previously stated that this model exhibits no phase transition. Let us show it (we will use the free energy characterization, but in this model the correlation decay characterization also holds):

Proposition 2.9. The infinite volume free density of the hard-core model on the family of paths $\mathcal{G}=\left\{P_{n}\right\}_{n \geq 1}$ is

$$
f(\lambda)=\frac{1+\sqrt{1+4 \lambda}}{2}
$$

Remark. Note that for $Z_{P_{n}}(1)$ is the number of independent sets on a path of $n$ vertices, which is the $n$-th Fibonacci number $F_{n}$ (starting with $F_{0}=F_{1}=1$ ). We know $F_{n}=\Theta\left(\phi^{n}\right)$, for $\phi:=(1+\sqrt{5}) / 2$, so $f(1)=\log F_{n} / n=\phi$, which is indeed the result we recover taking $\lambda=1$ in the previous formula. This connection is not surprising, since the partition function of the hard-core model on a path follows the same recurrence as Fibonacci's sequence for $\lambda=1$.

Proof. The key is that the partition function follows the recurrence

$$
Z_{P_{n}}(\lambda)=Z_{P_{n-1}}(\lambda)+\lambda Z_{P_{n-2}}(\lambda)
$$

That's because every independent set on $P_{n}$ can either contain vertex $n$ (in which case it can be though of as an independent set of $P_{n-2}$ which the extra weight of $\lambda$ given by vertex $n$ ), or it can not contain vertex $n$ (so we are left with an independent set of $P_{n-1}$ ).
Once we have this linear recurrence, we find the roots of the characteristic polynomial $x^{2}-x-\lambda$, which are

$$
\alpha_{1,2}=\frac{1 \pm \sqrt{1+4 \lambda}}{2}
$$

and then we know that we can express the general term as $Z_{P_{n}}(\lambda)=A \alpha_{1}^{n}+B \alpha_{2}^{n}$, for some constants $A, B>0$. The hard-core model is restricted to $\lambda \geq 0$, so we know that both roots are well-defined and that $\left|\alpha_{1}\right|>\left|\alpha_{2}\right|$, so in the limit the dominant term will be the one with $\alpha_{1}$ :

$$
f(\lambda)=\lim _{n \rightarrow \infty} \frac{1}{n} \log Z_{P_{n}}(\lambda)=\lim _{n \rightarrow \infty} \frac{1}{n} \log \left(A \alpha_{1}^{n}+B \alpha_{2}^{n}\right)=\alpha_{1}
$$

Corollary 2.9.1. The hard-core model on $\mathcal{G}=\left\{P_{n}\right\}_{n \geq 1}$ has no phase transition (in the sense of definition 2.13).

Proof. From the expression found above, we know $f(\lambda)$ is analytic for any $\lambda \geq 0$, so the model does not have any phase transition.

### 2.5.4 Infinite volume measures

Phase transitions only occur when we are dealing with infinite graphs, but we have only defined the notion of spin model for a finite graph. Thus, we want to find a good notion of limit for a sequence of spin models on growing subgraphs of an infinite graph. In particular, we fix a dimension $d$, and let $\Lambda_{n} \subset \mathbb{Z}^{d}$ be a box with sides of length $n$ in the infinite $d$-dimensional lattice. We want to define a notion of "infinite spin model" in $\mathbb{Z}^{d}$ such that the properties of the spin models on $\Lambda_{n}$ tend to the properties of the infinite spin model. Concretely, we would like that any local function (i.e. a
function that only depends on the spin of a finite number of vertices) has a well-defined limit when $n \rightarrow \infty$.

For a fixed $n$, the vertices on the boundary of $\Lambda_{n}$ have neighbors in $\mathbb{Z}^{d}$ that are not in $\Lambda_{n}$. If we just consider the spin model on $\Lambda_{n}$ on itself, forgetting about the fact that it is a subgraph of $\mathbb{Z}^{d}$, then that is equivalent to fixing the spin of the vertices from $Z^{d} \backslash \Lambda_{n}$ to not affect $\Lambda_{n}$ (for example, fix them to be unoccupied for the hard-core model). However, this decision is in some sense arbitrary, so we will consider more general boundary conditions, in which the vertices outside of $\Lambda_{n}$ that have some neighbor in $\Lambda_{n}$ are assigned some fixed spin from $\Omega$ (not necessarily the same for all of them).

For a finite $n$, the choice of boundary conditions will affect the marginals of the vertices inside $\Lambda_{n}$. However, one might hope that this effect fades as $n$ grows, so that any local function converges to a limit that does not depend on the boundary conditions.

This turns out to not be true in general, which leads us to our last characterization of phase transition:

Definition 2.14 (phase transition). We say that a spin model defined on $\mathcal{G}=\left\{\Lambda_{n}\right\}_{n \geq 1}$ (where $\Lambda_{n} \subset \mathbb{Z}^{d}$ is a cube with sides of length $n$ inside the $d$-dimensional infinite lattice) exhibits a phase transition if there exists a critical $\beta_{c}$ such that for $\beta<\beta_{c}$ there is a unique Gibbs measure on $\mathbb{Z}^{d}$ compatible with the measures on $\left\{\Lambda_{n}\right\}_{n \geq 1}$, while for $\beta>\beta_{c}$ there exist more than one (stemming from the choice of different boundary conditions in $\left\{\Lambda_{n}\right\}_{n \geq 1}$ ).

Remark. This definition can be extended to more general sequences of graphs $\mathcal{G}=\left\{G_{n}\right\}_{n \geq 1}$ as long as they satisfy that

- they are increasing: $G_{n} \subseteq G_{n+1}$
- they cover the whole lattice: $\bigcup_{n \geq 1} G_{n}=\mathbb{Z}^{d}$
- the number of vertices on the boundary is a vanishing fraction of the total: $\left|\partial G_{n}\right| /\left|G_{n}\right| \rightarrow 0$

Remark. We have not explained how to define Gibbs measures on infinite graphs such as $\mathbb{Z}^{d}$, or what does it mean for one such measure to be compatible with the Gibbs measures on $\left\{\Lambda_{n}\right\}_{n \geq 1}$. For a more complete explanation one can consult chapter 6 of [FV17], which approaches the subject from an extremely rigorous viewpoint, introducing a framework by Dobrushin, Lanford and Ruelle that is necessary to define infinite volume measures formally.

Example 2.7 (Ising model). We have already mentioned that the Ising model in 1 dimension exhibits no phase transition. That means that, for finite $\beta$, imposing a certain spin on the ends of a path does not affect the marginals of the vertices from the middle of the path, in the limit as the length of the path tends to infinity.

On the other hand, the Ising model in 2 dimensions does have a phase transition. In particular, one can prove that the boundary conditions with all boundary spins +1 or all boundary spins -1 induce
two different infinite volume measures on $\mathbb{Z}^{2}$, for $\beta>\beta_{c}:=\frac{1}{2} \log (1+\sqrt{2})$. This can be proven either with the explicit solution of the model given by Onsager, or without any explicit computation of the pressure as described in chapter 3 of [FV17].

## Chapter 3

## Approximate sampling and counting

### 3.1 Sampling and counting on spin models

Given a set of combinatorial objects $S$, two very natural problems are counting (i.e. computing the size of $S$ ) and uniform sampling (i.e. giving an algorithm that outputs a $X \sim \operatorname{Unif}(S)$ ). When the elements of $S$ are equipped with a weight $w: S \longrightarrow \mathbb{R}^{\geq 0}$, one can define the weighted version of these two problems: weighted counting becomes computing the sum of weights $\sum_{x \in S} w(x)$, and weighted sampling is defined as giving an algorithm that outputs a $X \sim \mu_{S}$, where $\mu_{S}(x):=$ $w(x) / \sum_{y \in S} w(y)^{1}$.

In the case of a spin model in a graph $G$, with a fixed inverse temperature $\beta$, the problem of weighted counting is akin to computing the partition function $Z_{G}(\beta)$, while the problem of weighted sampling consists on giving an algorithm that outputs a $X \sim \mu_{G, \beta}$.

Unless we restrict ourselves to very specific spin models (or very specific classes of graphs), both exact counting and sampling seem computationally intractable. Indeed, computing exactly $Z_{G}(\beta)$ is already \#P-hard for the Ising model (unless the values of $\beta$ and the external field satisfy a certain algebraic relation), as a consequence of Theorem 1.1 from [BG05], and this was generalized for spin models with arbitrary complex parameters by [CCL13]. For the case of the hard-core model, we know that the problem of counting independent sets of a general graph $G$ is \#P-complete, which is equivalent to computing $Z_{G}(1)$.

Remark. The \#P complexity class is defined as the problems that consist on counting the solutions to an NP problem (more formally, computing the number of accepting paths of a non-deterministic polynomial-time Turing machine). However, \#P is believed to be much more powerful than its decisional counterpart, because Toda's Theorem states that one can solve any problem from the polynomial hierarchy with only polynomially-many queries to a \#P oracle, and the polynomial hierarchy is believed to contain strictly NP.

[^3]Even if exact counting and sampling is hard in general, one hopes that we can still find approximate solutions to both problems. In general, the two notions of approximate counting algorithms that we use are the following:

Definition 3.1 (FPTAS). A FPTAS (or fully polynomial-time approximation scheme) is an algorithm that takes as an input an instance of a counting problem together with an $\varepsilon>0$ and outputs an $\varepsilon$-relative approximation of the solution in time polynomial in $n$ (the size of the input) and $1 / \varepsilon$.

Definition 3.2 (FPRAS). A FPRAS (or fully polynomial-time randomized approximation scheme) is a randomized algorithm that takes as an input an instance of a counting problem together with an $\varepsilon>0$ and outputs with probability $2 / 3$ an $\varepsilon$-relative approximation of the solution in time polynomial in $n$ and $1 / \varepsilon$.

Remark. The term fully-polynomial refers to the fact that the algorithm must be not just polynomial in the size of the input $n$, but also in the inverse error $1 / \varepsilon$. Other sources define FPTAS and FPRAS so that the time dependence on the error is restricted to poly $(\log (1 / \varepsilon))$ instead of poly $(1 / \varepsilon)$.

The constant $2 / 3$ in the definition of FPRAS is arbitrary, as the probability of success can be boosted to $1-\delta$ by repeating the algorithm $\mathcal{O}(\log (1 / \delta))$ times and taking the median of the outputs:

Lemma 3.1. Given $a \delta>0$ and a FPRAS that fails with probability at most $1 / 2-c$, for some $0<c<1 / 2$, one can construct a randomized algorithm that calls the FPRAS $\mathcal{O}(\log (1 / \delta))$ times and has probability of failure lower than $\delta$.

Proof. Let $c_{1}, \ldots, c_{t}$ be the outputs obtained by calling the FPRAS $t$ times, for some odd $t$ to be determined. Without loss of generality, suppose $c_{1} \leq \cdots \leq c_{t}$. Let $X_{i}$ be the indicator variable that $c_{i}$ constitutes a valid approximation to the correct answer $\hat{c}$. Note that the $X_{i}$ that take value 1 are consecutive, so the median of the $\left\{c_{i}\right\}_{i=1}^{t}$ will be guaranteed to be a valid approximation as long as $\sum X_{i}>t / 2$. By definition, each $X_{i}$ dominates a $\operatorname{Ber}(1 / 2+c)$, and the $X_{i}$ are mutually independent, so $\sum X_{i}$ dominates a $X \sim \operatorname{Bin}(t, 1 / 2+c)$. Hence,

$$
\operatorname{Pr}\left[\sum X_{i} \leq t / 2\right] \leq \operatorname{Pr}[X \leq t / 2] \leq \operatorname{Pr}[X \leq \mathbb{E}[X](1-c)]<e^{-2 c^{2} \mathbb{E}[X]^{2} / t}<e^{-2 c^{2}(1 / 2)^{2} t}=e^{-c^{2} t / 2}
$$

where we have used Hoeffding's inequality to bound the tail probability. We want the failure probability to be smaller than $\delta$, so we just have to choose $t$ such that

$$
e^{-c^{2} t / 2} \leq \delta \Longleftrightarrow t \geq \frac{2}{c^{2}} \log \left(\frac{1}{\delta}\right)
$$

For sampling, we define the notion of approximate as being close in terms of total variation distance:
Definition 3.3 (Fully polynomial-time approximate sampling scheme). Given a ground set $\Omega$ and a desired probability distribution $\mu: \Omega \longrightarrow[0,1]$, we define a fully polynomial-time approximate
sampling scheme as an algorithm that takes as input an $\varepsilon>0$ and outputs a sample $X \sim \nu$ for a certain distribution $\nu: \Omega \longrightarrow[0,1]$ such that $\|\mu-\nu\|_{\mathrm{TV}}<\varepsilon$. The algorithm is required to run in time polynomial in $n$ (not the size of $\Omega$, but the size of the elements $\omega \in \Omega$ ) and the inverse error $1 / \varepsilon$.

Remark. For spin models, we take as a ground set the set of spin configurations on a certain graph $G$ and as a desired distribution the Gibbs measure $\mu_{G, \beta}$, for some fixed inverse temperature $\beta$. The sampling algorithm must be polynomial in $n:=|V(G)|$ and $1 / \varepsilon$.

### 3.2 Self-reducibility

One might wonder why do we consider the problems of approximate counting and sampling at the same time. The reason is that there exists a self-reducibility condition due to Jerrum and Sinclair under which the two problems are equivalent. That means that for combinatorial structures that follow this self-reducibility condition, one can reduce approximate counting to approximate sampling and vice versa.

### 3.2.1 Unweighted problems

Let $\Sigma$ be a finite alphabet and let $\Sigma^{*}:=\bigcup_{n \geq 0} \Sigma^{n}$ be the corresponding set of all possible finite strings. We will define the notion of self-reducibility for a very general framework in which instances of a combinatorial problem are encoded as strings $x \in \Sigma^{*}$, and solutions are represented by polynomial-length certificates $y \in \Sigma^{*}$. We define a binary relation $\mathcal{R} \subseteq \Sigma^{*} \times \Sigma^{*}$ that contains the pairs $(x, y)$ such that $y$ constitutes a valid solution of instance $x$. We restrict ourselves to NP problems, that is, to relations $\mathcal{R}$ that satisfy:

- There exists a polynomial $p$ such that for all $(x, y) \in \mathcal{R},|y| \leq p(|x|)$.
- Given an arbitrary pair $(x, y) \in \Sigma^{*} \times \Sigma^{*}$, we can test whether $(x, y) \in \mathcal{R}$ in polynomial time on $|x|+|y|$.

Given an instance $x \in \Sigma^{*}$, we denote the set of associated solutions as $R(x):=\{y:(x, y) \in \mathcal{R}\}$. Note that we can assume (by adding padding) that all solutions of an instance $x \in \Sigma^{*}$ have the same size, which will be given by a length function $\ell: \Sigma^{*} \longrightarrow \mathbb{N}$ that is polynomially bounded (i.e. there exists some polynomial $p$ such that $\ell(x) \leq p(|x|)$ for any $\left.x \in \Sigma^{*}\right)$. Then, $y \in R(x) \Longrightarrow|y|=\ell(x)$. Remark. For the instances $x \in \Sigma^{*}$ with no solution (i.e. $R(x)=\emptyset$ ), it does not matter how we define $\ell(x)$. That includes the $x \in \Sigma^{*}$ that do not define a valid instance (which are formally equivalent to instances with no solution).

Definition 3.4 (self-reducible [Sin93]). We say that a relation $\mathcal{R}$ satisfying the previous constraints is self-reducible if
(i) Given an $x \in \Sigma^{*}$, we can compute $\ell(x)$ in polynomial time.
(ii) There exist polynomial time computable functions $\psi: \Sigma^{*} \times \Sigma^{*} \longrightarrow \Sigma^{*}$ and $\sigma: \Sigma^{*} \longrightarrow \mathbb{N}$ such that
(a) $\sigma(x)=\mathcal{O}(\log |x|)$
(b) $\sigma(x)=0 \Longrightarrow \ell(x)=0, \quad \forall x \in \Sigma^{*}$
(c) $|\psi(x, w)| \leq|x|, \quad \forall x, w \in \Sigma^{*}$
(d) $\ell(\psi(x, w))=\max \{\ell(x)-|w|, 0\}, \quad \forall x, w \in \Sigma^{*}$
and such that the set of solutions of $x$ can be expressed as

$$
R(x)=\bigcup_{\substack{w \in \Sigma^{*} \\|w|=\sigma(x)}}\{w \tilde{y}: \tilde{y} \in R(\psi(x, w))\}
$$

Remark. The way to interpret self-reducibility intuitively is that, given an instance $x \in \Sigma^{*}$ and a prefix $w$, we have a procedure $\psi$ that generates another instance of the problem $\psi(x, w)$ such that all solutions of $x$ that start with $w$ will have the form $w \tilde{y}$, where $\tilde{y} \in R(\psi(x, w))$. In that case, $\sigma(x)$ represents the size of the prefix $w$.

Under this interpretation, condition (a) bounds the size of the prefix, so we have to consider at most $\mathcal{O}(|x|)$ different prefixes at each step; conditions (b) and (d) guarantee that each reduction decreases the size of the solution, so we can iterate until $\ell(x)=0$, at which point we only have to check if the empty string is a valid solution (this can be done in polynomial time because we are assuming the problem is in NP); finally, condition (c) guarantees that the size of the instance does not increase after the reduction.

Example 3.1. An example of a self-reducible counting problem is computing the number of independent sets of a graph $G$. Considering alphabet $\Sigma=\{0,1\}$, we can encode the input as the flattened adjacency matrix of $G$, a binary string of length $n^{2}$, where $n$ is the number of vertices of the graph. The solution certificates can be encoded as a string of length $n$, where position $i$ has a 1 if vertex $i$ belongs to the independent set. It is trivial to see that this is a valid certificate, as $|y|=\sqrt{|x|}=\operatorname{poly}(|x|)$, and given a pair $(x, y)$ we can check whether $y$ constitutes a valid independent set of the graph encoded in $x$ in time $\mathcal{O}(|x|)$.

Then, the size of the solution is easily computable $(\ell(x):=\sqrt{|x|}$, except if $|x|$ is not a perfect power, in which case the instance is not valid). To perform the reduction, we iterate over the prefixes of length $\sigma(x)=1$. If $w=0$, that means that we are not adding vertex $v_{1}$ to the independent set, so the reduced instance $\psi(x, w)$ is simply the graph $G \backslash\left\{v_{1}\right\}$. If $w=1$, we are adding vertex $v_{1}$ to the independent set, so we must delete all neighbors. The problem is that we can not simply take $\psi(x, w)=G \backslash N\left[v_{1}\right]$, as then the concatenation of the solutions would have the wrong size. However, there are many easy fixes, such as taking $\psi(x, w)=G \backslash\left\{v_{1}\right\}$ and using the diagonal of
the adjacency matrix to store which vertices have been "eliminated" (for those we only consider the case $w=0$ when we delete them).

The motivation for self-reducibility is that approximate sampling and counting are equivalent for self-reducible problems:

Theorem 3.2 (Theorems 1.10 and 1.14 of [Sin93]). Let $\mathcal{R}$ be a self-reducible relation on alphabet $\Sigma$. Then the following are equivalent:
(i) There exists a FPRAS that counts the size of $R(x)$ for a given $x \in \Sigma^{*}$.
(ii) There exists a fully polynomial-time approximate sampling scheme that outputs a $y \sim \operatorname{Unif}(R(x))$, for a given $x \in \Sigma^{*}$.

### 3.2.2 Weighted problems

The concept of self-reducibility and the equivalence result of Theorem 3.2 can be easily extended to weighted counting and non-uniform sampling. For weighted problems, we consider that we have a polynomial time computable function $W: \Sigma^{*} \times \Sigma^{*} \longrightarrow \mathbb{R}$ that assigns a weight to each pair $(x, y)$ with $y \in R(x)$. In this case the goal is not to compute the size of $R(x)$ but to compute the sum of weights: $Z_{\mathcal{R}, W}(x):=\sum_{y \in R(x)} W(x, y)$. The non-uniform sampling problem is defined analogously by requiring that the output follows a probability distribution $\mu_{x}: R(x) \longrightarrow[0,1]$ with $\mu_{x}(y):=W(x, y) / Z_{\mathcal{R}, W}(x)$.
Definition 3.5 (weighted relation, partition function). A weighted relation is a pair of a relation $\mathcal{R}$ and a weight function $W: \Sigma^{*} \times \Sigma^{*} \longrightarrow \mathbb{R}$. We define the partition function of the weighted relation as the function that gives the sum of weights of the solutions corresponding to each instance:

$$
\begin{aligned}
Z_{\mathcal{R}, W}: \Sigma^{*} & \longrightarrow \mathbb{R} \\
x & \longmapsto \sum_{y \in R(x)} W(x, y)
\end{aligned}
$$

Definition 3.6 (self-reducible [Sin93]). We say that a weighted relation $(\mathcal{R}, W)$ is self-reducible if the relation $\mathcal{R}$ is self-reducible and there exists a polynomial time computable function $g: \Sigma^{*} \times$ $\Sigma^{*} \times \mathbb{R} \longrightarrow \mathbb{R}$ such that

$$
Z_{\mathcal{R}, W}(x)=\sum_{\substack{w \in \Sigma^{*} \\|w|=\sigma(x)}} g\left(x, w, Z_{\mathcal{R}, W}(\psi(x, w))\right.
$$

for all $x \in \Sigma^{*}$, where $\psi$ and $\sigma$ are the functions given by the definition of self-reducibility of $\mathcal{R}$. Remark. Intuitively, the condition tells us that, given a prefix $w$, the sum of weights of the solutions of instance $x$ that start with $w$ only depends on the sum of weights of the solutions of the reduced instance $\psi(x, w)$.

Example 3.2. In the previous subsection we showed that counting independent sets on graphs is a self-reducible relation. Here we will show that computing the partition function of the hardcore model (i.e. the weighted version of counting independent sets) is self-reducible as a weighted relation.

Suppose that we have an instance $x \in \Sigma^{*}$ representing a graph $G$, with $V(G) \neq \emptyset$, and let $\lambda \in \mathbb{R}$ be the fugacity of the hard-core model. We want to compute the partition function $Z_{G}(\lambda)$. We can reduce the computation to smaller graphs by using that

$$
Z_{G}(\lambda)=\sum_{I \in \mathcal{I}(G)} \lambda^{|I|}=Z_{G \backslash\left\{v_{1}\right\}}(\lambda)+\lambda \cdot Z_{G \backslash N\left[v_{1}\right]}(\lambda)
$$

where the first term corresponds to the independent sets that do not contain $v_{1}$, while the second term corresponds to the independent sets that contain $v_{1}$. Using the same encoding and functions $\psi, \sigma$ as in example 3.1 (including the trick of encoding eliminated vertices in the diagonal of the adjacency matrix of $\psi(G, 1)$ ) we can then define

$$
\begin{aligned}
g: \Sigma^{*} \times \Sigma^{*} \times \mathbb{R} & \longrightarrow \mathbb{R} \\
(G, 0, z) & \longmapsto z \\
(G, 1, z) & \longmapsto \lambda z
\end{aligned}
$$

so that the self-reducibility condition is satisfied.

We have an analogue to Theorem 3.2 for the weighted case:
Theorem 3.3 (Corollary 3.16 from [Sin93]). Let $(\mathcal{R}, W)$ be a self-reducible weighted relation on alphabet $\Sigma$. Then the following are equivalent:
(i) There exists a FPRAS that computes $Z_{\mathcal{R}, W}(x)$ for a given $x \in \Sigma^{*}$.
(ii) There exists a fully polynomial-time approximate sampling scheme that, given a $x \in \Sigma^{*}$, outputs a $y \sim \mu_{x}$, where $\mu_{x}: R(x) \longrightarrow[0,1]$ is the probability distribution given by $\mu_{x}(y):=$ $W(x, y) / Z_{\mathcal{R}, W}(x)$.

### 3.3 Decay of correlation (Weitz's method)

In this section we describe how correlation decay can be used to construct an FPTAS for the partition function. We illustrate the method using the hard-core model, but the same results can be extended to more general 2 -spin models, as described in [SS19.

In particular, we show how to prove the following result by Weitz:

Theorem 3.4 (Theorem 2.7 from Wei06]). For a fixed $\Delta \geq 1$ and for any $\lambda<\lambda_{c}(\Delta):=(\Delta-$ $1)^{\Delta-1} /(\Delta-2)^{\Delta}$, there exists an FPTAS for computing $Z_{G}(\lambda)$, for any graph $G$ with maximum degree $\Delta$.

### 3.3.1 Recursive approach

The first key idea is that we can reduce the problem of estimating the partition function $Z_{G}(\lambda)$ to the problem of estimating the marginals $\mu_{G, v}:=\operatorname{Pr}_{G}[v \in I]$. That's because, we can pick an arbitrary vertex $v \in V(G)$ and express $Z_{G}(\lambda)$ in terms of the marginal of $v$ and the partition function of a smaller graph:

$$
\mu_{G, v}=\frac{1}{Z_{G}(\lambda)} \sum_{\substack{I \in \mathcal{I}(G) \\ I \ni v}} \lambda^{|I|}=\frac{1}{Z_{G}(\lambda)} \lambda \cdot Z_{G \backslash N[v]}(\lambda)
$$

We can repeat the procedure, picking a $v^{\prime} \in V(G \backslash N[v])$, until at the end we will have expressed $Z_{G}(\lambda)$ in terms of the reciprocals of at most $n$ marginal probabilities. Using this formula, we need a relative error smaller than $\varepsilon / n$ in the marginals to estimate $Z_{G}(\lambda)$ up to a relative error of $\varepsilon$. This increases the runtime by a factor of $n$, which still fits the requirements of an FPTAS.

The next key idea is that we can reduce the problem from a general graph $G$ to a certain tree $T_{\text {SAW }}$, that we construct from $G$. This is particularly useful because the marginals of a tree can be calculated very easily in a recursive manner, by iterating over the subtrees rooted at the children. We can express this recursion in terms of ratios of marginals:

Definition 3.7 (ratio of marginals). Let $G$ be a graph and let $v$ be a certain vertex. We define the ratio of marginals at $v$ as

$$
R_{G, v}:=\frac{\operatorname{Pr}[v \in I]}{\operatorname{Pr}[v \notin I]}=\frac{\mu_{G, v}}{1-\mu_{G, v}}
$$

If $\mu_{G, v}=1$, we take $R_{G, v}=+\infty$. Observe that $\mu_{G, v}=R_{G, v} /\left(1+R_{G, v}\right)$, so we do not lose any information by working with the ratios.

The recursive relationship is the following:
Proposition 3.5. Let $T$ be a tree. Let $v$ be a vertex of $T$, with neighbors $u_{1}, \ldots, u_{d}$. For $i \in[d]$, let $T_{i}$ be the subtree rooted at $u_{i}$. Then,

$$
R_{T, v}=\lambda \prod_{i=1}^{d} \frac{1}{1+R_{T_{i}, u_{i}}}
$$

Proof. For a fixed vertex $v$ in a graph $G$, let $Z_{G, v}^{+}(\lambda)$ be the partition function restricted to the independent sets $I$ with $v \in I$, and let $Z_{G, v}^{-}(\lambda)$ be the partition function restricted to the independent
sets $I$ with $v \notin I$. Note that $Z_{G}(\lambda)=Z_{G, v}^{+}(\lambda)+Z_{G, v}^{-}(\lambda)$ and that $R_{G, v}=Z_{G, v}^{+}(\lambda) / Z_{G, v}^{-}(\lambda)$. Then,

$$
R_{G, v}=\frac{Z_{G, v}^{+}(\lambda)}{Z_{G, v}^{-}(\lambda)}=\frac{\lambda \prod_{i=1}^{d} Z_{T_{i}, u_{i}}^{-}(\lambda)}{\prod_{i=1}^{d} Z_{T_{i}, u_{i}}(\lambda)}=\lambda \prod_{i=1}^{d} \frac{Z_{T_{i}, u_{i}}^{-}(\lambda)}{Z_{T_{i}, u_{i}}^{+}(\lambda)+Z_{T_{i}, u_{i}}^{-}(\lambda)}=\lambda \prod_{i=1}^{d} \frac{1}{1+R_{T_{i}, u_{i}}}
$$

Remark. Note that if we fix the spin of a certain subset of vertices $\Lambda$, then the ratio of marginals still follows the same recursive relation. We will denote by $R_{G, v}^{\sigma_{\Lambda}}$ the ratio of marginals given the fixed spins $\sigma_{\Lambda}: \Lambda \longrightarrow \Omega$.

### 3.3.2 Self-avoiding walk tree

The tree that we will construct will be based on unfolding all the possible self-avoiding walks starting at a certain vertex $v$, and pruning the branch every time we close a cycle. The pruning will be done by fixing a certain spin on the vertex that closes the cycle.

Definition 3.8 (self-avoiding walk tree). Given a graph $G$, with ordered edges $e_{1}<\cdots<e_{m}$, and given a specific vertex $v \in V(G)$, we define the self-avoiding walk tree rooted at $v$, as the tree $T_{\text {SAW }}$ formed by all the simple paths (i.e. not repeating an edge) starting at $v$, in which the paths are truncated once a vertex is repeated. Besides, when we truncate a path we assign a fixed spin to the leaf ( 1 if the edge that started the cycle is smaller than the edge that finished the cycle, and 0 otherwise).

Example 3.3. One can see an example of the construction of $T_{\text {SAW }}$ in figure 3.1. Here we are choosing the vertex $a$ as the root and considering the order on edges induced by the lexicographic order on vertices $a<\cdots<f$. Notice that, we only ever have to compare incident edges (i.e. that share a vertex), so the order on vertices induces a well-defined order on incident edges (i.e. an edge is smaller if its non-repeated vertex is smaller).

As an example, on branch $a-c-d-a$, we are assigning the leaf to be occupied, as the edge that started the cycle $(a-c)$ is smaller than the edge that ended it $(d-a)$. The same cycle is transversed on branch $a-d-c-a$, but here we are assigning the lead to be unoccupied, as the edge that starts the cycle $(a-d)$ is bigger than the edge that ends it $(c-a)$.

Remark. In the definition of $T_{\text {SAW }}$ we have given (and in figure 3.1) we are restricting ourselves to paths that do not repeat edges. For example, we do not consider the branch $a-b-a$. However, it does not actually matter. In the construction of $T_{\text {SAW }}$ we can assign the leaf to be unoccupied if the edge that starts the cycle is the same as the edge that ends the cycle, so branches like $a-b-a$ are effectively truncated at $a-b$.

Remark. Note that each vertex from $T_{\text {SAW }}$ corresponds to some vertex from the original graph $G$. If the original graph $G$ has some subset of vertices $\Lambda$ with fixed spins $\sigma_{\Lambda}$, we can construct the


Figure 3.1: SAW tree construction (figure from [SS19])
self-avoiding walk tree as usual and then fix the spins of all the copies of vertices from $\Lambda$. With a slight abuse of notation, we will still denote these fixed spins as $\sigma_{\Lambda}$.

Remark. Suppose we have a vertex $u \in V(G)$ that has a fixed spin $\sigma_{u}$. By the remark above, we fix the spin of all copies of $u$ in $T_{\mathrm{SAW}}$ to be $\sigma_{u}$ too. But what if one of these was a leaf that has its spin already fixed to the opposite value? Notice that such cases do not affect the marginal of the root of the tree, since if there is a copy of $u$ with fixed spin on $T_{\mathrm{SAW}}$, that means that there is an earlier copy of $u$ in the same branch (as $u$ is the beginning and end of the cycle). This copy will also have its spin fixed by $\sigma_{\Lambda}$, so the leaf copy of $u$ will be separated from the root by a vertex with fixed spin. Applying the Markov spatial property, that means that the choice of spin for the leaf does not affect the marginal of the root.

As we have already mentioned, the important property of $T_{\text {SAW }}$ is that the marginal of the root is equal to the marginal in the original graph $G$ :

Theorem 3.6 (Theorem 3.1 from Wei06]). Let $G$ be a graph, and let $v \in V(G)$. Pick an arbitrary order of the edges and let $T_{S A W}$ be the self-avoiding walk tree rooted at $v$. Then, for any activity $\lambda$ and for any set of vertices $\Lambda \subseteq V(G)$ with fixed spins $\sigma_{\Lambda}$, we have that $\mu_{G, v}^{\sigma_{\Lambda}}=\mu_{T_{\mathrm{SAW}}, v}^{\sigma_{\Lambda}}$.

Proof. Let $u_{1}, \ldots, u_{d}$ be the neighbors of $v$ in $T_{\text {SAW }}$ (they correspond one to one to the neighbors of $v$ in $G$ ). Suppose without loss of generality that the indices are chosen so $v u_{1}<\cdots<v u_{d}$ in the ordering of the edges of $G$. Let $\sigma_{\Lambda_{i}}$ be the restriction of the set of fixed spins $\sigma_{\Lambda}$ to $T_{i}$, the subtree of $T_{\mathrm{SAW}}$ rooted at $u_{i}$. Then, using Proposition 3.5, the marginal on $T_{\mathrm{SAW}}$ satisfies the recursion

$$
\begin{equation*}
R_{T_{\mathrm{SAW}}, v}^{\sigma_{\Lambda}}=\lambda \prod_{i=1}^{d} \frac{1}{1+R_{T_{i}, u_{i}}^{\sigma_{i}}} \tag{3.1}
\end{equation*}
$$

The idea of the proof is to define a recursive procedure on $G$ that allows us to calculate $R_{G, v}^{\sigma_{\Lambda}}$, and to show that this recursive procedure is equivalent to the one on $T_{\mathrm{SAW}}$ that uses the recursion above,
so $R_{G, v}^{\sigma_{\Lambda}}=R_{T_{\mathrm{SAW}}, v}^{\sigma_{\Lambda}}$.
The procedure is the following: we delete vertex $v$ from the graph and add $d$ copies $v_{1}, \ldots, v_{d}$, such that each $v_{i}$ is only connected to $u_{i}$. This creates another graph $G^{\prime}$. For $0 \leq i \leq d+1$, let $\tau_{i}$ denote the boundary conditions obtained by fixing vertices $v_{j}$ with $j<i$ to be occupied, and fixing vertices $v_{j}$ with $j>i$ to be unoccupied. Note that we don't fix the spin of $v_{j}$. Let $\sigma_{\Lambda} \tau_{i}$ denote the concatenation of both boundary conditions.

Note that fixing $v$ to be occupied in $G$ is the same as fixing $v_{1}, \ldots, v_{d}$ to be occupied in $G^{\prime}$ (and setting the activities of these vertices as $\sqrt[d]{\lambda}$ ). The same is true for fixing $v$ to be unoccupied. Therefore,

$$
R_{G, v}^{\sigma_{\Lambda}}=\frac{\operatorname{Pr}_{G}^{\sigma_{\Lambda}}[v \in I]}{\operatorname{Pr}_{G}^{\sigma_{\Lambda}}[v \notin I]}=\frac{\operatorname{Pr}_{G_{A}^{\prime}}^{\sigma_{A}}\left[v_{1}, \ldots, v_{d} \in I\right]}{\operatorname{Pr}_{G^{\prime}}^{\sigma_{A}}\left[v_{1}, \ldots, v_{d} \notin I\right]}
$$

By telescoping, we can express this quotient as product of ratios of marginals:

$$
\begin{aligned}
\frac{\operatorname{Pr}_{G^{\prime}}^{\sigma_{\Lambda}}\left[v_{1}, \ldots, v_{d} \in I\right]}{\operatorname{Pr}_{G^{\prime}}^{\sigma_{A}}\left[v_{1}, \ldots, v_{d} \notin I\right]} & =\prod_{i=1}^{d} \frac{\operatorname{Pr}_{G^{\prime}}^{\sigma_{\lambda}}\left[v_{1}, \ldots, v_{i} \in I, v_{i+1}, \ldots, v_{d} \notin I\right]}{\operatorname{Pr}_{G^{\prime}}^{\sigma_{\lambda}}\left[v_{1}, \ldots, v_{i-1} \in I, v_{i}, \ldots, v_{d} \notin I\right]}= \\
& =\prod_{i=1}^{d} \frac{\lambda^{(i-1) / d} \cdot \operatorname{Pr}_{G^{\prime}}^{\sigma_{\Lambda} \tau_{i}}\left[v_{i} \in I\right]}{\lambda^{(i-1) / d} \cdot \operatorname{Pr}_{G^{\prime}}^{\sigma_{\Lambda} \tau_{i}}\left[v_{i} \notin I\right]}=\prod_{i=1}^{d} R_{G^{\prime}, v_{i}}^{\sigma_{A} \tau_{i}}
\end{aligned}
$$

Then, as $v_{i}$ only has one neighbor in $G^{\prime}$, the recursion formula for trees holds as well:

$$
R_{G^{\prime}, v_{i}}^{\sigma_{\Delta} \tau_{i}}=\sqrt[d]{\lambda} \cdot \frac{1}{1+R_{G^{\prime} \backslash\left\{v_{i}\right\}, u_{i}}^{\sigma_{\Lambda} \tau_{i}}}
$$

so putting all together we obtain

$$
\begin{equation*}
R_{G, v}^{\sigma_{\Lambda}}=\lambda \prod_{i=1}^{d} \frac{1}{1+R_{G^{\prime} \backslash\left\{v_{i}\right\}, u_{i}}^{\sigma_{\Lambda} \sigma_{i}}} \tag{3.2}
\end{equation*}
$$

Note that $G^{\prime} \backslash\left\{v_{i}\right\}$ has $d-1$ more vertices than $G$ (as we have turned vertex $v$ into the $d$ copies $v_{1}, \ldots, v_{d}$ ). The key is that the spin of all those has been fixed by $\tau_{i}$, so the number of vertices without fixed spin has actually decreased by one. Hence, after iterating this recursion at most $n$ times, we will get to the base case in which all spins are fixed.

Inspecting equations 3.2 and 3.1 one can see that the recursive formula is the same. It remains to prove that the further steps of the recursion will also coincide. In order to do so, notice that the recursion on $G^{\prime} \backslash\left\{v_{i}\right\}$ will proceed in the same way as in $T_{i}$ until we repeat one of the vertices. Assume the repeated vertex is $v$ (otherwise we change the names of the variables so $v$ is the repeated vertex, $u_{1}, \ldots, u_{d}$ are its neighbours and so on). Let $v \rightarrow u_{i} \rightarrow \cdots \rightarrow u_{j} \rightarrow v$ be the path on $T_{\text {SAW }}$. We know that in $T_{\text {SAW }}$ the path will end with the last copy of vertex $v$ having fixed spin. In particular, it will be occupied if edge $v u_{i}$ is smaller than $v u_{j}$ and unoccupied if $v u_{i}$ is bigger than
$v u_{j}$. But we have named $u_{1}, \ldots u_{d}$ so that $v u_{i}<v u_{j} \Longleftrightarrow i<j$, so the copy of $v$ will be occupied if $i<j$ and unoccupied if $i>j$. That's exactly the condition that we imposed on $G^{\prime}$ by $\tau_{i}$, so the recursion will stop in the same place and with the same boundary condition.

Hence, $R_{G, v}^{\sigma_{\Lambda}}=R_{T_{\mathrm{SAW}}, v}^{\sigma_{\Lambda}}$, and therefore the marginals must also be the same.
To recapitulate, we have reduced the problem of finding an FPTAS for $Z_{G}(\lambda)$ to finding an FPTAS for the marginals of the form $\mu_{G, v}$. We have then proved that there exists a tree $T_{\mathrm{SAW}}$ such that $\mu_{G, v}=\mu_{T_{\text {SAW }}, v}$, and shown a recursive procedure to calculate $\mu_{T_{\text {SAW }}, v}$.

Remark. Technically, the reduction from computing $Z_{G}(\lambda)$ to computing the marginals requires that we are able to compute the marginals not just on $G$ but on any subgraph of $G$. Thus, we require that the class of graphs that we are working with is closed under taking subgraphs. That is true for graphs of maximum degree at most $\Delta$, which is the class covered by Theorem 3.4 .

### 3.3.3 Spatial mixing

The problem is that $T_{\text {SAW }}$ can have by construction up to an exponential number of vertices, so we can't apply the recursive formula directly. Here is where we use correlation decay. Correlation decay tells us that the effect on the marginal of the root of vertices that are far away is exponentially decreasing on the distance. That means we can truncate the process after logarithmic depth to get a polynomially small error on the marginal. The number of vertex visited will then be $\Delta^{\mathcal{O}(\log n)}=$ $n^{\mathcal{O}(\log \Delta)}$, where $\Delta$ is the maximum degree of $T_{\text {SAW }}$. Notice that, by definition, $T_{\text {SAW }}$ has at most the same degree as the original graph $G$, so this gives an FPTAS for graphs $G$ of constant maximum degree.

First we need to extend the notion of correlation decay to subsets of vertices of arbitrary size:
Definition 3.9 (weak spatial mixing). We say that a spin model on a graph family $\mathcal{G}$ exhibits weak spatial mixing with exponential decay (or WSM) if there exist constants $A$ and $B$ such that

$$
\left|\mu_{G, v}^{\sigma_{\Lambda}}-\mu_{G, v}^{\tau_{\Lambda}}\right| \leq A e^{-B \operatorname{dist}(v, \Lambda)}
$$

for any $G \in \mathcal{G}$, for any $v \in V(G)$, and for any pair of spin assignments $\sigma_{\Lambda}, \tau_{\Lambda}$ on a subset of vertices $\Lambda \subset V(G)$.

Remark. Note that weak spatial mixing can be thought of as extending definition 2.10 to multiple vertices. That's because

$$
\begin{aligned}
|\kappa(u, v)| & =|\operatorname{Pr}[u \in I, v \in I]-\operatorname{Pr}[u \in I] \cdot \operatorname{Pr}[v \in I]|= \\
& =|\operatorname{Pr}[u \in I \mid v \in I]-\operatorname{Pr}[u \in I]| \cdot \operatorname{Pr}[v \in I] \leq \\
& \leq|\operatorname{Pr}[u \in I \mid v \in I]-\operatorname{Pr}[u \in I \mid v \notin I]|
\end{aligned}
$$

so weak spatial mixing (for $\Lambda$ consisting of 1 vertex) implies exponential decay of correlations (as stated in definition 2.10.

In fact, for the hard-core model, weak spatial mixing for $\Lambda$ of size 1 also implies weak spatial mixing for general $\Lambda$, as long as the neighborhoods of $G$ grow subexponentially with distance. That's a corollary of the monotonicity argument in section 4 of Wei06.

We need in fact a slightly stronger condition:
Definition 3.10 (strong spatial mixing). We say that a spin model on a graph family $\mathcal{G}$ exhibits strong spatial mixing with exponential decay (or SSM) if there exist constants $A$ and $B$ such that

$$
\left|\mu_{G, v}^{\sigma_{\Lambda}}-\mu_{G, v}^{\tau_{\Lambda}}\right| \leq A e^{-B \operatorname{dist}(v, \tilde{\Lambda})}
$$

for any $G \in \mathcal{G}$, for any $v \in V(G)$, and for any pair of spin assignments $\sigma_{\Lambda}, \tau_{\Lambda}$ on a subset of vertices $\Lambda \subset V(G)$, which disagree on $\tilde{\Lambda} \subseteq \Lambda$.

Remark. Intuitively, SSM says that it does not matter if we fix the spin of a vertex very close to $v$, as long as this spin is fixed to the same value by both $\sigma_{\Lambda}$ and $\tau_{\Lambda}$. This is not true in general, even if WSM holds. That's because fixing close spins can modify the distribution of the marginal of $v$ so that it is more highly correlated with distant spins.

If our graph $G$ satisfies SSM, then we can obtain the FPTAS of Theorem 3.4,
Lemma 3.7. Let $\lambda$ be such that the hard-core model on $G$ exhibits strong spatial mixing with an exponential decay rate. Then, there exists an FPTAS to approximate $Z_{G}(\lambda)$.

Proof. As explained in section 3.3.1, we can reduce the problem of finding an FPTAS for $Z_{G}(\lambda)$ to finding an FPTAS for $\mu_{G, v}$. In turn, the marginal can be computed from the ratio of marginals $R_{G, v}$ :

$$
R_{G, v}=\frac{\mu_{G, v}}{1-\mu_{G, v}} \Longrightarrow \mu_{G, v}=\frac{1}{1+1 / R_{G, v}}
$$

Note that from this formula we can deduce that the relative error in $\mu_{G, v}$ is at most the relative error in $R_{G, v}$ (because $0 \leq R_{G, v} \leq+\infty$ so the relative error decreases ${ }^{2}$ when summing 1 ). Therefore, we can reduce the problem to finding an FPTAS for $R_{G, v}$, or equivalently $R_{T_{\text {SAW }, v}}$ (using Theorem 3.6).

Suppose that, for some $\ell \in \mathbb{N}$, we truncate the calculation of $R_{T_{\text {SAW }}, v}$ at the $\ell$-th level of recursion. Note that, in the recursion formula from equation 3.1, the ratios at two consecutive depths are inversely related (when the ratio at one level increases, the ratio at the next level decreases, and vice versa). Thus, we can obtain a lower and upper bound of $R_{T \mathrm{SAW}, v}$ by setting the ratios at level $\ell$ all to 0 and all to $+\infty$. Let $R_{\ell}^{+}$and $R_{\ell}^{-}$be these bounds, such that $R_{\ell}^{-} \leq R_{T_{\mathrm{SAW}}, v} \leq R_{\ell}^{+}$.

[^4]Note too that $\mu_{G, v}$ is an increasing function in $R_{G, v}$, so the marginals corresponding to the bounds on $R$ bound the exact value of the marginal:

$$
\mu_{\ell}^{-} \leq \mu_{T_{\mathrm{SAW}}, v} \leq \mu_{\ell}^{+}
$$

By the SSM condition, the difference in the marginals from fixing the spins at level $\ell$ is at most $A e^{-B \ell}$ for some constants $A$ and $B$. Then, for $\ell$ such that $A e^{-B \ell} \leq \varepsilon$, any of $\mu_{\ell}^{-}$or $\mu_{\ell}^{+}$will constitute a valid $\varepsilon$-approximation of $\mu_{G, 2}{ }^{3}$. The optimal value of $\ell$ is

$$
\ell=\frac{1}{B} \log \frac{A}{\varepsilon}
$$

The number of vertices visited from the $T_{\mathrm{SAW}}$ is bounded by $\Delta^{\ell}$, so the runtime will be polynomial in $1 / \varepsilon$, as desired.

Note that the optimal value of $\ell$ depends on the values of $A$ and $B$ from the SSM condition. In case these values are unknown, we can still apply the same algorithm, trying out all values from $\ell=1$ upwards, until finding one such that the difference between $\left|\mu_{\ell}^{+}-\mu_{\ell}^{-}\right|$is low enough. This does not change the runtime, since $\Delta+\cdots+\Delta^{\ell}=\mathcal{O}\left(\Delta^{\ell}\right)$ still (for fixed $\Delta$ ).

Remark. Note that the runtime of the algorithm does not depend on the size of the graph $G$. That's because we have hidden a factor of $n^{2}$ in the reduction between the FPTAS for $Z_{G}(\lambda)$ and the FPTAS for $\mu_{G, v}$. To guarantee an $\varepsilon$-approximation of $Z_{G}(\lambda)$ we need to approximate each of the at most $n$ marginals to $\varepsilon / n$-relative error, so we get an extra $n^{2}$ factor.

### 3.3.4 Uniqueness threshold for the $\Delta$-regular tree

In virtue of Lemma 3.7, in order to prove Theorem 3.4 it's enough to prove that the hard-core model on $G$ exhibits strong spatial mixing. The final key idea from Weitz's method is that we can get SSM in a $G$ of maximum degree $\Delta$ if we know there's WSM in $T_{\Delta}$, the $\Delta$-regular infinite tree.

Lemma 3.8. Suppose that, for a certain $\Delta$ and $\lambda$, the hard-core model on the $\Delta$-regular infinite tree $T_{\Delta}$ exhibits strong spatial mixing with exponential decay. Then, the hard-core model also exhibits strong spatial mixing with exponential decay in any $G$ of maximum degree $\Delta$.

Lemma 3.9. Suppose that, for a certain $\Delta$ and $\lambda$, the hard-core model on the $\Delta$-regular infinite tree $T_{\Delta}$ exhibits weak spatial mixing with exponential decay. Then, it also exhibits strong spatial mixing with exponential decay.

Remark. One can consider a more general definition of WSM and SSM where there is no requirement of exponential decay, and instead we ask that $\left|\mu_{G, v}^{\sigma_{\Lambda}}-\mu_{G, v}^{\tau_{\Lambda}}\right| \leq f(\operatorname{dist}(v, \Lambda))$ for some function $f$ : $\mathbb{N} \longrightarrow \mathbb{R}^{+}$that tends to 0 as the distance increases. In that case, Lemma 3.8 still holds (SSM with

[^5]rate $f$ in $T_{\Delta}$ implies SSM with rate $f$ in $G$ ), but Lemma 3.9 no longer does (WSM with rate $f$ in $T_{\Delta}$ implies SSM with a higher rate $\left.C(\lambda, \Delta) \cdot f\right)$. What happens behind the scenes in Lemma 3.9 is that the constant factor $C(\lambda, \Delta)$ is getting absorbed into the constant $A$ from the definition of SSM with exponential decay.

Proof. (Lemma 3.8) Let $G$ be a graph of maximum degree $\Delta$, and let $v$ be a vertex from $G$. We construct the self-avoiding walk tree $T_{\text {SAW }}$ rooted at $v$. Note that this tree has maximum degree $\Delta$, so it is a subgraph of $T_{\Delta}$. Furthermore, we can embed $T_{\text {SAW }}$ in $T_{\Delta}$ with the additional constraint that the roots coincide. Under one such embedding, let $\omega$ be the boundary conditions that fix the spin of each vertex in $V\left(T_{\Delta}\right) \backslash V\left(T_{\mathrm{SAW}}\right)$ to be unoccupied. Then, for any set of fixed spins $\sigma_{\Lambda}$,

$$
\mu_{G, v}^{\sigma_{\Lambda}}=\mu_{T_{\mathrm{SAW}}, v}^{\sigma_{\Lambda}}=\mu_{T_{\Delta}, v}^{\sigma_{\Lambda} \circ \omega}
$$

where $\sigma_{\Lambda} \circ \omega$ denotes the composition of both boundary conditions (they are vertex-disjoint so we do not have to worry about one vertex being assigned two different spins). Thus, SSM in $T_{\Delta}$ with a certain decay rate implies SSM in $G$ with the same decay rate.

Proof. (Lemma 3.9) Suppose we have two different spin assignments $\sigma_{\Lambda}$ and $\tau_{\Lambda}$, for $\Lambda \subset V\left(T_{\Delta}\right)$. Let $\tilde{\Lambda}=\left\{u \in \Lambda: \sigma_{u} \neq \tau_{u}\right\}$ be the set of vertices in which they disagree. In order to prove SSM from WSM, we need to show that fixing the spins of vertices from $\Lambda \backslash \tilde{\Lambda}$ does not augment significantly the sensitivity of $\mu_{T_{\Delta}, v}$ to setting the spins on $\tilde{\Lambda}$.

Note that we can suppose that all vertices with fixed spins are set to be unoccupied, as setting $\sigma_{u}=1$ for some vertex $u$ is equivalent to setting $\sigma_{w}=0$ for all $w \in N(u)$ (in terms of the effect on $\left.\mu_{T_{\Delta}, v}\right)$. At the same time, setting a vertex $u$ to be unocuppied is the same as setting the activity parameter $\lambda_{u}=0$ (for the multivariate extension of the hard-core model, where every vertex has its own activity).

Through some involved computations, Weitz goes on to prove that, in fact, the influence on the marginal decreases for any decrease in the activity of the vertices $4_{4}^{4}$. For more details one can consult section 4 of Wei06.

The values of $\lambda$ for which $T_{\Delta}$ exhibits weak spatial mixing were actually well-known prior to Weitz's article (for an early source, see Kel85):

Proposition 3.10. Let $T_{\Delta}$ be the infinite $\Delta$-regular tree. Let $\lambda_{c}(\Delta)=(\Delta-1)^{\Delta-1} /(\Delta-2)^{\Delta}$. Then, the hard-core model on $T_{d}$ with fugacity $\lambda$

- exhibits weak spatial mixing with exponential decay if $\lambda<\lambda_{c}$, while
- it does not exhibit weak spatial mixing at any rate of decay for $\lambda>\lambda_{c}$.

[^6]In particular, one can prove that for $\lambda>\lambda_{c}$ the boundary conditions "all vertices at depth $r$ occupied" and "all vertices at depth $r$ unoccupied" induce two different infinite volume measures, in the limit as $r \rightarrow \infty$.

Proof. See Kel85 for a proof and Per22 for a discussion of the connection with the notion of uniqueness of the infinite volume measure.

This was the last ingredient needed for the construction of the FPTAS. To sum up, the proof goes as following:

Proof. (Theorem 3.4) Let $\lambda<\lambda_{c}(\Delta)$, for some fixed $\Delta$. By Proposition 3.10, the hard-core model on $T_{\Delta}$ exhibits weak spatial mixing with exponential decay so, by Lemma 3.9, it also exhibits strong spatial mixing with exponential decay. Then, Lemma 3.8 implies that any $G$ with maximum degree $\Delta$ also exhibits SSM with exponential decay. That means that we can apply Lemma 3.7 to find an FPTAS for $Z_{G}(\lambda)$.

Note that, apart from the positive result for $\lambda<\lambda_{c}$, Proposition 3.10, also tells us that WSM does not hold when $\lambda>\lambda_{c}$. This rules out extending Weitz's method to this regime. However, this does not automatically disprove the existence of an FPTAS for this values of $\lambda$, as there could be other methods to construct the algorithm not based on correlation decay. Nonetheless, Sly and Sun proved in 2014 that the threshold of Weitz is almost optimal:

Theorem 3.11 (Theorem 2 from [SS14]). Unless $R P=N P$, there is no FPRAS for computing $Z_{G}(\lambda)$ in the hard-core model with activity $\lambda>\lambda_{c}(\Delta)$.

Remark. Note that Theorem 3.11 not only rules out the existence of an FPTAS but also of an FPRAS. That does not happen in general: there are problems for which there exists randomized algorithms that can not be derandomized efficiently. In this problem, however, randomized and deterministic algorithms are equally powerful.

Together, theorems 3.4 and 3.11 give a complete picture of the complexity of approximating $Z_{G}(\lambda)$ for the hard-core model on graphs with constant maximum degree, except at the critical point $\lambda=\lambda_{c}$, for which there is no definitive result yet.

### 3.4 Power series approximation (Barvinok's method)

In this section we explain another method for constructing an FPTAS for the partition function $Z_{G}(\lambda)$, based on truncating the Taylor expansion of its logarithm. This method has been pionereed by Barvinok, who also wrote a recent monograph on the topic (see [Bar19]). In contrast with Weitz's method, here we do not make use of any information about the spin model, so it could be used too
to approximate a general complex polynomial $P(z)$, provided that it satisfies the assumptions from Lemma 3.12.

Suppose we have a polynomial $P(z)=\sum_{k=0}^{n} a_{k} z^{k}$, with coefficients $a_{k} \in \mathbb{C}$. For a fixed value of $z$, we want to approximate this polynomial up to $\varepsilon$-relative error, for a certain $\varepsilon>0$. If the coefficients are easy to compute, the problem is trivial, but we suppose that the $k$-th coefficient takes time $\Theta\left(n^{k}\right)$ to compute (as it is the case for the hard-core model, in which we can count the number of independent sets of size $k$ by iterating naively over all possible subsets of size $k$ ).

The main idea of Barvinok's method is to approximate instead $\log P(z)$. The Taylor expansion of $\log P$ around 0 gives us a power series

$$
\log P(z)=\sum_{j \geq 0} b_{j} z^{j}
$$

for some coefficients $b_{j} \in \mathbb{C}$. Let $T_{k}(z):=\sum_{j=0}^{k} b_{j} z^{j}$ be the $k$-th order truncation of the Taylor expansion. One can prove that $\left\{T_{k}\right\}_{k \geq 0}$ converges to $\log P(z)$ with error exponentially decreasing in $k$, as long as $P(z)$ has a zero-free disk around 0 :

Lemma 3.12 ([Bar19]). Let $P(z): \mathbb{C} \longrightarrow \mathbb{C}$ be a polynomial of degree $n$ with independent term $p_{0} \in \mathbb{R}^{+}$. Suppose there exist $R>0$ and $\delta>0$ such that $P(z) \neq 0$ for all $z \in B(0,(1+\delta) R)$. For $a z \in \overline{B(0, R)}$, consider the Taylor series of $\log P$ at $z$ expanded around 0 , and let $T_{k}(z)$ be its $k$-th order truncation. Then, $\left\{T_{k}(z)\right\}_{k \geq 1}$ converges exponentially to $\log P(z)$, i.e. there exist constants $A(\delta)$ and $B(\delta)$ independent of $z$ and $n$ such that

$$
\left|\log P(z)-T_{k}(z)\right| \leq A n e^{-B k}
$$

for all $k \in \mathbb{Z}^{+}$.
Remark. When working in the complex plane one has to be careful about how the logarithms are defined. Luckily, the zero-free condition of $P(z)$ allows us to define $\log P(z)$ analytically in $\overline{B(0, R)}$ by taking

$$
\begin{equation*}
\log P(z):=\log p_{0}+\sum_{j=1}^{n} \log \left(1-\frac{z}{\xi_{j}}\right) \tag{3.3}
\end{equation*}
$$

where $\xi_{j}$ are the zeros of $P(z)$. We can take the principal branch of the logarithm in each of the terms since $p_{0} \in \mathbb{R}^{+}$and $\left|z / \xi_{j}\right| \leq 1 /(1+\delta)<1$, so $\Re\left(1-z / \xi_{j}\right)>0$.

Notice that, if we interpret the logarithm as a formal power series, by defining

$$
\log (x):=\sum_{k \geq 1}(-1)^{k+1} \frac{x^{k}}{k},
$$

then both the LHS and the RHS of 3.3 correspond to the same formal power series on $z 5$. Therefore, the Taylor series of $\log P(z)$, understood as a formal power series, will have the same coefficients as the Taylor series of the RHS of 3.3 . Hence, we can work with one or the other indistinctly.

Proof. As explained in the previous remark, the Taylor series of $\log P(z)$ will be given by

$$
\log P(z)=\log p_{0}+\sum_{j=1}^{n} \sum_{\ell \geq 1}-\frac{1}{\ell}\left(\frac{z}{\xi_{j}}\right)^{\ell}
$$

Therefore, the residue after substracting the terms of order at most $k$ will be

$$
\left|\log P(z)-T_{k}(z)\right| \leq \sum_{j=1}^{n} \sum_{\ell \geq k+1} \frac{1}{\ell}\left|\frac{z}{\xi_{j}}\right|^{\ell}
$$

Since $P$ has no zeros in $B(0,(1+\delta) R)$ and $z \in \overline{B(0, R)}$, we have that $\left|z / \xi_{j}\right| \leq 1 /(1+\delta)$, so

$$
\begin{aligned}
\left|\log P(z)-T_{k}(z)\right| & \leq \sum_{j=1}^{n} \sum_{\ell \geq k+1} \frac{1}{\ell}\left(\frac{1}{1+\delta}\right)^{\ell} \leq n \sum_{\ell \geq k+1}\left(\frac{1}{1+\delta}\right)^{\ell} \\
& =n\left(\frac{1}{1+\delta}\right)^{k} \frac{1 /(1+\delta)}{1-1 /(1+\delta)}=\frac{n}{\delta} e^{-\log (1+\delta) k}
\end{aligned}
$$

Therefore, we can take $A(\delta):=1 / \delta$ and $B(\delta):=\log (1+\delta)$.

The general procedure for designing an FPTAS with this lemma is:

1. Compute coefficients $a_{0}, \ldots, a_{k}$ of polynomial $P(z)$ (for some $k=\Theta(\log (n / \varepsilon))$ that will be given a precise value later).
2. From these, compute $b_{0}, \ldots, b_{k}$, the coefficients of the Taylor series of $\log P(z)$ around $z=0$.
3. Evaluate the truncated Taylor series $T_{k}(z)$ and output $e^{T_{k}(z)}$ as the approximation of $P(z)$.

With this general procedure we can proof a slightly weaker form of Theorem 3.4 but without using any of the correlation decay tools from the original proof of Weitz. We will use the following zero-freeness result from Shearer:

Lemma 3.13 (She85 ${ }^{6}$ ). Let $Z_{G}(\lambda)$ be the partition function of the hard-core model on a graph $G$ of maximum degree $\Delta$. Then, $Z_{G}(\lambda) \neq 0$ for any $\lambda \in \mathbb{C}$ with $|\lambda| \leq \tilde{\lambda}_{c}:=(\Delta-1)^{\Delta-1} / \Delta^{\Delta}$.

[^7]Theorem 3.14 (weaker form of Theorem 3.4). For a fixed $\Delta \geq 1$ and a fixed $\eta>0$, there exists an FPTAS for computing the partition function of the hard-core model $Z_{G}(\lambda)$ for any graph $G$ with maximum degree $\Delta$ and any $\lambda \leq(1-\eta) \tilde{\lambda}_{c}(\Delta)$, where $\tilde{\lambda}_{c}(\Delta):=(\Delta-1)^{\Delta-1} / \Delta^{\Delta}$.

Proof. We will start from the end. We want $e^{T_{k}(\lambda)}$ to be an $\varepsilon$-relative approximation of $Z_{G}(\lambda)$. We may assume $\varepsilon<1$, in which case it can be shown with basic calculus that $e^{\varepsilon / 2} \leq 1+\varepsilon$. Thus, it is enough to choose $k$ such that

$$
\left|T_{k}(\lambda)-\log \left(Z_{G}(\lambda)\right)\right| \leq \varepsilon / 2
$$

as this ensures that

$$
e^{\left|T_{k}(\lambda)-\log Z_{G}(\lambda)\right|} \leq e^{\varepsilon / 2} \leq 1+\varepsilon
$$

We obtain Equation 3.4 from Lemma 3.12, using for the zero-freeness Lemma 3.13. That tells us that we need $k$ such that

$$
\left|T_{k}(\lambda)-\log Z_{G}(\lambda)\right| \leq A n e^{-B k} \leq \varepsilon / 2 \Longleftrightarrow k \geq \frac{1}{B} \log \frac{2 A n}{\varepsilon}
$$

As mentioned before, the naive algorithm for computing the $j$-th coefficient of $Z_{G}(\lambda)$, has runtime $\mathcal{O}\left(n^{j}\right)$. Thus, computing the first $k$ coefficients would give an algorithm with runtime $n^{\mathcal{O}(\log (n / \varepsilon))}$ which is not polynomial on $n / \varepsilon$. Luckily, we can use a result by Patel and Regts [PR17] that proved that one can compute the first $k$ coefficients in time $\operatorname{poly}(n / \varepsilon){ }^{7}$.

Once we have computed the first coefficients of $Z_{G}(\lambda)$, we can use those to find the coefficients of the Taylor series of $\log Z_{G}(\lambda)$, by solving a linear system. Let $Z_{G}(\lambda)=\sum a_{j} \lambda^{j}$, and let $\log Z_{G}(\lambda)=$ $\sum b_{j} \lambda^{j}$. Then,

$$
\begin{gathered}
\sum j b_{j} \lambda^{j-1}=\frac{d}{d \lambda} \log Z_{G}(\lambda)=\frac{Z_{G}^{\prime}(\lambda)}{Z_{G}(\lambda)}=\frac{\sum j a_{j} \lambda^{j-1}}{\sum a_{j} \lambda^{j}} \Longrightarrow \\
\Longrightarrow \sum_{j \geq 1} j a_{j} \lambda^{j-1}=\sum_{j \geq 1} \sum_{i \geq 0} a_{i} \lambda^{i} b_{j} j \lambda^{j-1}=\sum_{i \geq 0} \sum_{j \geq 0} a_{i} b_{j+1}(j+1) \lambda^{i+j}
\end{gathered}
$$

Equating the terms with the same power of $\lambda$ on each side, we obtain a system of $k$ equations with variables $b_{1}, \ldots, b_{k}$ and coefficients that can be computed from $a_{0}, \ldots, a_{k}$. The first coefficient $b_{0}$ does not appear on the system, but can be obtained simply by $b_{0}=\log Z_{G}(0)=\log a_{0}$.

Remark. In comparison with Weitz's result, the result proven with Barvinok's method is slightly weaker, but it is a much more general procedure, that does not require much insight about the nature of the spin model (aside from proving the zero-freeness of the partition function).

[^8]
## Chapter 4

## Existence guarantees for colorings

### 4.1 Colorings with fixed color sizes

In the next chapter we study the problem of sampling proper colorings with color classes of fixed size. Before that, it is pertinent to consider under which conditions do such colorings exist.

Definition 4.1 ( $\mathbf{n}$-colorable). Fix $q \in \mathbb{Z}^{+}$and let $\mathbf{n}=\left(n_{1}, \ldots, n_{q}\right) \in \mathbb{Z}^{q}$, with $n_{i} \geq 1$ for all $i \in[q]$. We say a graph $G$ is $\mathbf{n}$-colorable if there exists a proper coloring $\chi: V(G) \longrightarrow[q]$ such that $|\{v \in V(G): \chi(v)=i\}|=n_{i}$ for all $i \in[q]$. That is, there exists a coloring in which there are $n_{1}$ vertices of color $1, n_{2}$ vertices of color 2 , and so on.

If we want to find a general result on the existence of $\mathbf{n}$-colorings, we must first impose some restrictions on the graph $G$, since for example $K_{n}$ does not accept any n-coloring except for the trivial one $\mathbf{n}=(1, \ldots, 1)$. A natural restriction is to impose that the maximum degree of the graph is smaller than a certain $\Delta:=\Delta(n)$. Thus, in the remaining of this chapter we will assume that $G$ is a graph of maximum degree $\Delta(G) \leq \Delta$.

Since every color class must be an independent set, all $n_{i}$ will be upper-bounded by the independence number $\alpha(G)$. In particular, if we want to derive a general result for all graphs of maximum degree $\Delta$, we need that $n_{i} \leq\lceil n /(\Delta+1)\rceil$, as the union of cliques $G=K_{\Delta+1} \sqcup \cdots \sqcup K_{\Delta+1} \sqcup K_{r}$ (where $r:=n \bmod (\Delta+1))$ has $\alpha(G)=\lceil n /(\Delta+1)\rceil$.

This bound is tight in the sense that there exists no other $G$ of maximum degree $\leq \Delta$ with smaller independence number, because we can always find an independent set of size $\lceil n /(\Delta+1)\rceil$ by the naive greedy algorithm (repeatedly adding an arbitrary vertex to the independent set and deleting its neighbours from the graph).

However, this does not guarantee that for any $\mathbf{n}$ with $n_{i} \leq\lceil n /(\Delta+1)\rceil$ there exists an $\mathbf{n}$-coloring, since after finding an independent set $I_{1}$ of size $n_{1}$ for color 1 , we are left with $\tilde{n}:=n-n_{1}$ vertices, while the new maximum degree $\tilde{\Delta}:=\Delta\left(G\left[V \backslash I_{1}\right]\right)$ might not have decreased at all. Thus, the
condition $n_{2} \leq\lceil\tilde{n} /(\tilde{\Delta}+1)\rceil$ might not hold.
Nevertheless, we conjecture that it's always possible to find a coloring if all $n_{i} \leq\lfloor n /(\Delta+1)\rfloor$ :
Conjecture 4.1. Let $G$ be a graph with $n$ vertices and maximum degree at most $\Delta$. Let $\mathbf{n}=$ $\left(n_{1}, \ldots, n_{q}\right) \in \mathbb{Z}^{q}$ be the desired color class sizes, with $\sum n_{i}=n$ and $1 \leq n_{i} \leq\lfloor n /(\Delta+1)\rfloor$ for all $i \in[q]$. Then $G$ is $\mathbf{n}$-colorable.

Remark. Though it is not explicitly required in the statement, notice that the two conditions $n_{i} \leq\lfloor n /(\Delta+1)\rfloor$ and $n=\sum n_{i}$ imply that the number of colors $q$ has to be at least $\Delta+1$.

Notice too that the conjecture can not be extended to $n_{i} \leq\lceil n /(\Delta+1)\rceil$, as the union of cliques $G=K_{\Delta+1} \sqcup \cdots \sqcup K_{\Delta+1} \sqcup K_{r}$ (for any $1 \leq r<\Delta+1$ ) would be a counterexample. That's because every color class of size $\lceil n /(\Delta+1)\rceil$ must contain a vertex from the $r$-clique, so at most there are $r$ of them.

However, we conjecture that this is the most limiting counterexample, in the sense that if we have $n=s(\Delta+1)+r$, we can always $\mathbf{n}$-color the graph if at most $r$ of the $n_{i}$ 's have size $\lceil n /(\Delta+1)\rceil=s+1$ (and the rest have size at most $\lfloor n /(\Delta+1)\rfloor=s$ ):

Conjecture 4.2. Let $G$ be a graph with $n$ vertices and maximum degree at most $\Delta$. Let $s$ and $r$ be the unique integers such that $n=s(\Delta+1)+r$ and $0 \leq r<\Delta+1$. Then, $G$ is $\mathbf{n}$-colorable for any $\mathbf{n}=$ $\left(n_{1}, \ldots, n_{q}\right) \in \mathbb{Z}^{q}$ such that $\sum_{i} n_{i}=n, 1 \leq n_{i} \leq s+1$ for all $i \in[q]$, and $\left|\left\{i \in[q]: n_{i}=s+1\right\}\right| \leq r$.

Remark. The last condition is saying that there can be at most $r$ color classes with size $s+1$, where $r$ is the residue of dividing $n$ by $\Delta+1$ and $s$ is the quotient rounded down. As commented before, this is tight for the union of cliques $G=\underbrace{K_{\Delta+1} \sqcup \cdots \sqcup K_{\Delta+1}}_{s} \sqcup K_{r}$ which does not have any colouring with more than $r$ color classes of size $s+1$.

There are two pieces of evidence in favor of these conjectures:

1. Conjecture 4.1 is a weaker corollary of Seymour's Conjecture on powers of Hamiltonian cycles, which was proved for sufficiently large $n$ by Komlós, Sárközy and Szemerédi in [KSS98].
2. One would expect that the hardest case to prove is when we have $q=\Delta+1$ colors and all the $n_{i}$ are either $\lceil n /(\Delta+1)\rceil$ or $\lfloor n /(\Delta+1)\rfloor$. However, this is equivalent to a conjecture of Erdös which was proved by Hajnal and Szemerédi in 1970 HS70] and has been known since as the Hajnal-Szemerédi Theorem on equitable colorings.

In the next two sections we will explore these two pieces of evidence. In particular, we will explain in detail a simpler proof of the Hajnal-Szemerédi Theorem found by Kierstead and Kostochka KK08, and we will discuss the difficulties of adapting this proof for Conjecture 4.1 .

### 4.2 Seymour's Conjecture

Definition 4.2 (Power of a graph). Let $G$ be a graph. We define the $k$-th power of $G$ as the graph formed by adding edges in between every pair of vertices $u, v$ with $d_{G}(u, v) \leq k$. In particular, the second power of a graph is called its square.

Seymour's Conjecture states that if the minimum degree of the graph is large enough, then the graph must contain a power of a Hamiltonian cycle. Historically, it was first formulated in the case $k=2$ by Pósa:

Conjecture 4.3 (Pósa). Let $n$ be the number of vertices of $G$. If $\delta(G) \geq 2 n / 3$, then $G$ must contain the square of a Hamiltonian cycle.

This conjecture in itself can be seen as a generalization of Dirac's Theorem, which states that any graph with $\delta(G) \geq n / 2$ must have a Hamiltonian cycle.

In 1974, Seymour conjectured that Pósa's Conjecture could be extended to higher powers:
Conjecture 4.4 (Seymour Sey74). Let $G$ be a graph with $n$ vertices, and let $k \in \mathbb{Z}^{+}$. If $\delta(G) \geq$ $\frac{k}{k+1} n$, then $G$ must contain the $k$-th power of a Hamiltonian cycle.

In particular, note that the case $k=1$ is Dirac's Theorem, while the case $k=2$ is Pósa's Conjecture.
Pósa's Conjecture, while not proven in its entirety, has been proven for graphs with $\delta(G)=$ $\left(\frac{2}{3}+\varepsilon\right) n+C(\varepsilon)$ FK95]. It has also been proven for the case where we only require the square of a Hamiltonian path, not a Hamiltonian cycle [FK96. In 1998, Seymour's Conjecture was proven for large enough $n$ by Komlós, Sárközy and Szemerédi KSS98] (extending a previous result on Pósa's Conjecture from two years prior [KSS96]), using the regularity method of the latter author. However, the general case remains open despite the conjecture being almost 50 years old.

We can relate Seymour's Conjecture to our coloring problem, by applying Seymour's Conjecture on the complement of the graph:

Proposition 4.5. Seymour's Conjecture (Conjecture 4.4) implies Conjecture 4.1.

Proof. Let $G$ be a graph with $n$ vertices and maximum degree at most $\Delta$. Let $n=s(\Delta+1)+r$, with $0 \leq r<\Delta+1$. In that case, Conjecture 4.1 states that for any $\mathbf{n} \in \mathbb{Z}^{q}$, with coordinates $1 \leq n_{i} \leq s$ and summing to $n$, we can get an $\mathbf{n}$-coloring of the graph. The idea is to apply Seymour's Conjecture to guarantee that $\bar{G}$ has the $(s-1)$ th-power of a Hamiltonian cycle. That would mean that there exists an ordering of the vertices of $G$ such that each vertex is not adjacent to any of the next $s-1$ or the previous $s-1$ vertices. Thus, we can find a proper coloring by taking the color classes to be contiguous subsets of vertices according to this ordering.

To apply Seymour's Theorem with $k=s-1$, we need $\delta(\bar{G}) \geq \frac{k}{k+1} n=\frac{s-1}{s} n$. Using that $\delta(\bar{G})=n-1-\Delta(G)$ and that $\Delta(G) \leq \Delta$, we have that

$$
\delta(\bar{G}) \geq n-(\Delta+1)=n-\left\lfloor\frac{n}{s}\right\rfloor \geq n\left(\frac{s-1}{s}\right)
$$

as desired.
Remark. It is not obvious whether Seymour's Conjecture implies the second form of the conjecture (Conjecture 4.2), which is stronger. Applying Seymour's Conjecture directly we only get the (s-1)th power of a Hamiltonian cycle, so we can't guarantee that we can find any color class of size $s+1$.

The usual trick to solve this problem would be to apply Seymour's Conjecture to the graph $\tilde{G}:=$ $G \sqcup K_{\Delta+1-r}$, which gives us the $s$-th power of a Hamiltonian cycle, and then discard the extra vertices of the clique we added. This way we can find an equitable $(\Delta+1)$-coloring (see the next section for the definition). Indeed, if we divide the Hamiltonian cycle into chunks of size $s+1$, we'll find that $\Delta+1-r$ of those have an extra vertex in them (which we discard, obtaining a color class of size $s$ ), while $r$ of them do not have an extra vertex (so we can take them to be the color classes of size $s+1$ ). Notice there can not be two extra vertices at distance less than $s$ in the cycle, since they are adjacent in $G$.

However, if we want to find a coloring where there are some color classes of size $s+1$ and some others of size strictly less than $s$ (as required by Conjecture 4.2), it might happen that we are not able to pack the small color classes in the space between classes of size $s+1$, rendering the previous approach invalid.

### 4.3 Equitable colorings

A special case of Conjecture 4.2 which appears frequently in real-life applications ${ }^{1}$ is the existence of equitable colorings.

Definition 4.3 (Equitable coloring). A $k$-coloring of a graph is called equitable if the sizes of the color classes differ at most by one. Equivalently, an equitable $k$-coloring is a coloring in which each color class has size either $\lfloor n / k\rfloor$ or $\lceil n / k\rceil$.

It is interesting to note that, in contrast to normal colorings, the existence of an equitable $k$-coloring for a fixed graph $G$ is not a monotone property in $k$. That is, there exists graphs such that there exists an equitable $k_{1}$-coloring but no equitable $k_{2}$-coloring, for some $k_{1}<k_{2}$. An easy example is the complete bipartite graph with odd number of vertices on each side: $K_{2 m+1,2 m+1}$. This graph is

[^9]equitably 2-colorable, since we can paint the two sides of the partition with opposite colors, but it has no equitable $(2 m+1)$-coloring, since its complement does not have a perfect matching.

This particular case also provides an example of a graph that has no equitable $\Delta(G)$-coloring. However, in 1964, Paul Erdös conjectured that any graph $G$ has an equitable $(\Delta(G)+1)$-coloring. Remark. Note that if all graphs $G$ have an equitable $(\Delta(G)+1)$-coloring, that automatically implies that all graphs with $\Delta(G) \leq \Delta$ have an equitable ( $\Delta+1$ )-coloring. Thus, we do not have to worry about the non-monotonicity issues mentioned earlier. That follows easily by induction on $\Delta-\Delta(G)$ : if we have a graph with $\Delta(G)+1<n$, we can add an edge to a vertex of maximum degree and apply the induction hypothesis to get a coloring, because the coloring will still be proper after removing the edge. If $\Delta(G)+1=n$ (so we can't add any edge to the vertex of maximum degree), the color classes have size at most 1 , so any assignment is a proper coloring.

This conjecture was proven by Hajnal and Szemerédi in 1970, becoming known as the HajnalSzemerédi Theorem:

Theorem 4.6 (Hajnal-Szemerédi [HS70]). Let $G$ be a graph of maximum degree at most $\Delta$. Then, $G$ has an equitable $(\Delta+1)$-coloring.

The original proof of the theorem is quite complicated, but there exists a much shorter proof published by Kierstead and Kostochka in 2008 [KK08]. In the rest of the section we will explain in detail the strategy that they follow, as we hope it will be useful for elucidating the difficulties that one finds when trying to extend their argument to prove Conjectures 4.1 and 4.2 .

Lemma 4.7. Let $n$ be the number of vertices of $G$. It suffices to prove the theorem for the case when $\Delta+1$ divides $n$.

Proof. Suppose we have proven the theorem for the case when $n$ is divisible by $\Delta+1$. We'll show that then the theorem also holds for a general $n$. Let $G$ be a graph of maximum degree at most $\Delta$ with $n=s(\Delta+1)+r$ vertices, where $0<r<\Delta+1$. Define a new graph $\tilde{G}=G \sqcup K_{\Delta+1-r}$ formed by adding a clique to $G$. This new graph has $n+(\Delta+1-r)=(s+1)(\Delta+1)$ vertices and degree at most $\Delta$, so by the hypothesis it must have an equitable $(\Delta+1)$-coloring $\tilde{\chi}$.

Let $\chi:=\left.\tilde{\chi}\right|_{G}$ be the restriction of that coloring to the original graph $G$. Since all the vertices in $\tilde{G}-G$ are pairwise adjacent, they must belong each to a different color class of $\tilde{\chi}$. Thus, the color classes of $\chi$ will have either the same number of vertices as in $\tilde{\chi}$, or one vertex less. Since all color classes of $\tilde{\chi}$ have $s+1$ vertices, the color classes of $\chi$ will have either $s$ or $s+1$ vertices. Thus, $\chi$ is an equitable coloring of $G$.

Thanks to this lemma, from now on we will assume that $G$ has $n=s(\Delta+1)$ vertices, for some $s \in \mathbb{Z}^{+}$. Thus, we want to find a $(\Delta+1)$-coloring in which every color class has size $s$. The idea of the proof will be that, by induction on the number of edges, we can assume we have a coloring that is almost equitable (in the sense that all color classes have size $s$ except two of them, which are
off by 1). By studying the structural properties of this type of colorings, we will prove that there exists some local change that allows us to transform it into an equitable coloring of $G$.

Definition 4.4 (nearly-equitable coloring). We say that $\chi: V(G) \longrightarrow[\Delta+1]$ is a nearly-equitable coloring if there exist $i_{+}, i_{-} \in[\Delta+1]$ such that

$$
\left|\chi^{-1}(i)\right|= \begin{cases}s, & \text { if } i \neq i_{+}, i_{-} \\ s+1, & \text { if } i=i_{+} \\ s-1, & \text { if } i=i_{-}\end{cases}
$$

for all $i \in[\Delta+1]$. We will use $V_{i}$ to refer to the set of vertices with color $i$, and $V_{+}, V_{-}$for the sets of vertices with color $i_{+}$and $i_{-}$, respectively.

Definition 4.5 (movable vertex, accessible color). Given a nearly-equitable coloring $\chi$ of $G$, we say that a vertex $v$ is movable to color $i$ if $v$ is not adjacent to any vertex of color $i$. That is, $v$ is movable to $i$ if setting $\chi(v) \leftarrow i$ does not create any conflict.

Let $H_{G, \chi}$ be the digraph with a vertex for each color (i.e. $V(H):=[\Delta+1]$ ) and with an arc $i \rightarrow j$ if there exists some vertex with color $i$ that is movable to color $j$. We say that a color $i$ is accessible if there exists a directed path in $H$ that goes from $i$ to $i_{-}$. Note that, by definition, $i_{-}$is always accessible.

Intuitively, if $i$ is an accessible color, that means that we can transfer a vertex from $i$ to $i_{-}$. Indeed, let $i=i_{1} \rightarrow \cdots \rightarrow i_{k}=i_{-}$be a simple path from $i$ to $i_{-}$in $H$. For every $j \in[k-1]$, let $v_{j}$ be a vertex with color $i_{j}$ that is movable to color $i_{j+1}$. Then, we can set $\chi\left(v_{j}\right) \leftarrow i_{j+1}$ for all $j \in[k-1]$, obtaining a coloring in which color class $i$ has one vertex less and color class $i_{-}$has one vertex more. Thus, if $i_{+}$were accessible, we would be able to transform the nearly-equitable coloring into the equitable coloring that we desire.

Given a general nearly-equitable coloring $\chi$, there is no guarantee of $i_{+}$being accessible. However, we will be able to prove that there is some kind of local change that either reduces the number of non-accessible colors by 1 , or allows us to construct directly an equitable coloring. Thus, after performing this local change a finite number of times, we will be able to get an equitable coloring of $G$.

Let $\mathcal{A}$ and $\mathcal{B}$ be the set of accessible and non-accessible colors. Let $q:=|\mathcal{B}|$ and $m:=|\mathcal{A}|-1$. By definition, $q+m+1=\Delta+1$, so $q+m=\Delta$. Let $A:=\bigcup_{i \in \mathcal{A}} V_{i}$ and $B:=\bigcup_{i \in \mathcal{B}} V_{i}$ be the sets of the vertices that are painted with colors from $\mathcal{A}$ and $\mathcal{B}$, respectively. Since we are assuming that $i_{+} \in \mathcal{B}$, we have that $|A|=(m+1) s-1$ and $|B|=q s+1$.

Lemma 4.8. There exists at least one other accessible color apart from $i_{-}$(that is, $m \geq 1$ ).

Proof. If $i_{-}$was the only accessible color, then $|B|=\Delta s+1$. But every $y \in B$ must be adjacent
to some vertex in $V_{-}$(otherwise $y$ would be movable to color $i_{-}$), so $|B| \leq\left|E\left(V_{-}, B\right)\right| \leq \Delta\left|V_{-}\right|=$ $\Delta(s-1)$, reaching a contradiction.

In a later step of the proof, we will find a certain vertex $z \in V_{j}$ for some color $j \in \mathcal{A}$, and change its color. We would like to chose $j$ so that when we change the color of any $z \in V_{j}$ all other colors from $\mathcal{A}$ keep being accessible. This motivates us to define terminal colors, the colors from which we can safely remove vertices without affecting the accessibility of any other color:

Definition 4.6 (terminal color). Given a color $j \in \mathcal{A}$, let

$$
\mathcal{A}_{j}^{\prime}:=\left\{i \in \mathcal{A} \backslash\{j\}: \nexists \text { path from } i \text { to } i_{-} \text {in } H[\mathcal{A} \backslash\{j\}]\right\} .
$$

We say that a color $j \in \mathcal{A}$ is terminal if $\mathcal{A}_{j}^{\prime}=\emptyset$.
Remark. There always exists at least one terminal color. To prove it, notice that we can construct a directed graph $\tilde{H}$ where the vertices are the colors from $\mathcal{A}$ and there is an edge $i \rightarrow j$ if all paths from $i$ to $i_{-}$in $H$ go through $j$. This vertex has no cycles, since otherwise we would have that there exist $i \neq j$ such that all paths from $i$ to $i_{-}$in $H$ go through $j$ and all paths from $j$ to $i_{-}$go through $i$. Any directed acyclic graph has a vertex with no incoming edges (the first one in a topological order), and this vertex will be a terminal color.

Definition 4.7. Let $j^{*}:=\underset{\text { non-terminal }}{\arg \min }\left|\mathcal{A}_{j}^{\prime}\right|$ be the non-terminal color that minimizes the number of disconnected colors. Let $\mathcal{A}^{\prime}:=\mathcal{A}_{j^{*}}^{\prime}$ and let $t:=\left|\mathcal{A}^{\prime}\right|$. Also, let $A^{\prime}:=\bigcup_{j \in \mathcal{A}^{\prime}} V_{j}$ be the vertices with color from $\mathcal{A}^{\prime}$.

Remark. Note that there is always some non-terminal color, because $\left|\mathcal{A}_{i_{-}}^{\prime}\right|=m \geq 1$.
We have defined $\mathcal{A}^{\prime}$ this way because then any $j \in \mathcal{A}^{\prime}$ is terminal (otherwise $\left|\mathcal{A}_{j}^{\prime}\right|<\left|\mathcal{A}_{j^{*}}^{\prime}\right|$, contradicting the minimality condition). However, we do not use at any other point the minimality, so any other $j$ such that $\mathcal{A}_{j}^{\prime}$ only has terminal colors would also have sufficed.
Next we prove a series of lemmas that will guarantee that we can find a $z \in A^{\prime}$ that allows us to do the local change.

Lemma 4.9. For all $z \in A^{\prime}, d_{B}(z) \leq q+t$.

Proof. By definition of $\mathcal{A}^{\prime}, z$ must be adjacent to vertices from all colors in $\mathcal{A} \backslash\left(\mathcal{A}^{\prime} \cup\left\{j^{*}\right\}\right)$, because otherwise $z$ would be movable to some color in $\mathcal{A} \backslash\left(\mathcal{A}^{\prime} \cup\left\{j^{*}\right\}\right)$, and from there it would be movable to color $i_{-}$without passing through color $j^{*}$. Thus, $d_{A}(z) \geq m+1-(t+1)=m-t$, so

$$
d_{B}(z)=\Delta-d_{A}(z) \leq(\Delta-m)+t=q+t
$$

Definition 4.8 (solo edges, solo vertices, solo neighbours). Let $z \in V_{j}$ for some color $j \in \mathcal{A}^{\prime}$, and let $y \in B$. We say that the edge $z y$ is a solo edge if $N_{V_{j}}(y)=\{z\}$ (i.e. $z$ is only neighbour of $y$ with color $j$, so we will be able to set $\chi(y) \leftarrow j$ if we recolor first $z$ with some other color). We refer to vertices that are the endpoints of some solo edge as solo vertices, and we say that two solo vertices that share a solo edge are solo neighbours of each other. We denote the set of solo neighbours of $z \in \mathcal{A}^{\prime}$ and $y \in B$ as $S_{z}$ and $S^{y}$, respectively.

Remark. We say that $y$ is a solo neighbor of $z$ if the edge $z y$ is a solo edge, but note that there might be neighbors of $z$ that are solo vertices but that are not solo neighbors of $z$ (because the edge $z y$ is not a solo edge).

Lemma 4.10. For any $y \in B,\left|S^{y}\right| \geq t-q+d_{B}(y)+1$.

Proof. Let $j \in \mathcal{A}^{\prime}$. If $j \notin S^{y}$, then $y$ has at least two neighbors in $V_{j}$. Thus,

$$
\left|S^{y}\right| \geq t-\left|\left\{j \in \mathcal{A}: d_{V_{j}}(y) \geq 2\right\}\right|
$$

Since the total degree of $y$ is at most $\Delta$,

$$
\Delta \geq d_{B}(y)+|\mathcal{A}|+\left|\left\{j \in \mathcal{A}: d_{V_{j}}(y) \geq 2\right\}\right| \Longrightarrow\left|\left\{j \in \mathcal{A}: d_{V_{j}}(y) \geq 2\right\}\right| \leq q-1-d_{B}(y)
$$

Plugging this into the previous expression yields the desired bound.
Lemma 4.11. If there exists a color $j \in \mathcal{A}^{\prime}$ such that no solo vertex $z \in V_{j}$ is movable to a color from $\mathcal{A} \backslash\{j\}$, then all $y \in B$ must be solo vertices, and we have that $t>q$.

Proof. The fact that all $y \in B$ are solo vertices follows from plugging $t>q$ into the previous lemma (we even get the stronger result $\left|S^{y}\right|>d_{B}(y)+1>0$ ). To see that $t>q$, we count the edges in between $V_{j}$ and $B$ in two ways.

Let $S$ be the set of solo vertices from $V_{j}$. Let $D:=V_{j} \backslash S$. By definition of $B$, no $y \in B$ is movable to color $j$, so every $y$ has a neighbor in $V_{j}$. Those that have exactly one neighbor must be from $N_{B}(S)$, since their neighbor in $V_{j}$ must be solo (however, note that some solo $z \in V_{j}$ can have a non-solo neighbor in $B$ ). Therefore,

$$
\left|E\left(V_{j}, B\right)\right| \geq|B|+\left(|B|-\left|N_{B}(S)\right|\right)=2(q s+1)-\left|N_{B}(S)\right|
$$

The condition that no $z \in V_{j}$ is movable to $\mathcal{A} \backslash\{j\}$ implies that it must be adjacent to at least one vertex from each of the $m$ other colors in $\mathcal{A}$. Thus, $d_{A}(z) \geq m$ and $d_{B}(z) \leq \Delta-m=q$. Using this, we get that $N_{B}(S) \leq q|S|$, so

$$
\left|E\left(V_{j}, B\right)\right| \geq 2(q s+1)-q|S|=q s+q|D|+2>q s+q|D|
$$

where we have used that $s=\left|V_{j}\right|=|S|+|D|$. On the other hand,

$$
\left|E\left(V_{j}, B\right)\right|=|E(S, B)|+|E(D, B)| \leq q|S|+(q+t)|D|=q s+t|D|
$$

where we have used that the maximum degree of $z \in V_{j}$ is at most $q$ if $z$ is solo (by the previous argument), and at most $q+t$ in general (by Lemma 4.9). Putting the two inequalities together, we get that

$$
q s+q|D|<\left|E\left(V_{j}, B\right)\right| \leq q s+t|D| \Longrightarrow q<t
$$

Lemma 4.12. Under the same hypothesis as Lemma 4.11, there must be a color $j \in \mathcal{A}^{\prime}$ and a solo vertex $z \in V_{j}$ such that $z$ has two solo neighbours $y_{1}, y_{2} \in B$ that are not adjacent.

Proof. Suppose not. As in Lemma 4.11, the proof will be based on double counting the edges between $A^{\prime}$ and $B$, but this time we will weight each edge depending on how many solo neighbors does the endpoint on $A^{\prime}$ have. Let $\mu: A^{\prime} \times B \longrightarrow \mathbb{R}^{\geq 0}$ be the weight function defined by

$$
\mu(z, y):= \begin{cases}q /\left|S_{z}\right|, & \text { if } z y \text { is a solo edge } \\ 0, & \text { otherwise }\end{cases}
$$

First, since every $z \in A^{\prime}$ has $\left|S_{z}\right|$ solo neighbors,

$$
\mu\left(A^{\prime}, B\right):=\sum_{z \in A^{\prime}} \sum_{y \in B} \mu(z, y)=\sum_{z \in A^{\prime}}\left|S_{z}\right| \frac{q}{\left|S_{z}\right|} \leq q\left|A^{\prime}\right|=q s t
$$

On the other hand, if we let $c_{y}:=\max _{z}\left|S_{z}\right|$ among all solo neighbors $z$ of a fixed $y \in B$, we get that

$$
\mu\left(A^{\prime}, B\right)=\sum_{y \in B} \mu\left(A^{\prime}, y\right) \geq \sum_{y \in B}\left|S^{y}\right| \frac{q}{c_{y}}
$$

By hypothesis, all solo neighbors of a fixed $z$ form a clique, so $c_{y}=\max _{z}\left|S_{z}\right| \leq d_{B}(y)+1$. Hence, using Lemma 4.10 ,

$$
\left|S^{y}\right| \geq t-q+d_{B}(y)+1 \geq t-q+c_{y}
$$

so

$$
\mu\left(A^{\prime}, B\right) \geq \sum_{y \in B}\left(t-q+c_{y}\right) \frac{q}{c_{y}} \geq \sum_{y \in B}(t-q) \frac{q}{c_{y}}+q \geq \sum_{y \in B} t-q+q \geq t|B|=t(q s+1)
$$

where we have used that $t-q \geq 0$ (by Lemma 4.11) and that $q / c_{y} \geq 1$. This follows from the
fact that any $y \in B$ must be adjacent to a vertex from every color class in $\mathcal{A}^{\prime}$ (in order to not be movable), so

$$
d_{A}(y) \geq m+1 \Longrightarrow d_{B}(y) \leq q-1 \Longrightarrow q-1 \geq d_{B}(y) \geq c_{y}-1 \Longrightarrow q \geq c_{y}
$$

We have seen that $t(q s+1) \leq \mu\left(A^{\prime}, B\right) \leq t q s$, which (since $t>0$ by definition) constitutes a contradiction. Therefore, the assumption that all the solo neighbors from every $z$ form a clique must be incorrect.

We end this section by proving Theorem 4.6, since this last lemma gives us a sufficient condition for the inductive argument that we sketched before to work:

Proof. (Theorem 4.6). By Lemma 4.7, we may assume that the graph has $n=s(\Delta+1)$ vertices, where $s \in \mathbb{Z}^{+}$. The proof proceeds by induction on the number of edges of the graph. For $|E(G)|=0$, all colorings are proper so there is nothing to prove. Now, for the inductive step, take an arbitrary edge $e=x y \in E(G)$ and find an equitable coloring $\chi^{\prime}$ of $G-e$. If $\chi^{\prime}(x) \neq \chi^{\prime}(y)$, this also constitutes a proper coloring of $G$, so we are finished. Otherwise, find a color $c \notin \chi^{\prime}(N(x))$ and set $\chi^{\prime}(x) \leftarrow c$ (the existence of such a color is guaranteed by the fact that we have $\Delta+1$ possible colors, while $|N(x)| \leq \Delta(G) \leq \Delta)$. With this change, $\chi^{\prime}$ will be a nearly-equitable coloring, in which all color classes will have $s$ vertices with the exception of colors $i_{+}$and $i_{-}$, that will have $s+1$ and $s-1$ colors, respectively.

We build the accessibility digraph $H$, and we let $q:=|\mathcal{B}|$ be the number of non-accessible colors. As explained before, if $i_{+}$is accessible we are done, since we can exchange colors among a simple path between $i_{+}$and $i_{-}$, getting an equitable coloring.

Otherwise, by Lemma 4.12, there either exists a color $j \in \mathcal{A}^{\prime}$ and a solo vertex $z \in V_{j}$ such that $z$ is movable to $\mathcal{A} \backslash\{j\}$, or there exists a color $j \in \mathcal{A}^{\prime}$ and a solo vertex $z \in V_{j}$ such that $z$ has two non-adjacent solo neighbors $y_{1}$ and $y_{2}$.

In the first case, let $y$ be one of the solo neighbors of $z$. By hypothesis we can move $z$ to a color from $\mathcal{A} \backslash\{z\}$, and then transfer a vertex from this color to $i_{-}$(having moved $z$ does not affect the accessibility of any other color, since $j \in \mathcal{A}^{\prime}$, so it is terminal). Once we have moved $z$ out of $V_{j}$, we can recolor vertex $y$ with color $j$ without creating any conflict, since $z y$ was a solo edge. Hence, all color classes of $\mathcal{A}$ are now of size $s$. We can recolor the rest of the graph with the inductive hypothesis. Recall that all vertices in $B \backslash\{y\}$ have to be adjacent to some vertex from every one of the $m+1$ color classes in $\mathcal{A}$, since otherwise we would be able to move them to that color. Therefore, for any $\tilde{y} \in B \backslash\{y\}, d_{A}(\tilde{y}) \geq m+1$ so

$$
d_{B \backslash\{y\}}(\tilde{y}) \leq d_{B}(\tilde{y}) \leq \Delta-(m+1)=q-1
$$

Hence, $B \backslash\{y\}$ induces a graph with $(q s+1)-1=q s$ vertices and maximum degree $\leq q-1$. By
the inductive hypothesis ${ }^{2}$, this graph is equitably $q$-colorable, which together with the coloring on $A \cup\{y\}$ gives us an equitable $(\Delta+1)$-coloring of the whole graph $G$.

In the second case, we also move $y_{1}$ to color $j$. This creates a conflict with $z$ that we can not solve as in the previous case, because $z$ is not movable to any color in $\mathcal{A} \backslash\{j\}$. However, this also implies that $d_{A}(z) \geq m$, so $d_{B \backslash\{y\}}(z) \leq q-1$. Hence, there exists some color in $\mathcal{B}$ to which we can now move $z$. After this change, the coloring in $\mathcal{B}$ might not even be nearly-equitable, but by the same argument of the previous case, we can recolor it using the induction hypothesis to obtain a nearly-equitable $q$-coloring where all colors have $s$ vertices except one that has $s+1$. Thus, the coloring of the whole graph is still nearly-equitable after the change. The difference is that now $z$ is no longer colored with color $j$, so $y_{2}$ (that was a solo neighbor of $z$ ) is now movable to color $j$. Then, the nearly-equitable coloring that we have obtained has one non-accessible color less than the nearly-equitable coloring we started with.

Therefore, in the first case we obtain directly the equitable coloring we are looking for, while in the second case we decrease the number of non-accessible colors by 1 . Thus, after repeating this procedure at most $q$ times, $i_{+}$becomes accessible and we are able to obtain an equitable coloring.

The main difficulty in adapting Kierstead and Kostochka's proof to Conjecture 4.1 is that we do not have any lower bound on the size of the color classes, so the arguments based on double counting edges do not work.

Intuitively, it seems that having color classes of smaller size would only give us more leeway to find a proper coloring, but we have not been able to find an alternative argument for proving the analogous results to Lemmas 4.11 and 4.12 .

[^10]
## Chapter 5

## Sampling objects of fixed size

In chapter 3 we have discussed the problem of approximating the partition function $Z_{G}(\beta)$ (or, equivalently, sampling a configuration $\left.\sigma \sim \mu_{G, \beta}\right)$. Note that, for spin models in finite graphs, we can always express the partition function as a polynomial $Z_{G}(\lambda)$, by defining the fugacity in terms of $\beta$ appropiately and re-scaling if necessary the Hamiltonian.

Then, as a natural extension to the problem of approximating $Z_{G}(\lambda)$, we can ask whether we can compute approximately the $k$-th coefficient of $Z_{G}(\lambda)$, for some specific $\lambda$ and $k$. In sampling terms, this corresponds to asking for a sampling algorithm that gives us a configuration $\sigma$ distributed uniformly among all the ones with $\mathcal{H}(\sigma)=k$, for a certain $k$.

For the case of independent sets, we will describe the advances that have happened in the last 2 years, that have led to an almost complete solution of the problem. For the case of colorings, very little is known yet, but we sketch a future plan of research, using the same general ideas that are behind the new results on independent sets.

### 5.1 Independent sets

In the hard-core model, the partition function is $Z_{G}(\lambda)=\sum_{k=0}^{n} i_{k}(G) \lambda^{k}$, so the problem of approximating the $k$-th coefficient $\left[\lambda^{k}\right] Z_{G}(\lambda)$ is the same as approximately counting the number of independent sets of size $k$.

Instead of working with the size of the independent set, we will work with the density with respect to the total number of vertices: $\alpha:=k / n$. It turns out that there exists a critical value of density beyond which the problem becomes intractable:

Theorem 5.1 (Theorem 1 from [DP23). For fixed $\Delta$, there exists a critical density $\alpha_{c}(\Delta):=$ $\lambda_{c}(\Delta) /\left(1+(\Delta+1) \lambda_{c}(\Delta)\right)$ such that

- for $\alpha<\alpha_{c}$, there exists an FPRAS for computing $i_{\lfloor\alpha n\rfloor}(G)$ for the class of graphs of maximum
degree $\Delta$.
- for $\alpha>\alpha_{c}$, unless $N P=R P$, there exists no FPRAS for computing $i_{\lfloor\alpha n\rfloor}(G)$ for the class of graphs of maximum degree $\Delta$.

Remark. The critical density $\alpha_{c}(\Delta)$ is expressed in function of the critical fugacity $\lambda_{c}(\Delta):=(\Delta-$ $1)^{\Delta-1} /(\Delta-2)^{\Delta}$, which we have seen in chapter 3 that constitutes the threshold for approximating $Z_{G}(\lambda)$ for graphs of maximum degree $\Delta$. Furthermore, one might notice that $\lambda /(1+(\Delta+1) \lambda)$ is the expected density of an independent set drawn according to the hard-core model in $K_{\Delta+1}$. It can be proven that the graph $K_{\Delta+1}$ is the one that minimizes this quantity over all graphs of maximum degree $\Delta$ (though not explicitly mentioned, it can be derived from [CR13, c.f. Exercise 13 from [Per22]). Thus, a qualitative interpretation of Theorem 5.1 is that we can only sample independent sets that would be of "below-average size" at the maximum "tractable fugacity" (i.e. the maximum fugacity at which we can approximate $Z_{G}(\lambda)$ efficiently).

In their original paper, Davies and Perkins left the question of finding an FPTAS as an open problem, but it was resolved shortly after by the second author together with Jain, Sah and Sawhney:

Theorem 5.2 (Theorem 1.2 from [JPSS21]). For a fixed maximum degree $\Delta$ and a fixed $\delta>0$, there exists an FPTAS that computes $i_{\lfloor\alpha n\rfloor}(G)$ for any $\alpha \leq(1-\delta) \alpha_{c}(\Delta)$ and any $G$ of maximum degree $\Delta$.

The proof used in this second paper is the main inspiration behind the research plan that we describe in the next section to construct an approximate randomized sampler of colorings with fixed color sizes.

### 5.2 Colorings

### 5.2.1 Description of the model

We will now turn our attention to the problem of sampling colorings with given color class sizes. Recall from the previous chapter that, for a given $\mathbf{n}=\left(n_{1}, \ldots, n_{q}\right) \in\left(\mathbb{Z}^{+}\right)^{q}$ and a graph $G$ with $n:=\sum n_{i}$ vertices, we defined an $\mathbf{n}$-coloring of $G$ as a proper coloring of the vertices of $G$ such that for each $i \in[q]$ there are exactly $n_{i}$ vertices painted with color $i$.

Using this notation, we would like to find an algorithm that, given a graph $G$ and a vector $\mathbf{n}$ as inputs, together with a tolerance value $\varepsilon>0$, returns an $\mathbf{n}$-coloring of $G$ chosen approximately uniformly at random (i.e. within total variation distance $\varepsilon$ of the uniform distribution on the set of all possible $\mathbf{n}$-colorings). By the self-reducibility property from chapter 3, that's equivalent to finding an FPTAS that computes the number of $\mathbf{n}$-colorings within a given relative error $\varepsilon>0$. In fact, even just obtaining a randomized sampler (or equivalently, an FPRAS) would already constitute an important advance compared with the current state of the art.

In the previous chapter we explored what conditions do we need to impose on the $n_{i}$ so that we can guarantee the existence of an $\mathbf{n}$-coloring for any graph $G$ with a given maximum degree. From now on, we will assume that the given $\mathbf{n}$ and $G$ always allow us to find at least one such coloring, so the expected outcome of the algorithm is always well-defined.

This problem can be seen as a natural generalization of the problem of sampling an independent set of a given size, since sampling a $q$-coloring is akin to sampling $q$ disjoint independent sets. Indeed, we will follow a very similar framework to the one from the previous section, where instead of studying the random variable $X=|I|$, the size of an independent set $I$ chosen according to the the hard-core model, we will study the random vector $X=\left(X_{1}, \ldots, X_{q}\right)^{T}$, the color sizes from a $q$-coloring chosen according to the Potts model (with hard constraints). However, the interaction between the different colors presents some difficulties that do not appear in the univariate case.

Definition 5.1 (Potts model with hard constraints). Given a graph $G$ and a positive integer $q$, let $\sigma: V(G) \longrightarrow[q]$ be an assignment of one of $q$ different spins (that we will refer to as colors) to each vertex of $G$, and let $\Sigma$ be the set of all possible assignments. Given $q$ parameters $\lambda_{1}, \ldots, \lambda_{q} \in \mathbb{R}^{+}$, we define a probability distribution on $\Sigma$ where each $\sigma \in \Sigma$ is chosen with probability

$$
\mu_{G, \lambda}(\sigma) \propto \begin{cases}\prod_{v \in V} \lambda_{\sigma_{v}}, & \text { if } \sigma \text { is a proper coloring } \\ 0, & \text { otherwise }\end{cases}
$$

This measure corresponds to the Potts model with an external field that interacts differently with each of the $q$ spins (spins with greater $\lambda_{i}$ are favored) and with a hard constraint on the edges (so configurations with monochromatic edges have infinite energy, and their Gibbs measure vanishes). Sometimes we will refer to the activity parameters together as $\boldsymbol{\lambda}:=\left(\lambda_{1}, \ldots, \lambda_{q}\right)^{T}$, and denote the partition function of the model as $Z(\boldsymbol{\lambda})$ or $Z\left(\lambda_{1}, \ldots, \lambda_{q}\right)$ indistinctly. For a fixed $\boldsymbol{\lambda}$, we will denote by $\mathbf{X}=\left(X_{1}, \ldots, X_{q}\right)^{T}$ the random vector of color class sizes according to this model. That is, $\mathbf{X}$ is a random variable with the following distribution:

$$
\operatorname{Pr}\left[\mathbf{X}=\left(x_{1}, \ldots, x_{q}\right)^{T}\right]:=\sum_{\substack{\sigma \in \Sigma: \forall i \\\left|\sigma^{-1}(i)\right|=x_{i}}} \mu_{G, \boldsymbol{\lambda}}(\sigma)=\frac{c_{x_{1}, \ldots, x_{q}} \lambda_{1}^{x_{1}} \cdots \lambda_{q}^{x_{q}}}{Z(\boldsymbol{\lambda})}
$$

where $c_{x_{1}, \ldots, x_{q}}$ is the number of colorings (i.e. spin assignments) that have $x_{i}$ vertices with color $i$ for each $i \in[q]$.

Note that the $X_{i}$ are not independent, and in fact have negative correlation (due to the fact that $X_{1}+\cdots+X_{q}=n$ ). Besides, the colors are not indistinguishable, since the $\lambda_{i}$ might be different for each one. However, for the case were all the activities are equal, we can actually characterize their correlation matrix:

Proposition 5.3. Suppose $\boldsymbol{\lambda}=(\lambda, \ldots, \lambda)$ for some $\lambda \in \mathbb{R}^{+}$. Let $\sigma^{2}:=\operatorname{Var} X_{1}$. Then,

$$
\operatorname{Cov} \mathbf{X}=\sigma^{2} \cdot\left(\begin{array}{ccccc}
1 & \frac{-1}{q-1} & \cdots & \cdots & \frac{-1}{q-1} \\
\frac{-1}{q-1} & 1 & \ddots & & \vdots \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
\vdots & & \ddots & 1 & \frac{-1}{q-1} \\
\frac{-1}{q-1} & \cdots & \cdots & \frac{-1}{q-1} & 1
\end{array}\right)=\frac{\sigma^{2}}{q-1}\left(q \cdot \mathbb{I}_{q}-\mathbf{1} \cdot \mathbf{1}^{T}\right)
$$

Proof. In the case where $\boldsymbol{\lambda}$ is a constant vector, $\mu_{G, \boldsymbol{\lambda}}$ is symmetric with respect to the $X_{i}$, so it is clear that $\operatorname{Var} X_{1}=\cdots=\operatorname{Var} X_{q}=\sigma^{2}$. Besides, even if we condition on the value of a certain $X_{i}$, all the $X_{j}$ with $j \neq i$ still are indistinguishable and have the same distribution, so $\operatorname{Cov}\left[X_{i}, X_{j}\right]=\operatorname{Cov}\left[X_{i}, X_{k}\right]$ for all $j, k \neq i$. Therefore, as $\operatorname{Cov} X$ is symmetric, the values outside of the diagonal are all equal to each other. Let $c \in \mathbb{R}$ be the value that they take.

Using that $X_{1}+\cdots+X_{q}=n$, we have

$$
\begin{aligned}
\operatorname{Var} X_{i} & =\operatorname{Cov}\left[X_{i}, n-\sum_{j \neq i} X_{j}\right]=\mathbb{E}\left[X_{i}\left(n-\sum_{j \neq i} X_{j}\right)\right]-\mathbb{E}\left[X_{i}\right] \mathbb{E}\left[n-\sum_{j \neq i} X_{j}\right]= \\
& =-\sum_{j \neq i}\left(\mathbb{E}\left[X_{i} X_{j}\right]-\mathbb{E}\left[X_{i}\right] \mathbb{E}\left[X_{j}\right]\right)=-(q-1) c
\end{aligned}
$$

Thus, $c=-\frac{\sigma^{2}}{q-1}$, and the covariance matrix takes the claimed form.

### 5.2.2 Future directions

Our plan to construct a sampler for colorings with given color sizes is the following:

1. Find a zero-free region for $Z_{G}(\boldsymbol{\lambda})$ around 1. It does not need to be strictly a disk, as we can apply a transformation to the domain before applying Barvinok's argument, as they do in SS19.
2. Use the zero-free region to prove a multivariate Central Limit Theorem for an $X \sim \mu_{G, \boldsymbol{\lambda}}$, for $\boldsymbol{\lambda}$ in a (maybe smaller) disk around $\mathbf{1}$.
3. From the Central Limit Theorem, derive a Local Central Limit Theorem, by combining bounds on the characteristic function with the Fourier inversion arguments from the proof of Theorem 20 from JPP22.
4. Use the Local Central Limit Theorem together with an FPRAS of the partition function to find an FPRAS for the number of colorings of a given size, as it is done in JPSS21 for the hard-core model.

For step 1, current zero-free regions in the Potts model are for the case where there is no hardconstraint and instead each monochromatic edge is penalized by a factor of $\omega$, for some $\omega \in \mathbb{C}$. In that case, there are zero-free results for $Z_{G}(\omega)$ (under a model with fixed homogeneous fugacity $\boldsymbol{\lambda}=(1, \ldots, 1)$, but it is not clear how to translate them into zero-free results on $Z_{G}(\boldsymbol{\lambda})$, where we take the fugacity of each vertex to be different and we set $\omega=0$.

We believe to have solved step 2, using an argument inspired by the techniques from GLP16. However, we are still unsure about some of the technical details, so we will refrain from claiming the result yet.

For step 4, we need an FPRAS for the partition function. At first we thought that we could use the same method as in 3.14 , as Lemma 3.12 can be extended to the multivariate case, by defining an appropriate auxiliary univariate polynomial that is zero-free in a disk around 0 :

Lemma 5.4. Let $P(\mathbf{z}): \mathbb{C}^{q} \longrightarrow \mathbb{C}$ be a multivariate polynomial with degree $N$ (we are defining the degree of a monomial as the sum of the degrees of each variable) and independent term $p_{0} \in \mathbb{R}^{+}$. Suppose there exist $R>0, \varepsilon>0$ and $\mathbf{z}_{\mathbf{0}} \in \mathbb{C}^{q}$ such that $P(\mathbf{z}) \neq 0$ for all $\mathbf{z} \in B\left(\mathbf{z}_{\mathbf{0}},(1+\varepsilon) R\right)$. For $a$ $\mathbf{z} \in \overline{B\left(\mathbf{z}_{\mathbf{0}}, R\right)}$, consider the Taylor series of $\log P$ at $\mathbf{z}$ expanded around $\mathbf{z}_{\mathbf{0}}$, and let $T_{k}(\mathbf{z})$ be its $k$-th order truncation. Then, $\left\{T_{k}(\mathbf{z})\right\}_{k \geq 1}$ converges exponentially to $\log P(\mathbf{z})$, i.e. there exist constants $A(\varepsilon)$ and $B(\varepsilon)$ independent of $\mathbf{z}$ and $N$ such that

$$
\left|\log P(\mathbf{z})-T_{k}(\mathbf{z})\right| \leq A N e^{-B k}
$$

Proof. Fix a certain $\mathbf{z} \in \overline{B\left(\mathbf{z}_{\mathbf{0}}, R\right)}$. We define an auxiliary univariate polynomial $\tilde{P}_{\mathbf{z}}(t): \mathbb{C} \longrightarrow \mathbb{C}$ such that $\tilde{P}_{\mathbf{z}}(t):=P\left((1-t) \mathbf{z}_{\mathbf{0}}+t \mathbf{z}\right)$. Then, we have that $\tilde{P}_{\mathbf{z}}(0)=P\left(\mathbf{z}_{\mathbf{0}}\right)$ and $\tilde{P}_{\mathbf{z}}(1)=P(\mathbf{z})$. Besides, we know that $\tilde{P}_{\mathbf{z}}(t) \neq 0$ for all $t \in B(0,1+\varepsilon)$, since P is zero-free in $B\left(\mathbf{z}_{\mathbf{0}},(1+\varepsilon) R\right)$ and

$$
\left\|\left((1-t) \mathbf{z}_{\mathbf{0}}+t \mathbf{z}\right)-\mathbf{z}_{\mathbf{0}}\right\|=|t| \cdot\left\|\mathbf{z}-\mathbf{z}_{\mathbf{0}}\right\| \leq|t| R<(1+\varepsilon) R
$$

Therefore, using Lemma 3.12 , there exist $A(\varepsilon)$ and $B(\varepsilon)$ such that

$$
\left|\log \tilde{P}_{\mathbf{z}}(t)-\tilde{T}_{k, \mathbf{z}}(t)\right| \leq A N e^{-B k}
$$

for any $t \in \overline{B(0,1)}$, where $k \in \mathbb{Z}^{+}$and $\tilde{T}_{k, \mathbf{z}}$ is the $k$-th order truncation of the Taylor series of $\log \tilde{P}_{\mathbf{z}}$. In particular, for $t=1, \log \tilde{P}_{\mathbf{z}}(1)=\log P(\mathbf{z})$ and $\tilde{T}_{k, \mathbf{z}}(1)=T_{k}(\mathbf{z})$, so we obtain the desired result.

Remark. In the previous proof we claimed that $\tilde{T}_{k, \mathbf{z}}(1)=T_{k}(\mathbf{z})$. This follows from a simple (but tedious) computation. On the one hand, the multivariate Taylor series of $\log P$ is

$$
T_{k}(\mathbf{z})=\sum_{m \geq 0}^{k} \frac{1}{m!} \sum_{i_{1}, \ldots, i_{m}=1}^{q} \frac{\partial^{m} \log P}{\partial z_{i_{1}} \cdots \partial z_{i_{m}}}(\mathbf{z}) \cdot \prod_{j=1}^{m}\left(z_{i_{j}}-z_{0, i_{j}}\right)
$$

On the other hand, the univariate Taylor series of $\log \tilde{P}_{\mathbf{z}}$ is

$$
\tilde{T}_{k, \mathbf{z}}\left(t_{0}\right)=\sum_{m \geq 0}^{k} \frac{t_{0}^{m}}{m!} \frac{d^{m}}{d t^{m}}\left(\log P\left(\mathbf{z}_{\mathbf{0}}+t\left(\mathbf{z}-\mathbf{z}_{\mathbf{0}}\right)\right)\right)\left(t_{0}\right)
$$

Therefore, in order to prove that $T_{k}(\mathbf{z})=\tilde{T}_{k, \mathbf{z}}(1)$, it is enough to show that

$$
\frac{d^{m}}{d t^{m}}\left(\log P\left(\mathbf{z}_{\mathbf{0}}+t\left(\mathbf{z}-\mathbf{z}_{\mathbf{0}}\right)\right)\right)=\sum_{i_{1}, \ldots, i_{m}=1}^{q} \frac{\partial^{m} \log P}{\partial z_{i_{1}} \cdots \partial z_{i_{m}}}\left(\mathbf{z}_{\mathbf{0}}+t\left(\mathbf{z}-\mathbf{z}_{\mathbf{0}}\right)\right) \prod_{j=1}^{m}\left(z_{i_{j}}-z_{0, i_{j}}\right)
$$

We can prove it by induction on $m$. For the base case $m=0$, both sides reduce to $\log P\left(\mathbf{z}_{\mathbf{0}}+t(\mathbf{z}-\right.$ $\left.\mathbf{z}_{\mathbf{0}}\right)$ ). Now, suppose that the claim is true for a certain $m \geq 0$. Then,

$$
\begin{aligned}
\frac{d^{m+1}}{d t^{m+1}} & \left(\log P\left(\mathbf{z}_{\mathbf{0}}+t\left(\mathbf{z}-\mathbf{z}_{\mathbf{0}}\right)\right)\right)=\frac{d}{d t}\left(\sum_{i_{1}, \ldots, i_{m}=1}^{q} \frac{\partial^{m} \log P}{\partial z_{i_{1}} \cdots \partial z_{i_{m}}}\left(\mathbf{z}_{\mathbf{0}}+t\left(\mathbf{z}-\mathbf{z}_{\mathbf{0}}\right)\right) \prod_{j=1}^{m}\left(z_{i_{j}}-z_{0, i_{j}}\right)\right)= \\
& =\sum_{i_{1}, \ldots, i_{m}=1}^{q} \prod_{j=1}^{m}\left(z_{i_{j}}-z_{0, i_{j}}\right) \sum_{i_{m+1}=1}^{q}\left(z_{i_{m+1}}-z_{0, i_{m+1}}\right) \frac{\partial}{\partial z_{i_{m+1}}} \frac{\partial^{m} \log P}{\partial z_{i_{1}} \cdots \partial z_{i_{m}}}\left(\mathbf{z}_{\mathbf{0}}+t\left(\mathbf{z}-\mathbf{z}_{\mathbf{0}}\right)\right)= \\
& =\sum_{i_{1}, \ldots i_{m+1}=1}^{q} \prod_{j=1}^{m+1}\left(z_{i_{j}}-z_{0, i_{j}}\right) \frac{\partial^{m+1} \log P}{\partial z_{i_{1}} \cdots \partial z_{i_{m+1}}}\left(\mathbf{z}_{\mathbf{0}}+t\left(\mathbf{z}-\mathbf{z}_{\mathbf{0}}\right)\right)
\end{aligned}
$$

so the claim also holds for $m+1$.
However, we find several difficulties when adapting the argument to the multivariate case. The foremost one is that the partition function from the Potts model does not satisfy the BIGCP condition from [PR17], so we can not use their result to compute the first $\Theta(\log (n / \varepsilon))$ coefficients in time $\operatorname{poly}(n / \varepsilon)$.

An alternative approach, that might provide better results, is to use the Monte Carlo Markov Chain method, which is based on constructing a Markov Chain on the space of spin configurations that has the desired distribution as its equilibrium distribution, and then proving that the mixing time of the Markov Chain is logarithmic in the size of the state space, so the chain mixes after poly $(n / \varepsilon)$-many steps. This approach gives us a very simple implementation of an FPRAS, but it is usually very hard to prove that the chain mixes fast.

In fact, for general $q$-colorings it is believed that the Glauber dynamics Markov Chain should be rapidly mixing as long as $q \geq \Delta+2$, but the currently best-known bound is $q \geq(11 / 6-\delta) \Delta$, for some constant $\delta>0\left[\mathrm{CDM}^{+} 18\right]$.

The Glauber dynamics does not work for coloring with fixed color sizes, as the sizes of the colors change arbitrarily during the execution of the algorithm. However, results for objects with fixed sizes are not unheard of with this approach. As an example, a very recent (10th of May!) preprint claims to have proved that a certain Markov Chain for the hard-core model that preserves the size
of the independent set mixes rapidly for any size $k \leq(1-\delta) n \alpha_{c}(\Delta)$ JMPV23, matching the result of Theorem 5.2, and resolving a conjecture from [DP23].

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[^0]:    ${ }^{1}$ We could also consider a more general model in which we also include $k$-way interactions, for $k>2$. Then, the graph $G$ would be substituted with a non-uniform hypergraph, and the Hamiltonian could potentially have a contribution from every hyperedge of this hypergraph.

[^1]:    ${ }^{2}$ We will not consider the case where $\beta<0$, as then the temperature would be negative and the analogy would be broken.

[^2]:    ${ }^{3}$ If one wants to extend it to $q$-spin systems, for $q>2$, then marginals can no longer be expressed as a scalar, but as a probability distribution on the set of spins, so the definitions are more cumbersome.

[^3]:    ${ }^{1}$ The problem of weighted sampling is only well-defined if at least one of the weights is non-zero.

[^4]:    ${ }^{2}$ Technically that's except in the case $R_{G, v}=+\infty$, in which it stays the same.

[^5]:    ${ }^{3}$ If we want to minimize the error, we can choose the mean, while if we want to give one-sided error we can choose either the lower or the upper bound.

[^6]:    ${ }^{4}$ That's provided that in the beginning the activities were all the same. Otherwise one can find counterexamples.

[^7]:    ${ }^{5}$ Because $P(z)=p_{0} \prod_{j}\left(1-z / \xi_{j}\right)$ and the logarithm as a formal power series also satisfies the typical property of $\log \left(z_{1} z_{2}\right)=\log \left(z_{1}\right)+\log \left(z_{2}\right)$.
    ${ }^{6}$ The original result in Shearer's paper She85 is stated in terms of sufficient conditions for the LLL to hold. One can check $\mathrm{SS05}$ or Per 22 for an explanation of the relation between the Local Lemma and the zeros of the independence polynomial of a graph of bounded maximum degree.

[^8]:    ${ }^{7}$ In fact, they prove it for a larger class of polynomials called bounded induced graph counting polynomials, of which the independence polynomial is a particular case.

[^9]:    ${ }^{1}$ That's because it models the problem of distributing $n$ equally-time-consuming duties as evenly as possible among $k$ people (or threads, or servers, ...), where some pairs of duties are restricted and can't be performed by the same person.

[^10]:    ${ }^{2}$ We can apply the induction hypothesis because $G[B \backslash\{y\}]$ has less edges than $G$. For example, it does not contain the edge $z y$.

