Analyzing Boltzmann Samplers for Bose–Einstein Condensates with Dirichlet Generating Functions

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Abstract

Boltzmann sampling is commonly used to uniformly sample objects of a particular size from large combinatorial sets. For this technique to be effective, one needs to prove that (1) the sampling procedure is efficient and (2) objects of the desired size are generated with sufficiently high probability. We use this approach to give a provably efficient sampling algorithm for a class of weighted integer partitions related to Bose–Einstein condensation from statistical physics. Our sampling algorithm is a probabilistic interpretation of the ordinary generating function for these objects, derived from the symbolic method of analytic combinatorics. Using the Khintchine-Meinardus probabilistic method to bound the rejection rate of our Boltzmann sampler through singularity analysis of Dirichlet generating functions, we offer an alternative approach to analyze Boltzmann samplers for objects with multiplicative structure.

1 Introduction

Bose–Einstein condensation occurs when subatomic particles known as bosons are cooled to nearly absolute zero. These particles behave as waves due to their quantum nature and as their temperature decreases, their wavelength increases. At low enough temperature, the size of the waves exceeds the average distance between two particles and a constant fraction of bosons enter their ground state. These particles then coalesce into a single collective quantum wave called a *Bose–Einstein condensate* (BEC). Incredibly, this quantum phenomenon can be observed at the macroscopic scale.

In statistical physics, such thermodynamic systems are often modeled in one of three settings: the *micro-canonical ensemble*, where both the number of particles

and the total energy in the system are kept constant, the canonical ensemble, where the number of particles is constant but the energy is allowed to vary, and the grand canonical ensemble, where both the number of particles and energy can vary. A substantial amount of research has focused on understanding the asymptotic behavior of BECs in the microcanonical and canonical ensembles [8, 9]. Here, we give a provably efficient algorithm for uniformly sampling BEC configurations from the microcanonical ensemble in the low-temperature regime when the number of particles is at least the total energy in the system. This allows us to explore thermodynamic properties of systems with thousands of non-interacting bosons instead of relying solely on its limiting behavior.

Random sampling is widely used across scientific disciplines when exact solutions are unavailable. In many settings, Boltzmann samplers have proven particularly useful for sampling combinatorial objects of a fixed size. The state space \mathcal{C} includes configurations of all sizes, and the Boltzmann distribution assigns a configuration $\gamma \in \mathcal{C}$ probability $\mathbb{P}_{\lambda}(\gamma) = \lambda^k/Z$, where k is the size of γ , Z is the normalizing constant, and $\lambda \in \mathbb{R}_{>0}$ is a parameter of the system that biases the distribution toward configurations of the desired size. Boltzmann sampling is effective if the sampling procedure is efficient on $(\mathcal{C}, \mathbb{P})$ and rejection sampling (i.e., outputting objects of the desired size and rejecting all others) succeeds with high enough probability to produce samples of the correct size in expected polynomial time.

A useful example to demonstrate the effectiveness of Boltzmann sampling is integer partitions, which arise across many areas of mathematics and physics (see, e.g., [3, 19, 24]) and turn out to be closely related to BECs. An integer partition of a nonnegative integer n is a nonincreasing sequence of positive integers that sums to n. The simplest method for uniformly generating random partitions of n relies on exact counting. Nijenhuis and Wilf [23] gave a dynamic programming algorithm for enumerating partitions of n, which naturally extends to a sampling algorithm that requires $O(n^{2.5})$ time and space. However, no suitable closed-form expression for the number of integer partitions of n is known, thus limiting the usefulness of this approach.

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Alternatively, we can use Boltzmann sampling to generate integer partitions that are biased to have size close to n, augmented with rejection sampling to output only partitions of the desired size. Arratia and Tavaré [2] showed that integer partitions and many other objects with multiplicative generating functions can be sampled from Boltzmann distributions using independent random processes. Duchon et al. [11] generalized their approach to a systematic Boltzmann sampling framework using ideas from analytic combinatorics, yielding a Boltzmann sampler for integer partitions of varying size with time and space complexity linear in the size of partition produced. They suggest tuning λ so that the expected size of the generated object is n, which empirically gives a useful rejection rate. Leveraging additional symmetries of partitions, Arratia and DeSalvo [1] gave a sampling algorithm that runs in expected $O(\sqrt{n})$ time and space. Taking a completely different approach, Bhakta et al. [5] recently gave the first rigorous Markov chain for sampling partitions, again utilizing Boltzmann sampling to generate samples of a desired size.

While Boltzmann sampling has been shown to be quite effective on a vast collection of problems in statistical physics and combinatorics, several applications lack a proof that samples will be generated from close to the Boltzmann distribution, and even more lack rigorous arguments showing that rejection sampling will be efficient in expectation. In this paper we give an provably efficient Boltzmann sampler for BECs and rigorously bound its rejection rate through singularity analysis of Dirichlet generating functions. Our techniques naturally extend to many families of weighted partitions, which generalize integer partitions and BECs.

Bose-Einstein Condensates We study Bose-Einstein condensation in an idealized microcanonical setting with limited interactions between particles. In the physics community this represents configurations of zero-spin particles in a d-dimensional isotropic harmonic trap in the absence of two-body interactions and particle-photon interaction. We focus on the case d=3, but the results generalize to higher dimensions. Combinatorially, we interpret BECs as weighted partitions with $b_k = {k+3-1 \choose 3-1}$ types of summands of size k. The b_k summands correspond to the degenerate energy states of a boson with energy k. We view such energy states as multisets of three different colors with cardinality k. BEC configurations are unordered collections of bosons and can be understood as multisets of bosons, or equivalently weighted partitions. We represent BECs graphically by coloring Young diagrams. Each column corresponds to the energy state of a particle, and the columns are sorted lexicographically to give a partition of particles. In the microcanonical ensemble with m particles and energy n, the number of particles in their ground state is m minus the width of the Young diagram. Bose–Einstein condensation occurs when the width of the average Young diagram is at most a constant fraction of m.

In the language of analytic combinatorics, BECs are the combinatorial class $MSET(MSET_{\geq 1}(3\mathcal{Z}))$. For example, if n=2 there are 12 possible configurations. When there is one particle with energy 2 we have $\{\{1,1\}\}, \{\{1,2\}\}, \{\{1,3\}\}, \{\{2,2\}\}, \{\{2,3\}\}, \{\{3,3\}\},$ and when there are two particles each with energy 1 we have $\{\{1\}, \{1\}\}, \{\{1\}, \{2\}\}, \{\{1\}, \{3\}\}, \{\{2\}, \{2\}\}\}$ $\{\{2\}, \{3\}\}, \{\{3\}, \{3\}\}$. If n=3 there are 38 possible configurations: 10 if there is one particle with energy 3, 18 that emerge for the Young diagram with shape (2,1) when one particle has energy 2 and one has energy 1 (Figure 1), and 10 when there are three particles with energy 1.

1.2 Results Our complexity analysis follows the conventions in [7, 13] and assumes a real-arithmetic model of computation, an oracle that evaluates a generating function within its radius of convergence in constant time, and a root-finding oracle. We give a new method for rigorously analyzing algorithms that sample from the Bose–Einstein distribution in low-temperature microcanonical ensembles when the number of particles exceeds the total energy. In particular, we give a provably efficient algorithm for uniformly sampling BECs by constructing a linear-time Boltzmann sampler using the framework established in [13], and then bounding its rejection rate through singularity analysis of an associated Dirichlet generating function.

THEOREM 1.1. There exists a uniform sampling algorithm for Bose–Einstein condensates of size n that runs in expected $O(n^{1.625})$ time and uses O(n) space.

This algorithm generates samples of size n exactly from the uniform distribution in expected polynomial time. This allows us, for example, to rigorously study the expected width of Young diagrams arising from random configurations (or, equivalently, the fraction of particles in a BEC in their ground state) without relying on the limiting properties given in [26].

The singularity analysis used in the proofs generalizes to a broader family of weighted partitions, including integer partitions and plane partitions [7]. Let a positive integer sequence of degree r be a sequence of positive integers $(b_k)_{k=1}^{\infty}$ such that $b_k = p(k)$ for some polynomial $p(x) = a_0 + a_1x + \cdots + a_rx^r \in \mathbb{R}[x]$ with $\deg(p) = r$.

 $[\]overline{}^1$ In this setting each weighted partition of size n uniquely corresponds to a BEC configuration in the microcanonical ensemble.



Figure 1: Young diagrams of Bose–Einstein condensates with shape (2,1), where the colors (gray, green, blue) correspond to the numbers (1,2,3).

We show how the rightmost pole of the Dirichlet generating function for $(b_k)_{k=1}^{\infty}$ and its residue relate to p(x), which we then use to establish rigorous rejection rates for Boltzmann sampling.

THEOREM 1.2. There exists a uniform sampling algorithm for any class of weighted partitions parameterized by a positive integer sequence of degree r for objects of size n that runs in expected $O(n^{r+1+(r+3)/(2r+4)})$ time and uses O(n) space.

For a fixed degree r, the number of samples needed in expectation is $O(n^{(r+3)/(2r+4)})$, which is asymptotically tight by Theorem 2.1. In particular, when r=0 (as in the case of integer partitions) we need $O(n^{3/4})$ samples, and as $r\to\infty$ the number of required samples converges to $O(\sqrt{n})$. Independently, DeSalvo and Menz [10] recently developed a new probabilistic model that gives a central limit theorem for the same family of weighted partitions and circumvents singularity analysis of Dirichlet generating functions.

1.3 Techniques Probabilistic interpretations of ordinary generating functions for weighted partitions are useful for producing samples from Boltzmann distributions in polynomial time [2, 13], but rejection sampling is not always guaranteed to be efficient. We use the Khintchine–Meinardus probabilistic method [15, 16, 17] to establish that rejection sampling is efficient for a broad class of weighted partitions that includes BECs. We also use the Boltzmann sampling framework based on the symbolic method from analytic combinatorics to give a improved algorithms for BECs, instead of simply using a geometric random variable for each degenerate energy state (Theorem 1.1 vs. Theorem 1.2 with r=2).

The goal of the Khintchine–Meinardus probabilistic is to asymptotically enumerate combinatorial objects through singularity analysis of Dirichlet generating functions. For algorithmic purposes, it is useful for bounding rejection rates. Only recently were such techniques extended to handle Dirichlet series with multiple poles on the real axis [16], which is a necessary advancement for analyzing BECs and other weighted partitions parameterized by non-constant integer sequences. In this paper, we show that the Dirichlet series for classes of weighted partitions parameterized by positive integer sequences are linear combinations of shifted Riemann zeta functions, and thus amenable to singularity analy-

sis. Using bounds for the Riemann zeta function from analytic number theory, we show that the local limit theorem in [16] holds for BECs. We also view the parameterizing polynomial p(x) as a Newton-interpolating polynomial to lower bound the residue of the rightmost pole of the Dirichlet generating functions, which leads to a more convenient lemma for rejection rates.

Additionally, we develop a tail inequality for the negative binomial distribution (Lemma 3.8) that is empirically much tighter than a Chernoff-type inequality when used in the analysis of a subroutine of the main sampling algorithm. We also believe the singularity analysis of Dirichlet series in this paper will be valuable for a wide variety of sampling problems in computer science when the objects of interest can be decomposed into non-interacting components and when transfer theorems for ordinary generating functions do not work.

2 Preliminaries

We start by introducing fundamental ideas about Boltzmann samplers for combinatorial classes. Then we use the symbolic method to define Bose–Einstein condensates and present a local limit theorem from the Khintchine–Meinardus probabilistic method for weighted partitions. These are the main components of our analysis.

2.1 Boltzmann Sampling A combinatorial class \mathcal{C} is a finite or countably infinite set equipped with a size function $|\cdot|: \mathcal{C} \to \mathbb{Z}_{\geq 0}$ such that the number of elements of any given size is finite. For a given class \mathcal{C} , let c_n be the number of elements of size n. The counting sequence of \mathcal{C} is the integer sequence $(c_n)_{n=0}^{\infty}$, and the ordinary generating function of \mathcal{C} is

$$C(z) = \sum_{n=0}^{\infty} c_n z^n = \sum_{\gamma \in \mathcal{C}} z^{|\gamma|}.$$

DEFINITION 2.1. The Boltzmann distribution of a class C parameterized by $\lambda \in (0, \rho_C)$ is the probability distribution, for all $\gamma \in C$, defined as

$$\mathbb{P}_{\lambda}(\gamma) = \frac{\lambda^{|\gamma|}}{C(\lambda)},$$

where ρ_C is the radius of convergence of C(z).

Definition 2.2. A Boltzmann sampler $\Gamma C(\lambda)$ is an

algorithm that generates objects from a class C according the Boltzmann distribution with parameter λ .

The size of an object generated by $\Gamma C(\lambda)$ is a random variable denoted by U with the probability distribution

$$\mathbb{P}_{\lambda}(U=n) = \frac{c_n \lambda^n}{C(\lambda)}.$$

All objects of size n occur with equal probability, so if $\Gamma C(\lambda)$ returns an object γ of size n, then γ is a uniform random sample among all size n objects in \mathcal{C} . Therefore, we can use rejection sampling to generate objects of size n uniformly at random. For this technique to be effective, we need both an efficient sampling algorithm over the pair $(\mathcal{C}, \mathbb{P}_{\lambda})$ and a provably low rate of rejection.

Assuming that C is infinite and $c_0 \neq 0$, we maximize the probability of generating an object of size $n \geq 1$ by tuning the Boltzmann sampler so that $\mathbb{E}_{\lambda}[U] = n$ and denote this solution by λ_n . To see why this strategy works, observe that

(2.1)
$$\frac{\mathrm{d}}{\mathrm{d}\lambda} \mathbb{P}_{\lambda}(U=n) = \frac{c_n \lambda^{n-1}}{C(\lambda)} (n - \mathbb{E}_{\lambda}[U]),$$

where $\mathbb{E}_{\lambda}[U] = \lambda C'(\lambda)/C(\lambda)$. Because \mathcal{C} contains objects of varying size, we have

(2.2)
$$\frac{\mathrm{d}}{\mathrm{d}\lambda} \mathbb{E}_{\lambda}[U] = \frac{\mathrm{Var}_{\lambda}(U)}{\lambda} > 0.$$

Thus $\mathbb{E}_{\lambda}[U]$ is strictly increasing, so λ_n is unique. Together with (2.1), this implies that $\mathbb{P}_{\lambda}(U=n)$ is maximized at λ_n . The equality in (2.2) is a property of Boltzmann distributions [11], and the inequality is true because $\lambda \in (0, \rho_C)$ and U is a nonconstant random variable.

2.2 Symbolic Method We use the symbolic method of analytic combinatorics to construct the class of Bose–Einstein condensates and then utilize the Boltzmann sampling framework developed in [11, 12, 13]. The primitive combinatorial classes in the symbolic method are the neutral class \mathcal{E} and the atomic class \mathcal{E} . The class \mathcal{E} contains a single element of size 0 called a neutral object, and the class \mathcal{Z} contains a single element of size 1 called an atom. Neutral objects are used to mark objects as different, and atoms are combined to form combinatorial objects. We can express a rich family of discrete structures using these primitive classes with the following operators.

DEFINITION 2.3. The combinatorial sum of A and B is $C = A + B = (\mathcal{E}_1 \times A) \cup (\mathcal{E}_2 \times B)$, where \mathcal{E}_1 and \mathcal{E}_2 are different neutral classes. The size of an element in C is the same as in its class of origin, and the ordinary generating function for C is C(z) = A(z) + B(z).

DEFINITION 2.4. The Cartesian product of \mathcal{A} and \mathcal{B} is $\mathcal{C} = \mathcal{A} \times \mathcal{B} = \{(\alpha, \beta) : \alpha \in \mathcal{A}, \beta \in \mathcal{B}\}$. The size of the pair $\gamma = (\alpha, \beta) \in \mathcal{C}$ is defined as $|\gamma|_{\mathcal{C}} = |\alpha|_{\mathcal{A}} + |\beta|_{\mathcal{B}}$, and the generating function for \mathcal{C} is C(z) = A(z)B(z).

DEFINITION 2.5. The sequence operator of a class \mathcal{B} with $b_0 = 0$ is the infinite sum $\mathcal{C} = \text{SEQ}(\mathcal{B}) = \mathcal{E} + \mathcal{B} + (\mathcal{B} \times \mathcal{B}) + (\mathcal{B} \times \mathcal{B} \times \mathcal{B}) + \cdots$. The generating function for \mathcal{C} is $C(z) = \sum_{k=0}^{\infty} B(z)^k = (1 - B(z))^{-1}$.

DEFINITION 2.6. The multiset operator of a class \mathcal{B} with $b_0 = 0$ is $\mathcal{C} = \text{MSet}(\mathcal{B}) = \prod_{\beta \in \mathcal{B}} \text{Seq}(\{\beta\})$. The generating function for \mathcal{C} is

2.3)
$$C(z) = \prod_{\beta \in \mathcal{B}} \left(1 - z^{|\beta|}\right)^{-1}$$
$$= \prod_{k=1}^{\infty} \left(1 - z^k\right)^{-b_k}$$
$$= \prod_{k=1}^{\infty} \exp\left(\frac{1}{k}B(z^k)\right).$$

The final equality is an exp-log transform [14].

Multisets are essential to our analysis because they demonstrate how Bose–Einstein condensates decompose into combinatorial atoms. Bose–Einstein condensates and integer partitions are generalized by weighted partitions, which are the central objects in the Khintchine–Meinardus probabilistic method.

DEFINITION 2.7. The class C of weighted partitions with b_k different types of summands of size $k \geq 1$ is implicitly defined by the generating function

$$C(z) = \sum_{n=0}^{\infty} c_n z^n = \prod_{k=1}^{\infty} (1 - z^k)^{-b_k}.$$

Equivalently, C = MSet(B) is parameterized by the class B of permissible summands.

From here onward, we use C to denote classes of weighted partitions and B to denote the corresponding class of summands. For uniform sampling, it is beneficial to work with the truncated class of weighted partitions C_n with the generating function

$$C_n(z) = \prod_{k=1}^n (1 - z^k)^{-b_k},$$

since it completely contains the target set of objects of size n. Analogously, we define a random variable for the size of an object produced by a Boltzmann sampler for the truncated class \mathcal{C}_n .

DEFINITION 2.8. Let U_n denote the random variable for the size of an object generated by $\Gamma C_n(\lambda)$.

Equipped the notions of weighted partitions and the symbolic method, we can easily construct Bose– Einstein condensates in a way that is amenable to efficient uniform sampling.

DEFINITION 2.9. Bose–Einstein condensates are weighted partitions with the parameters $b_k = \binom{k+2}{2}$. In the language of analytic combinatorics they are the combinatorial class $MSet(MSet)(3\mathbb{Z})$.

The parameterizing class $\mathrm{MSeT}_{\geq 1}(3\mathcal{Z})$ is the set of all nonempty multisets of 3 different colored atoms. There are $\binom{k+3-1}{3-1}$ such multisets of size k, each corresponding to a different summand. From a physics point of view, multisets of size k in $\mathrm{MSeT}_{\geq 1}(3\mathcal{Z})$ are isomorphic to the three-dimensional degenerage energy states of a boson with energy k. A Bose–Einstien condensate is an unordered collection of bosons, so an object of size n in $\mathrm{MSet}(\mathrm{MSet}_{\geq 1}(3\mathcal{Z}))$ uniquely corresponds to a Bose–Einstein condensate with total energy n.

2.3 Khintchine-Meinardus Probabilistic Method

Under somewhat restrictive conditions, Meinardus [22] established an asymptotic equivalence between the number of weighted partitions c_n and the analytic behavior of the Dirichlet series

$$D(s) = \sum_{k=1}^{\infty} b_k k^{-s},$$

using the saddle-point method [14], where $s = \sigma + it$ is a complex variable. Granovsky, Stark, and Erlihson [17] extended Meinardus' theorem to new multiplicative combinatorial objects using Khintchine's probabilistic method [21]. Granovsky and Stark [16] later generalized their results to weighted partitions such that D(s) has multiple singularities on the positive real axis, which includes the class of Bose–Einstein condensates. To use the Khintchine–Meinardus probabilistic method for weighted partitions, we must show that the series D(s) satisfies the following conditions:

(I) The Dirichlet series D(s) has $r \geq 1$ simple poles at real positions $0 < \rho_1 < \rho_2 < \cdots < \rho_r$ with positive residues A_1, A_2, \ldots, A_r , and it is analytic in the half-plane $\sigma > \rho_r > 0$. Moreover, there is a constant $0 < C_0 \leq 1$ such that the function D(s) has a meromorphic continuation to the half-plane

$$\mathcal{H} = \{s : \sigma \geq -C_0\},\$$

on which it is analytic except for above the r simple poles.

(II) There is a constant $C_1 > 0$ such that

$$D(s) = O(|t|^{C_1}),$$

uniformly for $s = \sigma + it \in \mathcal{H}$, as $t \to \infty$.

(III) For $\delta > 0$ small enough and some $\varepsilon > 0$,

$$2\sum_{k=1}^{\infty} b_k e^{-k\delta} \sin^2(\pi k\alpha) \ge \mathcal{M}\left(1 + \frac{\rho_r}{2} + \varepsilon\right) |\log \delta|,$$

for all
$$\sqrt{\delta} \le |\alpha| \le 1/2$$
 and $\mathcal{M} = 4/\log 5$.

The local limit theorem that follows is the crux of the proof for [16, Theorem 1]. We use it to prove asymptotically tight rejection rates for our Boltzmann sampler as a function of the rightmost pole of D(s). In the statement, $\Gamma(z)$ is the gamma function and $\zeta(s)$ is the Riemann zeta function.

THEOREM 2.1. ([16]) If conditions (I)-(III) hold,

$$\mathbb{P}_{\lambda_n}(U_n = n) \sim \frac{1}{\sqrt{2\pi \text{Var}(U_n)}}$$
$$\sim \frac{1}{\sqrt{2\pi K_2}} \left(\frac{K_2}{\rho_r + 1}\right)^{\frac{2+\rho_r}{2(\rho_r + 1)}} n^{-\frac{2+\rho_r}{2(\rho_r + 1)}},$$

as $n \to \infty$, where $K_2 = A_r \Gamma(\rho_r + 2) \zeta(\rho_r + 1)$ is a constant.

3 Sampling Bose-Einstein Condensates

We can now present our main algorithm for uniformly sampling Bose–Einstein condensates. We bound the rejection rate of its underlying Boltzmann sampler using singularity analysis of a Dirichlet generating function and then analyze the complexity of the overall algorithm to prove Theorem 1.1.

Algorithm 1 Uniform sampling algorithm for BECs.

1: **procedure** RANDOMBEC(n)
2: $\lambda_n \leftarrow \operatorname{Solve} \sum_{k=1}^n k \binom{k+2}{2} \lambda^k / (1 - \lambda^k) = n$ 3: **repeat**4: $\gamma \leftarrow \Gamma \operatorname{MSET}[\operatorname{MSET}_{1...n}(3\mathcal{Z})](\lambda_n)$ 5: **until** $|\gamma| = n$ 6: **return** γ

Before discussing the Boltzmann samplers in Algorithm 1, we define several probability distributions that are fundamental to the following subroutines.

DEFINITION 3.1. Let Geometric(λ) denote the geometric distribution with success probability λ and probability density function $\mathbb{P}_{\lambda}(k) = (1 - \lambda)^k \lambda$, for all $k \in \mathbb{Z}_{\geq 0}$.

DEFINITION 3.2. Let Poisson(λ) denote the Poisson distribution with rate parameter λ and probability density function $\mathbb{P}_{\lambda}(k) = e^{-\lambda} \lambda^k / k!$, for all $k \in \mathbb{Z}_{\geq 0}$. The zero-truncated Poisson distribution Poisson $_{\geq 1}(\lambda)$ with rate parameter λ has the probability density function $\mathbb{P}_{\lambda}(k) = \lambda^k / ((e^{\lambda} - 1)k!)$.

DEFINITION 3.3. Let NegativeBinomial (r, λ) denote the negative binomial distribution with r failures, success probability λ , and probability density function $\mathbb{P}_{\lambda}(k) = \binom{k+r-1}{r-1} \lambda^k (1-\lambda)^r$, for all integers $k \in \mathbb{Z}_{\geq 0}$. The zero-truncated negative binomial distribution is NegativeBinomial $_{\geq 1}(r, \lambda)$.

One of the two main subroutines in Algorithm 1 is a template Boltzmann sampler for the class MSET(A), where A is any combinatorial class with $a_0 = 0$. This algorithm repeatedly calls the Boltzmann sampler of the input class $\Gamma A(\lambda^k)$ (for various values of k) and is part of the Boltzmann sampling framework for combinatorial classes that can be constructed with the symbolic method [13].

Algorithm 2 Boltzmann sampler for MSet(A).

```
1: procedure \Gamma MSET[A](\lambda)
           \gamma \leftarrow \text{Empty associative array}
 2:
           k_0 \leftarrow \text{MAXINDEX}(A, \lambda)
 3:
           for k = 1 to k_0 do
 4:
                 if k < k_0 then
 5:
                      m \leftarrow \text{Poisson}(A(\lambda^k)/k)
 6:
 7:
                      m \leftarrow \text{Poisson}_{>1}(A(\lambda^k)/k)
 8:
                 for j = 1 to m do
 9:
                      \alpha \leftarrow \Gamma A(\lambda^k)
10:
                      \gamma[\alpha] \leftarrow \gamma[\alpha] + k
11:
12:
           return \gamma
```

In particular, Algorithm 2 is a manifestation of the generating function for weighted partitions. It captures the exp-log transform in (2.3) by using the property that a geometric random variable can be decomposed into an infinite sum of independent, scaled Poisson random variables. We direct the reader to the proof of [13, Proposition 2.1] for more details. The function Maxindex(A, λ) samples from the distribution with cumulative density function

(3.4)
$$\mathbb{P}_{\lambda}(U \leq k) = \frac{\prod_{j=1}^{k} \exp\left(\frac{1}{j} A(\lambda^{j})\right)}{\prod_{j=1}^{\infty} \exp\left(\frac{1}{j} A(\lambda^{j})\right)}$$
$$= \prod_{j=k+1}^{\infty} \exp\left(-\frac{1}{j} A(\lambda^{j})\right),$$

for all integers $k \geq 1$. Note that we give the corrected expression for (3.4) that originally appeared in [7].

PROPOSITION 3.1. ([13]) Algorithm 2 is a valid Boltzmann sampler for MSET(\mathcal{A}). Moreover, if the time and space complexities of $\Gamma A(\lambda)$ are, in the worst case, linear in the size of the object produced, the time and space complexities of Algorithm 2 are also linear in the size of the object produced.

The second subroutine in Algorithm 1 is a Boltzmann sampler for the nonempty multisets of d different colored atoms with size at most n. This parameterizes the truncated class of Bose–Einstein condensates when d=3, and it is necessary for the Khintchine–Meinardus probabilistic method. It suffices to use the Boltzmann sampler $\Gamma MSET_{\geq 1}(d\mathcal{Z})$ and rejection sampling by Lemma 3.5.

Algorithm 3 Boltzmann sampler for multisets.

```
1: procedure \Gamma MSET_{1..n}(d\mathcal{Z})(\lambda)

2: repeat

3: m \leftarrow \text{NegativeBinomial}_{\geq 1}(d, \lambda)

4: until m \leq n

5: return RANDOMMULTISET(m, d)
```

The crucial observation in Algorithm 3 is that a negative binomial experiment with d failures can be interpreted as a multiset of d different colored atoms using the classical combinatorial idea of stars and bars. For a given experiment, a successful trial adds an atom of the current color and a failure is a bar that separates atoms of different colors. Once m is determined, the function RANDOMMULTISET(m,d) returns one of the $\binom{m+d-1}{d-1}$ multisets of size m uniformly at random.

3.1 Tuning the Boltzmann Sampler The factorization of the generating function for weighted partitions has a useful probabilistic interpretation in the context of Boltzmann sampling. We can iterate over all types of summands of size at most n and use independent geometric random variables to determine how many parts each type contributes to the final object [2, 13]. It follows that the random variable for the size of the object drawn from the Boltzmann sampler is

$$U_n = \sum_{k=1}^n \sum_{j=1}^{b_k} k Y_{k,j},$$

where $Y_{k,j} \sim \text{Geometric}(1 - \lambda^k)$.

Lemma 3.1. We have

$$\mathbb{E}_{\lambda}[U_n] = \sum_{k=1}^n k b_k \left(\frac{\lambda^k}{1 - \lambda^k}\right).$$

Proof. The result follows from the linearity of expectation and the mean of the variables $Y_{k,j}$.

Since $\mathbb{E}_{\lambda}[U_n]$ is strictly increasing (2.2), we can use Lemma 3.1 and a root-finding algorithm such as the bisection method to compute an ε -approximation of λ_n in time $O(n\log(\varepsilon^{-1}))$. In this paper, however, we assume an oracle that returns the exact value of λ_n in constant time and defer the numerical analysis needed for the accuracy of the ε -approximation. Since we are dealing with analytic functions, a quantitative statement about the continuity of the local limit theorem near λ_n should be achievable.

3.2 Rejection Rate of Algorithm 1 We generalize the analysis in this subsection from Bose–Einstein condensates to the class of weighted partitions parameterized by a positive integer sequence of degree r. We show that Theorem 2.1 holds for all such weighted partitions and bound the residue of the rightmost pole of the series D(s) to give rejection rates for these Boltzmann samplers as a function of the degree r.

DEFINITION 3.4. Let a positive integer sequence of degree r be a sequence of positive integers $(b_k)_{k=1}^{\infty}$ such that $b_k = p(k)$ for some polynomial

$$p(x) = a_0 + a_1 x + \dots + a_r x^r \in \mathbb{R}[x],$$

with deg(p) = r.

To interface with the Khintchine–Meinardus probabilistic method, we apply results from analytic number theory about the Riemann zeta function. The Riemann zeta function $\zeta(s)$, $s=\sigma+it$, is defined as the analytic continuation of the convergent series $\zeta(s)=\sum_{n=1}^{\infty}1/n^s$, for all $\sigma>1$, into the entire complex plane. The only singularity of $\zeta(s)$ is a simple pole at s=1.

The following lemma shows that the Dirichlet generating function D(s) for $(b_k)_{k=1}^{\infty}$ is a linear combination of Riemann zeta functions that are translated and scaled by the coefficients of p(x). With this, we can easily compute the residues of the poles of D(s) and satisfy conditions (I)–(III).

LEMMA 3.2. If $(b_k)_{k=1}^{\infty}$ is a positive integer sequence of degree r, its Dirichlet generating series is

$$D(s) = \sum_{k=0}^{r} a_k \zeta(s-k),$$

which satisfies conditions (I)–(III). Moreover, D(s) has at most r+1 simple poles on the positive real axis at positions $\rho_k = k+1$ with residue $A_k = a_k$ if and only if $a_k \neq 0$, for $k \in \{0, 1, \ldots, r\}$.

Proof. The Riemann zeta function converges uniformly and is analytic on $\mathbb{C} \setminus \{1\}$, so

$$D(s) = \sum_{k=1}^{\infty} \frac{b_k}{k^s}$$

$$= \sum_{k=1}^{\infty} \frac{a_0 + a_1 k + \dots + a_r k^r}{k^s}$$

$$= \sum_{k=0}^{r} a_k \zeta(s - k).$$

As $\zeta(s)$ has a simple pole at s=1 with residue 1, the claim about the poles of D(s) follows, and condition (I) is satisfied by letting $C_0=1$. For condition (II), we let $C_1=2+r$ since D(s) is a linear combination of shifted zeta functions and use [4, Section 8.2]:

$$\zeta(s) = \begin{cases} O(t^{1/2 - \sigma}) & \text{if } \sigma < 0, \\ O(t) & \text{if } 0 \le \sigma \le 1, \\ O(1) & \text{if } 1 < \sigma. \end{cases}$$

To show condition (III), we use an approach similar to the proof of [17, Lemma 1], which employs the following inequality of Karatsuba and Voronin [20, Section 4.2, Lemma 1] for trigonometric sums related to the Riemann zeta function: For all positive integers m,

$$(3.5) \qquad 2\sum_{k=1}^{m}\sin^2(\pi k\alpha) \ge m\left(1 - \min\left(1, \frac{1}{2m|\alpha|}\right)\right).$$

By assumption, $(b_k)_{k=1}^{\infty}$ is a sequence of positive integers and $0 < \sqrt{\delta} \le |\alpha| \le 1/2$, so

$$2\sum_{k=1}^{\infty} b_k e^{-k\delta} \sin^2(\pi k\alpha) \ge 2\sum_{k=1}^{m} e^{-k\delta} \sin^2(\pi k\alpha)$$
$$\ge e^{-m\delta} m \left(1 - \min\left(1, \frac{1}{2m|\alpha|}\right)\right).$$

Using (3.5), we let $m = \lceil 1/(2|\alpha|) + 1/\delta \rceil \ge 1$ so that

$$2\sum_{k=1}^{\infty} b_k e^{-k\delta} \sin^2(\pi k\alpha) \ge e^{-m\delta} \left(m - \frac{1}{2|\alpha|} \right)$$
$$\ge e^{-\left(\frac{1}{2|\alpha|} + \frac{1}{\delta} + 1\right)\delta} \delta^{-1}$$
$$> e^{-\left(\frac{\sqrt{\delta}}{2} + 1 + \delta\right)} \delta^{-1}.$$

Recall that the position of the pole $\rho_r = r + 1$ is fixed and \mathcal{M} is constant. It follows that

$$e^{-\left(\frac{\sqrt{\delta}}{2}+1+\delta\right)}\frac{1}{\delta|\log\delta|} \geq \mathcal{M}\Big(1+\frac{\rho_r}{2}+\varepsilon\Big),$$

for δ sufficiently small and $\varepsilon = 1$.

To conveniently use Theorem 2.1 in the analysis of Algorithm 1, we lower bound the rightmost residue A_r using Lemma 3.2 and the method of finite differences. In particular, we bound the coefficients of p(x) in the binomial basis as illustrated in [6]. Define the forward difference operator Δ to be

$$\Delta p(x) = p(x+1) - p(x).$$

Higher order differences are given by

$$\Delta^{n} p(x) = \Delta^{n-1} p(x+1) - \Delta^{n-1} p(x).$$

Viewing p(x) as a Newton interpolating polynomial, we can write

$$p(x) = \sum_{j=0}^{r} \Delta^{j} p(0) \binom{x}{j}.$$

LEMMA 3.3. ([25]) Let $p(x) \in \mathbb{R}[x]$ be a polynomial of degree r. We have $p(n) \in \mathbb{Z}$, for all $n \in \mathbb{Z}$, if and only if $\Delta^{j}p(0) \in \mathbb{Z}$, for all $0 \le j \le r$.

LEMMA 3.4. Let $(b_k)_{k=1}^{\infty}$ be any positive integer sequence of degree r. For n sufficiently large,

$$\mathbb{P}_{\lambda_n}(U_n = n) \ge \frac{1}{2\sqrt{2\pi}}((r+2)n)^{-\frac{r+3}{2(r+2)}}.$$

Proof. Theorem 2.1 holds for U_n by Lemma 3.2. By assumption $(b_k)_{k=1}^{\infty}$ is a positive integer sequence of degree r, so Lemma 3.3 implies that p(x) has integral coefficients $\Delta^j p(0)$ in the binomial basis. Thus, $\Delta^r p(0)$ is a positive integer, which implies that

$$a_r \ge \frac{1}{r!}$$
.

The residue $A_r = a_r$ by Lemma 3.2, so we can K_2 by

$$K_2 = A_r \Gamma(\rho_r + 2) \zeta(\rho_r + 1)$$

$$\geq \frac{1}{r!} (r+2)!$$

$$\geq 1.$$

since $\rho_r = r + 1$ and $\zeta(n) \ge 1$, for all $n \ge 2$. It follows that for $\varepsilon = 1/2$ and n sufficiently large, we have

$$\mathbb{P}_{\lambda_n}(U_n = n) \ge (1 - \varepsilon) \frac{1}{\sqrt{2\pi K_2}} \left(\frac{K_2}{(\rho_r + 1)n}\right)^{\frac{2 + \rho_r}{2(\rho_r + 1)}}$$

$$\ge \frac{1}{2\sqrt{2\pi}} K_2^{\frac{1}{2(r+2)}} ((r+2)n)^{-\frac{r+3}{2(r+2)}}$$

$$\ge \frac{1}{2\sqrt{2\pi}} ((r+2)n)^{-\frac{r+3}{2(r+2)}},$$

as desired.

3.3 Proving the Main Theorems Recall that we follow the convention of using the real-arithmetic model of computation and an oracle that evaluates a generating function within its radius of convergence in constant time [7, 13]. A consequence of this is that we can iteratively sample an integer m from the distributions Geometric(λ), Poisson(λ), MaxIndex(A, λ), etc., in O(m) time. We restate Theorem 1.1 and Theorem 1.2 for convenience.

THEOREM 1.1. There exists a uniform sampling algorithm for Bose–Einstein condensates of size n that runs in expected $O(n^{1.625})$ time and uses O(n) space.

Proof. We analyze the complexities of Algorithm 1. In the tuning step, we can compute the exact value of λ_n in O(1) time using a root-finding oracle and Lemma 3.1. (We can compute an ε -approximation in time $O(n \log(\varepsilon^{-1}))$.) We invoke the Boltzmann sampler Γ MSET[MSET_{1...n}(3 \mathbb{Z})](λ_n) at most $O(n^{5/8})$ times in expectation by Lemma 3.4, and we implement this Boltzmann sampler using Algorithm 2 and Algorithm 3. Lemma 3.5 ensures that the time and space complexities of Algorithm 3 are linear in the size of the object produced. Algorithm 2 runs in expected O(n) time and space by Proposition 3.1 and our choice of λ_n . Thus, Algorithm 1 runs in expected O(n) time and uses expected O(n) space.

To use deterministic O(n) space, we modify the Boltzmann sampler to reject partially constructed objects if their size is at least 2n. By Markov's inequality, this refined Boltzmann sampler outputs objects of size less than 2n from a new Boltzmann distribution with probability at least

$$1 - \mathbb{P}_{\lambda_n}(U_n \ge 2n) \ge 1 - \frac{\mathbb{E}_{\lambda_n}[U_n]}{2n}$$
$$= \frac{1}{2}.$$

Thus, at most a constant number of trials are needed in expectation to sample from the tail-truncated Boltzmann distribution.

The singularity analysis in Theorem 1.1 generalizes to the setting of weighted partitions parameterized by a positive integer sequence of degree r, but we need to use a different Boltzmann sampler. The truncated class C_n of weighted partitions has the generating function $C_n(z) = \prod_{k=1}^n (1-z^k)^{-b_k}$, so we can use independent geometric random variables to sample the number of parts each type of summand contributes to the final configuration. See the Boltzmann samplers for the Cartesian product and sequence operator in [13] for more details.

THEOREM 1.2. There exists a uniform sampling algorithm for any class of weighted partitions parameterized by a positive integer sequence of degree r for objects of size n that runs in expected $O(n^{r+1+(r+3)/(2r+4)})$ time and uses O(n) space.

Proof. The tuning step is the same as in the proof of Theorem 1.1. This Boltzmann algorithm samples from $\sum_{k=1}^{n} b_k = O(n^{r+1})$ geometric distributions, each taking time and space proportional to the number they output. The total number of geometric trials across all $O(n^{r+1})$ distributions is O(n) by our choice of λ_n . Using Markov's inequality again, we guarantee that the algorithm uses deterministic O(n) space. Lemma 3.4 gives a rejection rate of $O(n^{3/4})$.

3.4 Rejection Rate of Algorithm 3 Lemma 3.5 shows that the rejection sampling in Algorithm 3 takes a constant number of trials in expectation each time it is called as a subroutine by Algorithm 2. We generalize our analysis from the case d=3 (Bose–Einstein condensates) to $d \geq 1$ so that our arguments involving negative binomial distributions will be useful in other contexts. In particular, we develop a simple but effective tail inequality for negative binomial random variables (Lemma 3.8) parameterized by high success probabilities that outperforms the standard Chernoff-type inequality in this setting.

Throughout this subsection let $[n] = \{1, 2, ..., n\}$ and V be a random variable for the size of an object drawn from $\Gamma \text{MSeT}_{\geq 1}(d\mathcal{Z})(\lambda)$. The ordinary generating function for $\mathcal{B} = \text{MSeT}(d\mathcal{Z})$ (the multisets of d distinct atoms) is

$$B(z) = \sum_{k=0}^{\infty} {k+d-1 \choose d-1} z^k = \frac{1}{(1-z)^d},$$

so we have $V \sim \text{NegativeBinomial}_{\geq 1}(d, \lambda)$. Similarly, assume that $W \sim \text{NegativeBinomial}(d, \lambda)$.

LEMMA 3.5. For n sufficiently large and all $k \in [n]$,

$$\mathbb{P}_{\lambda_n^k}(V \le n) \ge \frac{1}{2}.$$

We use three lemmas to prove Lemma 3.5. First, Lemma 3.6 shows that it suffices to lower bound the success probability of Algorithm 3 for k=1 instead of all $k \in [n]$. Recall that the probability mass function for W is

(3.6)
$$\mathbb{P}_{\lambda}(W=k) = \binom{k+d-1}{d-1} \lambda^k (1-\lambda)^d,$$

The cumulative distribution function for W is

$$(3.7) \mathbb{P}_{\lambda}(W \le k) = 1 - I_{\lambda}(k+1, d),$$

where $I_{\lambda}(a,b)$ is the regularized incomplete beta function defined as

$$I_{\lambda}(a,b) = \frac{B_{\lambda}(a,b)}{B_{1}(a,b)},$$

with

$$B_{\lambda}(a,b) = \int_{0}^{\lambda} t^{a-1} (1-t)^{b-1} dt.$$

Lemma 3.6. For all $k \in [n]$, we have

$$\mathbb{P}_{\lambda_n^k}(V \leq n) \geq \mathbb{P}_{\lambda_n}(V \leq n).$$

Proof. Using (3.6) and (3.7), observe that

$$\begin{split} \mathbb{P}_{\lambda_n^k}(V \leq n) &= \frac{\mathbb{P}_{\lambda_n^k}(W \leq n) - \mathbb{P}_{\lambda_n^k}(W = 0)}{1 - \mathbb{P}_{\lambda_n^k}(W = 0)} \\ &= \frac{(1 - I_{\lambda_n^k}(n + 1, d)) - (1 - \lambda_n^k)^d}{1 - (1 - \lambda_n^k)^d} \\ &= 1 - \frac{I_{\lambda_n^k}(n + 1, d)}{1 - (1 - \lambda_n^k)^d}. \end{split}$$

Since the integrand of the beta function $t^{a-1}(1-t)^{b-1}$ is positive on (0,1) and $0 < \lambda_n < 1$, we have

$$1 - \frac{I_{\lambda_n^k}(n+1,d)}{1 - (1 - \lambda_n^k)^d} \ge 1 - \frac{I_{\lambda_n}(n+1,d)}{1 - (1 - \lambda_n)^d}$$

for all $k \in [n]$.

Thus, we only need to analyze the rejection rate when sampling from the zero-truncated distribution NegativeBinomial_{>1} (d, λ_n) .

Second, Lemma 3.7 gives an upper bound and lower bound for λ_n using an asymptotic formula from the Khintchine–Meinardus probabilistic method.

LEMMA 3.7. For $MSet(MSet_{1..n}(d\mathcal{Z}))$ and n sufficiently large, we have

$$\exp\left(-2n^{-\frac{1}{d+1}}\right) \le \lambda_n \le \exp\left(-\frac{1}{2}n^{-\frac{1}{d+1}}\right).$$

Proof. Let $\lambda_n = e^{-\delta_n}$. Equation (32) in [16] asserts that as $n \to \infty$.

$$\delta_n \sim (A_r \Gamma(\rho_r) \zeta(\rho_r + 1) \rho_r)^{\frac{1}{\rho_r + 1}} n^{-\frac{1}{\rho_r + 1}}.$$

In this instance, r = d - 1 and $\rho_r = d$. It follows that $A_r = 1/(d-1)!$ and $\Gamma(\rho_r) = (d-1)!$, so

$$\delta_n \sim (\zeta(d+1)d)^{\frac{1}{d+1}} n^{-\frac{1}{d+1}}$$

as $n \to \infty$. Therefore, for any $\varepsilon > 0$ and n sufficiently large, we have

$$\delta_n \ge (1 - \varepsilon)(\zeta(d+1)d)^{\frac{1}{d+1}} n^{-\frac{1}{d+1}},$$

and

$$\delta_n \le (1+\varepsilon)(\zeta(d+1)d)^{\frac{1}{d+1}}n^{-\frac{1}{d+1}}.$$

The result follows from the fact $1 \le \zeta(d+1) \le \pi^2/6$ and by letting $\varepsilon = 1/3$.

Third, Lemma 3.8 is a tail inequality for negative binomial random variables. Although our derivation is easily understood using standard techniques in enumerative combinatorics, the inequality captures an ample amount of probability mass for all integers $n \geq 0$. It is empirically much tighter than a Chernoff-type inequality in this setting as $n \to \infty$ and $\lambda_n \to 1$.

LEMMA 3.8. (NEGATIVE BINOMIAL TAIL INEQUALITY) Assume $W \sim \text{NegativeBinomial}(d, \lambda)$. For all $n \geq 0$,

$$\mathbb{P}(W > n) \le 1 - \left(1 - \lambda^{n/d}\right)^d.$$

Proof. Let $m = \lfloor n/d \rfloor$ and observe that

$$\sum_{k=0}^{n} {k+d-1 \choose d-1} \lambda^k \ge \left(\sum_{k=0}^{m} \lambda^k\right)^d.$$

This inequality has a direct combinatorial interpretation in terms of weak d-compositions. The left-hand side is the truncated ordinary generating function for weak compositions of k into d parts, and the right-hand side is the truncated ordinary generating function for weak compositions of k into d parts of size at most m. It follows that

$$\left(\sum_{k=0}^{m} \lambda^{k}\right)^{d} = \left(\frac{1-\lambda^{m+1}}{1-\lambda}\right)^{d}$$

$$\geq \left(1-\lambda^{n/d}\right)^{d} (1-\lambda)^{-d},$$

since $0 < \lambda < 1$. Therefore, by (3.6) we have

$$\mathbb{P}(W > n) = 1 - \mathbb{P}(W \le n)$$

$$= 1 - \sum_{k=0}^{n} {k+d-1 \choose d-1} \lambda^k (1-\lambda)^d$$

$$\le 1 - \left(1 - \lambda^{n/d}\right)^d,$$

as desired.

Combining the prerequisite lemmas and using the definition of the probability mass function for the negative binomial distribution, we prove Lemma 3.5.

Proof of Lemma 3.5. It suffices to consider the case when k = 1 by Lemma 3.6. By Lemma 3.8 and (3.6),

$$\mathbb{P}_{\lambda_n}(V \le n) = \frac{\mathbb{P}_{\lambda_n}(W \in [n])}{\mathbb{P}_{\lambda_n}(W \ge 1)}$$
$$\ge \mathbb{P}_{\lambda_n}(W \le n) - \mathbb{P}_{\lambda_n}(W = 0)$$
$$\ge \left(1 - \lambda_n^{n/d}\right)^d - (1 - \lambda_n)^d.$$

Substituting the upper and lower bounds for λ_n given in Lemma 3.7, it follows that

$$\left(1 - \lambda_n^{n/d}\right)^d - (1 - \lambda_n)^d \ge \left(1 - \exp\left(-\frac{1}{2d}n^{\frac{d}{d+1}}\right)\right)^d$$
$$-\left(1 - \exp\left(-2n^{-\frac{1}{d+1}}\right)\right)^d$$
$$\ge \frac{1}{2},$$

for n sufficiently large, because

$$\lim_{n \to \infty} \exp\left(-n^{\frac{d}{d+1}}\right) = 0,$$

and

$$\lim_{n \to \infty} \exp\left(-n^{-\frac{1}{d+1}}\right) = 1.$$

This completes the proof.

4 Conclusion

We have shown how to analyze the complexity of Boltzmann samplers for a family of weighted partitions (including Bose-Einstein condensates) through the singularity analysis of Dirichlet generating functions. In particular, we relate the degree of the polynomial parameterizing the sequence $(b_k)_{k=1}^{\infty}$ to the rejection rate of our algorithms through a local limit theorem in [16]. The main observation in our analysis is that the Dirichlet generating function for a positive integer sequence of degree r is a linear combination of shifted Riemann zeta functions. This allows us to use results from analytic number theory to conveniently analyze the poles of these functions. Other ideas in our analysis using a Newton interpolating polynomial to bound residues, and developing a negative binomial tail inequality to analyze an intermediate rejection rate.

Future directions of this work include analyzing these algorithms in the interval or floating-point arithmetic models of computation, instead of the real-arithmetic model. The primary question to address is how accurate the approximation of λ_n must be in order to maintain a similar rejection rate, since λ_n approaches an essential singularity of the generating function C(z).

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